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Towards a Godement Calculus for Dinatural Transformations

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Contents

Abstract

Dinatural transformations, which have been used to interpret the second-order λ-calculus as well as derivations in intuitionistic logic and multiplicative linear logic, fail to compose in general; this has been known since they were discovered by Dubuc and Street in 1970. Many ad hoc solutions to this remarkable shortcoming have been found, but a general theory of compositionality was missing. In this thesis we show how acyclicity of certain graphs associated to these transformations is a sufficient and essentially necessary condition that ensures that the composite of two arbitrary dinatural transformations is in turn dinatural. This leads (not straightforwardly) to the definition of a generalised functor category, whose objects are functors of mixed variance in many variables, and whose morphisms are transformations that happen to be dinatural only in some of their variables.

We also define a notion of horizontal composition for dinatural transformations, extending the well-known version for natural transformations, and prove it is associative and unitary. Horizontal composition embodies substitution of functors into transformations and vice-versa, and is intuitively reflected from the string-diagram point of view by substitution of graphs into graphs.

This work represents the first, fundamental steps towards a Godement-like calculus of dinatural transformations as sought originally by Kelly, with the intention then to apply it to describe coherence problems abstractly. There are still fundamental difficulties that are yet to be overcome in order to achieve such a calculus, and these will be the subject of future work; however, our contribution places us well in track on the path traced by Kelly towards a Godement calculus for dinatural transformations.

Introduction

Dinatural transformations are the generalisation of one of the very pillars of Category Theory: *natural transformations.* As such, they are ubiquitous in Mathematics and Computer Science, in particular in the fields of logic and theory of programming languages. One of their most prominent applications is giving the correct categorical semantics for the notion of *parametric polymorphism* in second-order λ-calculus [BFSS90], but numerous studies have been conducted about them, as we shall see later on.

Despite the crucial role they play in Category Theory and Theoretical Computer Science, they suffer from a troublesome shortcoming: they do not compose. This remarkable problem has haunted mathematicians and computer scientists alike for several decades since they were introduced by Dubuc and Street in [DS70]. There are certain conditions, known already to their discoverers, under which two dinatural transformations φ and ψ compose: if either of them is natural, or if a certain square happens to be a pullback or a pushout, then the composite $\psi \circ \varphi$ turns out to be dinatural. However, these are far from being satisfactory solutions for the compositionality problem, for either they are too restrictive (as in the first case), or they speak of properties enjoyed not by φ and ψ themselves, but rather by other structures, namely one of the functors involved.

So far, only *ad hoc* solutions for restricted classes of dinatural transformations have been found and a proper compositional calculus of dinaturals has never been formalised. The first contribution of this thesis is to finally solve the compositionality problem of dinatural transformations in its full generality. We shall see in Chapter 1 how we revealed the inherent computational nature of dinaturals by using *Petri Nets* as string diagrams for them, and reducing the compositionality problem to a matter of reachability of certain configurations in *acyclic* Petri Nets. Moreover, we also defined a notion of *horizontal* composition (Chapter 2), extending the well-known version for natural transformations, and proved it is associative and unitary, cf. [MS18]. Finally, we obtained a working definition of a category of mixed-variance functors and (partially) dinatural transformations (Chapter 3) using the vertical compositionality result, together with a category of *formal substitutions* entailing horizontal composition; the connection between the two is expressed by an adjunction. These results are the first steps towards a generalised Godement calculus, sought—but never achieved—by Kelly in order to solve the coherence problem in its complete generality [Kel72b].

The origins

Natural transformations and the Godement calculus. Functors and natural transformations are among the fundamental notions of Category Theory, and indeed they appear in the first article in which categories were treated in their own right by Eilenberg and Mac Lane [EM45]. Functors provide a way to translate objects of a category $\mathbb{C}$ into objects of a category $\mathbb{D}$ while respecting composition: they are, essentially, "homomorphisms" of categories, in the typical sense of "preserving the algebraic structure", namely composition. In the same way, natural transformations are homomorphisms of functors: given functors $F, G \colon \mathbb{C} \to \mathbb{D}$, a natural transformation $\varphi \colon F \to G$ is a family of morphisms $(\varphi_A \colon F(A) \to G(A))_{A \in \mathbb{C}}$ in $\mathbb{D}$ such that for all $f \colon A \to B$ morphism in $\mathbb{C}$ the following square commutes:

$$\begin{tikzcd}
F(A) \arrow[r, "\varphi_A"] \arrow[d, "F(f)"'] & G(A) \arrow[d, "G(f)"] \\
F(B) \arrow[r, "\varphi_B"] & G(B)
\end{tikzcd}$$

Hence such a φ "transforms" images of objects along F into images of objects along G, coherently with the images of morphisms along F and G. This essentially means that natural transformations are operations that act *uniformly*, independently of the specific structure of the objects A, B or their images. For example, given an arbitrary set A, we can always define the diagonal map $\delta_A \colon A \to A \times A$ that maps $a \in A$ into the pair (a, a). This operation does not depend on the very nature of A, and it is indeed a natural transformation from the identity functor to the diagonal functor on $\mathbb{S}$et (this can be generalised to an arbitrary category with finite products).

Functors can be composed, and so can natural transformations. In fact, the latter can compose in not just one, but *two* different ways: vertically and horizontally. For if we have natural transformations $F \xrightarrow{\varphi} G \xrightarrow{\psi} H$, with $F, G, H \colon \mathbb{C} \to \mathbb{D}$, then we can consider the family of morphisms $\psi \circ \varphi$ defined as

$$\psi \circ \varphi = (\psi_A \circ \varphi_A)_{A \in \mathbb{C}}$$

and it is immediate to see that it is still a natural transformation $F \to H$. Here $\psi \circ \varphi$ is the vertical composite of φ and ψ, and it is easily proven that $\circ$ is associative and unitary. Now, if in addition to φ above we also have functors $V \colon \mathbb{B} \to \mathbb{C}$ and $U \colon \mathbb{D} \to \mathbb{E}$, that is we are in the following situation:

$$\begin{tikzcd}
\mathbb{B} \arrow[r, "V"] & \mathbb{C} \arrow[r, bend left, "F"] \arrow[r, bend right, "G"'] \arrow[r, phantom, "\Downarrow\varphi"] & \mathbb{D} \arrow[r, "U"] & \mathbb{E}
\end{tikzcd}$$

we can compose U and V with φ in what is called *whiskering*, to obtain a natural transformation $U * \varphi * V : UFV \longrightarrow UGV$ defined as

$$U * \varphi * V = \big(U(\varphi_{V(A)})\big)_{A \in \mathbb{B}}.$$

If U (respectively, V) is the identity functor, we shall simply write $\varphi * V$ (respectively, $U * \varphi$). Godement [God58] individuated some simple properties relating whiskering with vertical composition of natural transformations and sequential composition of functors, the famous *five rules of the functorial calculus*, which we report from the original source.

Theorem (Godement Calculus). *Let F, G, U and V be functors, and φ, ψ natural transformations.*

(I) In the following situation:

$$\begin{tikzcd} \bullet \arrow[r, bend left] \arrow[r, bend right] \arrow[r, phantom, "\Downarrow\varphi"] & \bullet \arrow[r, "V"] & \bullet \arrow[r, "U"] & \bullet \end{tikzcd}$$

we have $(UV) * \varphi = U * (V * \varphi)$;

(II) If

$$\begin{tikzcd} \bullet \arrow[r, "V"] & \bullet \arrow[r, "U"] & \bullet \arrow[r, bend left] \arrow[r, bend right] \arrow[r, phantom, "\Downarrow\varphi"] & \bullet \end{tikzcd}$$

then $\varphi * (UV) = (\varphi * U) * V$;

(III) If

$$\begin{tikzcd} \bullet \arrow[r, "V"] & \bullet \arrow[r, bend left] \arrow[r, bend right] \arrow[r, phantom, "\Downarrow\varphi"] & \bullet \arrow[r, "U"] & \bullet \end{tikzcd}$$

then $(U * \varphi) * V = U * (\varphi * V) = U * \varphi * V$;

(IV) If

$$\begin{tikzcd} \bullet \arrow[r, "V"] & \bullet \arrow[r, bend left=60] \arrow[r] \arrow[r, bend right=60] \arrow[r, phantom, shift left=3ex, "\Downarrow\varphi"] \arrow[r, phantom, shift right=3ex, "\Downarrow\psi"] & \bullet \arrow[r, "U"] & \bullet \end{tikzcd}$$

then $U * (\psi \circ \varphi) * V = (U * \psi * V) \circ (U * \varphi * V)$;

(V) If

$$\begin{tikzcd} \bullet \arrow[r, bend left, "F"] \arrow[r, bend right, "G"'] \arrow[r, phantom, "\Downarrow\varphi"] & \bullet \arrow[r, bend left, "U"] \arrow[r, bend right, "V"'] \arrow[r, phantom, "\Downarrow\psi"] & \bullet \end{tikzcd}$$

then $(\psi * G) \circ (U * \varphi) = (V * \varphi) \circ (\psi * F)$.

In slightly more modern terminology, the *horizontal composition* of two transformations φ and ψ as in the following situation:

$$
\begin{tikzcd}
\mathbb{C} \arrow[r, bend left, "F"] \arrow[r, bend right, "G"'] \arrow[r, phantom, "\Downarrow\varphi"] & \mathbb{D} \arrow[r, bend left, "U"] \arrow[r, bend right, "V"'] \arrow[r, phantom, "\Downarrow\psi"] & \mathbb{E}
\end{tikzcd}
$$

is defined to be either side of the equation in (V), and denoted by $\psi * \varphi$: it is therefore the transformation $UF \to VG$ whose A-th component, for $A \in \mathbb{C}$, is either leg of the following square, which commutes by virtue of the naturality of ψ:

$$
\begin{tikzcd}
UF(A) \arrow[r, "\psi_{F(A)}"] \arrow[d, "U(\varphi_A)"'] & VF(A) \arrow[d, "V(\varphi_A)"] \\
UG(A) \arrow[r, "\psi_{G(A)}"] & UG(A)
\end{tikzcd}
$$

It turns out that horizontal composition is associative and unitary; moreover, it is coherent with vertical composition in the following sense. Suppose we are in the situation depicted below:

$$
\begin{tikzcd}
\mathbb{C} \arrow[r, bend left=60] \arrow[r] \arrow[r, bend right=60] \arrow[r, phantom, shift left=3ex, "\Downarrow\varphi"] \arrow[r, phantom, shift right=3ex, "\Downarrow\psi"] & \mathbb{D} \arrow[r, bend left=60] \arrow[r] \arrow[r, bend right=60] \arrow[r, phantom, shift left=3ex, "\Downarrow\varphi'"] \arrow[r, phantom, shift right=3ex, "\Downarrow\psi'"] & \mathbb{E}
\end{tikzcd}
$$

with φ, ψ, φ' and ψ' natural transformations. Then one can prove the following identity (the *interchange law*) as a consequence of the naturality of φ, ψ, φ' and ψ':

$$(\psi' \circ \varphi') * (\psi \circ \varphi) = (\psi' * \psi) \circ (\varphi' * \varphi),$$

which makes the category $\mathbb{C}\mathrm{at}$ of small categories, functors and natural transformations a 2-category. In fact, under the hypothesis of associativity and unitarity of $\circ$, we have that the five rules of the Godement calculus are *equivalent* to the interchange law together with associativity and unitarity of horizontal composition (in the sense that assuming the five Godement rules one can prove the properties of horizontal composition without referring to naturality conditions, and vice versa). Hence why in the literature (for example, in [EK66] and [Kel72a]) the Godement calculus is usually intended as the set of two operations on natural transformations, vertical and horizontal composition, both of which being associative and unitary and satisfying the interchange law.

Extraordinary natural transformations. Of course one can expand the Godement calculus to contravariant functors and functors of many variables by using dual categories and product of categories. However, Eilenberg and Kelly [EK66] recognised that there are interesting situations not covered by the notion of natural transformation. Take again the category $\mathbb{S}\mathrm{et}$ (or any cartesian closed category). For every pair of sets A and B, denote by $A \Rightarrow B$ the set of all functions from A to B. ($(-) \Rightarrow (-)$ is a functor $\mathbb{S}\mathrm{et}^{\mathrm{op}} \times \mathbb{S}\mathrm{et} \to \mathbb{S}\mathrm{et}$, contravariant in its first argument and covariant in the second.) We have the evaluation function

$$\begin{array}{ccc} A \times (A \Rightarrow B) & \xrightarrow{eval_{A,B}} & B \\ (a, f) & \longmapsto & f(a) \end{array}$$

and therefore a family of morphisms $eval = (eval_{A,B})_{A,B \in \mathbb{S}\mathrm{et}}$. If we fix the set A, as a family in B it is indeed a natural transformation; if we fix B though, the assignment $A \longmapsto A \times (A \Rightarrow B)$ is not even a functor, because A appears both covariantly and contravariantly at once. However, the following *is* indeed a functor:

$$\begin{array}{ccc} \mathbb{S}\mathrm{et} \times \mathbb{S}\mathrm{et}^{\mathrm{op}} \times \mathbb{S}\mathrm{et} & \xrightarrow{F} & \mathbb{S}\mathrm{et} \\ (X, Y, Z) & \longmapsto & X \times (Y \Rightarrow Z) \end{array}$$

and $eval_{-,B}$ still satisfies a “universal equational property” that resembles naturality: for all $f \colon A \to A'$, the following square commutes:

$$\begin{tikzcd} A \times (A' \Rightarrow B) \arrow[r, "1 \times (f \Rightarrow 1)"] \arrow[d, "f \times (1 \Rightarrow 1)"'] & A \times (A \Rightarrow B) \arrow[d, "eval_{A,B}"] \\ A' \times (A' \Rightarrow B) \arrow[r, "eval_{A',B}"] & B \end{tikzcd}$$

Notice how the f “jumps”, as it were, from the covariant to the contravariant argument of F in the two legs of the square. Eilenberg and Kelly designed a generalised notion of natural transformation, which are now known as *extranatural transformations*, to take into account transformations like *eval*.

Definition ([EK66])**.** Let $F \colon \mathbb{A} \times \mathbb{B}^{\mathrm{op}} \times \mathbb{B} \to \mathbb{E}$, $G \colon \mathbb{A} \times \mathbb{C}^{\mathrm{op}} \times \mathbb{C} \to \mathbb{E}$ be functors. An *extranatural* transformation $\varphi \colon F \to G$ is a family of morphisms in $\mathbb{E}$

$$\varphi = (\varphi_{A,B,C} \colon F(A, B, B) \to G(A, C, C))_{A \in \mathbb{A}, B \in \mathbb{B}, C \in \mathbb{C}}$$

such that for all $f \colon A \to A'$, $g \colon B \to B'$, $h \colon C \to C'$ in $\mathbb{A}$, $\mathbb{B}$ and $\mathbb{C}$ respectively, the following diagrams commute:

$$\begin{tikzcd} F(A, B, B) \arrow[r, "\varphi_{A,B,C}"] \arrow[d, "F(f,1,1)"'] & G(A, C, C) \arrow[d, "G(f,1,1)"] \\ F(A', B, B) \arrow[r, "\varphi_{A',B,C}"] & G(A', C, C) \end{tikzcd} \qquad \begin{tikzcd} F(A, B', B) \arrow[r, "F(1,g,1)"] \arrow[d, "F(1,1,g)"'] & F(A, B, B) \arrow[d, "\varphi_{A,B,C}"] \\ F(A, B', B') \arrow[r, "\varphi_{A,B',C}"] & G(A, C, C) \end{tikzcd}$$

$$\begin{tikzcd}
F(A,B,B) \arrow[r, "\varphi_{A,B,C}"] \arrow[d, "\varphi_{A,B,C'}"'] & G(A,C,C) \arrow[d, "G(1,1,h)"] \\
G(A,C',C') \arrow[r, "G(1,h,1)"] & G(A,C,C')
\end{tikzcd} \qquad \square$$

If we take $\mathbb{B}$ and $\mathbb{C}$ to be the terminal category, then we are left with the usual naturality square; this is why we say that φ is "natural in A" and "properly extranatural" in B and C. This also shows that an extranatural transformation can depend on fewer than three variables. At the same time, if we replace $\mathbb{A}$, $\mathbb{B}$ and $\mathbb{C}$ with products $\mathbb{A}_1 \times \cdots \times \mathbb{A}_n$, $\mathbb{B}_1 \times \cdots \times \mathbb{B}_t$ and $\mathbb{C}_1 \times \cdots \times \mathbb{C}_s$, then we obtain a definition of extranaturality for families of morphisms

$$\varphi_{A_1,\dots,A_n,B_1,\dots,B_t,C_1,\dots,C_s} \colon F(A_1 \dots A_n, B_1 \dots B_t, B_1 \dots B_t) \to \\ \to G(A_1 \dots A_n, C_1 \dots C_s, C_1 \dots C_s).$$

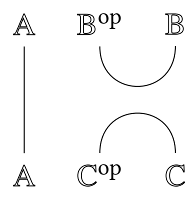
This means that extranatural transformations can depend on an arbitrary number of variables, but with a crucial constraint: every variable has to appear *exactly twice* between F and G; either once in F and once in G like the A_i's, or twice in F and never in G like the B_i's, or twice in G and never in F like the C_i's.

Extranatural transformations, however, share the same fate of dinaturals: they do not compose. For if $H \colon \mathbb{A} \times \mathbb{D}^{\mathrm{op}} \times \mathbb{D} \to \mathbb{E}$ is a functor and $\psi_{A,C,D} \colon G(A,C,C) \to H(A,D,D)$ is extranatural, then the composition

$$F(A,B,B) \xrightarrow{\varphi_{A,B,C}} G(A,C,C) \xrightarrow{\psi_{A,C,D}} H(A,D,D)$$

is a family of morphisms depending on A, B, C and D, therefore is not a well-defined extranatural transformation $F \to H$, as C never appears in any of these functors. Even if we allowed for variables to either appear twice or not at all, the above family would be (extra)natural in C only when it is constant in C, which in general is not true (Example (1.15) shows transformations φ and ψ with $\mathbb{A} = \mathbb{B} = \mathbb{D} = \mathbb{I}$, $\mathbb{I}$ being the terminal category, whose composite is not constant, hence not extranatural).

Nevertheless, Eilenberg and Kelly found a sufficient and also essentially necessary condition for φ and ψ to compose, by associating to each of them a *graph* (the archetype of a string diagram) whose vertices are the categories involved by F, G and H, and the links connect the vertices corresponding to those arguments of F, G and H that are set to be equal when we write the general components of φ and ψ. For a $\varphi_{A,B,C} \colon F(A,B,B) \to G(A,C,C)$ then, its graph would be:



Eilenberg and Kelly's result asserts that if the composite graph of φ and ψ is *acyclic*, then the composite transformation is again extranatural, see Theorem (1.37) and discussion afterwards. The condition of acyclicity will be central to our compositionality result for dinatural transformations (Theorem (1.38)).

Dinatural transformations. Four years after Eilenberg and Kelly's paper, Dubuc and Street introduced the notion of *dinatural transformation* for the first time in [DS70], as a common setting for natural and properly extranatural transformations.

Definition ([DS70])**.** Let $F \colon \mathbb{C}^{\mathrm{op}} \times \mathbb{C} \to \mathbb{D}$ and $G \colon \mathbb{C}^{\mathrm{op}} \times \mathbb{C} \to \mathbb{D}$ be functors. A *dinatural transformation* $\varphi \colon F \to G$ is a family of morphisms in $\mathbb{D}$

$$\varphi = (\varphi_A \colon F(A,A) \to G(A,A))_{A \in \mathbb{C}}$$

such that for all $f \colon A \to B$ in $\mathbb{C}$, the following hexagon commutes:

$$\begin{tikzcd} & F(A,A) \arrow[r, "\varphi_A"] & G(A,A) \arrow[dr, "G(1,f)"] & \\ F(B,A) \arrow[ur, "F(f,1)"] \arrow[dr, "F(1,f)"'] & & & G(A,B) \\ & F(B,B) \arrow[r, "\varphi_B"'] & G(B,B) \arrow[ur, "G(f,1)"'] & \end{tikzcd}$$ □

The reason for which they are called *di*natural is that their components are arrows between the values of the functors computed on the diagonal. In [DS70], the authors provide some results studying the connections between naturals and dinaturals, and a few examples of dinatural transformations occurring in Category Theory; a particularly interesting one is given by the *Church numerals*: for any category $\mathbb{C}$, if

$$\mathrm{Hom}_{\mathbb{C}} \colon \mathbb{C}^{\mathrm{op}} \times \mathbb{C} \to \mathbb{S}\mathrm{et}$$

is the Hom-functor and n is a natural number, the family of morphisms

$$n_A \colon \mathrm{Hom}_{\mathbb{C}}(A,A) \to \mathrm{Hom}_{\mathbb{C}}(A,A)$$

given by $n_A(f) = f^n$, that is the n-th iterated composition of f with itself, is dinatural. (See Example (1.12) for more details.)

If $\varphi \colon F \to G$ is dinatural, and F and G are both dummy in the first variable, then φ is in fact natural; if F or G is constant, then φ is properly extranatural. In particular, dinatural transformations do not compose, since extranaturals do not either, but the reason for which they do not is even more striking: consider $\psi \colon G \to H$ dinatural and the composite family $\psi \circ \varphi = (\psi_A \circ \varphi_A)_{A \in \mathbb{C}}$. Saying that $\psi \circ \varphi$ is dinatural means that the outer hexagon in the following diagram commutes for all $f\colon A \to B$:

$$
\begin{tikzcd}
 & F(A,A) \arrow[rr, "\varphi_A"] & & G(A,A) \arrow[rr, "\psi_A"] \arrow[dr, "G(1,f)"] & & H(A,A) \arrow[dr, "H(1,f)"] & \\
F(B,A) \arrow[ur, "F(f,1)"] \arrow[dr, "F(1,f)"'] & & G(B,A) \arrow[ur, "G(f,1)"] \arrow[dr, "G(1,f)"'] & & G(A,B) & & H(A,B) \\
 & F(B,B) \arrow[rr, "\varphi_B"'] & & G(B,B) \arrow[rr, "\psi_B"'] \arrow[ur, "G(f,1)"'] & & H(B,B) \arrow[ur, "H(f,1)"'] &
\end{tikzcd}
$$

There is no way, in general, to infer the commutativity of the outer hexagon from that of the two inner ones. Yet, as we shall see, dinatural transformations are a key categorical tool in the semantics of programming languages.

Ad hoc compositionality in denotational semantics

Denotational semantics is a methodology in Computer Science that gives mathematical meaning to programming languages. It assigns to each expression in the language a mathematical structure, its *denotation*, often of an algebraic nature: by understanding the mathematical properties of these structures, one automatically understands the computational properties of their counterparts.

A crucial feature of denotational semantics is the compositionality paradigm: the mathematical denotation of a composite program has to be given in terms of the denotations of its minor parts. This allows us to study arbitrarily complex programs by first decomposing them and analysing the smaller blocks they are made of, and then composing their interpretations in the mathematical world, as it were.

Despite the fact that dinatural transformations fail to compose, they have been found extremely useful in denotational semantics. We now explore how computer scientists have managed to get round the problem of compositionality in a few examples of applications of dinatural transformations in the semantics of programming languages.

Parametric polymorphism. *Polymorphism* is a feature of many typed programming languages, whereby some functions are defined over multiple types at once. For example, say that f is a function of argument α which returns objects of type β: f has then type $\alpha \Rightarrow \beta$. Given a list L of type $\mathrm{List}(\alpha)$, we can imagine a function *map* which applies f to each element of L, yielding therefore a new list L' of type $\mathrm{List}(\beta)$. We have then that *map* is a polymorphic function of type

$$(\alpha \Rightarrow \beta, \mathrm{List}(\alpha)) \Rightarrow \mathrm{List}(\beta).$$

The algorithm defining *map* is completely independent of α and β: no matter their nature, *map* acts in the exact same way on arbitrary inputs of the appropriate type. This is an instance of what Strachey called *parametric* polymorphism [Str67]. Strachey distinguished also another notion of polymorphism, named *ad hoc* polymorphism, to refer to those polymorphic functions whose algorithm does change when we instantiate them at different types. The typical arithmetic operators, such as +, fall into this category: the algorithm computing the sum of two integers differs from the one that adds together two floating-point numbers.

From the mathematical point of view, an extension of the typed λ-calculus that allows for variable types, that is a higher-order λ-calculus, was independently developed by Girard [Gir72] (which he called *System F*) and Reynolds [Rey74]; the latter proposed it as a syntax for Strachey's parametric polymorphism. The semantics of this calculus though has a particularly difficult story: Reynolds [Rey83] suggested that it might have a set-theoretical interpretation, but later [Rey84] showed that the only set model is trivial. However, Pitts [Pit87] proved that if we limit ourselves in the realm of *constructive* (intuitionistic) set theory, then it is indeed possible to give proper models to the Girard-Reynolds calculus.

The starting point of Bainbridge, Girard, Scedrov and Scott [BFSS90] was indeed to understand how to interpret the terms of the polymorphic λ-calculus without using set models. They looked at the polymorphic identity term, which is

$$\Lambda\alpha.\, (\lambda x^{\alpha}.\, x) \colon \forall\alpha.\, (\alpha \Rightarrow \alpha).$$

This means that $\Lambda\alpha.\, (\lambda x^{\alpha}.\, x)[A] = \lambda x^{A}.\, x$: once the polymorphic identity is instantiated at a type A we obtain the simply-typed identity function on A. Hence $\Lambda\alpha.\, (\lambda x^{\alpha}.\, x)$ is a *type-indexed family of identity functions.*

One would therefore be tempted to define $\forall\alpha.\, (\alpha \Rightarrow \alpha)$ as the product $\Pi_A(A \Rightarrow A)$ over all types, but such a product is simply too big: it also contains those *ad hoc* elements that do not comply with the parametricity paradigm. In [Rey83], Reynolds proposes to consider only parametric elements of this product by means of certain invariance conditions, that capture Strachey's intuition, in the context of a set-theoretical model which, as we said, does not exist.

Bainbridge et al.'s approach was to interpret the uniformity conditions of parametric terms as *naturality* conditions: they interpreted types as functors and terms as natural transformations, all defined over a fixed cartesian closed category $\mathbb{C}$ of "ground" types. In particular, the function space $\alpha \Rightarrow \beta$ is interpreted by the internal hom-functor $(-) \Rightarrow (-) \colon \mathbb{C}^{\mathrm{op}} \times \mathbb{C} \to \mathbb{C}$, which is contravariant in its first argument and covariant in the second. This immediately poses a problem: we need more than mere natural transformations, as they are defined between covariant functors only. *Dinatural transformations* are precisely what we require: in [BFSS90] the authors gave a semantic approximation to Strachey's notion of parametric polymorphism by means of certain dinatural transformations over a specific cartesian closed category. (In particular, the type $\forall\alpha.\, (\alpha \Rightarrow \alpha)$ is interpreted using the *end* [Yon60] of the hom-functor, which involves a universal dinatural transformation.)

But how did they tackle the "most perverse aspect of the calculus of dinatural transformations" (*sic*), namely the failure of composition? The answer is: with ad hoc arrangements. They took $\mathbb{C}$ to be the category $\mathbb{P}$er of partial equivalence relations (that is, symmetric and transitive relations) over the natural numbers and they considered particular families of morphisms, called *realizable families*, between functors of mixed variance over $\mathbb{P}$er. The authors did not know if realizable families were automatically dinatural (Freyd, Robinson and Rosolini gave sufficient conditions for the dinaturality of realizable families in [FRR92]), but they proved that realizable dinatural transformations do compose by using a crucial property of $\mathbb{P}$er: namely the fact that every morphism in $\mathbb{P}$er can be decomposed into isomorphisms and "I-maps", for I a specific subcategory of $\mathbb{P}$er, see [BFSS90, Proposition 2.4]. They then showed that the realizable families used to interpret the terms of the polymorphic λ-calculus are all dinatural, hence, as far as they were concerned, the compositionality problem of dinatural transformations posed no further issues.

Intuitionistic logic and λ-calculus. Girard, Scedrov and Scott [GSS92] interpreted the simply typed λ-calculus with type variables, that is essentially the fragment of the Girard-Reynolds calculus where type variables are quantified only *implicitly* over all the possible types (but the quantification is not encoded into the syntax of the calculus), using the same "recipe" provided in [BFSS90], but in an *arbitrary* cartesian closed category $\mathbb{C}$. Hence, types are mixed-variance functors and terms are families of morphisms, all built using the cartesian closed structure of $\mathbb{C}$: such functors and transformations are called *definable*. The two main results are that definable transformations are actually dinatural and they always compose; an important consequence of this is that well-formed terms provably satisfy dinaturality equations in the λ-calculus, in addition to those given by axiom, like the β-η rules. (We shall discuss the example of the dinaturality equation for *filter* in the next paragraph, on p. 16.)

Girard, Scedrov and Scott made use of the Curry-Howard correspondence [GLT89] to translate valid λ-terms in normal form into normal natural deduction proofs in intuitionistic logic. Such proofs arise from (possibly many) cut-free proofs in the sequent calculus, which in turn translate to certain closed λ-terms: these terms yield the definable transformations mentioned above. They proved that definable transformations are always dinatural by induction on *cut-free* Gentzen sequent proofs: they analysed each inference rule of the intuitionistic sequent calculus, except—crucially—the cut rule, and assuming a dinatural transformation is given for every premiss of the rule, they constructed a transformation interpreting the conclusion and proved that it is still dinatural. (The axiom is interpreted by an identity natural transformation; the other rules by making use of the cartesian closed structure.) They showed the dinaturality of the resulting transformation "by hand", as it were, but in fact one can easily apply the compositionality theorem (1.38) proved in this thesis to their case: it is very easy to see that the graph of the transformations associated with the conclusion of each rule is always acyclic, hence dinatural.

The key to circumvent the compositionality problem of dinatural transformations was indeed the ability to ignore the cut rule:

$$\frac{\Gamma \vdash A \quad \Delta, A \vdash B}{\Gamma, \Delta \vdash B}$$

For simplicity, suppose Δ is empty, and suppose that $\varphi \colon F \to G$ is the dinatural transformation interpreting the sequent $\Gamma \vdash A$, while $\psi \colon G \to H$ interprets $A \vdash B$. The obvious transformation interpreting the conclusion is indeed $\psi \circ \varphi$, which in general is not dinatural (and indeed, if we try to draw their graphs, they can well form cycles upon composition). However, thanks to Gentzen's cut-elimination theorem, and the fact that a cut-elimination step yields β-η equivalent terms (hence equal families of morphisms), there is no need to consider the cut-rule, as $\psi \circ \varphi$ above is equal to another transformation arising from a cut-free derivation, hence dinatural.

It is clear, then, that all that Girard, Scedrov and Scott proved (far from being of little importance!) is that the dinatural transformations arising from the cartesian closed structure of a category always compose, and given that such transformations are all they were interested in, they were satisfied with the result. Blute [Blu93] generalised their result for multiplicative Linear Logic [Gir87], both classical and intuitionistic. In his case, therefore, he interpreted deductions as families of morphisms in a symmetric monoidal closed (intuitionistic case) or $*$-autonomous category (classical) $\mathbb{C}$, using the closed structure of $\mathbb{C}$; he then proved they compose again by using a cut-elimination technique in a similar way to [GSS92]. As we have mentioned at the beginning, this thesis takes a very different approach: we shall consider *arbitrary* dinatural transformations φ and ψ between functors of arbitrary variance over arbitrary categories, and we will find a sufficient condition for the dinaturality of $\psi \circ \varphi$ that generalises Eilenberg and Kelly's result about extranatural transformations.

Dinaturality and parametricity. A similar result to Girard et al. about dinaturality of polymorphic terms had already been noticed by Wadler [Wad89] in his famous *Theorems for free!*. In there, Wadler gave a *relational* semantics of the polymorphic λ-calculus and proved it satisfies *parametricity*, in the following sense: if one instantiates a term of a polymorphic type at two related types, then the two values obtained are themselves related. He then showed how to deduce, using parametricity, equational properties "for free" satisfied by every term of a given type, for arbitrary types. Take, for example, the polymorphic function *filter*, of type

$$\forall \alpha. \big((\alpha \Rightarrow \mathbb{B}\mathrm{ool}, \mathrm{List}(\alpha)) \Rightarrow \mathrm{List}(\alpha)\big)$$

which, given a property $p \colon \alpha \Rightarrow \mathbb{B}\mathrm{ool}$ and a list L of type $\mathrm{List}(\alpha)$, returns a list L' obtained from L by keeping only those elements of L that satisfy p. The "theorem for free" that Wadler found says that for every function $f \colon A \Rightarrow B$, $p \colon A \Rightarrow \mathbb{B}\mathrm{ool}$

and for every list $L\colon \mathrm{List}(A)$ we have, if we denote, for short, by f^* the function $\mathit{map}[A,B](f,\cdot)\colon \mathrm{List}(A) \Rightarrow \mathrm{List}(B)$,

$$f^*\big(\mathit{filter}[A](p \circ f, L)\big) = \mathit{filter}[B]\big(p, f^*(L)\big).$$

This equational property is, in fact, a dinaturality equation, as it is tantamount to the commutativity of the following hexagon (in $\mathbb{S}\mathrm{et}$, say):

$$\begin{tikzcd}
& (A \Rightarrow \mathbb{B}\mathrm{ool}) \times \mathrm{List}(A) \arrow[r, "\mathit{filter}[A]"] & \mathrm{List}(A) \arrow[dr, "f^*"] & \\
(B \Rightarrow \mathbb{B}\mathrm{ool}) \times \mathrm{List}(A) \arrow[ur, "(f \Rightarrow \mathbb{B}\mathrm{ool}) \times 1"] \arrow[dr, "1 \times f^*"'] & & & \mathrm{List}(B) \\
& (B \Rightarrow \mathbb{B}\mathrm{ool}) \times \mathrm{List}(B) \arrow[r, "\mathit{filter}[B]"'] & \mathrm{List}(B) \arrow[ur, "1"'] &
\end{tikzcd}$$

Later on, Plotkin and Abadi [PA93] formally proved that dinaturality is a consequence of relational parametricity.

Dinaturality in System F. As we said, Girard et al. gave an interpretation of term judgments in the simply-typed λ-calculus with type variables (with no explicit quantifications over the types) using dinatural transformations over an arbitrary cartesian closed category $\mathbb{C}$. In particular, if $\mathbb{C}$ is the syntactic category generated by the calculus, then we have that every valid term is indeed a dinatural transformation. What happens if we consider the full second-order λ-calculus, that is Girard's System F? Lataillade [Lat09] showed that *not every term* in System F, seen as a family of morphisms in the syntactic category generated by the calculus, is in fact dinatural. For example, the term

$$t = \lambda x^{\forall Y.(Y \Rightarrow Y)}.\, \lambda y^X.\, (x[X])(y),$$

which is valid, is not dinatural in X, in the sense that the family of terms $\big(t[A/X]\big)_A$ is not a dinatural transformation in the syntactic category. Indeed, for it to be dinatural it should be the case that, for all valid terms $f\colon B \to C$,

$$\lambda x^{\forall Y.(Y \Rightarrow Y)}.\, \lambda y^B.\, f\big((x[B])(y)\big) = \lambda x^{\forall Y.(Y \Rightarrow Y)}.\, \lambda y^B.\, (x[C])(f(y))$$

which is not true in general. The criterion found by Lataillade is very simple: a term is dinatural in X if and only if its normal form contains no type instantiation where X appears as a free variable. (In our t above, X is free and appears in a type instantiation.)

Note that this is not in contrast with Bainbridge et al.'s [BFSS90] result. What they proved was that *every* valid term generates a dinatural transformation, that is true, but *over a specific model*, namely the category $\mathbb{P}\mathrm{er}$ of partial equivalence relations on $\mathbb{N}$. Lataillade's result is, in fact, stronger: he put himself in the free category generated by the calculus, hence anything that is dinatural in Lataillade's sense is dinatural in *any* model of System F; but saying that a term s is not dinatural in the syntactic category does not mean that s is not dinatural in any model. Indeed, our t above, interpreted using realizable dinatural transformations in $\mathbb{P}$er, is dinatural by Bainbridge et al.'s theorem. This means, therefore, that although not every valid term is provably dinatural in System F, it is not inconsistent to *impose* dinaturality (for example, by requiring relational parametricity as in [PA93]).

Other applications of dinatural transformations

Structural polymorphism. A few years after his paper with Bainbridge, Scedrov and Scott, Freyd [Fre93] used a different approach to give a semantics of parametric polymorphism: instead of considering "mixed-variance" natural transformations (that is, dinatural), he generalised the concept of functor, introducing the notion of *structor*. Given categories $\mathbb{A}$ and $\mathbb{B}$, a structor S from $\mathbb{A}$ to $\mathbb{B}$ is a function from the morphisms of $\mathbb{A}$ to the spans in $\mathbb{B}$ that carries a map $f : A \to B$ to

$$S(A) \xleftarrow{l(f)} S(f) \xrightarrow{r(f)} S(B),$$

where if f is an identity, then the span above consists only of identity morphisms, and the objects $S(A)$ and $S(B)$ depend only on A and B respectively. A transformation of structors from S to $T : \mathbb{A} \to \mathbb{B}$ is a family of morphisms in B indexed by the morphisms of $\mathbb{A}$:

$$(\varphi_f : S(f) \to T(f))_{f : A \to B}$$

such that for all $f : A \to B$ the following diagram commutes:

$$\begin{tikzcd} S(A) \arrow[d, "\varphi_{id_A}"'] & S(f) \arrow[l] \arrow[r] \arrow[d, "\varphi_f"] & S(B) \arrow[d, "\varphi_{id_B}"] \\ T(A) & T(f) \arrow[l] \arrow[r] & T(B) \end{tikzcd}$$

Structor transformations do compose, of course. One can see ordinary covariant functors $F : \mathbb{A} \to \mathbb{B}$ as structors sending $f : A \to B$ to

$$F(A) \xleftarrow{id} F(A) \xrightarrow{F(f)} F(B)$$

and contravariant functors $G : \mathbb{A}^{\mathrm{op}} \to \mathbb{B}$ as structors mapping $f : A \to B$ to

$$G(A) \xleftarrow{G(f)} G(B) \xrightarrow{id} G(B).$$

Ordinary natural transformations between covariant functors are in natural correspondence with the transformations of the associated structors.

Given a functor $F\colon \mathbb{A}^{\mathrm{op}} \times \mathbb{A} \to \mathbb{B}$, F gives rise to two structors: its *left diagonalization* $\blacktriangledown F$, that sends $f\colon A \to B$ to

$$F(A,A) \xleftarrow{F(f,id_A)} F(B,A) \xrightarrow{F(id_B,f)} F(B,B)$$

and, if it exists, its *right diagonalization*, $F\blacktriangledown$, that sends $f\colon A \to B$ to the top-left span of the pullback diagram:

$$\begin{tikzcd} F\blacktriangledown(f) \arrow[r] \arrow[d] & F(B,B) \arrow[d, "F(f,id_B)"] \\ F(A,A) \arrow[r, "F(id_A,f)"] & F(A,B) \end{tikzcd}$$

Then if $\mathbb{B}$ has pullbacks, it can be easily seen that the dinatural transformations $F \to G$ are in natural correspondence with the structor transformations $\blacktriangledown F \to G\blacktriangledown$. Hence, dinaturals are transformations between structors of a particular shape.

Freyd's way to bypass the compositionality problem of dinatural transformations when interpreting the polymorphic λ-calculus is to use structors and structor transformations instead. He proved that if $\mathbb{B}$ is cartesian closed with pullbacks then so is the category of structors from $\mathbb{A}$ to $\mathbb{B}$, for any $\mathbb{A}$. This means that one can interpret the simply-typed λ-calculus with type variables (like Girard, Scedrov and Scott did in [GSS92]) using the cartesian closed structure of endo-structors and transformations between them over an arbitrary cartesian closed category with pullbacks.

To interpret quantified types, Freyd introduced the notion of *binding* of a structor $S\colon \mathbb{A} \to \mathbb{B}$, when it exists, as an object of $\mathbb{B}$, denoted $\forall X.\, S(X)$, together with a canonical structor transformation $\forall X.\, S(X) \to S$. It is very reminiscent of the notion of end of a functor, and indeed if $F\colon \mathbb{A}^{\mathrm{op}} \times \mathbb{A} \to \mathbb{B}$ is an ordinary functor, its end is precisely the binding of $\blacktriangledown F$. Freyd finally interpreted the second-order λ-calculus using *realizable* structors and realizable transformations between them (appropriately defined) over the category of partial equivalence relations on $\mathbb{N}$, by showing that the category of realizable endo-structors is indeed cartesian closed with pullbacks and that every realizable endo-structor has a binding.

Dinatural numbers. Paré and Román [PR98], inspired by how Bainbridge, Girard, Scedrov and Scott circumvented the compositionality problem of dinatural transformations by working in a specific category ($\mathbb{P}$er) where the transformations they were interested in do compose, due to their special form and the peculiar properties of $\mathbb{P}$er, wondered how much one can say about dinaturals over nice categories like $\mathbb{S}$et. In particular, they focused on the following question: we have seen that natural numbers define dinatural transformations $\mathrm{Hom}_{\mathbb{C}} \to \mathrm{Hom}_{\mathbb{C}}$ by iterated composition for any category $\mathbb{C}$; is it true that *every* dinatural transformation $\varphi\colon \mathrm{Hom}_{\mathbb{C}} \to \mathrm{Hom}_{\mathbb{C}}$ is of the form $\varphi_A(f) = f^n$ for some n natural number, if $\mathbb{C} = \mathbb{S}\mathrm{et}$?

They answered this question negatively by showing a counterexample. However, they introduced a stronger notion of dinatural transformation suggested by Barr, for which the answer to the question above is in fact yes; moreover, these dinaturals do compose. In more detail, a *Barr dinatural transformation* $\varphi\colon \mathbb{A}^{\mathrm{op}} \times \mathbb{A} \to \mathbb{B}$, for $\mathbb{B}$ a category with pullbacks, is a family of morphisms $\varphi_A\colon F(A,A) \to G(A,A)$ such that for all $f\colon A \to B$ in $\mathbb{A}$, the following diagram commutes:

$$\begin{tikzcd}
 & F(A,A) \arrow[r, "\varphi_A"] & G(A,A) \arrow[dr, "G(1{,}f)"] & \\
F_f \arrow[ur] \arrow[dr] & & & G(A,B) \\
 & F(B,B) \arrow[r, "\varphi_B"'] & G(B,B) \arrow[ur, "G(f{,}1)"'] &
\end{tikzcd}$$

where F_f is given by the pullback

$$\begin{tikzcd}
 & F(A,A) \arrow[dr, "F(1{,}f)"] & \\
F_f \arrow[ur] \arrow[dr] & & F(A,B) \\
 & F(B,B) \arrow[ur, "F(f{,}1)"'] &
\end{tikzcd}$$

It is clear that Barr dinaturals are dinaturals. However, the former do compose, thanks to the pullback property that gives a fill-in τ making everything in sight commute:

$$\begin{tikzcd}
 & F(A,A) \arrow[rr, "\varphi_A"] & & G(A,A) \arrow[dr] \arrow[rr, "\psi_A"] & & H(A,A) \arrow[dr] & \\
F_f \arrow[ur] \arrow[dr] \arrow[rr, dotted, "\tau"] & & G_f \arrow[ur] \arrow[dr] & & G(A,B) & & H(A,B) \\
 & F(B,B) \arrow[rr, "\varphi_B"'] & & G(B,B) \arrow[ur] \arrow[rr, "\psi_B"'] & & H(B,B) \arrow[ur] &
\end{tikzcd}$$

By spelling out the definition, a Barr dinatural transformation $\varphi\colon \mathrm{Hom}_{\mathbb{A}} \to \mathrm{Hom}_{\mathbb{A}}$ is a family of morphisms such that for all $k\colon A \to B$, $f\colon A \to A$ and $g\colon B \to B$, if

$k \circ f = g \circ k$ then $k \circ \varphi_A(f) = \varphi_B(g) \circ k$, that is:

$$\begin{tikzcd} A \arrow[r, "f"] \arrow[d, "k"'] & A \arrow[d, "k"] \\ B \arrow[r, "g"] & B \end{tikzcd} \text{ commutes} \Rightarrow \begin{tikzcd} A \arrow[r, "\varphi_A(f)"] \arrow[d, "k"'] & A \arrow[d, "k"] \\ B \arrow[r, "\varphi_B(g)"] & B \end{tikzcd} \text{ commutes.}$$

For example, $\varphi_A(f) = f^n$ is Barr dinatural, because if $k \circ f = g \circ k$ then $k \circ f^n = g^n \circ k$. In fact, every Barr dinatural transformation $\varphi\colon \mathrm{Hom}_{\mathbb{S}\mathrm{et}} \to \mathrm{Hom}_{\mathbb{S}\mathrm{et}}$ is of the form $\varphi_A(f) = f^n$, for n given uniquely by $\varphi_{\mathbb{N}}(s)(0)$, where $\mathbb{N}$ is the set of natural numbers and $s\colon \mathbb{N} \to \mathbb{N}$ is the successor function [PR98, Proposition 1, due to Barr].

Paré and Román rephrased Barr's result for arbitrary monoidal categories $\mathbb{A}$ with a *natural numbers object* [Law63], that is a diagram $I \xrightarrow{0} N \xrightarrow{s} N$ universal among diagrams of the form $A \xrightarrow{f} B \xrightarrow{g} B$, which is used to define an "internal" notion of iterative composition. Then they showed that there is a one-to-one correspondence between the elements of N (i.e. maps $I \to N$) and a specific subclass of Barr dinatural transformations, called *dinatural numbers.* (A dinatural number is a Barr dinatural transformation $\varphi\colon \mathrm{Hom}_{\mathbb{A}} \to \mathrm{Hom}_{\mathbb{A}}$ such that for all A and $g\colon B \to B$ we have $\varphi_{A\otimes B}(g) = id_A \otimes \varphi_B(g)$.) Dinatural numbers have a beautiful arithmetic that really does justice to their names: the transformation $\varphi_A\colon \mathrm{Hom}_{\mathbb{A}}(A,A) \to \mathrm{Hom}_{\mathbb{A}}(A,A)$ defined by $\varphi_A(f) = id_A$ for all $f\colon A \to A$ is a dinatural number, and we shall call it $\underline{0}$. Given a dinatural number φ, one can define $\sigma(\varphi)_A\colon \mathrm{Hom}_{\mathbb{A}}(A,A) \to \mathrm{Hom}_{\mathbb{A}}(A,A)$ as $\sigma(\varphi)_A(f) = f \circ \varphi_A(f)$ and prove it is also a dinatural number, playing the role of the successor of φ. Hence we can define the standard numerals: if n is an ordinary natural number, let $\underline{n} = \sigma(\sigma(\sigma(\dots(\underline{0})\dots)))$, where σ has been applied n times. Then $\underline{n}(f) = f \circ f \circ \dots \circ f$, n times.

The authors then studied the arithmetic of dinatural numbers, defining an operation of addition (that forms a commutative monoid on dinatural numbers with unit $\underline{0}$) and multiplication (monoid, but not commutative, with unit $\underline{1}$). If $\mathbb{A}$ is also closed, then also exponentiation is defined, satisfying some nice coherent properties with addition and multiplication.

Fixed point operators and dinaturality. Yet another application of dinatural transformations in Computer Science is given by *fixed point operators.* The work of Mulry and Simpson shows the intimate connection between the two notions, by demonstrating that the least fixed point operator is a dinatural transformation ([Mul90]) and in fact it is the only one, between the appropriate functors, in many categories of domains ([Sim93]).

Mulry set himself in the category of Scott domains (see, for example, [AJ95]) $\mathbb{D}\mathrm{om}$, where objects are algebraic, bounded cpos (directed-complete partial orders with a least element $\perp$) with countably many compact elements; morphisms are the Scott-continuous functions, i.e. monotone maps preserving directed sups. It is well known that $\mathbb{D}\mathrm{om}$ is cartesian closed and every map f has a least fixed point, namely $\bigvee_{n\in\mathbb{N}} f^n(\perp)$. A *natural numbers object* (nno) in a cartesian closed category $\mathbb{C}$ is now a diagram $1 \xrightarrow{0} N \xrightarrow{s} N$ universal with respect to any other data of the form $1 \xrightarrow{d} D \xrightarrow{F} D$. However, Huwig and Poigné [HP90] proved that any cartesian closed category with fixpoints and a natural numbers object is degenerate (that is, it reduces to a point): $\mathbb{D}\mathrm{om}$ therefore certainly does not have a nno. Although this could have cast doubt on the possibility of any intrinsic, explicit use of natural numbers in relation with fixed point operators, Mulry found a way around the problem: to use a slightly weaker notion of nno, that is what he called an *ordered-natural numbers object* (onno), which is the same as a nno except that it is required to be universal only with respect of data (d, F) with $d \le F(d)$. In $\mathbb{D}\mathrm{om}$ there is indeed a onno: the domain $\mathbb{N}^\infty$, with $0 \le 1 \le 2 \cdots \le \infty$ where $s(n) = n+1$ if $n \ne \infty$, $s(\infty) = \infty$.

Now, take a Scott-continuous function $F\colon D \to D$. By the universality of the onno $\mathbb{N}^\infty$, we have that there is a unique map $T(F)\colon \mathbb{N}^\infty \to D$ such that

$$\begin{tikzcd} 1 \arrow[r, "0"] \arrow[dr, "\perp"'] & \mathbb{N}^\infty \arrow[r, "s"] \arrow[d, "T(F)"] & \mathbb{N}^\infty \arrow[d, "T(F)"] \\ & D \arrow[r, "F"] & D \end{tikzcd}$$

commutes. Since $\perp \le F(\perp)$ and F is monotone, we have a chain $\perp \le F(\perp) \le F^2(\perp)\dots$ in D. By commutativity of the above diagram, we have that $T(F)(0) = \perp$, $T(F)(1) = F(\perp)$, $T(F)(2) = F^2(\perp)$ and so on. Since D is closed under directed sups, $\bigvee F^n(\perp)$ exists and equals $T(F)(\infty)$ by continuity of $T(F)$; moreover it is the least fixed point of F, as we already know. Now, it turns out that the map $T\colon (D \Rightarrow D) \to (D \Rightarrow D)$ is in fact Scott-continuous, hence a morphism in $\mathbb{D}\mathrm{om}$. Since evaluation is continuous, so is the map $\mathit{eval}_\infty\colon (\mathbb{N}^\infty \Rightarrow D) \to D$, evaluation at ∞. Therefore we have that if *lfp* denotes the least fixed point combinator,

$$\mathit{lfp} = \mathit{eval}_\infty \circ T.$$

Mulry then shows how *lfp* is indeed a dinatural transformation $\big((-) \Rightarrow (-)\big) \to \mathit{id}_{\mathbb{D}\mathrm{om}}$, see Example (1.13) for details of the proof. This is tantamount to saying that for any $f\colon D \to E$, $g\colon E \to D$,

$$\mathit{lfp}_E(f \circ g) = f(\mathit{lfp}_D(g \circ f)).$$

He comments that the dinaturality of *lfp* was discovered independently by Freyd (who did not use natural numbers objects) who also observed that *any* dinatural transformation $\big((-) \Rightarrow (-)\big) \to \mathit{id}_{\mathbb{D}\mathrm{om}}$ generates a family of fixpoint operators. For this reason, Simpson [Sim93] calls dinatural transformations between these two functors *fix-dinaturals*.

Although this result gives *lfp* a nice algebraic description as a dinatural transformation and makes evident the role of induction in its definition, Mulry wondered whether *lfp* can be characterised as the *unique* fix-dinatural transformation in some suitable categories of domains. Note that in the category of complete lattices and monotone functions there are at least two such dinatural transformations: the least fixed point and the greatest fixed point operators.

Simpson [Sim93] answered Mulry's question by giving a sufficient condition on subcategories of the category of algebraic cpos $\mathbb{A}\mathrm{lg}\mathbb{C}\mathrm{po}$ for the characterisation to hold, which we now briefly explain. Given an algebraic cpo D and a strict finite chain $C = \{c_0, c_1, \ldots, c_n\} \subseteq D$, with $\perp = c_0 < c_1 < \cdots < c_n$ and $n \geq 0$, he defined the *cokernel* (in $\mathbb{D}\mathrm{om}$) of C as the pushout of the inclusion $i \colon C \to D$ along itself:

$$\begin{tikzcd} C \arrow[r, "i"] \arrow[d, "i"'] \arrow[dr, phantom, "\ulcorner", very near start] & D \arrow[d, "-g"] \\ D \arrow[r, "g"] & E \end{tikzcd}$$

He showed that such a pushout exists by computing it explicitly: it is essentially two copies of D, where the elements of C have been identified, together with a particular order that goes "via the elements of C", as it were. More precisely, one can take E to be the following cpo:

$$E = \{(0,c) \mid c \in C\} \cup \{(1,d) \mid d \in D \setminus C\} \cup \{(-1,d) \mid d \in D \setminus C\},$$

ordered by:

$$(\sigma, d) \leq (\tau, e) \iff d \leq e \text{ and either } \sigma = \tau \text{ or there is } c \in C \text{ such that } d \leq c \leq e.$$

So one can perhaps imagine E as a cpo with the chain C in the middle and two copies of $D \setminus C$, one on its left and the other on its right: two elements d and e are comparable if either they are on the same side of C and are comparable in D, or they are on opposite sides but there is a common central element of C in between the two. The two functions g and $-g$ in the pushout above are defined as

$$g(d) = \begin{cases} (0,d) & d \in C \\ (1,d) & d \notin C \end{cases} \qquad -g(d) = \begin{cases} (0,d) & d \in C \\ (-1,d) & d \notin C \end{cases}$$

Simpson then showed that if D is algebraic, then so is E precisely if all the elements of C are compact. The main result is then the following: *if $\mathbb{K}$ is a cartesian closed full subcategory of* $\mathbb{A}\mathrm{lg}\mathbb{C}\mathrm{po}$ *that is closed under cokernels of strict finite chains of compact elements* (which means that for every algebraic cpo D in $\mathbb{K}$ and for every strict finite chain $C \subseteq D$ of compact elements the cokernel of $i \colon C \to D$ is in $\mathbb{K}$), *then the least fixed point operator lfp is the unique dinatural transformation* $\big((-) \Rightarrow (-)\big) \to id_{\mathbb{K}}$. (This result extends to all the categories of retractions of $\mathbb{K}$'s above, which are cartesian closed and full subcategories of $\mathbb{C}\mathrm{ont}\mathbb{C}\mathrm{po}$, the category of continuous cpos.)

It turns out that this condition is satisfied in many known categories of domains (see [Sim93, Corollary 5.2]), but not all of them: the category of algebraic (complete) lattices is not closed under cokernels of strict finite chains of compact elements. If $\mathbb{C}\mathrm{ont}\mathbb{CL}$ is the cartesian closed full subcategory of $\mathbb{C}\mathrm{ont}\mathbb{C}\mathrm{po}$ whose objects are continuous lattices, Simpson in fact proved that *lfp* is *not* the unique fix-dinatural transformation in any nontrivial cartesian closed full subcategory of $\mathbb{C}\mathrm{ont}\mathbb{CL}$, which includes the algebraic lattices as well.

Kelly's project for coherence problems

We have seen so far important examples and applications of dinatural transformations, and how in some cases the compositionality problem was handled. However, the real frame for the research presented in this thesis is Kelly's project to solve coherence problems abstractly [Kel72a; Kel72b].

The problem of coherence for a certain theory (like monoidal, monoidal closed…) consists in understanding which diagrams necessarily commute as a consequence of the axioms. One of the most famous results is Mac Lane's theorem on coherence for monoidal categories [Mac63]: every diagram built up only using associators and unitors, which are the data that come with the definition of monoidal category, commutes. One of the consequences of this fact is that every monoidal category is monoidally equivalent to a *strict* monoidal category, where associators and unitors are, in fact, identities. From the point of view of logic and semantics, what this tells us is that those operations that one regards as not important (what is sometimes referred to as *bureaucracy*) really are not important. Solving the coherence problem for a theory, therefore, is fundamental to the complete understanding of the theory itself.

Substitution. Coherence problems are concerned with categories carrying an extra structure: a collection of functors and natural transformations subject to various equational axioms. For example, in a monoidal category $\mathbb{A}$ we have $\otimes\colon \mathbb{A}^2 \to \mathbb{A}$, $I\colon \mathbb{A}^0 \to \mathbb{A}$; if $\mathbb{A}$ is also closed then we would have a functor of mixed variance $(-) \Rightarrow (-)\colon \mathbb{A}^{\mathrm{op}} \times \mathbb{A} \to \mathbb{A}$. The natural transformations that are part of the data, like associativity in the monoidal case:

$$\alpha_{A,B,C}\colon (A \otimes B) \otimes C \to A \otimes (B \otimes C),$$

connect not the basic functors directly, but rather functors obtained from them by *iterated substitution*. By "substitution" we mean the process where, given functors

$$K\colon \mathbb{A} \times \mathbb{B}^{\mathrm{op}} \times \mathbb{C} \to \mathbb{D}, \quad F\colon \mathbb{E} \times \mathbb{G} \to \mathbb{A}, \quad G\colon \mathbb{H} \times \mathbb{L}^{\mathrm{op}} \to \mathbb{B}, \quad H\colon \mathbb{M}^{\mathrm{op}} \to \mathbb{C}$$

we obtain the new functor

$$K(F, G^{\mathrm{op}}, H)\colon \mathbb{E} \times \mathbb{G} \times \mathbb{H}^{\mathrm{op}} \times \mathbb{L} \times \mathbb{M}^{\mathrm{op}} \to \mathbb{D}$$

sending (A, B, C, D, E) to $K(F(A, B), G^{\mathrm{op}}(C, D), H(E))$. Hence substitution generalises composition of functors, to which it reduces if we only consider one-variable functors. In the same way, the equational axioms for the structure, like the pentagonal axiom for monoidal categories:

$$\begin{tikzcd}
& (A\otimes B)\otimes(C\otimes D) \arrow[dr, "\alpha_{A,B,C\otimes D}"] & \\
\big((A\otimes B)\otimes C\big)\otimes D \arrow[ur, "\alpha_{A\otimes B,C,D}"] \arrow[d, "\alpha_{A,B,C}\otimes D"'] & & A\otimes\big(B\otimes(C\otimes D)\big) \\
\big(A\otimes(B\otimes C)\big)\otimes D \arrow[r, "\alpha_{A,B\otimes C,D}"'] & A\otimes\big((B\otimes C)\otimes D\big) \arrow[ur, "A\otimes\alpha_{B,C,D}"'] &
\end{tikzcd}$$

involve natural transformations obtained from the basic ones by “substituting functors into them and them into functors”, like $\alpha_{A\otimes B,C,D}$ and $\alpha_{A,B,C} \otimes D$ above.

By substitution of functors into transformations and transformations into functors we mean therefore a generalised *whiskering* operation or, more broadly, a generalised *horizontal composition* of transformations. For these reasons Kelly argued in [Kel72a] that an abstract theory of coherence requires “a tidy calculus of substitution” for functors of many variables and appropriately general kinds of natural transformations, generalising the usual Godement calculus for ordinary functors in one variable and ordinary natural transformations.

One could ask why bother introducing the notion of substitution, given that it is not primitive, as the functor $K(F, G^{\mathrm{op}}, H)$ above can be easily seen to be the usual composite $K \circ (F \times G^{\mathrm{op}} \times H)$. Kelly’s argument is that there is *no need* to consider functors whose codomain is a product of categories, like $F \times G^{\mathrm{op}} \times H$, or the twisting functor $T(A, B) = (B, A)$, or the diagonal functor $\Delta\colon \mathbb{A} \to \mathbb{A}\times\mathbb{A}$ given by $\Delta(A) = (A, A)$, if we consider substitution as an operation on its own. In fact, in some cases these functors are just not enough: take a cartesian closed category $\mathbb{A}$, and consider the diagonal transformation $\delta_A\colon A \to A \times A$, the symmetry $\gamma_{A,B}\colon A \times B \to B \times A$ and the evaluation transformation $eval_{A,B}\colon A \times (A \Rightarrow B) \to B$. It is true that we can see δ and γ as transformations $id_{\mathbb{A}} \to \Delta$ and $\times \to \times \circ T$, but, as we have already noticed, there is no way to involve Δ into the codomain of *eval*, given that the variable A appears covariantly and contravariantly. Kelly suggested, then, to use the same idea of *graph* for extranatural transformations that he had with Eilenberg in the aforementioned [EK66] to natural transformations as well; that is, he proposed to consider natural transformations $\varphi\colon F \to G$ between functors of many variables together with a graph $\Gamma(\varphi)$ that tells us which arguments of F and G are to be equated when we write down the general component of φ.

With the notion of “graph of a natural transformation”, Kelly constructed a full Godement calculus for covariant functors only. His starting point was the observation that the usual Godement calculus essentially asserts that $\mathbb{C}\mathrm{at}$ is a 2-category, as we have seen, but this is saying less than saying that $\mathbb{C}\mathrm{at}$ is actually *cartesian closed*, $- \times B$ having a right adjoint $[B, -]$ for $[B, C]$ the functor category. Since every cartesian closed category is enriched over itself, we have that $\mathbb{C}\mathrm{at}$ is a $\mathbb{C}\mathrm{at}$-category, which is just another way to say 2-category. Now, vertical composition of natural transformations is embodied in $[\mathbb{B}, \mathbb{C}]$, but composition of functors and horizontal composition of natural transformations are embodied in the functor

$$M : [\mathbb{B}, \mathbb{C}] \times [\mathbb{A}, \mathbb{B}] \to [\mathbb{A}, \mathbb{C}]$$

given by the closed structure (using the adjunction and the evaluation map twice). What Kelly does, therefore, is to create a generalised functor category $\{\mathbb{B}, \mathbb{C}\}$ over a category of graphs $\mathbb{P}$ and to show that the functor $\{-, -\}$ is the internal-hom of ${}^{\mathbb{C}\mathrm{at}}\!/_{\mathbb{P}}$, which is then monoidal closed (in fact, far from being cartesian or even symmetric), the left adjoint of $\{\mathbb{B}, -\}$ being denoted as $- \circ \mathbb{B}$. The analogue of the M above, now of the form $\{\mathbb{B}, \mathbb{C}\} \circ \{\mathbb{A}, \mathbb{B}\} \to \{\mathbb{A}, \mathbb{C}\}$, is what provides the desired substitution calculus, see §3.1 for a technical overview.

When trying to deal with the mixed-variance case, however, Kelly ran into problems. He considered the every-variable-twice extranatural transformations, and although he got "tantalizingly close", to use his words, to a sensible calculus, he could not find a way to define a category of graphs that can handle cycles in a proper way. This is the reason for the "I" in the title *Many-Variable Functorial Calculus, I* of [Kel72a]: he hoped to solve these issues in a future paper, which sadly has never seen the light of day. In this thesis we propose a category $\mathbb{G}$ of graphs for transformations of mixed variance that does handle loops, and we hope this can be the first step towards the fulfilment of Kelly's project.

An abstract approach to coherence. Armed with the substitution calculus built, at least in the covariant case, in [Kel72a], Kelly framed the coherence problem in [Kel72b] around the notion of substitution in the following terms. Given basic functors and appropriately natural transformations together with their graphs as above, we can consider the wider class of *allowable* transformations and functors obtained by unlimited composition and substitution. Now, if $\varphi, \psi : T \to S$ are two such allowable transformations with the same domain and codomain, it makes no sense to ask whether they are equal or not unless they have the same graphs, otherwise their general components would not have same domain and codomain objects (because if the graphs are different, then the arguments of T and S to be equated when writing down the general component of φ would be different than those required to be equal by ψ). One then might add a set of axioms requiring certain formally different pairs $\varphi, \psi : T \to S$ with the same graph to coincide (like the two legs of the pentagon axiom in monoidal categories above). The coherence problem for the given structure consists in deciding which other formally different allowable natural transformations necessarily coincide as a consequence of the axioms.

If in [Mac63] the coherence problem for monoidal categories was actually of the form "every diagram commutes", this is not the case for other examples, like [KM71], where Kelly and Mac Lane obtained only a partial result of the form "φ and ψ coincide if they have the same graphs and their domain and codomain are *proper*", that is belong to a specific subset of the allowable functors. An ideal solution to the coherence problem, however, would be to find necessary and sufficient conditions for two allowable transformations to coincide.

Kelly emphasises a crucial point: the allowable functors and natural transformations we have mentioned ought not to form a subcategory $\mathbb{A}\mathrm{ll}(\mathbb{A})$ of the generalised functor category $\{\mathbb{A},\mathbb{A}\}$, because two formally different allowable functors $Q, T \colon \mathbb{A}^n \to \mathbb{A}$ might fortuitously coincide in a particular model $\mathbb{A}$: hence, as Kelly said, "honest allowable transformations $\varphi \colon P \to Q$, $\psi \colon T \to S$ could be composed in $\{\mathbb{A},\mathbb{A}\}$ to form a freak allowable $\psi \circ \varphi$" not writeable in another model $\mathbb{B}$. What we need is therefore a *universal* $\mathbb{A}\mathrm{ll}$ whose objects are *formal* allowable functors and morphisms *formal* allowable natural transformations, completely independent of particular models $\mathbb{A}$. Then we would have that $\varphi = \psi$ in $\mathbb{A}\mathrm{ll}$ if and only if their realisations in $\mathbb{A}$ coincide for all models $\mathbb{A}$ of the theory at matter.

Kelly individuates this universal $\mathbb{A}\mathrm{ll}$ as a *club* $\mathbb{K}$. Without getting into details, a club is a category that admits formal substitution of objects into objects and morphisms into morphisms within itself ($\{\mathbb{A},\mathbb{A}\}$ is an example). To give an extra structure to a category $\mathbb{A}$ by listing basic data and axioms is then the same as giving a functor $\phi \colon \mathbb{K} \to \{\mathbb{A},\mathbb{A}\}$ or, equivalently by adjunction, an action $\theta \colon \mathbb{K} \circ \mathbb{A} \to \mathbb{A}$. What we called allowable functors and transformations would essentially be, in these terms, the objects and morphisms in the image of ϕ, and we have that $u = v$ in $\mathbb{K}$ if and only if $\phi(u) = \phi(v)$ for every model $\mathbb{A}$. All in all, therefore, solving the coherence problem for a given structure is tantamount to calculating the corresponding club $\mathbb{K}$. Moreover, understanding $\mathbb{K}$ also provides knowledge of the free-category-with-structure over $\mathbb{A}$, because the latter is precisely $\mathbb{K} \circ \mathbb{A}$.

In [Kel72b] Kelly shows how to explicitly build $\mathbb{K}$ from a set of generators and relations given by the basic functors and transformations provided by the basic data of the theory, at least in the fully covariant case. He also finds a way to partially discuss the case of transformations like Eilenberg and Kelly's ones, but only provided that the data ensures that no loops can arise upon composing the graphs of formal allowable transformations (in which case, though, there is no functor category $\{\mathbb{A},\mathbb{A}\}$). If loops can in fact happen, then the theory is said to be *not clubbable*, in the sense that we cannot describe its models in terms of a "universal" club.

Our contribution. What we have done in this thesis is, in fact, consider transformations between mixed-variance functors whose type is even more general than Eilenberg and Kelly's, corresponding to $\mathbb{G}^*$ in [Kel72a], recognising that they are a straightforward generalisation of dinatural transformations in many variables. We determine when they compose (Theorem (1.38), (3.31)) by means of a satisfactory property that sounds exactly like Eilenberg and Kelly's result: acyclicity is again the crucial—and only—requirement. We define a working notion of horizontal composition (Definition (2.6)), that we believe will play the role of substitution of dinaturals into dinaturals, precisely as horizontal composition of natural transformation does, as shown by Kelly in [Kel72a]. Next, we form a generalised functor category $\{\mathbb{B}, \mathbb{C}\}$ for these transformations (Definition (3.39)). Finally, we prove that $\{\mathbb{B}, -\}$ has indeed a left adjoint $- \circ \mathbb{B}$, which gives us the definition of a category of formal substitutions $\mathbb{A} \circ \mathbb{B}$ generalising Kelly's one. Although the road paved by Kelly towards a Godement calculus still stretches a long way, our work sets the first steps in the right direction for a full understanding of the compositionality properties of dinatural transformations, which hopefully will be achieved soon.

Notations. Throughout the thesis, $\mathbb{N}$ is the set of natural numbers, including 0, and we shall ambiguously write n for both the natural number n and the set $\{1, \dots, n\}$.

We denote by $\mathbb{I}$ the category with one object and one morphism. Let $\alpha \in \mathrm{List}\{+, -\}$, $|\alpha| = n$, with $|-|$ denoting the length function (and also the cardinality of an ordinary set). We refer to the i-th element of α as α_i. We denote by $\overline{\alpha}$ the list obtained from α by swapping the signs. Given a category $\mathbb{C}$, if $n \geq 1$, then we define $\mathbb{C}^\alpha = \mathbb{C}^{\alpha_1} \times \cdots \times \mathbb{C}^{\alpha_n}$, with $\mathbb{C}^+ = \mathbb{C}$ and $\mathbb{C}^- = \mathbb{C}^{\mathrm{op}}$, otherwise $\mathbb{C}^\alpha = \mathbb{I}$.

If $F \colon \mathbb{C}^\alpha \to \mathbb{D}$ is a functor, we define $F(A|B)$ to be the following object (if A, B are objects) or morphism (if they are morphisms) of $\mathbb{D}$:

$$F(A|B) = F(X_1, \dots, X_{|\alpha|}) \text{ where } X_i = \begin{cases} A & \alpha_i = - \\ B & \alpha_i = + \end{cases}$$

Also, we call $F^{\mathrm{op}} \colon \mathbb{C}^{\overline{\alpha}} \to \mathbb{D}^{\mathrm{op}}$ the *opposite functor*, which is the obvious functor that acts like F between opposite categories.

Composition of morphisms $f \colon A \to B$ and $g \colon B \to C$ will be denoted by $g \circ f$, gf or also $f ; g$. The identity morphism of an object A will be denoted by id_A, 1_A (possibly without subscripts, if there is no risk of confusion), or A itself.

If $f \colon X \to Y$ is a function of sets, and $Z \subseteq X$, we write $f_{\restriction Z} \colon Z \to Y$ for the restriction of f to Z. Given $y \in Y$, the *preimage* of y along f is denoted by $f^{-1}\{y\}$.

Chapter 1

Vertical compositionality

A FULL UNDERSTANDING of how and when dinatural transformations compose is, of course, the very first step towards a proper calculus of dinaturals. Regarding the *how*, the best thing to do is to introduce the notion of *transformation* (§1.1) between two functors, which is simply a family of morphisms that does not have to satisfy any naturality condition. (This simple idea is not, unsurprisingly, new: it appears, for example, in [PR97].) Following Kelly's principle [Kel72a] of having transformations equipped with a *graph* telling us which arguments of the functors involved are to be equated, we shall require that transformations have a *cospan* in $\mathbb{F}\mathrm{in}\mathbb{S}\mathrm{et}$ as part of their data; such a cospan will play the role of the graph of the transformation. In Chapter 3 we shall see how cospans are not quite enough, but for pedagogic simplicity and for clarity of exposure we shall use cospans in this chapter. Transformations then compose, and their graphs compose by computing pushouts in $\mathbb{F}\mathrm{in}\mathbb{S}\mathrm{et}$. The question now is: When is the dinaturality condition preserved, upon composition of transformations? We shall give an actual diagrammatic and computational flavour to our graphs, by interpreting them as *Petri Nets* (§1.2). By reading the dinaturality condition of a transformation as the firing of an enabled transition in the corresponding net, we will find a sufficient (§1.3) and "essentially necessary" (§1.4) condition for two dinatural transformations to compose, thus solving the compositionality problem in its full generality.

§1.1 Dinatural transformations

The category $\mathbb{C}\mathrm{o}\mathbb{S}\mathrm{pan}(\mathbb{C})$. The category $\mathbb{C}\mathrm{o}\mathbb{S}\mathrm{pan}(\mathbb{C})$, for a category $\mathbb{C}$ with pushouts, has been introduced for the first time by [Bén67] as an example of a *bicategory*, which is a weak version of 2-category where associativity and unitarity of composition only hold up to coherent isomorphism. We recall here the usual categorified version of it, obtained—as it is standard—by appropriately quotienting morphisms. For the purposes of this thesis, we are not interested in the 2-cells.

(1.1) Definition. Let $\mathbb{C}$ be a category with pushouts, $f = \left(A \xrightarrow{\sigma} X \xleftarrow{\tau} B\right)$ and $f' = \left(A \xrightarrow{\sigma'} X' \xleftarrow{\tau'} B\right)$ cospans in $\mathbb{C}$. We define an equivalence relation $\sim$ as follows:

$$f \sim f' \iff \exists \pi \colon X \to X' \text{ isomorphism such that } \begin{cases} \sigma' = \pi\sigma \\ \tau' = \pi\tau \end{cases} .$$

In this case, with little abuse of notation, we write $f' = \pi f$. We denote by $[f]$ or also $[\sigma, \tau]$ the equivalence class of f. □

The objects of $\mathbb{C}\mathrm{o}\mathbb{S}\mathrm{pan}(\mathbb{C})$ are the same as those of $\mathbb{C}$, while a morphism $[f] \colon A \to B$ is an equivalence class of cospans in $\mathbb{C}$ as in Definition (1.1):

$$f = \left(A \xrightarrow{\sigma} X \xleftarrow{\tau} B\right).$$

Composition of $[f]$ and $\left[g = \left(B \xrightarrow{\sigma'} Y \xleftarrow{\tau'} C\right)\right]$ is the equivalence class of the cospan $gf = (A \to Z \leftarrow C)$ got by computing the pushout of τ against σ':

(1.2)
$$\begin{tikzcd} & & C \arrow[d, "\tau'"] \\ & B \arrow[r, "\sigma'"] \arrow[d, "\tau"'] \arrow[dr, phantom, "\ulcorner"] & Y \arrow[d, dotted, "\xi"] \\ A \arrow[r, "\sigma"] & X \arrow[r, dotted, "\zeta"] & Z \end{tikzcd}$$

It is easy to see that composition is well defined using the universal property of pushouts. The identity morphism id_A is given by $\left[A \xrightarrow{id_A} A \xleftarrow{id_A} A\right]$.

Generalised dinatural transformations. We now introduce the notion of *transformation* between functors of arbitrary variance. It consists of a family of morphisms equipped with a cospan in $\mathbb{F}\mathrm{in}\mathbb{S}\mathrm{et}$ that tells which arguments of the functors involved are to be set equal when writing down the general component of the family of morphisms. We call this cospan the *type* of the transformation. This is the same idea described by Kelly in [Kel72a, p. 95].

(1.3) Definition. Let $\alpha, \beta \in \mathrm{List}\{+,-\}$, $F \colon \mathbb{C}^\alpha \to \mathbb{D}$, $G \colon \mathbb{C}^\beta \to \mathbb{D}$ functors. A *transformation* $\varphi \colon F \to G$ *of type* $f = \left(|\alpha| \xrightarrow{\sigma} k \xleftarrow{\tau} |\beta|\right)$ (with k positive integer) is a family of morphisms

$$\left(\varphi_{A_1,\dots,A_k} \colon F\left(A_{\sigma 1}, \dots, A_{\sigma|\alpha|}\right) \to G\left(A_{\tau 1}, \dots, A_{\tau|\beta|}\right)\right)_{(A_1 \dots A_k) \in \mathbb{C}^k}.$$

Given $\varphi' \colon F \to G$ of type f', we say that

$$\varphi \sim \varphi' \iff \exists \pi \colon k \to k \text{ isomorphism such that } \begin{cases} f' = \pi f \\ \varphi'_{A_1,\dots,A_k} = \varphi_{A_{\pi 1},\dots,A_{\pi k}} \end{cases} .$$

$\sim$ so defined is an equivalence relation and we denote by $[\varphi]$ the equivalence class of φ. Notice that σ and τ need not be surjective, so we may have unused variables. $\square$

(1.4) Remark. Two transformations are equivalent precisely when they differ only by a permutation of the indexes: they are "essentially the same". For this reason, from now on we shall drop an explicit reference to the equivalence class $[\varphi]$ and just reason with the representative φ, except when defining new operations on transformations, like the vertical composition below.

(1.5) Definition. Let $\varphi \colon F \to G$ of type f be a transformation as in Definition (1.3), $H \colon \mathbb{C}^\gamma \to \mathbb{D}$ and $\psi \colon G \to H$ a transformation of type $g = \left(|\beta| \xrightarrow{\sigma'} p \xleftarrow{\tau'} |\gamma|\right)$, so that we have, for all $B_1, \dots, B_p$,

$$\psi_{B_1,\dots,B_p} \colon G\left(B_{\sigma' 1}, \dots, B_{\sigma' |\beta|}\right) \to H\left(B_{\tau' 1}, \dots, B_{\tau' |\gamma|}\right).$$

The *vertical composition* $[\psi] \circ [\varphi]$ is defined as the equivalence class of $\psi \circ \varphi$, which is the transformation of type

$$gf = |\alpha| \xrightarrow{\zeta\sigma} q \xleftarrow{\xi\tau'} |\gamma|$$

where ζ and ξ are given by (1.2) and $(\psi \circ \varphi)_{C_1,\dots,C_q}$ is the composite:

$$\begin{array}{lll} F\left(C_{\zeta\sigma 1}, \dots, C_{\zeta\sigma|\alpha|}\right) \xrightarrow{\varphi_{C_{\zeta 1},\dots,C_{\zeta k}}} & G\left(C_{\zeta\tau 1}, \dots, C_{\zeta\tau|\beta|}\right) & \\ & \parallel & \\ & G\left(C_{\xi\sigma' 1}, \dots, C_{\xi\sigma'|\beta|}\right) \xrightarrow{\psi_{C_{\xi 1},\dots,C_{\xi p}}} & H\left(C_{\xi\tau' 1}, \dots, C_{\xi\tau'|\gamma|}\right) \end{array}$$

(Notice that by definition $\varphi_{C_{\zeta 1},\dots,C_{\zeta k}}$ requires that the i-th variable of F be the σi-th element of the list $(C_{\zeta 1}, \dots, C_{\zeta k})$, which is indeed $C_{\zeta\sigma i}$.) $\square$

(1.6) Definition. Consider $F \colon \mathbb{C}^\alpha \to \mathbb{D}$, $G \colon \mathbb{C}^\beta \to \mathbb{D}$, $\varphi \colon F \to G$ a transformation of type $|\alpha| \xrightarrow{\sigma} k \xleftarrow{\tau} |\beta|$ as in Definition (1.3). For $i \in \{1, \dots, k\}$, we say that φ is *dinatural in A_i* (or, more precisely, *in its i-th variable*) if and only if for all $A_1, \dots, A_{i-1}, A_{i+1}, \dots, A_k$ objects of $\mathbb{C}$ and for all $f \colon A \to B$ in $\mathbb{C}$ the following diagram commutes:

$$\begin{tikzcd}
& \cdot \arrow[r, "\varphi_{A_1,\dots,A_{i-1},B,A_{i+1},\dots,A_k}"] & \cdot \arrow[dr, "G(y_1,\dots,y_{|\beta|})"] & \\
\cdot \arrow[ur, "F(x_1,\dots,x_{|\alpha|})"] \arrow[dr, "F(x'_1,\dots,x'_{|\alpha|})"'] & & & \cdot \\
& \cdot \arrow[r, "\varphi_{A_1,\dots,A_{i-1},A,A_{i+1},\dots,A_k}"'] & \cdot \arrow[ur, "G(y'_1,\dots,y'_{|\beta|})"'] &
\end{tikzcd}$$

where

$$x_j = \begin{cases} f & \sigma j = i \wedge \alpha_j = + \\ id_B & \sigma j = i \wedge \alpha_j = - \\ id_{A_{\sigma j}} & \sigma j \neq i \end{cases} \qquad y_j = \begin{cases} id_B & \tau j = i \wedge \beta_j = + \\ f & \tau j = i \wedge \beta_j = - \\ id_{A_{\tau j}} & \tau j \neq i \end{cases}$$

$$x'_j = \begin{cases} id_A & \sigma j = i \wedge \alpha_j = + \\ f & \sigma j = i \wedge \alpha_j = - \\ id_{A_{\sigma j}} & \sigma j \neq i \end{cases} \qquad y'_j = \begin{cases} f & \tau j = i \wedge \beta_j = + \\ id_A & \tau j = i \wedge \beta_j = - \\ id_{A_{\tau j}} & \tau j \neq i \end{cases} \qquad \square$$

The condition $\sigma j = i$ means that in the domain of $\varphi_{A_1,\dots,A_k}$, A_i will be the j-th variable of F (by definition); the dinaturality condition asserts that, focusing only on the arguments of F and G which are involved by the i-th variable of the transformation φ, computing F on f in all the "positive" (that is, covariant) variables, followed by φ, followed by G computed on f in all the "negative" (that is, contravariant) variables, is the same as computing F on f in all the negative variables, followed by the appropriate component of φ, followed by G computed on f in all the positive variables.

(1.7) Remark. Definition (1.6) is a generalisation of the well known notion of dinatural transformation, which we can obtain when $\alpha = \beta = [-,+]$ and $k = 1$. Here we are allowing multiple variables at once and the possibility for F and G of having an arbitrary number of copies of $\mathbb{C}$ and $\mathbb{C}^{\mathrm{op}}$ in their domain, for each variable $i \in \{1,\dots,k\}$.

It is known that dinatural transformations generalise natural and extranatural ones. Here we make this fact explicit by defining the latter as particular cases of dinatural transformations where the functors and the type have a special shape: essentially, a dinatural transformation $\varphi \colon F \to G$ is natural in A_i if F and G are both covariant or both contravariant in the variables involved by A_i; φ is extranatural in A_i if one of the functors F and G does not involve the variable A_i while A_i appears both covariantly and contravariantly in the other.

(1.8) Definition. Let $\varphi \colon F \to G$ be a transformation as in Definition (1.3). $\varphi = \left(\varphi_{A_1,\dots,A_k}\right)$ is said to be *natural* in A_i if and only if

- it is dinatural in A_i;

- $\forall u \in \sigma^{-1}\{i\}.\, \forall v \in \tau^{-1}\{i\}.\, (\alpha_u = \beta_v = +) \vee (\alpha_u = \beta_v = -)$.

φ is called *extranatural* in A_i if and only if

- it is dinatural in A_i;

- $\bigl(\sigma^{-1}\{i\} = \varnothing \wedge \exists j_1, j_2 \in \tau^{-1}\{i\}.\, \beta_{j_1} \neq \beta_{j_2}\bigr) \vee$
  $\vee \bigl(\tau^{-1}\{i\} = \varnothing \wedge \exists i_1, i_2 \in \sigma^{-1}\{i\}.\, \alpha_{i_1} \neq \alpha_{i_2}\bigr)$. □

Notice that our notion of (extra)natural transformation is more general than the one given by Eilenberg and Kelly in [EK66], as we allow the arguments of F and G to be equated not just in pairs, but in an arbitrary number, according to σ and τ.

(1.9) Example. Suppose that $\mathbb{C}$ is a cartesian category, with $\times\colon \mathbb{C}\times\mathbb{C} \to \mathbb{C}$ the product functor. The diagonal transformation

$$\delta = (\delta_A \colon A \to A \times A)_{A \in \mathbb{C}},$$

classically a natural transformation from $id_{\mathbb{C}}$ to the diagonal functor, can be equivalently seen in our notations as a transformation $\delta\colon\ id_{\mathbb{C}} \to \times$ of type $1 \longrightarrow 1 \longleftarrow 2$. We have that δ is indeed natural in its only variable , because for all $f\colon A \to B$ the following diagram commutes:

$$\begin{tikzcd}
 & B \arrow[r, "\delta_B"] & B \times B \arrow[dr, "id_B \times id_B"] & \\
A \arrow[ur, "f"] \arrow[dr, "id_A"'] & & & B \times B \\
 & A \arrow[r, "\delta_A"] & A \times A \arrow[ur, "f \times f"'] &
\end{tikzcd}$$ □

(1.10) Example. Suppose that $\mathbb{C}$ is a cartesian closed category and consider the functor

$$\begin{array}{ccc} \mathbb{C} \times \mathbb{C}^{op} \times \mathbb{C} & \xrightarrow{\ T\ } & \mathbb{C} \\ (X,Y,Z) & \longmapsto & X \times (Y \Rightarrow Z) \end{array}$$

The evaluation $eval = \bigl(eval_{A,B} \colon A \times (A \Rightarrow B) \to B\bigr)_{A,B \in \mathbb{C}} : T \to id_{\mathbb{C}}$ is a transformation of type

$$\begin{tikzcd}[row sep=tiny]
3 \arrow[r] & 2 & 1 \arrow[l] \\
1 \arrow[r, mapsto] & 1 & 1 \arrow[dl, mapsto, bend right] \\
2 \arrow[ur, mapsto, bend right] & 2 & \\
3 \arrow[ur, mapsto, bend right] & &
\end{tikzcd}$$

which is extranatural in A and natural in B because the following hexagons commute for all $f\colon A \to A'$ and $g\colon B \to B'$:

$$\begin{tikzcd}
 & A' \times (A' \Rightarrow B) \arrow[r, "eval_{A',B}"] & B \arrow[dr, "1"] & \\
A \times (A' \Rightarrow B) \arrow[ur, "f\times(1\Rightarrow 1)"] \arrow[dr, "1\times(f\Rightarrow 1)"'] & & & B \\
 & A \times (A \Rightarrow B) \arrow[r, "eval_{A,B}"] & B \arrow[ur, "1"'] &
\end{tikzcd} \qquad \text{(extranaturality in } A\text{)}$$

$$\begin{tikzcd}
 & A \times (A \Rightarrow B') \arrow[r, "eval_{A,B'}"] & B' \arrow[dr, "1"] & \\
A \times (A \Rightarrow B) \arrow[ur, "1\times(1\Rightarrow g)"] \arrow[dr, "1\times(1\Rightarrow 1)"'] & & & B' \\
 & A \times (A \Rightarrow B) \arrow[r, "eval_{A,B}"] & B \arrow[ur, "g"'] &
\end{tikzcd} \qquad \text{(naturality in } B\text{)}$$

Indeed, the commutativity of the first hexagon above is equivalent to the following true equality in the internal language [Cro94] of $\mathbb{C}$:

$$\lambda a^A.\, \lambda h^{A' \Rightarrow B}.\, h(f(a)) = \lambda a^A.\, \lambda h^{A' \Rightarrow B}(h \circ f)(a),$$

while the second one to:

$$\lambda a^A.\, \lambda h^{A \Rightarrow B}.\, (f \circ h)(a) = \lambda a^A.\, \lambda h^{A \Rightarrow B} f(h(a)).$$ □

(1.11) Example. Suppose again that $\mathbb{C}$ is cartesian closed. With little abuse of notation, call $1\colon \mathbb{I} \to \mathbb{C}$ the constant functor with value the terminal object 1. Consider the transformation

$$\ulcorner id \urcorner \colon 1 \to (- \Rightarrow -)$$

of type $0 \longrightarrow 1 \longleftarrow 2$ where $\ulcorner id \urcorner_A$ is given by $\lambda x^A.\, x$ (known as the "name" of the identity of A). Then $\ulcorner id \urcorner$ is extranatural in its only variable: for all $f\colon A \to B$, the following square

$$\begin{tikzcd}
1 \arrow[r, "\ulcorner id \urcorner_A"] \arrow[d, "\ulcorner id \urcorner_B"'] & A \Rightarrow A \arrow[d, "1\Rightarrow f"] \\
B \Rightarrow B \arrow[r, "f\Rightarrow 1"] & A \Rightarrow B
\end{tikzcd}$$

commutes because that is equivalent to say that $f \circ id_A = id_B \circ f$. □

(1.12) Example. Call $\mathrm{Hom}_{\mathbb{C}}\colon \mathbb{C}^{\mathrm{op}} \times \mathbb{C} \to \mathbb{S}\mathrm{et}$ the hom-functor of $\mathbb{C}$. The n-th numeral ([DS70]) is the transformation $n\colon \mathrm{Hom}_{\mathbb{C}} \to \mathrm{Hom}_{\mathbb{C}}$ of type $2 \longrightarrow 1 \longleftarrow 2$ whose general component $n_A \colon \mathbb{C}(A,A) \to \mathbb{C}(A,A)$ is given, for $A \in \mathbb{A}$ and $g \colon A \to A$, by

$$n_A(g) = g^n,$$

with $0_A(g) = id_A$. Then n is dinatural because for all $f \colon A \to B$ the following hexagon commutes:

$$\begin{tikzcd}
& \mathbb{C}(B,B) \arrow[r, "n_B"] & \mathbb{C}(B,B) \arrow[dr, "-\circ f"] & \\
\mathbb{C}(B,A) \arrow[ur, "f\circ -"] \arrow[dr, "-\circ f"'] & & & \mathbb{C}(A,B) \\
& \mathbb{C}(A,A) \arrow[r, "n_A"] & \mathbb{C}(A,A) \arrow[ur, "f\circ -"'] &
\end{tikzcd}$$

It is indeed true that for $h \colon B \to A$, $(f \circ h)^n \circ f = f \circ (h \circ f)^n$: for $n = 0$ it follows from the identity axiom; for $n \geq 1$ it is a consequence of associativity of composition. □

(1.13) Example. (From [Sim93], cf. also [Mul90] and [BFSS90], Appendix 2.) Suppose $\mathbb{C}$ is a $\mathbb{PoSet}$-enriched category which is cartesian closed in the $\mathbb{PoSet}$-enriched sense and such that the functor $\mathbb{C}(1,-) \colon \mathbb{C} \to \mathbb{PoSet}$ is faithful. The latter requirement means that we can treat $\mathbb{C}$ as a category of partially ordered sets and monotone functions: in virtue of this, we shall use set-theoretic notation for global elements and function application.

Consider the transformation $Y \colon (- \Rightarrow -) \to id_{\mathbb{C}}$ of type $2 \longrightarrow 1 \longleftarrow 1$ where $Y_A \colon (A \Rightarrow A) \to A$ takes a morphism $h \colon A \to A$ into the least fixed-point of h, which concretely means that $Y_A(h) = h(Y_A(h))$ and that $x = h(x) \in A$ implies $Y_A(h) \leq x$. Then Y is dinatural, that is, the following hexagon commutes for all $f \colon A \to B$:

$$\begin{tikzcd}
& A \Rightarrow A \arrow[r, "Y_A"] & A \arrow[dr, "f"] & \\
B \Rightarrow A \arrow[ur, "f\Rightarrow 1"] \arrow[dr, "1\Rightarrow f"'] & & & B \\
& B \Rightarrow B \arrow[r, "Y_B"] & B \arrow[ur, "1"'] &
\end{tikzcd}$$

Indeed, let $g \colon B \to A$ and $x = f(Y_A(g \circ f))$. We have that x is a fixed point of $f \circ g$, because

$$(f \circ g)(x) = f\left((g \circ f)\left(Y_A\left(g \circ f\right)\right)\right) = f(Y_A(g \circ f)) = x,$$

hence $Y_B(f \circ g) \leq f(Y_A(g \circ f))$. Applying g, we obtain the inequality

$$g(Y_B(f \circ g)) \leq g(f(Y_A(g \circ f))) = Y_A(g \circ f).$$

It now suffices to repeat the same argument interchanging the roles of f and g to obtain that $f(Y_A(g \circ f)) \leq Y_B(f \circ g)$. Therefore $f(Y_A(g \circ f)) = Y_B(f \circ g)$, which means Y is dinatural. □

The compositionality problem. Dinatural transformations are mostly famous for what they *fail* to do: to compose. Indeed, consider two dinatural transformations $\varphi \colon F \to G$ and $\psi \colon G \to H$, both of type $2 \longrightarrow 1 \longleftarrow 2$, with $F, G, H \colon \mathbb{C}^{\mathrm{op}} \times \mathbb{C} \to \mathbb{D}$ say. The dinaturality of their composite $\psi \circ \varphi = (\psi_A \circ \varphi_A)_{A \in \mathbb{C}}$ is tantamount to saying that the outer hexagon in the following diagram commutes for all $f \colon A \to B$:

(1.14)
$$\begin{tikzcd}
 & F(A,A) \arrow[rr, "\varphi_A"] & & G(A,A) \arrow[rr, "\psi_A"] \arrow[dr, "G(1,f)"] & & H(A,A) \arrow[dr, "H(1,f)"] & \\
F(B,A) \arrow[ur, "F(f,1)"] \arrow[dr, "F(1,f)"'] & & G(B,A) \arrow[ur, "G(f,1)"] \arrow[dr, "G(1,f)"'] & & G(A,B) & & H(A,B) \\
 & F(B,B) \arrow[rr, "\varphi_B"'] & & G(B,B) \arrow[rr, "\psi_B"'] \arrow[ur, "G(f,1)"'] & & H(B,B) \arrow[ur, "H(f,1)"'] &
\end{tikzcd}$$

However, while both inner hexagons commute, the outer does not in general. The following is a classic counter-example.

(1.15) Example. Take $\mathbb{C} = \mathbb{S}\mathrm{et}$, $\varphi = \ulcorner id \urcorner$. The transformation $\psi \colon (- \Rightarrow -) \to \{0,1\}$ (here $\{0,1\}$ seen as a constant functor) of type $2 \longrightarrow 1 \longleftarrow 0$ where $\psi_A \colon (A \Rightarrow A) \to \{0,1\}$ returns 0 if the number of fixed points of its argument is even or infinite, and 1 if it is odd, is dinatural (in fact, extranatural). The reason for this is that, given $f \colon A \to B$ and $g \colon B \to A$, there is a bijective correspondence between the fixed points of $g \circ f$ and those of $f \circ g$. However, the composite $\psi \circ \varphi \colon 1 \to \{0,1\}$ is a non-constant family of morphisms between constant functors: it cannot be dinatural. □

It is known that there are certain conditions that guarantee the commutativity of (1.14). For example, if either φ or ψ is natural, then one of the two internal hexagons reduces to a square, and everything in sight commutes. Also, if the middle square happens to be a pullback, then there is a unique map from $F(B,A)$ to $G(B,A)$ that makes everything commutative:

$$\begin{tikzcd}
 & F(A,A) \arrow[rr, "\varphi_A"] & & G(A,A) \arrow[rr, "\psi_A"] \arrow[dr, "G(1,f)"] & & H(A,A) \arrow[dr, "H(1,f)"] & \\
F(B,A) \arrow[ur, "F(f,1)"] \arrow[dr, "F(1,f)"'] \arrow[rr, dotted, "!"] & & G(B,A) \arrow[ur, "G(f,1)"] \arrow[dr, "G(1,f)"'] & & G(A,B) & & H(A,B) \\
 & F(B,B) \arrow[rr, "\varphi_B"'] & & G(B,B) \arrow[rr, "\psi_B"'] \arrow[ur, "G(f,1)"'] & & H(B,B) \arrow[ur, "H(f,1)"'] &
\end{tikzcd}$$

Dually, if the middle square is a pushout, then the outer hexagon commutes. However, these are conditions that depend on the nature of the category $\mathbb{D}$ and the functor G, and *not* on the dinaturality of φ and ψ alone. We shall now work towards stating a sufficient condition for the dinaturality of $\psi \circ \varphi$ that does rely only on the "geometry", as it were, of φ and ψ.

The graph of a transformation. Given a transformation φ, we now define a graph that reflects its signature, which we shall use to solve the compositionality problem of dinatural transformations. This graph is, as a matter of fact, a *string diagram* for the transformation. String diagrams have been introduced by Eilenberg and Kelly in [EK66] (indeed our graphs are inspired by theirs) and have had a great success in the study of coherence problems ([Mac63],[KL80]) and monoidal categories in general ([JS91],[JSV96], a nice survey can be found in [Sel10]).

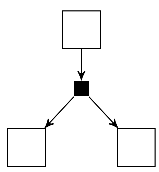
(1.16) Definition. Let $F \colon \mathbb{C}^\alpha \to \mathbb{D}$ and $G \colon \mathbb{C}^\beta \to \mathbb{D}$ be functors, and let $\varphi \colon F \to G$ be a transformation of type $|\alpha| \xrightarrow{\sigma} k \xleftarrow{\tau} |\beta|$. We define its *graph* $\Gamma(\varphi) = (P, T, \bullet(-), (-)\bullet)$ as a directed, bipartite graph as follows:

- $P = |\alpha| + |\beta|$ and $T = k$ are distinct finite sets of vertices;
- $\bullet(-), (-)\bullet \colon T \to \mathcal{P}(P)$ are the input and output functions for elements in T: there is an arc from p to t if and only if $p \in \bullet t$, and there is an arc from t to p if and only if $p \in t\bullet$. Indicating with $\iota_{|\alpha|} \colon |\alpha| \to P$ and $\iota_{|\beta|} \colon |\beta| \to P$ the injections defined as follows:
$$\iota_{|\alpha|}(x) = x, \quad \iota_{|\beta|}(x) = |\alpha| + x,$$
we have:
$$\begin{aligned} \bullet t &= \{\iota_{|\alpha|}(p) \mid \sigma(p) = t,\, \alpha_p = +\} \cup \{\iota_{|\beta|}(p) \mid \tau(p) = t,\, \beta_p = -\} \\ t\bullet &= \{\iota_{|\alpha|}(p) \mid \sigma(p) = t,\, \alpha_p = -\} \cup \{\iota_{|\beta|}(p) \mid \tau(p) = t,\, \beta_p = +\} \end{aligned}$$

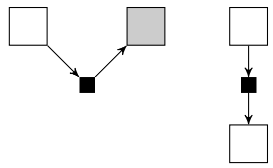
In other words, elements of P correspond to the arguments of F and G, while those of T to the variables of φ. For $t \in T$, its inputs are the covariant arguments of F and the contravariant arguments of G which are mapped by σ and τ to t; similarly for its outputs (swapping 'covariant' and 'contravariant'). □

Graphically, we draw elements of P as white or grey boxes (if corresponding to a covariant or contravariant argument of a functor, respectively), and elements of T as black squares. The boxes for the domain functor are drawn at the top, while those for the codomain at the bottom; the black boxes in the middle. The graphs of the transformations given in examples (1.9)-(1.13) are the following:

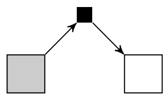
- $\delta = (\delta_A \colon A \to A \times A)_{A \in \mathbb{C}}$ (example (1.9)):



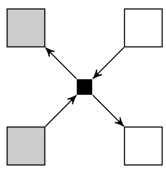
- $eval = \big(eval_{A,B} \colon A \times (A \Rightarrow B) \to B\big)_{A,B \in \mathbb{C}}$ (example (1.10)):



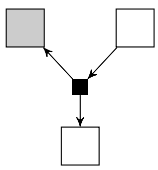
- $\ulcorner id \urcorner = (\ulcorner id \urcorner_A \colon 1 \to (A \Rightarrow A))_{A \in \mathbb{C}}$ (example (1.11)):



- $n = (n_A \colon \mathbb{C}(A,A) \to \mathbb{C}(A,A))_{A \in \mathbb{C}}$ (example (1.12)):



- $Y = (Y_A \colon (A \Rightarrow A) \to A)_{A \in \mathbb{C}}$ (example (1.13)):

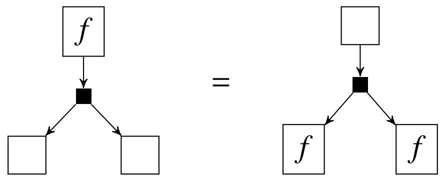


(1.17) Remark. Each connected component of $\Gamma(\varphi)$ corresponds to one variable of φ: the arguments of the domain and codomain of φ corresponding to (white, grey) boxes belonging to the same connected component are all computed on the same object, when we write down the general component of φ.

This graphical counterpart of a transformation $\varphi \colon F \to G$ permits us to represent, in an informal fashion, the dinaturality properties of φ. By writing inside a box a morphism f and reading a graph from top to bottom as "compute F in the morphisms as they are written in its corresponding boxes, compose that with an appropriate component of φ, and compose that with G computed in the morphisms as they are written in its boxes (treating an empty box as an identity)", we can express the commutativity of a dinaturality diagram as an informal equation of graphs. (We shall make this precise in §1.3.) For instance, the dinaturality of examples (1.9)-(1.13) can be depicted as follows, where the upper leg of the diagrams are the left-hand sides of the equations:

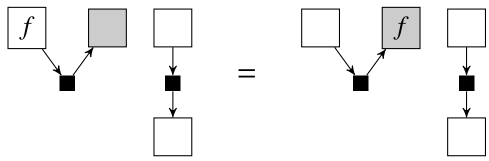
- $\delta = (\delta_A \colon A \to A \times A)_{A \in \mathbb{C}}$ (example (1.9)):

$$\begin{tikzcd} A \arrow[r, "f"] \arrow[d, "\delta_A"'] & B \arrow[d, "\delta_B"] \\ A \times A \arrow[r, "f \times f"] & B \times B \end{tikzcd}$$

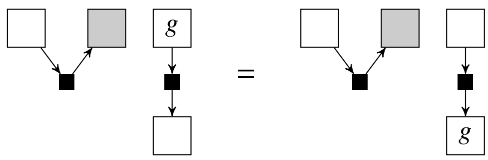


- $eval = \big(eval_{A,B} \colon A \times (A \Rightarrow B) \to B\big)_{A,B \in \mathbb{C}}$ (example (1.10)):

$$\begin{tikzcd} A \times (A' \Rightarrow B) \arrow[r, "f \times (1 \Rightarrow 1)"] \arrow[d, "1 \times (f \Rightarrow 1)"'] & A' \times (A' \Rightarrow B) \arrow[d, "eval_{A',B}"] \\ A \times (A \Rightarrow B) \arrow[r, "eval_{A,B}"] & B \end{tikzcd}$$

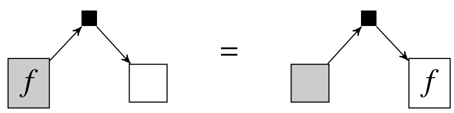


$$\begin{tikzcd} A \times (A \Rightarrow B) \arrow[r, "1 \times (1 \Rightarrow g)"] \arrow[d, "eval_{A,B}"'] & A \times (A \Rightarrow B') \arrow[d, "eval_{A,B'}"] \\ B \arrow[r, "g"] & B' \end{tikzcd}$$



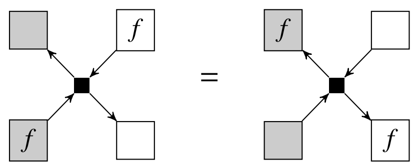
- $\ulcorner id \urcorner = (\ulcorner id \urcorner_A \colon 1 \to (A \Rightarrow A))_{A \in \mathbb{C}}$ (example (1.11)):

$$\begin{tikzcd} 1 \arrow[r, "\ulcorner id \urcorner_B"] \arrow[d, "\ulcorner id \urcorner_A"'] & B \Rightarrow B \arrow[d, "f \Rightarrow 1"] \\ A \Rightarrow A \arrow[r, "1 \Rightarrow f"] & A \Rightarrow B \end{tikzcd}$$



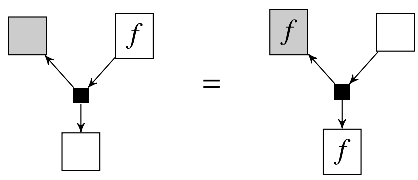
- $n = (n_A \colon \mathbb{C}(A,A) \to \mathbb{C}(A,A))_{A \in \mathbb{C}}$ (example (1.12)):

$$\begin{tikzcd} & \mathbb{C}(B,B) \arrow[r, "n_B"] & \mathbb{C}(B,B) \arrow[dr, "\mathbb{C}(f,1)"] & \\ \mathbb{C}(B,A) \arrow[ur, "\mathbb{C}(1,f)"] \arrow[dr, "\mathbb{C}(f,1)"'] & & & \mathbb{C}(A,B) \\ & \mathbb{C}(A,A) \arrow[r, "n_A"] & \mathbb{C}(A,A) \arrow[ur, "\mathbb{C}(1,f)"'] & \end{tikzcd}$$



- $Y = (Y_A \colon (A \Rightarrow A) \to A)_{A \in \mathbb{C}}$ (example (1.13)):

$$\begin{tikzcd} & B \Rightarrow B \arrow[r, "Y_B"] & B \arrow[dr, "1"] & \\ B \Rightarrow A \arrow[ur, "1 \Rightarrow f"] \arrow[dr, "f \Rightarrow 1"'] & & & B \\ & A \Rightarrow A \arrow[r, "Y_A"] & A \arrow[ur, "f"'] & \end{tikzcd}$$



All in all, the dinaturality condition becomes, in graphical terms, as follows: φ *is dinatural if and only if having in* $\Gamma(\varphi)$ *one* f *in all white boxes at the top and grey boxes at the bottom is the same as having one* f *in all grey boxes at the top and white boxes at the bottom.*

Not only does $\Gamma(\varphi)$ give an intuitive representation of the dinaturality properties of φ, but also of the process of composition of transformations. Given two transformations $\varphi\colon F \to G$ and $\psi\colon G \to H$ as in Definition (1.5), the act of computing the pushout (1.2) corresponds to "glueing together" $\Gamma(\varphi)$ and $\Gamma(\psi)$ along the boxes corresponding to the functor G (more precisely, one takes the disjoint union of $\Gamma(\varphi)$ and $\Gamma(\psi)$ and then identifies the G-boxes), obtaining a "temporary" graph $\Gamma^*(\psi \circ \varphi)$. The number of its connected components is, indeed, the result of the pushout. That being done, $\Gamma(\psi \circ \varphi)$ is obtained by collapsing each connected component of $\Gamma^*(\psi \circ \varphi)$ into a single black square together with the F- and H-boxes. The following example shows this process. The graph $\Gamma^*(\psi \circ \varphi)$ will play a crucial role into the compositionality problem of $\psi \circ \varphi$.

(1.18) Example. Suppose that $\mathbb{C}$ is cartesian closed, fix an object R in $\mathbb{C}$, consider functors

$$
\begin{array}{ccc}
\mathbb{C} \times \mathbb{C}^{\mathrm{op}} \xrightarrow{F} \mathbb{C} & \qquad \mathbb{C} \times \mathbb{C} \times \mathbb{C}^{\mathrm{op}} \xrightarrow{G} \mathbb{C} & \qquad \mathbb{C} \xrightarrow{H} \mathbb{C} \\
(A,B) \longmapsto A \times (B \Rightarrow R) & \qquad (A,B,C) \longmapsto A \times B \times (C \Rightarrow R) & \qquad A \longmapsto A \times R
\end{array}
$$

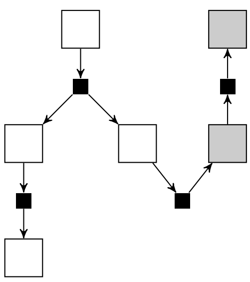
and transformations $\varphi = \delta \times id_{(-)\Rightarrow R}\colon F \to G$ and $\psi = id_{\mathbb{C}} \times eval_{(-),R}\colon G \to H$ of types, respectively,

$$
\begin{array}{ccccc}
2 & \xrightarrow{\sigma} & 2 & \xleftarrow{\tau} & 3 \\
1 & \longmapsto & 1 & \longleftarrow & 1 \\
2 & \longmapsto & 2 & \longleftarrow & 2 \\
 & & 1 & \longleftarrow & 3
\end{array}
\qquad \text{and} \qquad
\begin{array}{ccccc}
3 & \xrightarrow{\eta} & 2 & \xleftarrow{\theta} & 1 \\
1 & \longmapsto & 1 & \longleftarrow & 1 \\
2 & \longmapsto & 2 & & \\
3 & \longmapsto & 2 & &
\end{array}
$$

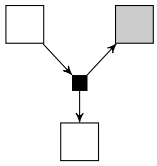
so that

$$\varphi_{A,B} = \delta_A \times id_{B\Rightarrow R}\colon F(A,B) \to G(A,A,B),\ \psi_{A,B} = id_A \times eval_{B,R}\colon G(A,B,B) \to H(A).$$

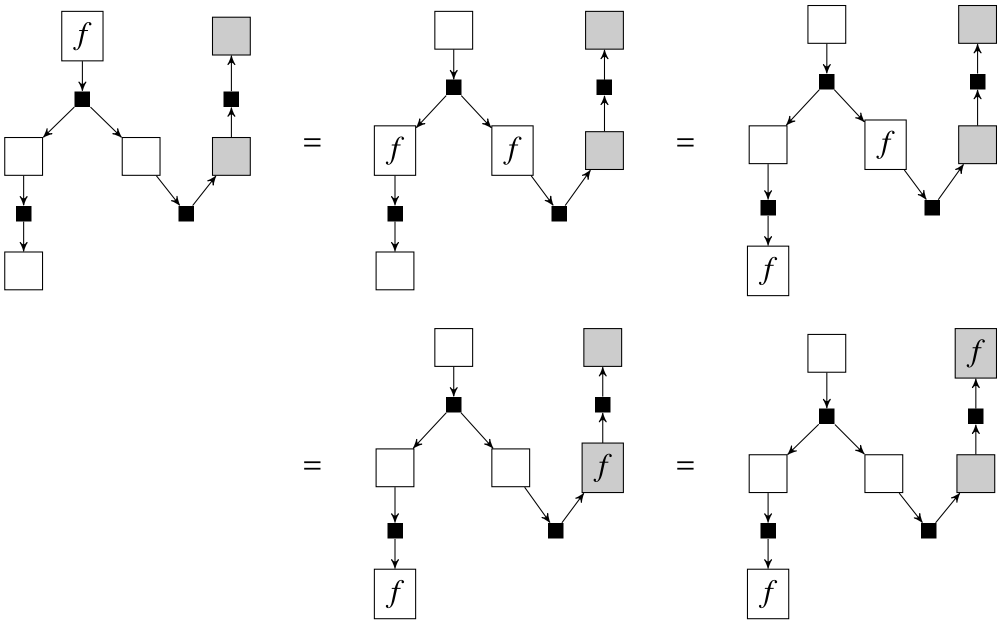
Then $\psi \circ \varphi$ has type $2 \longrightarrow 1 \longleftarrow 1$ and $\Gamma^*(\psi \circ \varphi)$ is:



The two upper boxes at the top correspond to the arguments of F, the three in the middle to the arguments of G, and the bottom one to the only argument of H. This is a connected graph (indeed, $\psi \circ \varphi$ depends only on one variable) and by collapsing it into a single black box we obtain $\Gamma(\psi \circ \varphi)$ as it is according to Definition (1.16):



We have that $\psi \circ \varphi$ is a (non-natural, non-extranatural) dinatural transformation. (This is one of the transformations studied by Girard, Scedrov and Scott in [GSS92].) The following string-diagrammatic argument proves that:



The first equation is due to naturality of φ in its first variable; the second to naturality of ψ in its first variable; the third to extranaturality of ψ in its second variable; the fourth equation holds by naturality of φ in its second variable. □

We shall solve the compositionality problem by interpreting $\Gamma^*(\psi \circ \varphi)$, for arbitrary transformations φ and ψ, as a Petri Net whose set of *places* is P and of *transitions* is T. The dinaturality of $\psi \circ \varphi$ will be expressed as a reachability problem. In order to do this, we first discuss some general properties of Petri Nets in the following section.

§1.2 Petri Nets

Petri Nets have been invented by Carl Adam Petri in 1962 in [Pet62], and have been used since then to model concurrent systems, resource sensitivity and many dynamic systems. A nice survey of their properties was written by Murata in [Mur89], to which we refer the reader for more details and examples. Here we shall limit ourselves only to the definitions and the properties of which we will make use in the thesis.

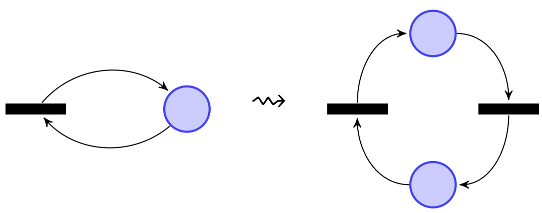
(1.19) Definition. A *Petri Net* N is a tuple $(P, T, \bullet(-), (-)\bullet)$ where P and T are distinct, finite sets, and $\bullet(-), (-)\bullet : T \to \mathcal{P}(P)$ are functions. For t a transition, $\bullet t$ is the set of *inputs* of t, and $t\bullet$ is the set of its *outputs*. Elements of P are called *places*, while elements of T are called *transitions*. A *marking* for N is a function $M : P \to \mathbb{N}$. □

Graphically, the elements of P and T are drawn as light-blue circles and black bars respectively. Notice that the graph of a transformation is, as a matter of fact, a Petri Net. We can represent a marking M by drawing, in each place p, $M(p)$ *tokens* (black dots). Note that there is only one arrow from a node to another.

With little abuse of notation, we extend the input and output notation for places too, where

$$\bullet p = \{t \in T \mid p \in t\bullet\}, \qquad p\bullet = \{t \in T \mid p \in \bullet t\}.$$

A pair of a place p and a transition t where p is both an input and an output of t is called *self-loop*. Without loss of generality, we shall only consider Petri Nets that contain no self-loops. Indeed, any self-loop can be transformed into a loop by introducing a new place and a new transition as follows:



(1.20) Definition. Let N be a Petri Net. A place p of N is said to be a *source* if $\bullet p = \varnothing$, whereas is said to be a *sink* if $p\bullet = \varnothing$. A source (or sink) place p is said to be *proper* if $p\bullet \neq \varnothing$ (or $\bullet p \neq \varnothing$, respectively). □

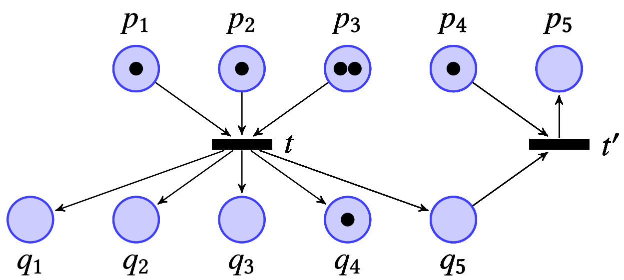
The firing rule. We can give a dynamic flavour to Petri Nets by allowing the tokens to "flow" through the nets, that is allowing markings to change according to the following *transition firing rule*.

(1.21) Definition. Let $N = (P, T, \bullet(-), (-)\bullet)$ be a Petri Net, and M a marking for N. A transition t is said to be *enabled* if for all $p \in \bullet t$ we have $M(p) \geq 1$. An enabled transition may *fire*; the firing of an enabled transition t removes one token from each

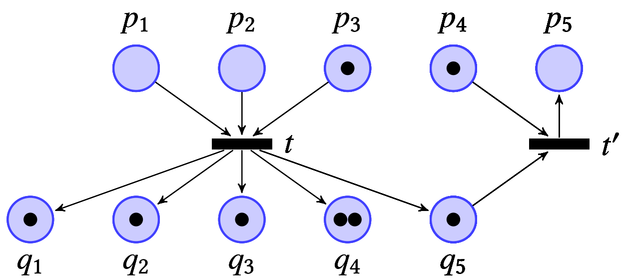
$p \in \bullet t$ and adds one token to each $p \in t\bullet$, generating the following new marking M':

$$M'(p) = \begin{cases} M(p) - 1 & p \in \bullet t \\ M(p) + 1 & p \in t\bullet \\ M(p) & \text{otherwise} \end{cases} \qquad \square$$

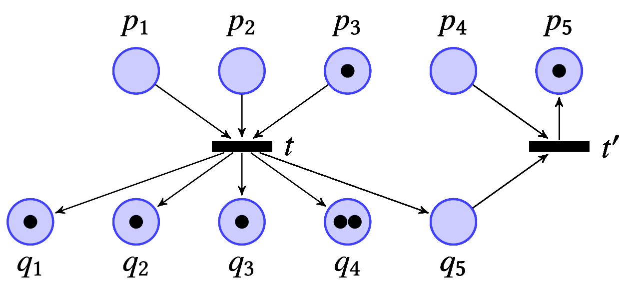
(1.22) Example. Consider the following net:



There are two transitions, t and t', but only t is enabled. Firing t will change the state of the net as follows:

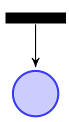


Now t is disabled, but t' is enabled, and by firing it we obtain:

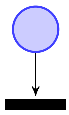


$\square$

(1.23) Remark. The following net is a legitimate one and its only transition is *always* enabled: all it does is create tokens out of nowhere, when it fires:



The following net instead destroys tokens, when its transition is enabled and it fires:



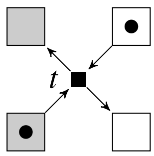
The reachability problem and dinaturality. Suppose we have a Petri Net N and an initial marking M_0. The firing of an enabled transition in N will change the distribution of tokens from M_0 to M_1, according to the firing transition rule, therefore a sequence of firings of enabled transitions yields a sequence of markings. A *firing sequence* is denoted by $\sigma = (t_0, \ldots, t_n)$ where the t_i's are transitions which fire.

(1.24) Definition. A marking M for a Petri Net N is said to be *reachable* from a marking M_0 if there exists a firing sequence $(t_0, \ldots, t_n)$ and markings $M_1, \ldots, M_n$ where M_i is obtained from M_{i-1} by firing transition t_i, for $i \in \{1, \ldots, n\}$, and $M_n = M$. □

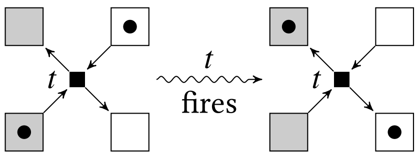
The reachability problem for Petri Nets consists in checking whether a marking M is or is not reachable from M_0. It has been shown that the reachability problem is decidable [Kos82; May81].

(1.25) Remark. Given a Petri Net N, consider the *reversed* net N^{op} obtained from N by reversing the direction of all the arrows. Then a marking M_d is reachable from M_0 in N if and only if M_0 is reachable from M_d in N^{op}.

(1.26) Remark. The crucial observation that will allow us to solve the compositionality problem for dinatural transformations is that the firing of an enabled transition in the graph of a dinatural transformation φ corresponds, under certain circumstances, to the dinaturality condition of φ in one of its variables. Take, for instance, the n-th numeral transformation (see example (1.12)). Call t the only transition, and consider the following marking M_0:

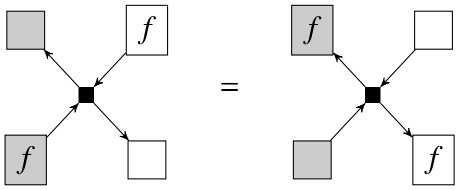


t is enabled, and once it fires we obtain the following marking M_1:



The striking resemblance with the graphical version of the dinaturality condition for

n is evident:



By treating the "morphism f in a box" as a "token in a place" of $\Gamma(n)$, we have seen that the firing of t generates an equation in $\mathbb{S}$et, namely the one that expresses the dinaturality of n.

Suppose now we have two composable transformations φ and ψ dinatural in all their variables, in a category $\mathbb{D}$. We shall make precise how certain markings of $\Gamma^*(\psi \circ \varphi)$ correspond to morphisms in $\mathbb{D}$, and how the firing of an enabled transition corresponds to applying the dinaturality of φ or ψ in one of their variables, thus creating an equation of morphisms in $\mathbb{D}$. Therefore, if the firing of a single transition generates an equality in the category, a sequence of firings of enabled transitions yields a chain of equalities. By individuating two markings M_0 and M_d, each corresponding to a leg of the dinaturality hexagon for $\psi \circ \varphi$ we want to prove is commutative, and by showing that M_d is reachable from M_0, we shall have proved that $\psi \circ \varphi$ is dinatural.

From an intellectual point of view, this approach reveals a remarkable connection between two disparate areas of research: Category Theory and Petri Nets. The practical advantage of reducing our compositionality problem of $\psi \circ \varphi$ to the reachability problem for certain markings in the Petri Net $\Gamma^*(\psi \circ \varphi)$ is that we can make use of the necessary and sufficient conditions for reachability which have already been studied in the past.

The incidence matrix of a Petri Net. The dynamics of Petri Nets is governed by a system of linear equations, which we now proceed to introduce. First of all, we associate a matrix to each Petri Net as follows. (Recall that we assume our nets do not contain self-loops.)

(1.27) Definition. Let N be a Petri Net with m places and n transitions. The *incidence matrix* $A = [a_{pt}]$ of N is a $m \times n$ matrix of integers where a_{pt} is the number of tokens changed in place p when transition t fires once, that is:

(1.28)
$$a_{pt} = \begin{cases} 1 & p \in t\bullet \\ -1 & p \in \bullet t \\ 0 & \text{otherwise} \end{cases} \qquad \square$$

In writing matrix equations, we write a marking M_k as an $m \times 1$ column vector, where the p-th entry of M_k denotes the number of tokens in place p immediately after the k-th firing in some firing sequence. The k-th *firing* or *control vector* u_k is a $n \times 1$ column vector made of all 0's except for one entry; a 1 in the t-th position indicating that transition t fires at the k-th firing. In fact, the t-th column of the incidence matrix A denotes the change of the marking as the result of firing transition t, therefore the following state equation for a Petri Net holds [Mur89]:

(1.29) $$M_k = M_{k-1} + Au_k, \qquad k = 1, 2, \ldots$$

Suppose now that a destination marking M_d is indeed reachable from M_0 through a firing sequence $\{u_1, \ldots, u_d\}$. Writing the state equation (1.29) for each $i = 1, \ldots, d$ and summing them, we obtain

$$M_d = M_0 + A \sum_{k=1}^{d} u_k$$

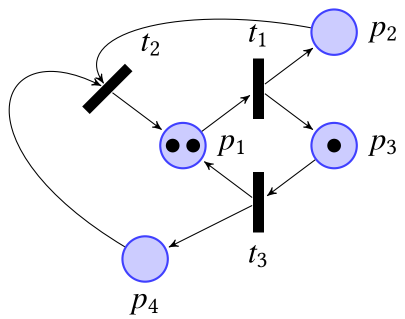
which can be rewritten as

(1.30) $$M_d = M_0 + Ax$$

where $x = \sum_{k=1}^{d} u_k$. x is therefore a $n \times 1$ column vector of non-negative integers and is called the *firing count vector*, whose t-th entry denotes the number of times that transition t must fire to transform M_0 into M_d. Notice though that x does not tell us in which order to fire the transitions to get from M_0 to M_d. We have then the following necessary condition for the reachability problem in arbitrary Petri Nets [Mur89].

(1.31) Theorem. *Let N be a Petri Net, M_0 and M_d markings for N. If M_d is reachable from M_0, then the system of linear equations with integer coefficients (1.30) has a non-negative integer solution.*

(1.32) Example. Consider the following Petri Net:



The state equation (1.29) is shown below, where the transition t_3 fires to result in the marking $M_1 = [3, 0, 0, 1]^T$ from $M_0 = [2, 0, 1, 0]^T$:

$$\begin{bmatrix} 3 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \\ 1 \\ 0 \end{bmatrix} + \begin{bmatrix} -1 & 1 & 1 \\ 1 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$ □

We now introduce the notion of (directed) path in a Petri Net, which we need in order to talk about acyclic Nets.

(1.33) Definition. Let N be a Petri Net. A *path* from a vertex v to a vertex w is a finite sequence of vertices $\pi = (v_0, \ldots, v_l)$ where $l \geq 1$, $v_0 = v$, $v_l = w$ and for all $i \in \{0, \ldots, l-1\}$ $v_{i+1} \in v_i{\bullet} \cup {\bullet}v_i$. Two vertices are said to be *connected* if there is a path from one to the other. If every vertex in N is connected with every other vertex, then N is said to be *weakly connected*.

A *directed path* from a vertex v to a vertex w is a finite sequence of vertices $\pi = (v_0, \ldots, v_l)$ such that $v = v_0$, $w = v_l$ and for all $i \in \{0, \ldots, l-1\}$ $v_{i+1} \in v_i{\bullet}$. In this case we say that the path π has length l. A directed path from a vertex to itself is called a *cycle*, or *loop*; if N does not have cycles, then it is said to be *acyclic*. Two vertices v and w are said to be *directly connected* if there is a directed path either from v to w or from w to v. □

The existence of a non-negative integer solution to equation (1.30) is in general only a necessary condition, but for *acyclic* Petri Nets it turns out to be also sufficient: if x is a non-negative integer solution for (1.30), then M_d is reachable from M_0 by firing each transition t exactly $x(t)$ times, as we can see in the following theorem.

(1.34) Theorem ([HI88]). *Let N be an acyclic Petri Net and A its incidence matrix, M_0, M_d markings for N. Then M_d is reachable from M_0 if and only if there is a non-negative integer solution x for the equation*

$$M_d = M_0 + Ax.$$

Proof. Only sufficiency has to be shown. Suppose there exists x vector of non-negative integers satisfying equation $M_d = M_0 + Ax$, call N_x the subnet of N consisting of all those transitions t such that $x(t) > 0$, together with their input and output places and connecting arcs. Denote by M_{0_x} the subvector of M_0 for places in N_x.

The subnet N_x is obviously acyclic. Claim: there is at least one transition t in N_x that is enabled in marking M_{0_x}. If there were not such a t, then consider any disabled transition s: there must be at least one token-free input place of s, say p_1. If p_1 is not a source, then it is the output of another disabled transition s'. Continue to back-track token-free input places of disabled transitions: this process will end, because of the acyclicity of N_x, at at least one token-free source place p. That means that $M_0(p) = 0$, and by definition of the incidence matrix A (1.28), we have $a_{pj} \leq 0$ for all j transitions in N_x, as p is not the output of any transition. However, there is at least one j_0 transition which has p as input, as we found p by back-tracking input places of non-firable transitions, hence $a_{pj_0} = -1$. Since $x(j) > 0$ for all j transitions in N_x, we have, if n is the total number of transitions,

$$0 \leq M_d(p) = 0 + (Ax)(p) = \sum_{j=1}^{n} a_{pj}\, x(j) < 0$$

which is a contradiction, hence the claim holds and there is indeed an enabled transition t in M_{0_x}. Now, fire t, call u_t the n-vector consisting of all 0's except for a 1 in the t-th entry, let the resulting marking be $M' = M_0 + Au_t$, and let $x' = x - u_t$: we have then $M_d = M' + Ax'$, with x' vector of non-negative integers, and the subnet $N_{x'}$ is still acyclic. Repeating this process until x' reduces to a zero vector will yield to a firing sequence that transforms M_0 in M_d. **Qed**

(1.35) Remark. The proof of Theorem (1.34) shown here is non-constructive; however, a constructive proof has been proposed in [SB02]: the idea is to classify the transitions in terms of how "far" they are from source places, and to notice that the incidence matrix can obtain a block-triangular structure by re-arranging the rows and columns accordingly. We refer the reader to [SB02] for more details.

§1.3 A sufficient condition for compositionality

We are now ready to apply the theory of Petri Nets to solve the problem of compositionality of arbitrary dinatural transformations. For the rest of this chapter, fix transformations $\varphi\colon F_1 \to F_2$ and $\psi\colon F_2 \to F_3$ where

- $F_i\colon \mathbb{C}^{\alpha^i} \to \mathbb{D}$ is a functor for all $i \in \{1,2,3\}$,
- φ and ψ have type, respectively,

$$|\alpha^1| \xrightarrow{\sigma_1} k_1 \xleftarrow{\tau_1} |\alpha^2| \qquad \text{and} \qquad |\alpha^2| \xrightarrow{\sigma_2} k_2 \xleftarrow{\tau_2} |\alpha^3|.$$

We shall establish a sufficient condition for the dinaturality of $\psi \circ \varphi$ in some of its variables. However, since we are interested in analysing the dinaturality of the composition in each of its variables *separately*, we start by assuming that $\psi \circ \varphi$ depends on only one variable, i.e. has type $|\alpha^1| \to 1 \leftarrow |\alpha^3|$, and that φ and ψ are dinatural in all their variables. In this case, we have to show that the following hexagon commutes for all $f\colon A \to B$, recalling from p.26 that $F_1(B|A)$ is the result of applying functor F_1 in B in all its contravariant arguments and in A in all its covariant ones:

(1.36)
$$\begin{tikzcd}
 & F_1(A|A) \arrow[r, "\varphi_{A\dots A}"] & F_2(A|A) \arrow[r, "\psi_{A\dots A}"] & F_3(A|A) \arrow[dr, "F_3(1|f)"] & \\
F_1(B|A) \arrow[ur, "F_1(f|1)"] \arrow[dr, "F_1(1|f)"'] & & & & F_3(A|B) \\
 & F_1(B|B) \arrow[r, "\varphi_{B\dots B}"'] & F_2(B|B) \arrow[r, "\psi_{B\dots B}"'] & F_3(B|B) \arrow[ur, "F_3(f|1)"'] &
\end{tikzcd}$$

The no-ramification case. Rephrasing Eilenberg and Kelly's work in [EK66] on what they called "generalised natural transformations" in our terms, they treated the case in which φ and ψ are either natural or extranatural in each variable and their graphs do not contain ramifications. This means that every variable of φ and ψ is used exactly twice when writing down their general components, or, in other words, the boxes in $\Gamma(\varphi)$ and $\Gamma(\psi)$ are linked in pairs. Examples (1.10), (1.11) are instances of Eilenberg-Kelly transformations. Indeed, their definition of graph of a transformation does not involve the black squares corresponding to the variables of the family of morphisms, since there was no need for that.

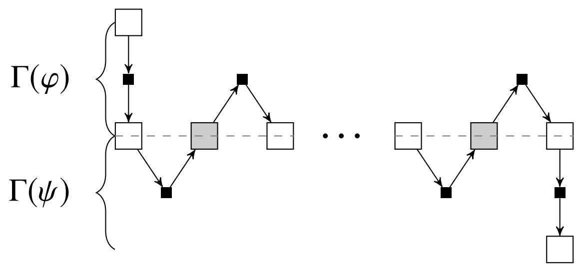
(Extra)natural transformations with no ramifications already do not compose in general, as example (1.15) applies. However, Eilenberg and Kelly individuated a sufficient and "essentially necessary" condition for composability, which in our notations is the following:

(1.37) Theorem (Eilenberg-Kelly, 1966). *Suppose φ and ψ are either natural or extranatural in all their variables, and $\Gamma(\varphi)$ and $\Gamma(\psi)$ contain no ramifications. If $\Gamma^*(\psi \circ \varphi)$ is acyclic, then $\psi \circ \varphi$ is either natural or extranatural.*

In their proof, they showed that there are only three possible schemes of cases for $\Gamma(\varphi)$ and $\Gamma(\psi)$ in order to have $\Gamma^*(\psi \circ \varphi)$ acyclic:

- "Yanking" case:

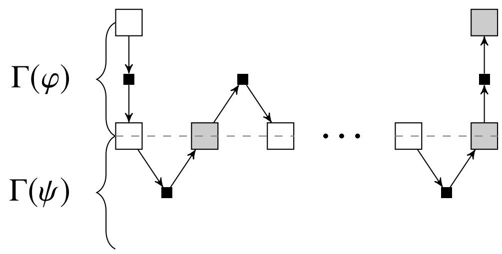
If



then $\psi \circ \varphi$ is natural.

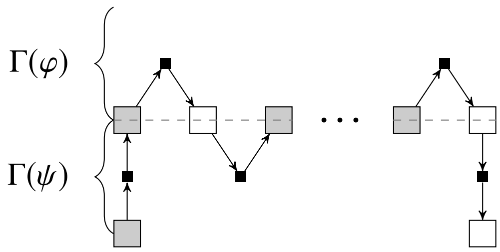
- "Stalactite" case:

If



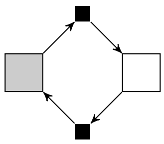
then $\psi \circ \varphi$ is extranatural.

- "Stalagmite" case:

If 

then $\psi \circ \varphi$ is extranatural.

Their proof is essentially combinatoric, but in fact it shows that "plugging" an f at the top left box in the first two cases and in the bottom left box in the last one, the f can "travel" through the graph in virtue of the (extra)naturality of φ and ψ in each of their variables, until it reaches the opposite end of the graph, no matter how many U-turns there are. The result is "essentially necessary" in the sense that if we do create a cycle upon constructing $\Gamma^*(\psi \circ \varphi)$, then that means we are in a situation like this:



where we have a transformation between constant functors, like in Example (1.15). Such a family of morphisms is (extra)natural precisely when it is constant (that is, if every component is equal to the same morphism).

The general case. What happens when we lift the hypothesis of no ramifications? Now Eilenberg and Kelly's proof is not useful any more, as there are not just three schemes of cases for $\Gamma(\varphi)$ and $\Gamma(\psi)$ so that $\Gamma^*(\psi \circ \varphi)$ is acyclic, but infinitely many. Nonetheless, the presence of cycles is clearly problematic for the same reasons as before, and by looking at acyclic examples, like (1.18), one can see that dinaturality is preserved. The result we want to prove is then the following direct generalisation of (1.37).

(1.38) Theorem. *Let φ and ψ be transformations which are dinatural in all their variables and such that $\psi \circ \varphi$ depends on only one variable. If $\Gamma^*(\psi \circ \varphi)$ is acyclic, then $\psi \circ \varphi$ is a dinatural transformation.*

As already said in Remark (1.26), the key to prove this theorem is to see $\Gamma^*(\psi \circ \varphi)$ as a Petri Net, reducing the dinaturality of $\psi \circ \varphi$ to the reachability problem for two markings we shall individuate and then using Theorem (1.34). We begin by unfolding the definition of $\Gamma^*(\psi \circ \varphi)$: we have $\Gamma^*(\psi \circ \varphi) = (P, T, \bullet(-), (-)\bullet)$ where $P = |\alpha^1| + |\alpha^2| + |\alpha^3|$, $T = k_1 + k_2$ and, indicating with $\iota_i \colon |\alpha^i| \to P$ and $\rho_i \colon k_i \to T$

the injections defined similarly to $\iota_{|\alpha|}$ and $\iota_{|\beta|}$ in (1.16),

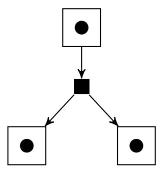
$$\textbf{(1.39)}\qquad \begin{aligned} \bullet(\rho_i(t)) &= \{\iota_i(p) \mid \sigma_i(p) = t,\ \alpha^i_p = +\} \cup \{\iota_{i+1}(p) \mid \tau_i(p) = t,\ \alpha^{i+1}_p = -\},\\ (\rho_i(t))\bullet &= \{\iota_i(p) \mid \sigma_i(p) = t,\ \alpha^i_p = -\} \cup \{\iota_{i+1}(p) \mid \tau_i(p) = t,\ \alpha^{i+1}_p = +\}. \end{aligned}$$

For the rest of this chapter, we shall reserve the names P and T for the sets of places and transitions of $\Gamma^*(\psi \circ \varphi)$.

(1.40) Remark. Since σ_i and τ_i are functions, we have that $|\bullet p|, |p\bullet| \leq 1$ and also that $|\bullet p \cup p\bullet| \geq 1$ for all $p \in P$. (In particular, every source or sink is proper.) With a little abuse of notation then, if $\bullet p = \{t\}$ then we shall simply write $\bullet p = t$, and similarly for $p\bullet$.

Labelled markings as morphisms. We now show how to formally translate certain markings of $\Gamma^*(\psi \circ \varphi)$ in actual morphisms of $\mathbb{D}$. The idea is to treat every token in the net as a fixed, arbitrary morphism $f\colon A \to B$ of $\mathbb{C}$ and then use the idea discussed in p. 38.

However, not all possible markings of $\Gamma^*(\psi \circ \varphi)$ have a corresponding morphism in $\mathbb{D}$ as such. For example, if M is a marking and p is a place such that $M(p) > 1$, it makes no sense to "compute a functor F_i in f twice" in the argument of F_i corresponding to p. Hence, only markings $M\colon P \to \{0,1\}$ can be considered. Moreover, we have to be careful with *where* the marking puts tokens: if a token corresponds to a morphism $f\colon A \to B$, we have to make sure that there are no two consecutive tokens (more in general, we have to make sure that there is at most one token in every directed path), otherwise a naive attempt to assign a morphism to that marking might end up with type-checking problems. For instance, consider the diagonal transformation in a Cartesian category (example (1.9)) and the following marking:



The token on the top white box should be interpreted as $id_{\mathbb{C}}(f)\colon A \to B$, hence the black middle box should correspond to the B-th component of the family δ, that is $\delta_B\colon B \to B \times B$. However, the bottom two white boxes are read as $f \times f\colon A \times A \to B \times B$, which cannot be composed with δ_B!

We therefore introduce the notion of *labelled marking*, which consists of a marking together with a labelling of the transitions, such that a certain coherence condition between the two is satisfied. This restraint will ensure that every labelled marking will be "translatable", as it were, into a morphism of $\mathbb{C}$. We will then use only *some* labelled markings to prove our compositionality theorem.

(1.41) Definition. Consider $f : A \to B$ a morphism in $\mathbb{C}$. A *labelled marking* for $\Gamma^*(\psi \circ \varphi)$ is a triple (M, L, f) where functions $M : P \to \{0, 1\}$ and $L : T \to \{A, B\}$ are such that for all $p \in P$

$$M(p) = 1 \Rightarrow L(\bullet p) = A,\ L(p\bullet) = B$$

$$M(p) = 0 \Rightarrow L(\bullet p) = L(p\bullet)$$

These conditions need to be satisfied only when they make sense; for example if $M(p) = 1$ and $\bullet p = \varnothing$, condition $L(\bullet p) = A$ is to be ignored. □

(1.42) Proposition. *If $(M, L, f : A \to B)$ is a labelled marking, then every directed path in $\Gamma^*(\psi \circ \varphi)$ contains at most one token. If π is a directed path containing one token, then every transition preceding the token is labelled with A, while every transition following it is labelled with B. If π does not contain any token, then every transition in π has the same label, either A or B.*

PROOF. We only prove the first statement; the rest follows from a similar argument. Suppose that there is a directed path $\pi = (v_0, \ldots, v_l)$ with $v_{i+1} \in v_i\bullet$ that contains two tokens, say one in place $p = v_0$ and one in place $q = v_l$ (l is even). Then $L(p\bullet) = B$ and $L(\bullet q) = A$. Now, $p\bullet = v_1$ and since we assumed π only contains two tokens, we have that $M(v_1\bullet) = M(v_2) = 0$. Hence, $L(v_3) = L(v_2\bullet) = L(\bullet v_2) = L(v_1) = L(p\bullet) = B$. By repeating the process, we have that $L(v_5) = \cdots = L(v_{l-1}) = B$, which is in contradiction with the fact that $A = L(\bullet q) = L(v_{l-1})$. QED

We are now ready to assign a morphism in $\mathbb{D}$ to every labelled marking by reading a token in a place as a morphism f in one of the arguments of a functor, while an empty place corresponds to the identity morphism of the label of the transition of which the place is an input or an output.

(1.43) Definition. Let $(M, L, f : A \to B)$ be a labelled marking. We define a morphism $\mu(M, L, f)$ in $\mathbb{D}$ as follows:

$$\mu(M, L, f) = F_1(x^1_1, \ldots, x^1_{|\alpha^1|}); \varphi_{X^1_1 \ldots X^1_{k_1}}; F_2(x^2_1, \ldots, x^2_{|\alpha^2|}); \psi_{X^2_1 \ldots X^2_{k_2}}; F_3(x^3_1, \ldots, x^3_{|\alpha^3|})$$

where

$$x^i_j = \begin{cases} f & M(\iota_i(j)) = 1 \\ id_{L(t)} & M(\iota_i(j)) = 0 \wedge t \in \bullet\iota_v(j) \cup \iota_v(j)\bullet \end{cases} \qquad X^i_j = L(\rho_i(j)).$$

for all $i \in \{1, 2, 3\}$ and $j \in \{1, \ldots, |\alpha^i|\}$. (Recall that $\iota_i : |\alpha^i| \to P$ and $\rho_i : k_i \to T$ are the injections defined similarly to $\iota_{|\alpha|}$ and $\iota_{|\beta|}$ in (1.16).) □

(1.44) Proposition. *$\mu(M, L, f)$ is indeed a morphism of $\mathbb{D}$.*

Proof. We prove that the morphisms $\mu(M, L, F)$ is made of are actually composable, by making use of the definition of labelled marking (1.41) and the explicit definition of $\Gamma^*(\psi \circ \varphi)$ (1.39). We only show that $codom\left(F_1(x^1_1, \ldots, x^1_{|\alpha^1|})\right) = dom\left(\varphi_{X^1_1,\ldots,X^1_{k_1}}\right)$, all the remaining equalities can be shown by an analogous argument.

We have $codom\left(F_1(x^1_1, \ldots, x^1_{|\alpha^1|})\right) = F_1(C_1, \ldots, C_{|\alpha^1|})$ where

$$C_j = \begin{cases} codom\left(x^1_j\right) & \alpha^1_j = + \\ dom\left(x^1_j\right) & \alpha^1_j = - \end{cases}$$

whereas

$$dom\left(\varphi_{X_1,\ldots,X_{k_1}}\right) = F_1\left(X^1_{\sigma_1 1}, \ldots, X^1_{\sigma_1|\alpha^1|}\right) = F_1\left(L(\rho_1\sigma_1 1), \ldots, L(\rho_1\sigma_1|\alpha^1|)\right)$$

and we prove that $C_j = L(\rho_1\sigma_1 j)$ for all $j \in \{1, \ldots, |\alpha^1|\}$.
Case $\alpha^1_j = +$. We have $C_j = codom\left(x_j\right)$, $\bullet\iota_1(j) = \varnothing$, $\iota_1(j)\bullet = \rho_1\sigma_1 j$.

- If $M(\iota_1 j) = 1$, then $x^1_j = f$ and $C_j = B$ while $L(\rho_1\sigma_1 j) = L((\iota_1 j)\bullet) = B$.
- If $M(\iota_1 j) = 0$, then $C_j = L((\iota_1 j)\bullet) = L(\rho_1\sigma_1 j)$.

Case $\alpha^1_j = -$. We have $C_j = dom\left(x_j\right)$, $\iota_1(j)\bullet = \varnothing$, $\bullet\iota_1(j) = \rho_1(\sigma_1 j)$.

- If $M(\iota_1 j) = 1$, then $C_j = A$ while $L(\rho_1\sigma_1 j) = L(\bullet(\iota_1 j)) = A$.
- If $M(\iota_1 j) = 0$, then $C_j = L(\bullet(\iota_1 j)) = L(\rho_1\sigma_1 j)$. **Qed**

What are the labelled markings corresponding to the two legs of diagram (1.36)? In the lower leg of the hexagon, f appears in all the covariant arguments of F_1 and the contravariant ones of F_3, which correspond in $\Gamma^*(\psi \circ \varphi)$ to those places which have no inputs (in Petri nets terminology, *sources*), and all variables of φ are equal to B; in the upper leg, f appears in those arguments corresponding to places with no outputs (*sinks*), and ψ is computed in A in each variable. Hence, the lower leg is $\mu(M_0, L_0, f)$ while the upper leg is $\mu(M_d, L_d, f)$, where:

(1.45)
$$M_0(p) = \begin{cases} 1 & \bullet p = \varnothing \\ 0 & \text{otherwise} \end{cases} \qquad M_d(p) = \begin{cases} 1 & p\bullet = \varnothing \\ 0 & \text{otherwise} \end{cases}$$
$$L_0(t) = B \qquad\qquad L_d(t) = A$$

for all $p \in P$ and $t \in T$. It is an immediate consequence of the definition that (M_0, L_0, f) and (M_d, L_d, f) so defined are labelled markings.

We aim to show that M_d is reachable from M_0 by means of a firing sequence that "preserves" the morphism $\mu(M_0, L_0, f)$. In order to do so, we now prove that firing a B-labelled transition in an arbitrary labelled marking (M, L, f) generates a new labelled marking, whose associated morphism in $\mathbb{D}$ is still equal to $\mu(M, L, f)$.

(1.46) Proposition. *Let (M, L, f) be a labelled marking, $t \in T$ an enabled transition such that $L(t) = B$. Consider*

$$\begin{array}{ccc} P \xrightarrow{M'} \{0,1\} & & T \xrightarrow{L'} \{A,B\} \\ p \mapsto \begin{cases} 0 & p \in \bullet t \\ 1 & p \in t\bullet \\ M(p) & \textit{otherwise} \end{cases} & & s \mapsto \begin{cases} A & s = t \\ L(s) & s \neq t \end{cases} \end{array} \tag{1.47}$$

Then (M', L', f) is a labelled marking and $\mu(M, L, f) = \mu(M', L', f)$.

Proof. By definition of labelled marking, if $t\bullet \neq \emptyset$ and $L(t) = B$ then $M(p) = 0$ for all $p \in t\bullet$, because if there were a $p \in t\bullet$ with $M(p) = 1$, then $L(t) = A$. M' is therefore the marking obtained from M when t fires once. We now show that (M', L', f) is a labelled marking.

Case $M'(p) = 1$. If $p \in t\bullet$, then $L'(\bullet p) = L'(t) = A$ and $L'(p\bullet) = L(p\bullet) = B$, the last equation is due to the fact that $M(p) = 0$, so $L(p\bullet) = L(\bullet p) = L(t) = B$ by hypothesis. If $p \notin t\bullet$, then $1 = M'(p) = M(p)$ and $\bullet p \neq t$. Since (M, L, f) is a labelled marking, we have that $L'(\bullet p) = L(\bullet p) = A$ and $L'(p\bullet) = L(p\bullet) = B$ because $p\bullet \neq t$ as if it were we would have $M'(p) = 0$ by definition of M'.

Case $M'(p) = 0$. If $p \in \bullet t$, then $L'(\bullet p) = L(\bullet p)$ (remember that we do not allow for self loops, that is $\bullet p \neq p\bullet$ for all places p) and since $M(p) = 1$ given that t is enabled in M, we have $L(\bullet p) = A = L'(t) = L'(p\bullet)$. If instead $p \notin \bullet t$, then $0 = M'(p) = M(p)$ and $p\bullet \neq t$. Since (M, L, f) is a labelled marking, we have that $L'(\bullet p) = L(\bullet p)$ as $\bullet p \neq t$ (otherwise we would have $M'(p) = 1$), moreover $L(\bullet p) = L(p\bullet) = L'(p\bullet)$.

We have now to prove that $\mu(M, L, f) = \mu(M', L', f)$. Since $t \in T$, we have $t = \rho_u(i)$ for some $u \in \{1, 2\}$ and $i \in \{1, \dots, k_u\}$. The fact that t is enabled in M, together with (1.39) and (1.43), ensures that, in the notations of Definition (1.43),

$$\begin{aligned} \sigma_u(j) = i \wedge \alpha_j^u = + &\Rightarrow x_j^u = f \\ \sigma_u(j) = i \wedge \alpha_j^u = - &\Rightarrow x_j^u = id_B \\ \tau_u(j) = i \wedge \alpha_j^{u+1} = + &\Rightarrow x_j^{u+1} = id_B \\ \tau_u(j) = i \wedge \alpha_j^{u+1} = - &\Rightarrow x_j^{u+1} = f \end{aligned}$$

hence we can apply the dinaturality of φ or ψ (if, respectively, $u = 1$ or $u = 2$) in its i-th variable. For the sake of simplicity, assume that $u = 1$: we obtain therefore a new morphism

$$F_1(y_1^1, \dots, y_{|\alpha^1|}^1); \varphi_{Y_1^1 \dots Y_{k_1}^1}; F_2(y_1^2, \dots, y_{|\alpha^2|}^2); \psi_{X_1^2 \dots X_{k_2}^2}; F_3(x_1^3, \dots, x_{|\alpha^3|}^3)$$

where

$$y_j^1 = \begin{cases} id_A & \sigma_1(j) = i \wedge \alpha_j^1 = + \\ f & \sigma_1(j) = i \wedge \alpha_j^1 = - \\ x_j^1 & \text{otherwise} \end{cases} \qquad y_j^2 = \begin{cases} f & \sigma_2(j) = i \wedge \alpha_j^2 = + \\ id_A & \sigma_2(j) = i \wedge \alpha_j^2 = - \\ x_j^2 & \text{otherwise} \end{cases}$$

$$Y_j^1 = \begin{cases} A & j = i \\ X_j^1 & j \neq i \end{cases}$$

On the other hand,

$$\mu(M', L', f) = F_1(z_1^1, \ldots, x_{|\alpha^1|}^1); \varphi_{Z_1^1 \ldots Z_{k_1}^1}; F_2(z_1^2, \ldots, z_{|\alpha^2|}^2); \psi_{X_1^2 \ldots X_{k_2}^2}; F_3(x_1^3, \ldots, x_{|\alpha^3|}^3)$$

where

$$z_j^\nu = \begin{cases} f & M'(\iota_\nu(j)) = 1 \\ id_{L'(s)} & M'(\iota_\nu(j)) = 0 \wedge s \in \bullet\iota_\nu(j) \cup \iota_\nu(j)\bullet \end{cases} \qquad Z_j^1 = L'(\rho_1(j))$$

for $\nu \in \{1,2\}$. Is it true that $y_j^\nu = z_j^\nu$ for all $\nu \in \{1,2\}$ and $j \in \{1, \ldots, |\alpha^\nu|\}$? We consider case $\nu = 1$. Call $p = \iota_1(j)$. Then

$$\begin{aligned} z_j^1 = f &\iff M'(p) = 1 \iff p \in t\bullet \vee (p \notin \bullet t \wedge M(p) = 1) \\ y_j^1 = f &\iff (\sigma_1(j) = i \wedge \alpha_j^1 = -) \vee (\sigma_1(j) \neq i \wedge M(p) = 1) \end{aligned}$$

Condition $p \in t\bullet$ is equivalent, by (1.39), to $\sigma_1(j) = i \wedge \alpha_j^1 = -$, whereas

$$p \notin \bullet t \wedge M(p) = 1 \iff (p \in t\bullet \vee \sigma_1(j) \neq i) \wedge M(p) = 1 \iff \sigma_1(j) \neq i \wedge M(p) = 1$$

the last equivalence following from the fact that $p \in t\bullet \wedge M(p) = 1$ is false, as remarked at the very beginning of this proof. Moreover, $z_j^1 \neq f$ precisely when $M'(p) = 0$, in which case $z_j^1 = id_{L'(s)}$ for $s \in \bullet p \cup p\bullet$. On the other hand,

$$y_j^1 \neq f \iff (\sigma_1(j) = i \wedge \alpha_j^1 = +) \vee (\sigma_1(j) \neq i \wedge M(p) = 0)$$

and in any case $y_j^1 \neq f$ means $y_j^1 = id_{L'(s)}$ for $s \in \bullet p \cup p\bullet$, as if $\sigma_1(j) = i \wedge \alpha_j^1 = -$ then $L'(\bullet p) = L'(t) = A$, and if $\sigma_1(j) \neq i \wedge M(p) = 0$ then $y_f^1 = x_j^1 = id_{L(s)} = id_{L'(s)}$, since $s \neq t$. Finally, condition $M'(p) = 0$ means that either $p \in \bullet t$, which is the same as saying that $\sigma_1(j) = i \wedge \alpha_j^1 = +$, or $p \notin t\bullet \wedge M(p) = 0$, which is equivalent to $\sigma_1(j) \neq i \wedge M(p) = 0$.

We have now only to check that $Y_j^1 = Z_j^1$ for all $j \in \{1, \ldots, k_1\}$. If $j = i$, then

$$Z_j^1 = L'(\rho_1 i) = L'(t) = A = Y_j^1$$

whereas if $j \neq i$ then $\rho_1 j \neq t$, therefore

$$Z^1_j = L'(\rho_1 j) = L(\rho_1 j) = Y^1_j.$$ **Qed**

It immediately follows that a sequence of firings of B-labelled transitions gives rise to a labelled marking whose associated morphism is still equal to the original one, as the following Proposition states.

(1.48) Proposition. *Let $\mu(M, L, f)$ be a labelled marking, M' a marking reachable from M by firing only B-labelled transitions $t_1, \ldots, t_m$, $L' \colon T \to \{A, B\}$ defined as:*

$$L'(s) = \begin{cases} A & s = t_i \text{ for some } i \in \{1, \ldots, m\} \\ L(s) & \text{otherwise} \end{cases}$$

Then (M', L', f) is a labelled marking and $\mu(M, L, f) = \mu(M', L', f)$.

(1.49) Remark. Although the previous Propositions hold for arbitrary labelled markings, we shall make use of them only for those markings that are "intermediate" in between (M_0, L_0, f) and (M_d, L_d, f). These intermediate markings are characterised by the fact that they put exactly one token in each directed path.

Now all we have to show is that M_d is reachable from M_0 (see (1.45)) by only firing B-labelled transitions: it is enough to make sure that each transition is fired at most once to satisfy this condition. Theorem (1.34) provides a necessary and sufficient condition for the reachability of M_d from M_0: find a vector x of non-negative integers that solves equation $M_d = M_0 + Ax$, with A the incidence matrix of $\Gamma^*(\psi \circ \varphi)$. Here x has length $k_1 + k_2$, which is the number of transitions in $\Gamma^*(\psi \circ \varphi)$, and $x(t)$ is the number of times transition t has to fire in order to transform M_0 into M_d. Hence, as long as we know how many times each transition should fire, and the resulting vector is a solution to (1.30), Theorem (1.34) ensures us that there is indeed a way to transform M_0 into M_d by firing each transition t exactly $x(t)$ times.

A necessary condition for x. We start by showing some necessary conditions for x to be a non-negative integer solution of $M_d = M_0 + Ax$: these conditions, together with the fact that we want $x(t) \leq 1$ for all t transitions as we have already observed, will lead us to find x explicitly. For reasons that will become clear in Chapter 3, it is useful to work abstractly in the general theory of Petri Nets. We now introduce a special class of Nets, to which our $\Gamma^*(\psi \circ \varphi)$ belongs (Remark (1.40)), where all places have at most one input and at most one output.

(1.50) Definition. A Petri Net is said to be *forward-backward conflict free* (FBCF) if for all p place $|\bullet p| \leq 1$ and $|p \bullet| \leq 1$. □

In this section we fix an arbitrary FBCF Petri Net N with m places and n transitions, call A its incidence matrix, and define markings M_0 and M_d as in (1.45). We recall again that M_0 puts one token in every source, while M_d in every sink; if p is a source and a sink at once (so it is a place "floating in space" as it were, not connected to any transition), then $M_0(p) = M_d(p)$. (Notice that such places do not exist in $\Gamma^*(\psi \circ \varphi)$, as all sources and sinks are proper.) We assume that M_d is indeed reachable from M_0 by means of a firing sequence $u_1, \dots, u_d$, with

$$x = \sum_{k=1}^{d} u_k \tag{1.51}$$

(each u_i is a $n \times 1$ vector consisting of $n-1$ zeros and one 1 in the entry which corresponds to the transition fired at step i). What can we infer about x?

(1.52) Remark. If N does not have any sources or sinks, then $M_0 = M_d$ and $x = [0, \dots, 0]$. For $N = \Gamma^*(\psi \circ \varphi)$, this would mean that $\psi \circ \varphi$ is a transformation between constant functors, which is dinatural precisely when it is a constant family of morphisms. Also if every source is also a sink, then $M_0 = M_d$ and $x = [0, \dots, 0]$ as well.

(1.53) Remark. By definition of incidence matrix, the p-th row of A is a $n \times 1$ vector that is null precisely if p has no inputs or outputs and, if p does have at least one input or output, then it is made of all zeros except for:

- exactly one 1 and one -1, when p has one input and one output,
- exactly one 1, when p has one input and no outputs (i.e. is a proper sink),
- exactly one -1, when p has one output and no inputs (i.e. is a proper source),

The following Lemma states a very simple remark: if there is at least one proper source or sink place in N, and M_d is reachable from M_0, then at least one transition must fire. Intuitively, if no transition fired, then the tokens in the proper source places (put there by M_0) would never move away from them, and the proper sink places would never be marked (as they should be in M_d).

(1.54) Lemma. *Suppose that N has at least one proper source or proper sink place. Then there is a transition t such that $x(t) > 0$.*

Proof. Define the $m \times 1$ vectors

$$M_k = M_{k-1} + Au_k \qquad k \in \{1, \dots, d\}.$$

Suppose that there is a proper source (sink) place p, and call t its only output (input). If, by contradiction, $x(t) = 0$, then $u_k(t) = 0$ for all k by definition of x (1.51). Hence $M_k(p) = M_{k-1}(p)$ for all $k \geq 1$: indeed,

$$(Au_k)(p) = \sum_{j=1}^{n} a_{pj}\, u_k(j)$$

and

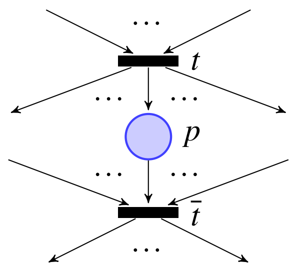
$$a_{pj} = \begin{cases} -1 & j = t \text{ and } p \text{ is a source} \\ +1 & j = t \text{ and } p \text{ is a sink} \\ 0 & \text{otherwise} \end{cases}$$

In any case, $\sum_{j=1}^{n} a_{pj}\, u_k(j) = \pm u_k(t) = 0$, hence $M_k(p) = M_{k-1}(p)$. This is in contradiction with $M_0(p) \neq M_d(p)$, be p a source or a sink place. **Qed**

We move on by observing that if M_d is reachable from M_0 and a particular transition fires at least once, then all transitions directly connected to it must fire as well: again intuitively, in order for a transition t to fire it must be enabled, hence those transitions which are between the source places and t must fire to move the tokens to the input places of t; moreover, if t fires, then also all those transitions "on the way" from t to the sink places must fire, otherwise some tokens would get stuck in the middle of the net, in disagreement with M_d.

(1.55) Lemma. *If there is a transition $\bar{t}$ such that $x(\bar{t}) > 0$, then $x(t) > 0$ for all transitions t connected to $\bar{t}$.*

Proof. If $\bar{t} = t$, there is nothing to prove. As every path can be split into a sequence of directed ones, it is enough to prove the lemma for those transitions t directly connected with $\bar{t}$. We prove that for all $l \geq 2$, for all t transition such that there is a path $\pi = (v_0, \dots, v_l)$ from t to $\bar{t}$ or from $\bar{t}$ to t it is the case that $x(t) > 0$, by induction on l, the length of π.
Case $l = 2$. Suppose $\pi = (t, p, \bar{t})$, that is we are in the situation



Define the $m \times 1$ vectors

$$M_k = M_{k-1} + Au_k \qquad k \in \{1, \dots, d\}.$$

The fact that $x(\bar{t}) > 0$ implies that there is a $k \in \{1, \dots, d\}$ such that $u_k(\bar{t}) = 1$, which is the same as saying that $\bar{t}$ fires at step k for some k. Necessarily then, $M_{k-1}(p) > 0$, otherwise $\bar{t}$ would be disabled and unable to fire at step k. (Notice that k cannot be 1, as $M_0(p) = 0$, but we do not need this additional information.) Now, suppose that t never fires, that is $x(t) = 0$: we prove that in this case $M_i(p) = 0$ for all $i \in \{1, \dots, d\}$ (i.e. p is never marked), which contradicts the fact that $M_{k-1}(p) > 0$, by finite induction on i. As we have already observed, $M_0(p) = 0$, what with p being neither a source nor a sink place; suppose that $M_{i-1}(p) = 0$ for a fixed $i \geq 1$: we have, by definition of M_i,

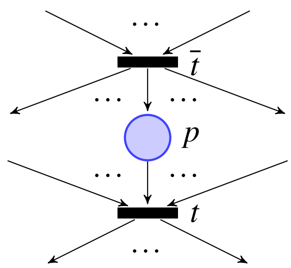
$$M_i(p) = M_{i-1}(p) + (Au_k)(p) = (Au_k)(p) = \sum_{j=1}^{n} A_{pj}\, u_i(j)$$

where

$$A_{pj} = \begin{cases} +1 & j = t \\ -1 & j = \bar{t} \\ 0 & \text{otherwise} \end{cases}$$

Therefore, $M_i(p) = u_i(t) - u_i(\bar{t}) = 0$ because $u_i(t) = 0$ as $x(t) = 0$ and because $u_i(\bar{t}) = 0$ as $M_{i-1}(p) = 0$, hence $\bar{t}$ cannot fire at step i.

If, instead, $\pi = (\bar{t}, p, t)$, then we are in the following situation:



Again, we have $u_k(\bar{t}) =$ for some k, which implies $M_k(p) > 0$. Suppose, by contradiction, that $x(t) = 0$: then $u_i(t) = 0$ for all i. We prove that $M_i(p) > 0$ for all $i \in \{k, \ldots, d\}$ by finite induction on i. The base case is already proven, suppose now $M_{i-1}(p) > 0$ for a fixed $i \geq k + 1$. Since

$$A_{pj} = \begin{cases} +1 & j = \bar{t} \\ -1 & j = t \\ 0 & \text{otherwise} \end{cases}$$

we have

$$M_i(p) = M_{i-1}(p) + u_i(\bar{t}) - u_i(t) = M_{i-1}(p) + u_i(\bar{t}) > 0$$

as $u_i(\bar{t}) \geq 0$.

Inductive step. Fix now $l \geq 2$, suppose that for all $k \leq l$, for all t transitions directly connected to $\bar{t}$ by a path of length k we have indeed $x(t) > 0$. Consider then a transition t directly connected to $\bar{t}$ by a path $\pi = (v_0, \ldots, v_{l+1})$ of length $l + 1$. Then the vertices v_2 and v_{l-1}, which are transitions, are such that $x(v_2) > 0$ and $x(v_{l-1}) > 0$ by inductive hypothesis. Hence, by the base case, also $x(t) > 0$, regardless of whether π is a path from t to $\bar{t}$ or vice versa. **Qed**

Combining Lemmas (1.54) and (1.55), we obtain the following necessary condition for reachability of M_d from M_0 in case N is weakly connected and has at least one proper source or sink.

(1.56) Theorem. *Suppose N is weakly connected and has at least one proper source or proper sink. If M_d is reachable from M_0 through a firing sequence $u_1, \dots, u_d$ and $x = \sum_{k=1}^{d} u_k$, then $x(t) > 0$ for all t transitions in N.*

The proof of Theorem (1.38). We have proved that in an arbitrary FBCF Petri Net N with at least one proper source or sink each transition has to fire at least once in order for M_d to be reachable from M_0. On the other hand, when $N = \Gamma^*(\psi \circ \varphi)$, we cannot fire any transition more than once, since we only want to fire B-labelled transitions. It is clear then that what we want is to fire every transition exactly once: the vector $x = [1, \dots, 1]$ is indeed the solution we are seeking.

(1.57) Theorem. *Let N be a FBCF Petri Net, M_0, M_d markings as in (1.45). If N is acyclic, then M_d is reachable from M_0 by firing each transition exactly once.*

Proof. Suppose N has m places and n transitions. Consider the $n \times 1$ vector $x = [1, \dots, 1]$. We have, by Remark (1.53),

$$(Ax)(p) = \sum_{j=1}^{n} A_{pj} = \begin{cases} -1 & p \text{ is a proper source} \\ +1 & p \text{ is a proper sink} \\ 0 & \text{otherwise.} \end{cases}$$

By definition of M_0 and M_d then,

$$M_0(p) + (Ax)(p) = \begin{cases} 1 - 1 & p \text{ is a proper source} \\ 0 + 1 & p \text{ is a proper sink} \\ 1 + 0 & p \text{ is a source and a sink} \\ 0 + 0 & \text{otherwise} \end{cases} = M_d(p).$$

By Theorem (1.34), we conclude. **Qed**

We are now ready to prove Theorem (1.38), which solves the compositionality problem of dinatural transformations.

Proof of Theorem (1.38). Let $f \colon A \to B$ be a morphism in $\mathbb{C}$, and define labelled markings (M_0, L_0, f) and (M_d, L_d, f) as in (1.41). Then $\mu(M_0, L_0, f)$ is the lower leg of (1.36), while $\mu(M_d, L_d, f)$ is the upper leg. By theorem (1.57), marking M_d is reachable from M_0 by firing each transition of $\Gamma^*(\psi \circ \varphi)$ exactly once, hence by only firing B-labelled transitions. By Proposition (1.48), we have that the dinaturality hexagon (1.36) commutes. **Qed**

Theorem (1.38) can then be straightforwardly generalised to the case in which $\psi \circ \varphi$ depends on n variables for an arbitrary n. Suppose then that the type of $\psi \circ \varphi$ is given by the following pushout:

(1.58)
$$\begin{tikzcd}
 & & {|\alpha^3|} \arrow[d, "\tau_2"] \\
 & {|\alpha^2|} \arrow[r, "\sigma_2"] \arrow[d, "\tau_1"'] \arrow[dr, phantom, "\ulcorner"] & k_2 \arrow[d, dotted, "\xi"] \\
{|\alpha^1|} \arrow[r, "\sigma_1"] & k_1 \arrow[r, dotted, "\zeta"] & n
\end{tikzcd}$$

$\Gamma^*(\psi \circ \varphi)$ now has n connected components, and a sufficient condition for the dinaturality of $\psi \circ \varphi$ in its i-th variable is that φ and ψ are dinatural in all those variables of theirs which are "involved", as it were, in the i-th connected component of $\Gamma^*(\psi \circ \varphi)$ *and* each such connected component is acyclic.

(1.59) Theorem. *In the notations above, let $i \in \{1, \dots, n\}$. If φ and ψ are dinatural in all their variables in, respectively, $\zeta^{-1}\{i\}$ and $\xi^{-1}\{i\}$ (with ζ and ξ given by the pushout (1.58)), and if the i-th connected component of $\Gamma^*(\psi \circ \varphi)$ is acyclic, then $\psi \circ \varphi$ is dinatural in its i-th variable.*

We conclude with a straightforward corollary.

(1.60) Corollary. *Let $\varphi \colon F \to G$ and $\psi \colon G \to H$ be transformations which are dinatural in all their variables. If $\Gamma^*(\psi \circ \varphi)$ is acyclic, then $\psi \circ \varphi$ is dinatural in all its variables.*

§1.4 A "necessary" condition for compositionality

Going back to the general theory of FBCF Petri Nets, Theorem (1.56) has also another consequence: if N is weakly connected, has at least one proper source or one proper sink and M_d is reachable from M_0, then N cannot contain any cycle. The reason is that all the transitions involved in any cycle cannot be enabled at any point, as the places in the loop will never be marked. We therefore obtain a sort of inverse of Theorem (1.57).

(1.61) Theorem. *Let N be weakly connected with at least one proper source or one proper sink place. If M_d is reachable from M_0, then N is acyclic.*

Proof. Suppose M_d is reachable from M_0 through a firing sequence $u_1, \dots, u_d$, define $x = \sum_{k=1}^{d} u_k$ and, as usual,

$$M_k = M_{k-1} + Au_k \qquad k \in \{1, \dots, d\}.$$

Suppose also that N contains a directed path $\pi = (v_0, \ldots, v_{2l})$ where $v_0 = v_{2l}$ is a place. We prove that for all $k \in \{1, \ldots, d\}$, for all $i = 0, \ldots, l$, $M_k(v_{2i}) = 0$ by finite induction on k. This implies that all the transitions in π will be forever disabled, contradicting Theorem (1.56).

Indeed, $M_0(v_{2i}) = 0$ for all i because v_{2i} is neither a source nor a sink place by definition of (circular) directed path. Suppose now that for all i, $M_{k-1}(v_{2i}) = 0$ for a fixed $k \geq 1$. Then, given an arbitrary i,

$$M_k(v_{2i}) = M_{k-1}(v_{2i}) + (Au_k)(v_{2i}) = u_k(v_{2i-1}) - u_k(v_{2i+1}) = 0$$

where $u_k(v_{2i-1}) = 0$ and $u_k(v_{2i+1}) = 0$ since, respectively, $M_{k-1}(v_{2i-2}) = 0$ and $M_{k-1}(v_{2i}) = 0$ by inductive hypothesis (so transitions v_{2i-1} and v_{2i+1} cannot fire at step k). **Qed**

In other words, if N contains a loop—in the hypothesis that N is weakly connected and has at least one proper source or sink place—then M_d is *not* reachable from M_0. In the case of $N = \Gamma^*(\psi \circ \varphi)$, given the correspondence between the dinaturality condition of φ and ψ in each of their variables and the firing of the corresponding transitions, this intuitively means that $\psi \circ \varphi$ cannot be proved to be dinatural as a sole consequence of the dinaturality of φ and ψ when $\Gamma^*(\psi \circ \varphi)$ is cyclic. Therefore, acyclicity is not only a *sufficient* condition for the dinaturality of the composite transformation, but also "essentially necessary": if the composite happens to be dinatural despite the cyclicity of the graph, then this is due to some "third" property, like the fact that certain squares of morphisms are pullbacks or pushouts (see discussion after example (1.15)). We prove this intuition formally by considering a syntactic category generated by the equations determined by the dinaturality conditions of φ and ψ, and by showing that in there $\psi \circ \varphi$ *is not* dinatural.

The syntactic category over a signature. We begin by recalling from [Mim11; Bur93; Str76] the concept of syntactic category over a given signature.

(1.62) Definition. A *signature* Σ is a tuple $(O, M, dom, codom)$ where O and M are sets, together with functions $dom, codom \colon M \to O$. O is the set of the *generators for objects*, M of *generators for morphisms*. The signature Σ generates a category $\mathbb{S}$ whose objects are the elements of O and morphisms are formal composite of elements of M and formal identity morphisms, quotiented by suitable laws ensuring associativity and unitarity of composition.

An *equational theory* is a tuple $(O, M, dom, codom, E, l, r)$ where $(O, M, dom, codom)$ is a signature, whereas E is a set of *relations*. Call M^* the set of morphisms of the category generated by the signature $(O, M, dom, codom)$: then $l, r \colon E \to M^*$ are functions such that $dom \circ l = dom \circ r$ and $codom \circ l = codom \circ r$.

The *syntactic category* over the equational theory $(O, M, dom, codom, E, l, r)$ is the category obtained from the category $\mathbb{S}$ generated by the signature $(O, M, dom, codom)$

by quotienting its morphisms by the smallest congruence $\equiv$, with respect to composition, such that $l(e) \equiv r(e)$ for all $e \in E$. □

Given now our category $\mathbb{C}$ and transformations φ and ψ as in §1.3 (dinatural in all their variables), where we suppose again that $\Gamma^*(\psi \circ \varphi)$ is connected, call

$$\mathbb{C}^+ = \mathbb{C} + \text{discrete category over } \{dom\,(x)\,, codom\,(x)\}$$

where x here will play the role of an "indeterminate morphism". $dom\,(x)$ and $codom\,(x)$ are, at the moment, just two additional objects which we add to $\mathbb{C}$ to get the category $\mathbb{C}^+$. Now, call $\mathbb{C}_x$ the free category over the equational theory $(O, M, dom, codom, E, l, r)$ where:

$$\begin{aligned}
O &= \{F_i(A_1, \dots, A_{|\alpha^i|}) \mid i \in \{1,2,3\},\ A_j \in \mathbb{C}^+\} \\
M &= \{F_i(a_1, \dots, a_{|\alpha^i|}) \mid i \in \{1,2,3\},\ a_j = x \text{ or } id_X \text{ for some } X \in \mathbb{C}^+\} \cup \\
&\quad \cup \{\varphi_{A_1,\dots,A_{k_1}} \mid A_j \in \mathbb{C}^+\} \cup \{\psi_{A_1,\dots,A_n} \mid A_j \in \mathbb{C}^+\}
\end{aligned}$$

and E consists of all those relations asserting functoriality of F_1, F_2 and F_3, together with the dinaturality conditions of φ and ψ on $x \colon dom\,(x) \to codom\,(x)$ in each of their variables. In other words, $\mathbb{C}_x$ is the syntactic category whose only morphisms are components of φ and ψ ranging over the objects of $\mathbb{C}^+$, together with the images along the functors F_i's of identity morphisms and x, which has been artificially added to $\mathbb{C}$. In $\mathbb{C}_x$, the only equations that hold, other than those given by the definition of category, are those obtained by functoriality conditions on the F_i's and by dinaturality conditions of φ and ψ.

For $f \colon A \to B$ morphism in $\mathbb{C}$, define the functor $S^f_x \colon \mathbb{C}_x \to \mathbb{D}$ which acts

- on objects by substituting $dom\,(x)$ with A and $codom\,(x)$ with B;

- on morphisms by substituting $x \colon dom\,(x) \to codom\,(x)$ with $f \colon A \to B$.

This is well defined for all f, as if $m_1 = m_2$ in $\mathbb{C}_x$ then $S^f_x(m_1) = S^f_x(m_2)$ in $\mathbb{D}$ because S^f_x preserves the equations of E, given that F_i's are indeed functors and φ and ψ are indeed dinatural in all their variables. Essentially, S^f_x instantiates the indeterminate morphism x in $\mathbb{C}_x$ with the *actual* morphism f of $\mathbb{C}$, and in doing so we come back to our usual $\mathbb{C}$.

We want to prove that if the dinaturality hexagon of $\psi \circ \varphi$ on morphism x commutes in $\mathbb{C}_x$, which implies (via use of S^f_x) that $\psi \circ \varphi$ is "really" dinatural and its dinaturality is due exclusively by dinaturality of φ and ψ and by functoriality of F_i's, then $\Gamma^*(\psi \circ \varphi)$ is acyclic.

(1.63) Theorem. *Consider the following diagram in $\mathbb{C}_x$, where for lack of space we* *abbreviate* $dom\,(x)$ *as* D_x *and* $codom\,(x)$ *as* C_x*:*

$$\textbf{(1.64)}\qquad \begin{tikzcd}[column sep=small] & F_1(D_x|D_x) \arrow[r, "\varphi_{D_x \dots D_x}"] & F_2(D_x|D_x) \arrow[r, "\psi_{D_x \dots D_x}"] & F_3(D_x|D_x) \arrow[dr, "F_3(1|x)"] & \\ F_1(C_x|D_x) \arrow[ur, "F_1(x|1)"] \arrow[dr, "F_1(1|x)"'] & & & & F_3(D_x|C_x) \\ & F_1(C_x|C_x) \arrow[r, "\varphi_{C_x \dots C_x}"'] & F_2(C_x|C_x) \arrow[r, "\psi_{C_x \dots C_x}"'] & F_3(C_x|C_x) \arrow[ur, "F_3(x|1)"'] & \end{tikzcd}$$

If this diagram commutes, then $\Gamma^*(\psi \circ \varphi)$ *is acyclic.*

Now, saying that (1.64) commutes in $\mathbb{C}_x$ is equivalent to having a (finite) chain of equations starting from the upper leg and ending at the lower one, where each equation is due to the dinaturality of φ or ψ in one of their variables:

$$\textbf{(1.65)}\qquad \begin{aligned} & F_1(x|1)\,;\,\varphi_{dom(x)\dots dom(x)}\,;\,\psi_{dom(x)\dots dom(x)}\,;\,F_3(1|x) \\ &= F_1(u^1_1,\dots,u^1_{|\alpha^1|})\,;\,\varphi_{X^1_1,\dots,X^1_{k_1}}\,;\,G(v^1_1,\dots,v^1_{|\alpha^2|})\,;\,\psi_{Y^1_1,\dots,Y^1_{k_2}}\,;\,H(w^1_1,\dots,w^1_{|\alpha^3|}) \\ &= F_1(u^2_1,\dots,u^2_{|\alpha^1|})\,;\,\varphi_{X^2_1,\dots,X^2_{k_1}}\,;\,G(v^2_1,\dots,v^2_{|\alpha^2|})\,;\,\psi_{Y^2_1,\dots,Y^2_{k_2}}\,;\,H(w^2_1,\dots,w^2_{|\alpha^3|}) \\ &= \dots \\ &= F_1(u^k_1,\dots,u^k_{|\alpha^1|})\,;\,\varphi_{X^k_1,\dots,X^k_{k_1}}\,;\,G(v^k_1,\dots,v^k_{|\alpha^2|})\,;\,\psi_{Y^k_1,\dots,Y^k_{k_2}}\,;\,H(w^k_1,\dots,w^k_{|\alpha^3|}) \\ &= F_1(1|x)\,;\,\varphi_{codom(x)\dots codom(x)}\,;\,\psi_{codom(x)\dots codom(x)}\,;\,F_3(x|1) \end{aligned}$$

By definition of generators of morphisms in $\mathbb{C}_x$, every u^i_j, v^i_j and w^i_j is either $id_{dom(x)}$, $id_{codom(x)}$ or x. Each morphism in the chain therefore corresponds to a labelled marking (M_i, L_i, x) where M_i puts one token in each place whose corresponding argument of F_1, F_2 or F_3 is x and 0 elsewhere; L_i assigns to each transition value $dom\,(x)$ or $codom\,(x)$ according to the corresponding variable of φ and ψ.

By orientating the equations from left to right, each equation corresponds to the firing of a single, enabled, $codom\,(x)$-labelled transition in $\Gamma^*(\psi \circ \varphi)$ *or* to the firing of a single, enabled, $dom\,(x)$-labelled transition in $\Gamma^*(\psi \circ \varphi)^{\mathrm{op}}$ (which is $\Gamma^*(\psi \circ \varphi)$ with all the arrows reversed). We have indeed to take into account that, of course, dinaturality conditions can be used to pass from one leg to the other of the dinaturality hexagon interchangeably.

Given N an arbitrary Petri Net, an enabled transition in N^{op} is, by definition, a transition t in N where each of its *outputs* contain at least one token. We say that t is *coenabled* in N and we call *unfiring* the act of removing one token from every output of t and adding one token to each of its inputs. The chain of equations (1.65) translates therefore into a chain of labelled markings (M_i, L_i, x), starting from (M_0, L_0, x) and ending with (M_d, L_d, x) with:

$$M_0(p) = \begin{cases} 1 & {}^\bullet p = \emptyset \\ 0 & \text{otherwise} \end{cases} \qquad M_d(p) = \begin{cases} 1 & p^\bullet = \emptyset \\ 0 & \text{otherwise} \end{cases}$$

(1.66)

$$L_0(t) = \mathit{codom}(x) \qquad L_d(t) = \mathit{dom}(x)$$

and where each labelled marking is obtained from the preceding one by either firing an enabled $\mathit{codom}(x)$-labelled transition or by unfiring a coenabled $\mathit{dom}(x)$-labelled transition.

The strategy we shall use to prove Theorem (1.63) is the following. First we prove that we can "eliminate" the unfirings in this chain, that is that we can individuate a sequence of firings of enabled $\mathit{codom}(x)$-labelled transitions from M_0 to M_d; in other words, we can rearrange equations (1.65) in a way that we only use dinaturality conditions "in one direction". This will show that M_d is reachable from M_0. We will then use Theorem (1.61) to imply that $\Gamma^*(\psi \circ \varphi)$ must necessarily be acyclic.

We prove the following *unfiring elimination* theorem in the hypothesis that we have an arbitrary sequence of labelled markings, starting from our (M_0, L_0, x) but ending with any labelled marking, where only one unfiring happens, and it happens at the very end. This is indeed sufficient for the elimination of *all* unfirings from the chain of equations (1.65) (as we can apply the argument to one initial segment at a time, starting from the one that ends with the first unfiring, applying unfiring elimination, repeat the argument with the initial segment ending with the second unfiring, and so on). The theorem essentially states that in such a situation we can find a new sequence of labelled markings *with same initial and final* labelled marking, where each (M_i, L_i, x) is obtained from the preceding one by firing an enabled, $\mathit{codom}(x)$-labelled transition. In the proof we show that this is possible by observing that the coenabled, $\mathit{dom}(x)$ transition that unfires at the last step is in fact one of the transitions that has fired earlier on: hence by avoiding firing it in the first place, we eliminate the problem.

(1.67) Theorem (Unfiring elimination)**.** *Let $(M_i, L_i, x)_{i \in \{0,\dots,k+1\}}$ be a sequence of labelled markings, with M_0, L_0 as in (1.66), and let y_i, for $i \in \{0, \dots, k-1\}$, be vectors of length $k_1 + k_2$ consisting of all 0's except for one 1, call t_i the corresponding transition. Call $A = [a_{pt}]$ the incidence matrix of $\Gamma^*(\psi \circ \varphi)$. Suppose that for all $i \in \{0, \dots, k-1\}$*

(i) $M_{i+1} = M_i + Ay_i$ *(M_{i+1} is obtained by firing t_i),*

(ii) $\forall p \in P. (a_{pt_i} = -1 \Rightarrow M_i(p) = 1)$ *(t_i is enabled in M_i),*

(iii) $\forall t \in T. \, L_{i+1}(t) = \begin{cases} \mathit{dom}(x) & t = t_i \\ L_i(t) & \text{otherwise} \end{cases}$ *(t_i becomes $\mathit{dom}(x)$-labelled after firing),*

(iv) $L_i(t_i) = \mathit{codom}(x)$ *(t_i is $\mathit{codom}(x)$ labelled before firing)*

(that is, the enabled, $\mathit{codom}(x)$- labelled transition t_i fires transforming M_i into M_{i+1} and its label changes to $\mathit{dom}(x)$). Consider vector y_k of length $k_1 + k_2$ consisting of all 0's except for one -1, call t_k the corresponding transition. Suppose that

(v) $M_{k+1} = M_k + Ay_k$

(vi) $\forall p \in P.\,(a_{pt_k} = 1 \Rightarrow M_k(p) = 1)$

(vii) $\forall t \in T.\, L_{k+1}(t) = \begin{cases} codom\,(x) & t = t_k \\ L_k(t) & otherwise \end{cases}$

(viii) $L_k(t_k) = dom\,(x)$

(that is, coenabled, $dom\,(x)$-labelled transition t_k unfires transforming M_k into M_{k+1} and its label changes to $codom\,(x)$).

Then there exists a sequence of labelled markings $(M'_i, L'_i, x)_{i\in\{0,\ldots,k'+1\}}$ and vectors $y'_0, \ldots, y'_{k'}$, each of which consists of all 0's except for one 1 at transition t'_i, such that $(M_0, L_0, x) = (M'_0, L'_0, x)$, $(M_{k+1}, L_{k+1}, x) = (M'_{k'+1}, L'_{k'+1}, x)$ and for all $i \in \{0, \ldots, k'\}$:

(1) $M'_{i+1} = M'_i + Ay'_i$

(2) $\forall p \in P.\,(a_{pt'_i} = -1 \Rightarrow M'_i(p) = 1)$

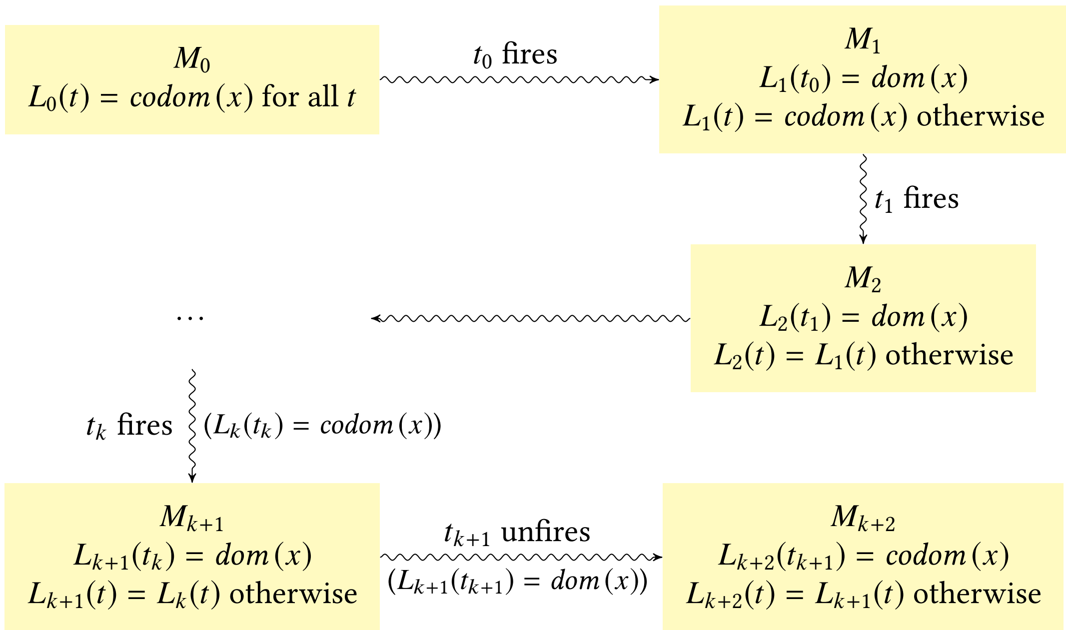
(3) $\forall t \in T.\, L'_{i+1}(t) = \begin{cases} dom\,(x) & t = t'_i \\ L'_i(t) & otherwise \end{cases}$

(4) $L'_i(t_i) = codom\,(x)$

Proof. Induction on k.

Case $k = 1$. We have three markings with accompanying labellings: M_0, where there is one token in each source and every transition has label $codom\,(x)$; M_1, obtained by firing a single enabled transition t_0 in M_0, with now $L_1(t_0) = dom\,(x)$; M_2, obtained by unfiring a coenabled, $dom\,(x)$-labelled transition t_1 in M_1, with $L_2(t_1) = codom\,(x)$. Necessarily then $t_0 = t_1$, because the only transition t such that $L_1(t) = dom\,(x)$ is t_0 itself. This means that we first fired and then unfired t_0: (M_0, L_0, x) and (M_2, L_2, x) are the same. Hence consider $k' = 0$, $M'_0 = M_0$, $L'_0 = L_0$, $y'_0 = y_0$ and $t'_0 = t_0$. Then conditions (1)-(4) are equivalent to (i)-(iv).

Inductive step. Let $k \geq 1$ and suppose the theorem is true for any sequence of labelled markings satisfying conditions (i)-(viii) of length less than or equal to $k + 1$. Let now $(M_i, L_i, x)_{i\in\{0,\ldots,k+2\}}$ be a sequence of labelled markings and $x_0, \ldots, x_{k+1}$ be vectors of length $k_1 + k_2$ as in the hypothesis of the theorem: for $i \in \{0, \ldots, k\}$, M_{i+1} is obtained from M_i by firing an enabled transition t_i with $L_i(t_i) = codom\,(x)$; L_{i+1} is the same as L_i except that now $L_{i+1}(t_i) = dom\,(x)$; whereas M_{k+2} is obtained from M_{k+1} by *unfiring* a coenabled transition t_{k+1}, where $L_{k+1}(t_{k+1}) = dom\,(x)$. The final labelling L_{k+2} differs from L_{k+1} only on t_{k+1}, where it has value $codom\,(x)$.



If $t_k = t_{k+1}$, then a similar argument to case $k = 1$ can be followed: we are in the presence of a series of firing of enabled transitions $t_0, \dots, t_k$, after which we unfire t_k, hence the sequence $(M_i, L_i, x)_{i \in \{0,\dots,k\}}$, where we avoided firing t_k altogether, is the desired solution.

If $t_k \neq t_{k+1}$, then we argue that we can first unfire t_{k+1} at stage (M_k, L_k) and then fire t_k. More precisely, we have

$$M_{k+2} = M_{k+1} + Ay_{k+1} = M_k + Ay_k + Ay_{k+1}$$

(where y_k has a 1 in position t_k, while y_{k+1} has a -1 in position t_{k+1}). Let:

- $\overline{M_{k+1}} = M_k + Ay_{k+1}$,
- $\overline{y_k} = y_{k+1}$, $\overline{y_{k+1}} = y_k$,
- $\overline{t_k} = t_{k+1}$, $\overline{t_{k+1}} = t_k$,
- $\overline{M_i} = M_i$ and $\overline{L_i} = L_i$ for $i \in \{0, \dots, k\}$, $\overline{y_i} = y_i$ for $i \in \{0, \dots, k-1\}$,
- $\overline{L_{k+1}}(t) = \begin{cases} codom\,(x) & t = \overline{t_k} \\ \overline{L_k}(t) & \text{otherwise} \end{cases}$

We want to show that the sequence of labelled markings $(\overline{M_i}, \overline{L_i}, x)_{i \in \{0,\dots,k+1\}}$ satisfies the hypotheses (i)–$(viii)$ of the theorem, so that we can apply the inductive hypothesis.

Now, conditions (i) – (iv) are already satisfied, since the labelled markings and the firing vectors have not changed. Condition (v) holds by definition of $\overline{M_{k+1}}$ and $\overline{y_k}$.

We now check that condition (vi) is true, that is $\forall p \in P.\, (a_{p\overline{t_k}} = 1 \Rightarrow \overline{M_k}(p) = 1)$. Let then $p \in P$ and suppose $a_{p\overline{t_k}} = 1$. Then $M_{k+1}(p) = 1$ because $a_{p\overline{t_{k+1}}} = a_{pt_k} = 1$ and (vi) holds for M_k. We have then:

$$1 = M_{k+1}(p) = M_k(p) + Ay_k(p) = M_k(p) + a_{pt_k}.$$

Since p is an output of $\overline{t_k} = t_{k+1}$, it cannot be an output of t_k as well (remember that we assumed $t_k \neq t_{k+1}$), so $a_{pt_k} \neq 1$. If it were the case that $a_{pt_k} = -1$, that is if p were an input of t_k and output of t_{k+1} at once, then necessarily $M_k(p) = 1$ (as t_k is enabled in M_k), hence

$$1 = M_k(p) + a_{pt_k} = 1 - 1 = 0$$

which is impossible. Therefore $a_{pt_k} = 0$ and $M_k(p) = M_{k+1}(p) = 1$.

Condition (vii) is satisfied by definition of $\overline{L_{k+1}}$. As per condition $(viii)$, we have:

$$\overline{L_k}(\overline{t_k}) = L_k(\overline{t_k}) = L_k(t_{k+1}) = L_{k+1}(t_{k+1}) = dom\,(x)\,.$$

(The penultimate equation is due to our assumption that $t_k \neq t_{k+1}$, whereas the last one by hypothesis.) Thus we can apply the inductive hypothesis and conclude the existence of a new sequence of labelled markings $(M'_i, L'_i, x)_{i\in\{0,\ldots,k'+1\}}$ and vectors $y'_0, \ldots, y'_{k'}$ with y'_i a vector 0 everywhere except in position t'_i, $(M_0, L_0, x) = (M'_0, L'_0, x)$, $(\overline{M_{k+1}}, \overline{L_{k+1}}, x) = (M'_{k'+1}, L'_{k'+1}, x)$ and satisfying conditions (1) – (4) for all $i \in \{0, \ldots, k'\}$. Define $M'_{k'+2} = M_{k+2}$ and

$$L'_{k'+2}(t) = \begin{cases} dom\,(x) & t = \overline{t_{k+1}} \\ L'_{k+1}(t) & \text{otherwise} \end{cases}$$

(hence we defined $t'_{k'+1} = \overline{t_{k+1}}$ and $y'_{k'+1} = \overline{y_{k+1}}$). All we have to do now is to show that

$$(M'_0, L'_0, x), \ldots, (M'_{k'+1}, L'_{k'+1}, x), (M'_{k'+2}, L'_{k'+2}, x)$$

is the sequence satisfying conditions (1) – (4) for all $i \in \{0, \ldots, k'+1\}$ which concludes the proof.

Only case $i = k'+1$ is left to check. Condition (1) requires $M'_{k'+2} = M'_{k'+1} + Ay'_{k'+1}$, which is true:

$$M'_{k'+2} = M_{k+2} = M_k + Ay_{k+1} + Ay_k = \overline{M_{k+1}} + A\overline{y_{k+1}} = M'_{k'+1} + Ay'_{k'+1}.$$

Condition (2) asks for transition $t'_{k'+1} = t_k$ to be enabled in $M'_{k'+1} = \overline{M_{k+1}}$. Let then $p \in P$ and suppose $a_{pt_k} = -1$ (that is, p is an input of t_k). We have to prove that $M'_{k'+1}(p) = 1$.

Now, $M'_{k'+1}(p) = M_k(p) + Ay_{k+1}(p)$. Since $y_{k+1} = (0, \ldots, 0, -1, 0, \ldots, 0)$ with the

-1 in position t_{k+1} and $a_{pt_k} = -1$, we have

$$Ay_{k+1}(p) = \Sigma_t a_p t y_{k+1}(t) = -a_{ptk+1}.$$

Since p is an input of t_k and $t_k \neq t_{k+1}$, necessarily $a_{pt_{k+1}} \neq -1$. If $a_{pt_{k+1}} = 1$, that is, if p were an output of t_{k+1}, then by hypothesis $M_{k+1}(p) = 1$ (as t_{k+1} is coenabled in M_{k+1}). On the other hand, since p is an input of t_k as well, and t_k is enabled in M_k, we have $M_k(p) = 1$. We have then:

$$1 = M_{k+1}(p) = M_k(p) + Ay_k(p) = 1 + a_{pt_k} = 1 - 1 = 0$$

which is impossible. Hence necessarily $a_{pt_{k+1}} = 0$, therefore

$$M'_{k+1}(p) = M_k(p) - a_{pt_{k+1}} = M_k(p) = 1.$$

Condition (3) is satisfied by definition of $L'_{k'+2}$. Finally, regarding condition (4):

$$L'_{k'+1}(t'_{k'+1}) = \overline{L_{k+1}}(\overline{t_{k+1}}) = \overline{L_{k+1}}(t_k) = \overline{L_k}(t_k) = L_k(t_k) = codom\,(x)\,.$$ **Qed**

As we have mentioned already in the discussion prior to Theorem (1.67), we have the following straightforward corollary.

(1.68) Corollary. *Let $(M_i, L_i, x)_{i\in\{0,\dots,k\}}$ be a sequence of labelled markings, with M_0, L_0 as in (1.66), where (M_{i+1}, L_{i+1}, x) is obtained from (M_i, L_i, x) by either firing an enabled, $codom\,(x)$-labelled transition t_i or by unfiring a coenabled, $dom\,(x)$-labelled transition t_i, and L_{i+1} differs from L_i only on t_i. Then M_k is reachable from M_0 by only firing enabled, $codom\,(x)$-labelled transitions.*

We can now then prove Theorem (1.63), which states how acyclicity of the composite graph is an "essentially necessary" condition for compositionality of dinatural transformations.

Proof of Theorem (1.57). We have already noticed how the chain of equations (1.65) translates into a sequence of labelled markings (M_i, L_i, x), starting from (M_0, L_0, x) and ending with (M_d, L_d, x) given by (1.66) satisfying the hypotheses of Corollary (1.68). Hence we can say that M_d is reachable from M_0. By Theorem (1.61), we conclude that $\Gamma^*(\psi \circ \varphi)$ has to be acyclic. **Qed**

Chapter 2

Horizontal compositionality

Horizontal composition of natural transformations is co-protagonist, together with vertical composition, in the classical Godement calculus. In this chapter we define a new operation of horizontal composition for dinatural transformations, generalising the well-known version for natural transformations. We also study its algebraic properties, proving it is associative and unitary. Remarkably, horizontal composition behaves better than vertical composition, as it is *always* defined between dinatural transformations of matching type. We begin in §2.1 with an analysis of the natural case in order to obtain a suitably general version for dinatural transformations. In §2.2 we prove that the result of the horizontal composition is in turn dinatural; moreover, we individuate a unit for the composition. In §2.3 we carefully build up the proof of associativity of horizontal composition, while in §2.4 we discuss the problem of compatibility with vertical composition.

§2.1 From the natural to the dinatural

Horizontal composition of natural transformations [Mac78] is a well-known operation which is rich in interesting properties: it is associative, unitary and compatible with vertical composition. As such, it makes $\mathbb{C}\mathrm{at}$ a strict 2-category. Also, it plays a crucial role in the calculus of substitution of functors and natural transformations developed by Kelly in [Kel72a]; in fact, as we have seen in the introduction, it is at the heart of Kelly's abstract approach to coherence. An appropriate generalisation of this notion for dinatural transformations seems to be absent in the literature: in this chapter we propose a working definition, as we shall see. The best place to start is to take a look at the usual definition for the natural case.

(2.1) Definition. Consider (classical) natural transformations

$$\begin{tikzcd} \mathbb{A} \arrow[r, bend left, "F"] \arrow[r, bend right, "G"'] \arrow[r, phantom, "\Downarrow\varphi"] & \mathbb{B} \arrow[r, bend left, "H"] \arrow[r, bend right, "K"'] \arrow[r, phantom, "\Downarrow\psi"] & \mathbb{C} \end{tikzcd}$$

The horizontal composition $\psi * \varphi \colon HF \to KG$ is the natural transformation whose A-th component, for $A \in \mathbb{A}$, is either leg of the following commutative square:

(2.2)
$$
\begin{tikzcd}
HF(A) \arrow[r, "\psi_{F(A)}"] \arrow[d, "H(\varphi_A)"'] & KF(A) \arrow[d, "K(\varphi_A)"] \\
HG(A) \arrow[r, "\psi_{G(A)}"] & KG(A)
\end{tikzcd}
$$
□

Now, the commutativity of (2.2) is due to the naturality of ψ; the fact that $\psi * \varphi$ is in turn a natural transformation is due to the naturality of both φ and ψ. However, in order to *define* the family of morphisms $\psi * \varphi$, all we have to do is to apply the naturality condition of ψ to the components of φ, one by one. We apply the very same idea to dinatural transformations, leading to the following preliminary definition for classical dinatural transformations.

(2.3) Definition. Let $\varphi \colon F \to G$ and $\psi \colon H \to K$ dinatural transformations of type $2 \longrightarrow 1 \longleftarrow 2$, where $F, G \colon \mathbb{A}^{\mathrm{op}} \times \mathbb{A} \to \mathbb{B}$ and $H, K \colon \mathbb{B}^{\mathrm{op}} \times \mathbb{B} \to \mathbb{C}$. The *horizontal composition* $\psi * \varphi$ is the family of morphisms

$$\big((\psi * \varphi)_A \colon H(G(A,A), F(A,A)) \to K(F(A,A), G(A,A))\big)_{A \in \mathbb{A}}$$

where the general component $(\psi * \varphi)_A$ is given, for any object $A \in \mathbb{A}$, by either leg of the following commutative hexagon:

$$
\begin{tikzcd}
& H(F(A,A),F(A,A)) \arrow[r, "\psi_{F(A,A)}"] & K(F(A,A),F(A,A)) \arrow[dr, "K(1{,}\varphi_A)"] & \\
H(G(A,A),F(A,A)) \arrow[ur, "H(\varphi_A{,}1)"] \arrow[dr, "H(1{,}\varphi_A)"'] & & & K(F(A,A),G(A,A)) \\
& H(G(A,A),G(A,A)) \arrow[r, "\psi_{G(A,A)}"] & K(G(A,A),G(A,A)) \arrow[ur, "K(\varphi_A{,}1)"'] &
\end{tikzcd}
$$
□

(2.4) Remark. In the same notations as in (2.3), suppose that F, G, H and K all factor through the second projection, that is there are functors $F', G' \colon \mathbb{A} \to \mathbb{B}$ and $H', K' \colon \mathbb{B} \to \mathbb{C}$ such that

$$
\begin{tikzcd}
& \mathbb{B} \\
\mathbb{A}^{\mathrm{op}} \times \mathbb{A} \arrow[ur, "F"] \arrow[r, "\pi_2"] \arrow[dr, "G"'] & \mathbb{A} \arrow[u, "F'"'] \arrow[d, "G"] \\
& \mathbb{B}
\end{tikzcd}
\quad \text{and} \quad
\begin{tikzcd}
& \mathbb{C} \\
\mathbb{B}^{\mathrm{op}} \times \mathbb{B} \arrow[ur, "H"] \arrow[r, "\pi_2"] \arrow[dr, "K"'] & \mathbb{A} \arrow[u, "H'"'] \arrow[d, "K"] \\
& \mathbb{C}
\end{tikzcd}
$$

commute. (In other words, suppose that they are "dummy" in their first variable.)

The dinaturality of φ and ψ is equivalent to the naturality of φ' and ψ', with $\varphi' = (\varphi_A \colon F'(A) \to G'(A))_{A\in\mathbb{A}}$ and $\psi' = (\psi_A \colon H'(A) \to K'(A))_{A\in\mathbb{A}}$ (as $F(A,A) = F'(A)$, etc.). In simpler terms, we have that φ and ψ are (classical) natural transformations. In this case, Definition (2.3) reduces to the usual Definition (2.1).

As in the classical natural case, we can deduce the dinaturality of $\psi * \varphi$ from the dinaturality of φ and ψ, as the following Theorem states. (Recall that for $F \colon \mathbb{A} \to \mathbb{B}$ a functor, $F^{\mathrm{op}} \colon \mathbb{A}^{\mathrm{op}} \to \mathbb{B}^{\mathrm{op}}$ is the obvious functor which behaves like F.)

(2.5) Theorem. *Let φ and ψ be dinatural transformations as in Definition (2.3). Then $\psi * \varphi$ is a dinatural transformation*

$$\psi * \varphi \colon H(G^{op}, F) \to K(F^{op}, G)$$

of type $4 \longrightarrow 1 \longleftarrow 4$, where $H(G^{op},F), K(F^{op},G) \colon \mathbb{A}^{[+,-,-,+]} \to \mathbb{C}$ are defined on objects as

$$\begin{aligned} H(G^{op},F)(A,B,C,D) &= H(G^{op}(A,B),F(C,D)) \\ K(F^{op},G)(A,B,C,D) &= K(F^{op}(A,B),G(C,D)) \end{aligned}$$

and similarly on morphisms.

Proof. The proof consists in showing that the diagram that asserts the dinaturality of $\psi * \varphi$ commutes: this is done in Figure 2.1. **Qed**

Note that the domain and codomain of $\psi*\varphi$ are the result of a particular substitution of functors as it appears in the Introduction at page 23.

The general definition. We can now proceed with the general definition, which involves transformations of arbitrary type. As the idea behind Definition (2.3) is to apply the dinaturality of ψ to the general component of φ in order to define $\psi * \varphi$, if ψ is a transformation with many variables, then we have many dinaturality conditions we can apply to φ, namely one for each variable of ψ in which ψ is dinatural. Hence, the general definition will depend on the variable of ψ we want to use. For the sake of simplicity, we shall consider only the one-category case, that is when all functors in the definition involve one category $\mathbb{C}$, in line with our approach in Chapter 1; the general case follows with no substantial complications except for a much heavier notation.

Notation. Given A, B and C objects of a category $\mathbb{C}$ with coproducts, and given $f \colon A \to C$ and $g \colon B \to C$, we denote by $[f,g] \colon A + B \to C$ the unique map granted by the universal property of $+$.

(2.6) Definition. Let $F \colon \mathbb{C}^\alpha \to \mathbb{C}$, $G \colon \mathbb{C}^\beta \to \mathbb{C}$, $H \colon \mathbb{C}^\gamma \to \mathbb{C}$, $K \colon \mathbb{C}^\delta \to \mathbb{C}$ be functors, $\varphi = (\varphi_{A_1,\dots,A_n}) \colon F \to G$ be a transformation of type $|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|$ and

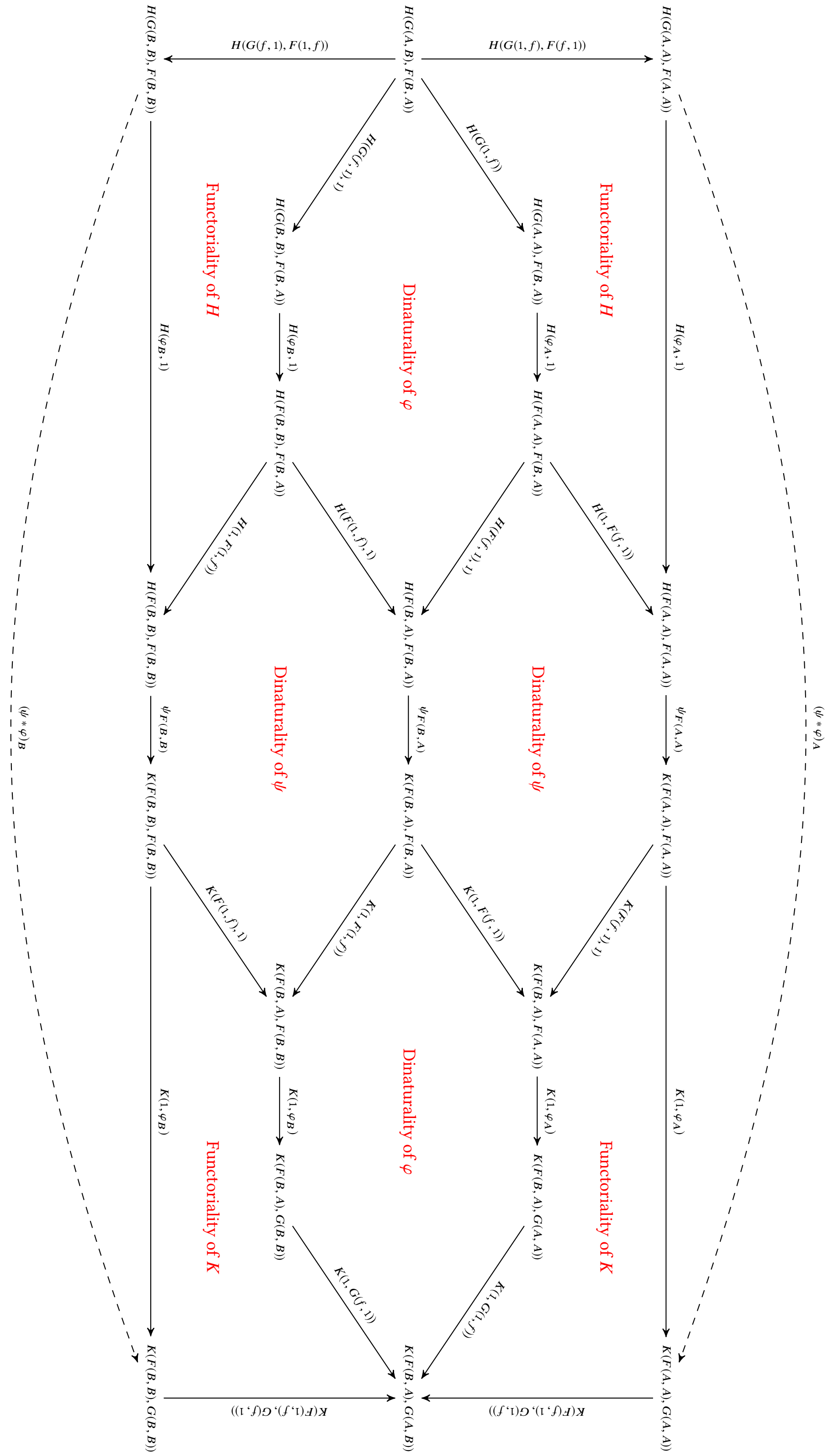


Figure 2.1 Proof of Theorem (2.5): dinaturality of horizontal composition in the classical case. Here $f : A \to B$.

$\psi = (\psi_{B_1,\dots,B_m}) \colon H \to K$ of type $|\gamma| \xrightarrow{\eta} m \xleftarrow{\theta} |\delta|$ a transformation which is dinatural in its i-th variable. Denoting with ++ the concatenation of a family of lists, let

$$H(X_1 \dots X_{|\gamma|}) \colon \mathbb{C}^{\mathop{++}\limits_{u=1}^{|\gamma|} \lambda^u} \to \mathbb{C}, \quad K(Y_1 \dots Y_{|\delta|}) \colon \mathbb{C}^{\mathop{++}\limits_{v=1}^{|\delta|} \mu^v} \to \mathbb{C}$$

be functors, defined similarly to $H(G^{\mathrm{op}}, F)$ and $K(F^{\mathrm{op}}, G)$ in Theorem (2.5), where for all $u \in \{1, \dots, |\gamma|\}$ and $v \in \{1, \dots, |\delta|\}$:

$$X_u = \begin{cases} F & \eta u = i \wedge \gamma_u = + \\ G^{\mathrm{op}} & \eta u = i \wedge \gamma_u = - \\ id_{\mathbb{C}^{\gamma_u}} & \eta u \neq i \end{cases} \qquad \lambda^u = \begin{cases} \alpha & \eta u = i \wedge \gamma_u = + \\ \overline{\beta}^* & \eta u = i \wedge \gamma_u = - \\ [\gamma_u] & \eta u \neq i \end{cases}$$

$$Y_v = \begin{cases} G & \theta v = i \wedge \delta_v = + \\ F^{\mathrm{op}} & \theta v = i \wedge \delta_v = - \\ id_{\mathbb{C}^{\delta_v}} & \theta v \neq i \end{cases} \qquad \mu^v = \begin{cases} \beta & \theta v = i \wedge \delta_v = + \\ \overline{\alpha} & \theta v = i \wedge \delta_v = - \\ [\delta_v] & \theta v \neq i \end{cases}$$

Define for all $u \in \{1, \dots, |\gamma|\}$ and $v \in \{1, \dots, |\delta|\}$ the following functions:

$$a_u = \begin{cases} \iota_n \sigma & \eta u = i \wedge \gamma_u = + \\ \iota_n \tau & \eta u = i \wedge \gamma_u = - \\ \iota_m K_{\eta u} & \eta u \neq i \end{cases} \qquad b_v = \begin{cases} \iota_n \tau & \theta v = i \wedge \delta_v = + \\ \iota_n \sigma & \theta v = i \wedge \delta_v = - \\ \iota_m K_{\theta v} & \theta v \neq i \end{cases}$$

with $K_{\eta u} \colon 1 \to m$ the constant function equal to ηu, while ι_n and ι_m are defined as:

$$\begin{array}{rcl} n & \xrightarrow{\iota_n} & (i-1) + n + (m-i) \\ x & \longmapsto & i - 1 + x \end{array} \qquad \begin{array}{rcl} m & \xrightarrow{\iota_m} & (i-1) + n + (m-i) \\ x & \longmapsto & \begin{cases} x & x < i \\ x + n - 1 & x \geq i \end{cases} \end{array}$$

The *i-th horizontal composition* $[\psi] \overset{i}{*} [\varphi]$ is the equivalence class of the transformation

$$\psi \overset{i}{*} \varphi \colon H(X_1 \dots X_{|\gamma|}) \to K(Y_1 \dots Y_{|\delta|})$$

of type

$$\sum_{u=1}^{|\gamma|} |\lambda^u| \xrightarrow{[a_1 \dots a_{|\gamma|}]} (i-1) + n + (m-i) \xleftarrow{[b_1 \dots b_{|\delta|}]} \sum_{v=1}^{|\delta|} |\mu^v|$$

whose general component, $(\psi \overset{i}{*} \varphi)_{B_1 \dots B_{i-1}, A_1 \dots A_n, B_{i+1} \dots B_m}$, is the diagonal of the commutative hexagon obtained by applying the dinaturality of ψ in its i-th variable to the

*Remember that for any $\beta \in \mathrm{List}\{+,-\}$ we denote $\overline{\beta}$ the list obtained from β by swapping the signs.

general component $\varphi_{A_1,\dots,A_n}$ of φ:

$$
\begin{tikzcd}
 & \cdot \arrow[rr, "\psi_{B_1\dots B_{i-1},G(A_{\tau 1}\dots A_{\tau|\beta|}),B_{i+1}\dots B_m}"] & & \cdot \arrow[dr, "K(y_1,\dots,y_{|\delta|})"] & \\
\cdot \arrow[ur, "H(x_1,\dots,x_{|\gamma|})"] \arrow[dr, "H(x'_1,\dots,x'_{|\gamma|})"'] \arrow[rrrr, dotted, "(\psi \overset{i}{*} \varphi)_{B_1\dots B_{i-1},A_1\dots A_n,B_{i+1}\dots B_m}"] & & & & \cdot \\
 & \cdot \arrow[rr, "\psi_{B_1\dots B_{i-1},F(A_{\sigma 1}\dots A_{\sigma|\alpha|}),B_{i+1}\dots B_m}"'] & & \cdot \arrow[ur, "K(y'_1,\dots,y'_{|\delta|})"'] &
\end{tikzcd}
$$

where

$$
x_u = \begin{cases} \varphi_{A_1,\dots,A_n} & \eta u = i \wedge \gamma_u = + \\ id_{G(A_{\tau 1}\dots A_{\tau|\beta|})} & \eta u = i \wedge \gamma_u = - \\ id_{B_{\eta u}} & \eta u \neq i \end{cases}
\qquad
y_v = \begin{cases} id_{G(A_{\tau 1}\dots A_{\tau|\beta|})} & \theta v = i \wedge \delta_v = + \\ \varphi_{A_1,\dots,A_n} & \theta v = i \wedge \delta_v = - \\ id_{B_{\theta v}} & \theta v \neq i \end{cases}
$$

$$
x'_u = \begin{cases} id_{F(A_{\sigma 1}\dots A_{\sigma|\alpha|})} & \eta u = i \wedge \gamma_u = + \\ \varphi_{A_1,\dots,A_n} & \eta u = i \wedge \gamma_u = - \\ id_{B_{\eta u}} & \eta u \neq i \end{cases}
\qquad
y_v = \begin{cases} \varphi_{A_1,\dots,A_n} & \theta v = i \wedge \delta_v = + \\ id_{F(A_{\sigma 1}\dots A_{\sigma|\alpha|})} & \theta v = i \wedge \delta_v = - \\ id_{B_{\theta v}} & \theta v \neq i \end{cases}
$$

$\square$

In other words, the domain of $\psi \overset{i}{*} \varphi$ is obtained by substituting the arguments of H (the domain of ψ) that are in the i-th connected component of $\Gamma(\psi)$ (which is the condition $\eta u = i$ in X_u) with F (the domain of φ) if they are covariant, and with G^{op} (the opposite of the codomain of φ) if they are contravariant; those arguments not in the i-th connected component are left untouched. Similarly the codomain. The type of $\psi \overset{i}{*} \varphi$ is obtained by replacing the i-th variable of ψ with all the variables of φ and adjusting the type of ψ with σ and τ to reflect this act. In the following example, we see what happens to $\Gamma(\varphi)$ and $\Gamma(\psi)$ upon horizontal composition.

(2.7) Example. Consider transformations δ and *eval* (see examples (1.9),(1.10)). In the notations of Definition (2.6), we have $F = id_{\mathbb{C}} \colon \mathbb{C} \to \mathbb{C}$, $G = \times \colon \mathbb{C}^{[+,+]} \to \mathbb{C}$, $H \colon \mathbb{C}^{[+,-,+]} \to \mathbb{C}$ defined as $H(X,Y,Z) = X \times (Y \Rightarrow Z)$ and $K = id_{\mathbb{C}} \colon \mathbb{C} \to \mathbb{C}$. The types of δ and *eval* are respectively

$$
\begin{tikzcd}
1 \arrow[r] & 1 & 2 \arrow[l]
\end{tikzcd}
\qquad \text{and} \qquad
\begin{tikzcd}[row sep=tiny]
3 \arrow[r] & 2 & 1 \arrow[l] \\
1 \arrow[r, mapsto] & 1 & 1 \arrow[dl, mapsto, bend right] \\
2 \arrow[ur, mapsto, bend right] & 2 & \\
3 \arrow[ur, mapsto, bend right] & &
\end{tikzcd}
$$

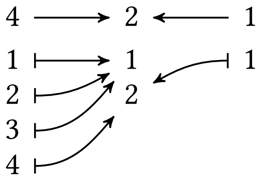
The transformation *eval* is extranatural in its first variable and natural in its second: we have two horizontal compositions. $(eval \overset{1}{*} \delta)_{A,B}$ is given by either leg of the following commutative square:

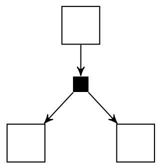
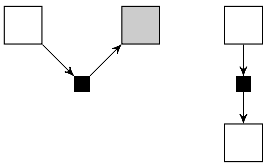
$$
\textbf{(2.8)} \qquad
\begin{tikzcd}
A \times \big((A \times A) \Rightarrow B\big) \arrow[r, "\delta_A \times (1 \Rightarrow 1)"] \arrow[d, "1 \times (\delta_A \Rightarrow 1)"'] & (A \times A) \times \big((A \times A) \Rightarrow B\big) \arrow[d, "eval_{A \times A, B}"] \\
A \times (A \Rightarrow B) \arrow[r, "eval_{A,B}"] & B
\end{tikzcd}
$$

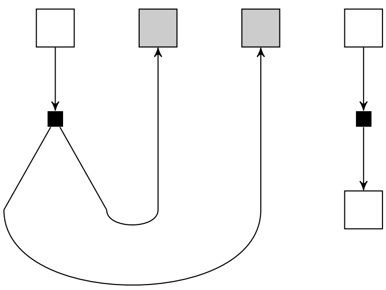
We have $eval \overset{1}{*} \delta \colon H(id_{\mathbb{C}}, \times, id_{\mathbb{C}}) \to id_{\mathbb{C}}(id_{\mathbb{C}})$ where $id_{\mathbb{C}}(id_{\mathbb{C}}) = id_{\mathbb{C}}$ and

$$
\begin{array}{ccc}
\mathbb{C}^{[+,-,-,+]} & \xrightarrow{H(id_{\mathbb{C}}, \times, id_{\mathbb{C}})} & \mathbb{C} \\
(X, Y, Z, W) & \longmapsto & X \times \big((Y \times Z) \Rightarrow W\big)
\end{array}
$$

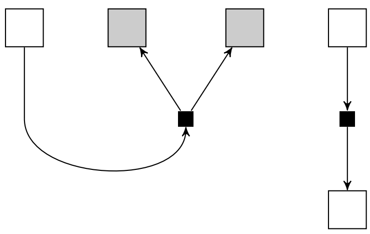
and it is of type



Intuitively, $\Gamma\Big(eval \overset{1}{*} \delta\Big)$ is obtained by substituting $\Gamma(\delta) =$  into the first connected component of $\Gamma(eval) =$  , by "bending", as it were, $\Gamma(\delta)$ into the U-turn that is the first connected component of $\Gamma(eval)$:

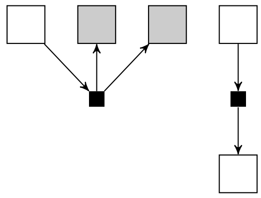


or



Here the first graph corresponds to the upper leg of (2.8), the second to the lower one. Notice how the component $eval_{A \times A, B}$ has now *two* wires, one per each A in the graph on the left. The result is therefore

$$\Gamma\Big(eval \overset{1}{*} \delta\Big) =$$



Turning now to the other possible horizontal composition, we have that $eval \overset{2}{*} \delta \colon H(id_{\mathbb{C}}, id_{\mathbb{C}}, id_{\mathbb{C}}) \to id_{\mathbb{C}}(\times)$ where $H(id_{\mathbb{C}}, id_{\mathbb{C}}, id_{\mathbb{C}}) = H$ and $id_{\mathbb{C}}(\times) = \times$ by definition; it is of type

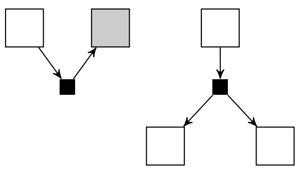
$$\begin{tikzcd}[row sep=tiny]
3 \arrow[r] & 2 & 2 \arrow[l] \\
1 \arrow[r, mapsto] & 1 & 1 \arrow[dl, mapsto, bend right] \\
2 \arrow[ur, mapsto, bend right] & 2 & 2 \arrow[l, mapsto] \\
3 \arrow[ur, mapsto, bend right] & &
\end{tikzcd}$$

and $(eval \overset{2}{*} \delta)_{A,B}$ is given by either leg of the following commutative square:

$$\begin{tikzcd}
A \times (A \Rightarrow B) \arrow[r, "1\times(1\Rightarrow\delta_B)"] \arrow[d, "eval_{A,B}"'] & A \times \big(A \Rightarrow (B \times B)\big) \arrow[d, "eval_{A,B\times B}"] \\
B \arrow[r, "\delta_B"] & B \times B
\end{tikzcd}$$

Substituting $\Gamma(\delta)$ into the second connected component of $\Gamma(eval)$, which is just a "straight line", results into the following graph:

$$\Gamma\Big(eval \overset{2}{*} \delta\Big) =$$



□

§2.2 Dinaturality of horizontal composition

We aim to prove here that our definition of horizontal composition, which we have already noticed generalises the well-known version for classical natural transformations (Remark (2.4)), is a closed operation on dinatural transformations. For the rest of this chapter, we shall fix transformations φ and ψ with the notations used in Definition (2.6) for their signature; we also fix the "names" of the variables of φ as $A_1, \dots, A_n$ and of ψ as $B_1, \dots, B_m$. In this spirit, i is a fixed element of $\{1, \dots, m\}$, we assume ψ to be dinatural in B_i and we shall sometimes refer to $\psi \overset{i}{*} \varphi$ also as $\psi \overset{B_i}{*} \varphi$.

As in the classical natural case (Definition (2.1)), only the dinaturality of ψ in B_i is needed to *define* the i-th horizontal composition of φ and ψ. Here we want to understand in which variables the i-th horizontal composition

$$\psi \overset{B_i}{*} \varphi = \big((\psi \overset{B_i}{*} \varphi)_{B_1 \ldots B_{i-1}, A_1 \ldots A_n, B_{i+1} \ldots B_m}\big)$$

itself is in turn dinatural. It is straightforward to see that $\psi \overset{B_i}{*} \varphi$ is dinatural in all its B-variables where ψ is dinatural, since the act of horizontally composing φ and ψ in B_i has not "perturbed" H, K and ψ in any way except in those arguments involved in the i-th connected component of $\Gamma(\psi)$, see example (2.7). Hence we have the following preliminary result.

(2.9) Proposition. *If ψ is dinatural in B_j, for $j \neq i$, then $\psi \overset{B_i}{*} \varphi$ is also dinatural in B_j.*

More interestingly, it turns out that $\psi \overset{B_i}{*} \varphi$ is also dinatural in all those A-variables where φ is dinatural in the first place. We aim then to prove the following Theorem.

(2.10) Theorem. *If φ is dinatural in its k-th variable and ψ in its i-th one, then $\psi \overset{i}{*} \varphi$ is dinatural in its $(i-1+k)$-th variable. In other words, if φ is dinatural in A_k and ψ in B_i, then $\psi \overset{B_i}{*} \varphi$ is dinatural in A_k.*

The proof of this theorem relies on the fact that we can reduce ourselves, without loss of generality, to Theorem (2.5). To prove that, we introduce the notion of *focalisation* of a transformation on one of its variables: essentially, the focalisation of a transformation ϕ is a transformation depending on only one variable between functors that have only one covariant and one contravariant argument, obtained by fixing all the parts of the data involving variables different from the one we are focusing on.

(2.11) Definition. Let $\phi = (\phi_{A_1,\ldots,A_p}) \colon T \to S$ be a transformation of type

$$|\alpha| \xrightarrow{\sigma} p \xleftarrow{\tau} |\beta|$$

with $T \colon \mathbb{C}^\alpha \to \mathbb{C}$ and $S \colon \mathbb{C}^\beta \to \mathbb{C}$. Fix $k \in \{1, \ldots, p\}$ and objects $A_1, \ldots, A_{k-1}, A_{k+1}, \ldots, A_p$ in $\mathbb{C}$. Consider functors $\overline{T}^k, \overline{S}^k \colon \mathbb{C}^{\mathrm{op}} \times \mathbb{C} \to \mathbb{C}$ defined by

$$\begin{aligned} \overline{T}^k(A,B) &= T(C_1, \ldots, C_{|\alpha|}) \\ \overline{S}^k(A,B) &= S(D_1, \ldots, D_{|\beta|}) \end{aligned}$$

where for every X object of $\mathbb{C}$

$$C_u = \begin{cases} B & \sigma u = k \wedge \alpha_u = + \\ A & \sigma u = k \wedge \alpha_u = - \\ A_{\sigma u} & \sigma u \neq k \end{cases} \qquad D_v = \begin{cases} B & \tau v = k \wedge \beta_v = + \\ A & \tau v = k \wedge \beta_v = - \\ A_{\tau v} & \tau v \neq k \end{cases}$$

The *focalisation of ϕ on its k-th variable* is the transformation

$$\overline{\phi}^k : \overline{T}^k \to \overline{S}^k$$

of type $2 \to 1 \leftarrow 2$ where

$$\overline{\phi}^k_X = \varphi_{A_1 \dots A_{k-1}, X, A_{k+1} \dots A_p}.$$

Sometimes we may write $\overline{\phi}^{A_k} : \overline{T}^{A_k} \to \overline{S}^{A_k}$ too, when we fix as $A_1, \dots, A_p$ the name of the variables of ϕ. □

(2.12) Remark. ϕ is dinatural in its k-th variable if and only if $\overline{\phi}^k$ is dinatural in its only variable for all objects $A_1, \dots, A_{k-1}, A_{k+1}, \dots, A_p$ fixed by the focalisation of ϕ.

The $\overline{(-)}^k$ construction depends on the $k-1$ objects we fix, but not to make the notation too heavy, we shall always call those (arbitrary) objects $A_1, \dots, A_{k-1}, A_{k+1}, \dots, A_n$ for $\overline{\varphi}^k$ and $B_1, \dots, B_{i-1}$, $B_{i+1}, \dots, B_m$ for $\overline{\psi}^i$.

(2.13) Remark. It immediately follows from the definitions of horizontal composition and of the $\overline{(-)}^i$, $\overline{(-)}^k$ constructions that

$$\left(\overline{\psi}^i * \overline{\varphi}^k\right)_X = (\psi \overset{i}{*} \varphi)_{B_1 \dots B_{i-1}, A_1 \dots A_{k-1}, X, A_{k+1} \dots A_n, B_{i+1} \dots B_m} = \left(\overline{\psi \overset{i}{*} \varphi}^{(i-1+k)}\right)_X .$$

(2.14) Lemma. *It is the case that $\psi \overset{i}{*} \varphi$ is dinatural in its $(i-1+k)$-th variable if and only if $\overline{\psi}^i * \overline{\varphi}^k$ is dinatural in its only variable for all objects $B_1, \dots, B_{i-1}$, $A_1, \dots, A_{k-1}$, $A_{k+1}, \dots, A_n$, $B_{i+1}, \dots, B_m$ in $\mathbb{C}$ fixed by the focalisations of φ and ψ.*

Proof. The proof consists in unwrapping the two definitions and showing that they require the exact same hexagon to commute.

Recall that $\varphi \colon F \to G$ and $\psi \colon H \to K$ have the following type:

$$|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta| \quad \text{and} \quad |\gamma| \xrightarrow{\eta} m \xleftarrow{\theta} |\delta|$$

We have that $\overline{\varphi}^k : \overline{F}^k \to \overline{G}^k, \overline{\psi}^i : \overline{H}^i \to \overline{K}^i$ are both transformations of type $2 \to 1 \leftarrow 2$ with $\overline{\psi}^i$ dinatural by Remark (2.12), since we assumed ψ to be dinatural in its i-th variable. Saying that $\overline{\psi}^i * \overline{\varphi}^k$ is dinatural for all objects $A_1, \dots, A_{k-1}$, $A_{k+1}, \dots, A_n$ and $B_1, \dots, B_{i-1}$, $B_{i+1}, \dots, B_m$ is equivalent to say that for all such A_j's and B_j's and for every $f\colon X \to Y$ morphism in $\mathbb{C}$

(2.15)
$$
\begin{tikzcd}
& \cdot \arrow[r, "\left(\overline{\psi}^i * \overline{\varphi}^k\right)_X"] & \cdot \arrow[dr, "\overline{K}^i\left(\overline{F}^{k\,\mathrm{op}},\overline{G}^k\right)(f,id_X,id_X,f)"] & \\
\cdot \arrow[ur, "\overline{H}^i\left(\overline{G}^{k\,\mathrm{op}},\overline{F}^k\right)(id_X,f,f,id_X)"] \arrow[dr, "\overline{H}^i\left(\overline{G}^{k\,\mathrm{op}},\overline{F}^k\right)(f,id_Y,id_Y,f)"'] & & & \cdot \\
& \cdot \arrow[r, "\left(\overline{\psi}^i * \overline{\varphi}^k\right)_Y"'] & \cdot \arrow[ur, "\overline{K}^i\left(\overline{F}^{k\,\mathrm{op}},\overline{G}^k\right)(id_Y,f,f,id_Y)"'] &
\end{tikzcd}
$$

Now,

$$\overline{H}^i\left(\overline{G}^{k\,\mathrm{op}},\overline{F}^k\right)(id_X,f,f,id_X) = \overline{H}^i\left(\overline{G}^{k\,\mathrm{op}}(id_X,f),\overline{F}^k(f,id_X)\right) = H(L_1,\dots,L_{|\gamma|})$$

where for $u \in \{1,\dots,|\gamma|\}$, $v \in \{1,\dots,|\alpha|\}$ and $w \in \{1,\dots,|\beta|\}$:

$$L_u = \begin{cases} \overline{F}^k(f,id_X) & \eta u = i \wedge \gamma_u = + \\ \overline{G}^{k\,\mathrm{op}}(id_X,f) & \eta u = i \wedge \gamma_u = - \\ id_{B_{\eta u}} & \eta u \neq i \end{cases} = \begin{cases} F(c_1^u,\dots,c_{|\alpha|}^u) & \eta u = i \wedge \gamma_u = + \\ G^{\mathrm{op}}(d_1^u,\dots,d_{|\beta|}^u) & \eta u = i \wedge \gamma_u = - \\ id_{B_{\eta u}} & \eta u \neq i \end{cases}$$

$$c_v^u = \begin{cases} id_X & \sigma v = k \wedge \alpha_v = + \\ f & \sigma v = k \wedge \alpha_v = - \\ id_{A_{\sigma v}} & \sigma v \neq k \end{cases} \qquad d_w^u = \begin{cases} f & \tau w = k \wedge \beta_w = + \\ id_X & \tau w = k \wedge \beta_w = - \\ id_{B_\eta u} & \tau_w \neq k \end{cases}$$

Similarly for $\overline{K}^i\left(\overline{F}^{k\,\mathrm{op}},\overline{G}^k\right)(f,id_X,id_X,f)$. By Definition (2.3), we have

$$\begin{aligned} \left(\overline{\psi}^i * \overline{\varphi}^k\right)_X &= \overline{H}^i\left((\overline{\varphi}^k)_X, id_{\overline{F}^k(X,X)}\right) \,;\, (\overline{\psi}^i)_{\overline{F}^k(X,X)} \,;\, \overline{K}^i\left(id_{\overline{F}^k(X,X)}, (\overline{\varphi}^k)_X\right) \\ &= H(x_1,\dots,x_{|\gamma|}) \,;\, \psi_{B_1\dots B_{i-1},F(O_1\dots O_{|\alpha|}),B_{i+1}\dots B_m} \,;\, K(y_1,\dots,y_{|\delta|}) \end{aligned}$$

with

$$x_u = \begin{cases} id_{F(O_1\dots O_{|\alpha|})} & \eta u = i \wedge \gamma_u = + \\ \varphi_{A_1\dots A_{k-1},X,A_{k+1}\dots A_n} & \eta u = i \wedge \gamma_u = - \\ id_{B_{\eta u}} & \eta u \neq i \end{cases} \qquad O_w = \begin{cases} X & \sigma w = k \\ A_{\sigma w} & \sigma w \neq k \end{cases}$$

$$y_v = \begin{cases} \varphi_{A_1\dots A_{k-1},X,A_{k+1}\dots A_n} & \theta v = i \wedge \delta_u = + \\ id_{F(O_1\dots O_{|\alpha|})} & \theta v = i \wedge \delta_u = - \\ id_{B_{\theta v}} & \theta v \neq i \end{cases}$$

Now, the dinaturality condition for $\psi \overset{i}{*} \varphi$ in its $(i-1+k)$-th variable asks for a certain hexagon depending on an arbitrary morphism $f \colon X \to Y$ to commute. One leg of this hexagon involves the component of $\psi \overset{i}{*} \varphi$ having X as its $(i-1+k)$-th variable, the other having Y instead. We analyse the former leg and show that it is equal to the corresponding leg (the upper one) of the dinaturality hexagon (2.15). It is the following composite of morphisms:

$$\begin{aligned}
&H(X_1,\dots,X_{|\gamma|})\left(r^1_1,\dots,r^1_{|\lambda^1|},\dots,r^{|\gamma|}_1,\dots,r^{|\gamma|}_{|\lambda^{|\gamma|}|}\right) \ ;\\
&\left(\psi \overset{i}{*} \varphi\right)_{B_1\dots B_{i-1},A_1\dots A_{k-1},X,A_{k+1}\dots A_n,B_{i+1}\dots B_m} \ ;\\
&K(Y_1,\dots,Y_{|\delta|})\left(s^1_1,\dots,s^1_{|\mu^1|},\dots,s^{|\delta|}_1,\dots,s^{|\delta|}_{|\mu^{|\delta|}|}\right)
\end{aligned}$$

where for all $u \in \{1,\dots,|\gamma|\}$, $v \in \{1,\dots,|\lambda^u|\}$, $x \in \{1,\dots(i-1)+n+(m-i)\}$ and functions ι_n and ι_m defined as in Definition (2.6):

$$X_u = \begin{cases} F & \eta u = i \wedge \gamma_u = + \\ G^{\mathrm{op}} & \eta u = i \wedge \gamma_u = - \\ id_{\mathbb{C}^{\gamma_u}} & \eta u \neq i \end{cases} \qquad \lambda^u = \begin{cases} \alpha & \eta u = i \wedge \gamma_u = + \\ \overline{\beta} & \eta u = i \wedge \gamma_u = - \\ [\gamma_u] & \eta u \neq i \end{cases}$$

$$a_u = \begin{cases} \iota_n \sigma & \eta u = i \wedge \gamma_u = + \\ \iota_n \tau & \eta u = i \wedge \gamma_u = - \\ \iota_m K_{\eta u} & \eta u \neq i \end{cases} \qquad V_x = \begin{cases} B_x & x < i \\ A_{x-(i-1)} & i \le x < i+n \\ B_{x-(n-1)} & x \ge i+n \end{cases}$$

$$r^u_v = \begin{cases} id_X & a_u(v) = i-1+k \wedge \lambda^u_v = + \\ f & a_u(v) = i-1+k \wedge \lambda^u_v = - \\ id_{V_{a_u(v)}} & a_u(v) \neq i-1+k \end{cases}$$

Therefore, to conclude we have to prove the following equalities:

- $H(L_1,\dots,L_{|\gamma|}) = H(X_1,\dots,X_{|\gamma|})\left(r^1_1,\dots,r^1_{|\lambda^1|},\dots,r^{|\gamma|}_1,\dots,r^{|\gamma|}_{|\lambda^{|\gamma|}|}\right)$,
- $\left(\overline{\psi}^i * \overline{\varphi}^k\right)_X = \left(\psi \overset{i}{*} \varphi\right)_{B_1\dots B_{i-1},A_1\dots A_{k-1},X,A_{k+1}\dots A_n,B_{i+1}\dots B_m}$,
- $\overline{K}^i\left(\overline{F}^{k\,\mathrm{op}},\overline{G}^k\right)(f, id_X, id_X, f) = K(Y_1,\dots,Y_{|\delta|})\left(s^1_1,\dots,s^1_{|\mu^1|},\dots,s^{|\delta|}_1,\dots,s^{|\delta|}_{|\mu^{|\delta|}|}\right)$.

We only prove the first equation: the third is analogous, while the second has already been observed in Remark (2.13). Now, by definition of $H(X_1,\dots,X_{|\gamma|})$, we have

$$\begin{aligned}
&H(X_1,\dots,X_{|\gamma|})\left(r^1_1,\dots,r^1_{|\lambda^1|},\dots,r^{|\gamma|}_1,\dots,r^{|\gamma|}_{|\lambda^{|\gamma|}|}\right) = \\
&= H\left(X_1(r^1_1,\dots,r^1_{|\lambda^1|}),\dots,X_{|\gamma|}(r^{|\gamma|}_1,\dots,r^{|\gamma|}_{|\lambda^{|\gamma|}|})\right)
\end{aligned}$$

We shall then prove that $L_u = X_u(r^u_1, \dots, r^u_{|\lambda^u|})$ for all $u \in \{1, \dots, |\gamma|\}$.
Case $\eta u = i \wedge \gamma u = +$. We have $L_u = F(c^u_1, \dots, c^u_{|\alpha|})$, $X_u = F$, $\lambda^u = \alpha$, $a_u = \iota_n \sigma$. Hence we have to prove that $c^u_v = r^u_v$ for all $v \in \{1, \dots, |\alpha|\}$.

Recall from (2.6) the definition of ι_n and ι_m:

$$
\begin{array}{rcl}
n & \xrightarrow{\iota_n} & (i-1)+n+(m-i) \\
x & \longmapsto & i-1+x
\end{array}
\qquad
\begin{array}{rcl}
m & \xrightarrow{\iota_m} & (i-1)+n+(m-i) \\
x & \longmapsto & \begin{cases} x & x < i \\ x-1+n & x \geq i \end{cases}
\end{array}
$$

Since $a_u = \iota_n \sigma$, we have $a_u(v) = \iota_n(\sigma v) = i-1+\sigma v$ hence condition $a_u(v) = k+i-1$ is equivalent to $\sigma v = k$. This immediately tells us that c^u_v and r^u_v coincide when $\sigma v = k$. When $\sigma v \neq k$, we have $c^u_v = id_{A_{\sigma v}}$ while $r^u_v = id_{V_{a_u(v)}}$. But

$$V_{a_u(v)} = V_{i-1+\sigma v}$$

and given that $1 \leq \sigma v \leq n$, we have $i \leq i-1+\sigma v \leq i-1+n < i+n$ hence

$$V_{i-1+\sigma v} = A_{i-1+\sigma v-(i-1)} = A_{\sigma v}.$$

Case $\eta u = i \wedge \gamma u = -$. We have $L_u = G^{\mathrm{op}}(d^u_1, \dots, d^u_{|\beta|})$, $X_u = G^{\mathrm{op}}$, $\lambda^u = \overline{\beta}$, $a_u = \iota_n \tau$. Similarly to the previous case, we prove that $d^u_v = r^u_v$ for all $v \in \{1, \dots, |\beta|\}$.

Now condition $a_u(v) = k+i-1$ is equivalent to $\tau v = k$, therefore d^u_v and r^u_v coincide when $\tau v = k$, because $\lambda^u_v = \overline{\beta}_v$ hence $\lambda^u_v = -$ if and only if $\beta_v = +$. When $\tau v \neq k$, again $V_{a_u(v)} = A_{\tau v}$ by definition of V_x because $a_u(v) = \tau v + i - 1$ is such that $i \leq i-1+\tau v < i+n$. Hence $d^u_v = r^u_v$.
Case $\eta u \neq i$. We have $L_u = id_{B_{\eta u}}$, $X_u = id_{\mathbb{C}^{\gamma u}}$, $\lambda^u = [\gamma_u]$, $a_u = \iota_m K_{\eta u}$. In particular $|\lambda^u| = 1$. We now show that $a_u(1) \neq i-1+k$, so that we can imply that $r^u_1 = id_{V_{a_u(1)}}$. We have:

$$a_u(1) = \iota_m K_{\eta u}(1) = \iota_m(\eta u) = \begin{cases} \eta u & \eta u < i \\ \eta u - 1 + n & \eta u > i \end{cases}$$

and, given that $1 \leq k \leq n$, we have that $i \leq i-1+k \leq i-1+n$. Hence, if $\eta u < i$ then $a_u(1) = \eta u < i-1+k$; if instead $\eta u > i$, then $a_u(1) = \eta u - 1 + n > i-1+n \geq i-1+k$. In any case, $a_u(1) \neq i-1+k$.

We now show that $L_u = r^u_1$, concluding the proof.

$$V_{a_u(1)} = \begin{cases} V_{\eta u} & \eta u < i \\ V_{\eta u - 1 + n} & \eta u > i \end{cases} = \begin{cases} B_{\eta u} & \eta u < i \\ B_{\eta u - 1 + n - (n-1)} & \eta u > i \end{cases} = B_{\eta u}$$

hence $id_{B_{\eta u}} = id_{V_{a_u(1)}}$, as required. **Qed**

We can now prove that horizontal composition preserves dinaturality.

Proof of Theorem (2.10). Consider transformations $\overline{\varphi}^k$ and $\overline{\psi}^i$. By Remark (2.12), they are both dinatural in their only variable. Hence, by Theorem (2.5), $\overline{\psi}^i * \overline{\varphi}^k$ is dinatural and by Lemma (2.14) we conclude. **Qed**

Unitarity. It is straightforward to see that horizontal composition has a left and a right unit, namely the identity (di)natural transformation on the appropriate identity functor.

(2.16) Theorem. *Let $T\colon \mathbb{C}^\alpha \to \mathbb{D}$, $S\colon \mathbb{C}^\beta \to \mathbb{D}$ be functors, and let $\phi\colon T \to S$ be a transformation of any type. Then*

$$id_{id_{\mathbb{D}}} * \phi = \phi.$$

If ϕ is dinatural in its i-th variable, for an appropriate i, then also

$$\phi \overset{i}{*} id_{id_{\mathbb{C}}} = \phi.$$

Proof. Direct consequence of the definition of horizontal composition. **Qed**

§2.3 Associativity of horizontal composition

Associativity is a crucial property of any respectable algebraic operation. It gives us the opportunity to safely compose not just two, but an arbitrarily long finite string of objects in whichever order we prefer: in other words, "bracketing does not matter". We begin by considering "classical" dinatural transformations $\varphi\colon F \to G$, $\psi\colon H \to K$ and $\chi\colon U \to V$, for $F, G, H, K, U, V\colon \mathbb{C}^{\mathrm{op}} \times \mathbb{C} \to \mathbb{C}$ functors, all of type $2 \twoheadrightarrow 1 \twoheadleftarrow 2$.

(2.17) Theorem. $\chi * (\psi * \varphi) = (\chi * \psi) * \varphi$.

Proof. We first prove that the two transformations have same domain and codomain functors. Since they both depend on one variable, this also immediately implies they have same type.

We have $\psi * \varphi\colon H(G^{\mathrm{op}}, F) \to K(F^{\mathrm{op}}, G)$, hence

$$\chi * (\psi * \varphi)\colon U\Big(K(F^{\mathrm{op}}, G)^{\mathrm{op}}, H(G^{\mathrm{op}}, F)\Big) \to V\Big(H(G^{\mathrm{op}}, F)^{\mathrm{op}}, K(F^{\mathrm{op}}, G)\Big).$$

Notice that $K(F^{\mathrm{op}}, G)^{\mathrm{op}} = K^{\mathrm{op}}(F, G^{\mathrm{op}})$ and $H(G^{\mathrm{op}}, F)^{\mathrm{op}} = H^{\mathrm{op}}(G, F^{\mathrm{op}})$. Next, we have $\chi * \psi\colon U(K^{\mathrm{op}}, H) \to V(H^{\mathrm{op}}, K)$. Given that $U(K^{\mathrm{op}}, H), V(H^{\mathrm{op}}, K)\colon \mathbb{C}^{[+,-,-,+]} \to \mathbb{C}$, we have

$$(\chi * \psi) * \varphi\colon \underbrace{U(K^{\mathrm{op}}, H)(F, G^{\mathrm{op}}, G^{\mathrm{op}}, F)}_{U\left(K^{\mathrm{op}}(F, G^{\mathrm{op}}), H(G^{\mathrm{op}}, F)\right)} \to \underbrace{V(H^{\mathrm{op}}, K)(G, F^{\mathrm{op}}, F^{\mathrm{op}}, G)}_{V\left(H^{\mathrm{op}}(G, F^{\mathrm{op}}), K(F^{\mathrm{op}}, G)\right)}.$$

This proves $\chi * (\psi * \varphi)$ and $(\chi * \psi) * \varphi$ have the same signature.

Only equality of the single components is left to show. Fix then an object A in $\mathbb{C}$. Figure 2.2 shows how to pass from $(\chi * \psi) * \varphi$ to $\chi * (\psi * \varphi)$ by pasting three commutative diagrams. In order to save space, we simply wrote "$H(G, F)$" instead of the proper "$H(G^{\mathrm{op}}(A, A), F(A, A))$" and similarly for all the other instances of functors in the nodes of the diagram in Figure 2.2; we also dropped the subscript for components of φ, ψ and χ when they appear as arrows, that is we simply wrote φ instead of φ_A, since there is only one object involved and there is no risk of confusion. **Qed**

We can now start discussing the general case for transformations with an arbitrary number of variables; we shall prove associativity by reducing ourselves to Theorem (2.17) using focalisation (see Definition (2.11)). For the rest of this section, fix transformations φ, ψ and χ, dinatural in all their variables, with signatures:

- $\varphi \colon F \to G$, for $F \colon \mathbb{C}^{\alpha} \to \mathbb{C}$ and $G \colon \mathbb{C}^{\beta} \to \mathbb{C}$, of type $|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|$;
- $\psi \colon H \to K$, for $H \colon \mathbb{C}^{\gamma} \to \mathbb{C}$ and $K \colon \mathbb{C}^{\delta} \to \mathbb{C}$, of type $|\gamma| \xrightarrow{\eta} m \xleftarrow{\theta} |\delta|$;
- $\chi \colon U \to V$, for $U \colon \mathbb{C}^{\varepsilon} \to \mathbb{C}$ and $V \colon \mathbb{C}^{\zeta} \to \mathbb{C}$, of type $|\varepsilon| \xrightarrow{\pi} l \xleftarrow{\omega} |\zeta|$

For sake of simplicity, let us fix the name of the variables for φ as $A_1, \dots, A_n$, for ψ as $B_1, \dots, B_m$ and for χ as $C_1, \dots, C_l$. In this spirit we also fix the variables of the horizontal compositions, so for $i \in \{1, \dots, m\}$, the variables of $\psi \overset{i}{*} \varphi$ are

$$B_1, \dots, B_{i-1}, A_1, \dots, A_n, B_{i+1}, \dots, B_m$$

while for $j \in \{1, \dots, l\}$ the variables of $\chi \overset{j}{*} \psi$ are

$$C_1, \dots, C_{j-1}, B_1, \dots, B_m, C_{j+1}, \dots, C_l.$$

The theorem asserting associativity of horizontal composition, which we prove in the rest of this section, is the following.

(2.18) Theorem. *For $i \in \{1, \dots, m\}$ and $j \in \{1, \dots, l\}$,*

$$\chi \overset{j}{*} \left(\psi \overset{i}{*} \varphi\right) = \left(\chi \overset{j}{*} \psi\right) \overset{j-1+i}{*} \varphi$$

or, in alternative notation,

$$\chi \overset{C_j}{*} \left(\psi \overset{B_i}{*} \varphi\right) = \left(\chi \overset{C_j}{*} \psi\right) \overset{B_i}{*} \varphi. \tag{2.19}$$

Notice, first of all, that both sides of (2.19) depend on the following variables:

$$C_1, \dots, C_{j-1}, B_1, \dots, B_{i-1}, A_1, \dots, A_n, B_{i+1}, \dots, B_m, C_{j+1}, \dots, C_l.$$

$$
\begin{tikzcd}
U(K(F,G),H(G,F)) \arrow[rr, "{U(K(1,\varphi),H(\varphi,1))}"] \arrow[d, "{U(K(1,\varphi),1)}"'] & & U(K(F,F),H(F,F)) \arrow[rr, "{U(\psi,1)}"] \arrow[d, phantom, "\text{Functoriality of } U"] & & U(H(F,F),H(F,F)) \arrow[d, "\chi"] & & & & \\
U(K(F,F),H(G,F)) \arrow[d, "{U(\psi,1)}"'] & & U(H(F,F),H(F,F)) \arrow[rr, "\chi"] \arrow[dd, phantom, "\text{Dinaturality of } \chi"] & & V(H(F,F),H(F,F)) \arrow[rr, "{V(1,\psi)}"] \arrow[drr, "{V(H(\varphi,1),1)}"] & & V(H(F,F),K(F,F)) \arrow[rr, "{V(H(\varphi,1),K(1,\varphi))}"] \arrow[drr, phantom, "\text{Functoriality of } V"] & & V(H(G,F),K(F,G)) \\
U(H(F,F),H(G,F)) \arrow[urr, "{U(1,H(\varphi,1))}"] \arrow[drr, "{U(H(\varphi,1),1)}"'] & & & & & & V(H(G,F),H(F,F)) \arrow[rr, "{V(1,\psi)}"] & & V(H(G,F),K(F,F)) \arrow[u, "{V(1,K(1,\varphi))}"'] \\
& & U(H(G,F),H(G,F)) \arrow[rr, "\chi"] & & V(H(G,F),H(G,F)) \arrow[urr, "{V(1,H(\varphi,1))}"'] & & & &
\end{tikzcd}
$$

Figure 2.2 Associativity of horizontal composition in the classical case. The upper leg is $(\chi * \psi) * \varphi$, whereas the lower one is $\chi * (\psi * \varphi)$.

Next, we compute their domain and codomain functors. We have that

$$\psi \overset{i}{*} \varphi \colon H(X_1, \dots, X_{|\gamma|}) \to K(Y_1, \dots, Y_{|\delta|})$$

(with the same notations as in Definition (2.6)). Hence

$$\chi \overset{C_j}{*} \left(\psi \overset{B_i}{*} \varphi\right) \colon U(W_1, \dots, W_{|\varepsilon|}) \to V(Z_1, \dots, Z_{|\zeta|})$$

with $U(W_1, \dots, W_{|\varepsilon|}) \colon \mathbb{C}^{\mathop{++}_{u=1}^{|\varepsilon|} \nu^u} \to \mathbb{C}$, $V(Z_1, \dots, Z_{|\zeta|}) \colon \mathbb{C}^{\mathop{++}_{u=1}^{|\zeta|} \xi^u} \to \mathbb{C}$ where

$$W_u = \begin{cases} H(X_1, \dots, X_{|\gamma|}) & \pi u = j \wedge \varepsilon_u = + \\ K(Y_1, \dots, Y_{|\delta|})^{\mathrm{op}} & \pi u = j \wedge \varepsilon_u = - \\ id_{\mathbb{C}^{\varepsilon_u}} & \pi u \neq j \end{cases} \qquad \nu^u = \begin{cases} \mathop{++}\limits_{u=1}^{|\gamma|} \lambda^u & \pi u = j \wedge \varepsilon_u = + \\ \overline{\mathop{++}\limits_{u=1}^{|\delta|} \mu^u} & \pi u = j \wedge \varepsilon_u = - \\ [\varepsilon_u] & \pi u \neq j \end{cases}$$

and similarly are defined Z_u and ξ^u (swapping $H(X_1, \dots, X_{|\gamma|})$ with $K(Y_1, \dots, Y_{|\delta|})$, ω with π, ε with ζ and so on).

To compute the domain and codomain of the right-hand side of (2.19), we need the complete signature of $\chi \overset{C_j}{*} \psi$, which we list now following Definition (2.6). We have

$$\chi \overset{C_j}{*} \psi \colon U(L_1, \dots, L_{|\varepsilon|}) \to V(M_1, \dots, M_{|\zeta|})$$

with $U(L_1, \dots, L_{|\varepsilon|}) \colon \mathbb{C}^{\mathop{++}_{u=1}^{|\varepsilon|} \rho^u} \to \mathbb{C}$, $V(M_1, \dots, M_{|\zeta|}) \colon \mathbb{C}^{\mathop{++}_{u=1}^{|\zeta|} \vartheta^u} \to \mathbb{C}$ where, as usual, if the u-th argument of U is "involved" by the j-th variable of χ (that is, if it belongs to the j-th connected component of $\Gamma(\chi)$), which means if $\pi u = j$, then L_u is either the domain or the codomain of ψ, depending whether the u-th argument of U is covariant ($\varepsilon_u = +$) or contravariant ($\varepsilon_u = -$); if instead $\pi u \neq j$, then we leave U untouched in its u-th argument. More precisely, we have:

$$L_u = \begin{cases} H & \pi u = j \wedge \varepsilon_u = + \\ K^{\mathrm{op}} & \pi u = j \wedge \varepsilon_u = - \\ id_{\mathbb{C}^{\varepsilon_u}} & \pi u \neq j \end{cases} \qquad \rho^u = \begin{cases} \gamma & \pi u = j \wedge \varepsilon_u = + \\ \overline{\delta} & \pi u = j \wedge \varepsilon_u = - \\ [\varepsilon_u] & \pi u \neq j \end{cases}$$

$$M_u = \begin{cases} K & \omega u = j \wedge \zeta_u = + \\ H^{\mathrm{op}} & \omega u = j \wedge \zeta_u = - \\ id_{\mathbb{C}^{\zeta_u}} & \omega u \neq j \end{cases} \qquad \vartheta^u = \begin{cases} \delta & \omega u = j \wedge \zeta_u = + \\ \overline{\gamma} & \omega u = j \wedge \zeta_u = - \\ [\zeta_u] & \omega u \neq j \end{cases}$$

$$\chi \overset{C_j}{*} \psi \text{ has type } \sum_{u=1}^{|\varepsilon|} |\rho^u| \xrightarrow{[c_1,\ldots,c_{|\varepsilon|}]} (j-1)+m+(l-j) \xleftarrow{[d_1,\ldots,d_{|\zeta|}]} \sum_{u=1}^{|\zeta|} |\vartheta^u| \quad \text{with}$$

$$c_u = \begin{cases} \iota_m \eta & \pi u = j \wedge \varepsilon_u = + \\ \iota_m \theta & \pi u = j \wedge \varepsilon_u = - \\ \iota_l K_{\pi u}{}^{\dagger} & \pi u \neq j \end{cases} \qquad d_u = \begin{cases} \iota_m \theta & \omega u = j \wedge \zeta_u = + \\ \iota_m \eta & \omega u = j \wedge \zeta_u = - \\ \iota_l K_{\omega u} & \omega u \neq j \end{cases}$$

$$\begin{array}{rcl} m & \xrightarrow{\iota_m} & (j-1)+m+(l-j) \\ x & \longmapsto & x+j-1 \end{array} \qquad \begin{array}{rcl} l & \xrightarrow{\iota_l} & (j-1)+m+(l-j) \\ x & \longmapsto & \begin{cases} x & x \leq j \\ x+m-1 & x > j \end{cases} \end{array}$$

Therefore, the domain and codomain of $\left(\chi \overset{C_j}{*} \psi\right) \overset{B_i}{*} \varphi$ are, respectively:

$$U(L_1,\ldots,L_{|\varepsilon|})(P^1_1,\ldots,P^1_{|\rho^1|},\ldots,P^{|\varepsilon|}_1,\ldots,P^{|\varepsilon|}_{|\rho^{|\varepsilon|}|}) \quad \text{and}$$
$$V(M_1,\ldots,M_{|\zeta|})(Q^1_1,\ldots,Q^1_{|\vartheta^1|},\ldots,Q^{|\zeta|}_1,\ldots,Q^{|\zeta|}_{|\vartheta^{|\zeta|}|})$$

where

$$P^u_v = \begin{cases} F & c_u(v) = j-1+i \wedge \rho^u_v = + \\ G^{\mathrm{op}} & c_u(v) = j-1+i \wedge \rho^u_v = - \\ id_{\mathbb{C}^{\rho^u_v}} & c_u(v) \neq j-1+i \end{cases} \qquad Q^u_v = \begin{cases} G & d_u(v) = j-1+i \wedge \vartheta^u_v = + \\ F^{\mathrm{op}} & d_u(v) = j-1+i \wedge \vartheta^u_v = - \\ id_{\mathbb{C}^{\vartheta^u_v}} & d_u(v) \neq j-1+i \end{cases}$$

(Remember that B_i is the $(j-1+i)$-th variable of $\chi \overset{C_j}{*} \psi$. The use of an upper and lower index helps us to keep track of which c_u and d_u to use: it is a heavy but working notation.) Denoting the domain of $\left(\chi \overset{C_j}{*} \psi\right) \overset{B_i}{*} \varphi$ as $U(L(P))$ for short, we have

$$U(L(P)) \colon \mathbb{C}^{\overset{|\varepsilon|}{\underset{u=1}{+\!+}} \left(\overset{|\rho^u|}{\underset{v=1}{+\!+}} w^u_v \right)} \to \mathbb{D}$$

where

$$w^u_v = \begin{cases} \alpha & c_u(v) = j-1+i \wedge \rho^u_v = + \\ \overline{\beta} & c_u(v) = j-1+i \wedge \rho^u_v = - \\ [\rho^u_v] & c_u(v) \neq j-1+i \end{cases}$$

and similarly for $V(M(Q))$. Now we are ready to prove the following Lemma.

(2.20) Lemma. *The transformations $\chi \overset{C_j}{*} \left(\psi \overset{B_i}{*} \varphi\right)$ and $\left(\chi \overset{C_j}{*} \psi\right) \overset{B_i}{*} \varphi$ have same domain, codomain and type.*

† $K_{\pi u} \colon 1 \to l$ is the constant function equal to πu.

Proof. One can prove that $\mathop{+\!\!+}\limits_{u=1}^{|\varepsilon|}\left(\mathop{+\!\!+}\limits_{v=1}^{|\rho^u|} w^u_v\right) = \mathop{+\!\!+}\limits_{u=1}^{|\varepsilon|} \nu^u$ by showing that $\mathop{+\!\!+}\limits_{v=1}^{|\rho^u|} w^u_v = \nu^u$ for all $u \in \{1, \ldots, |\varepsilon|\}$, analysing each of the three cases for ηu that define ν^u.

Next, we have that

$$U(L(P)) = U\Big(L_1\big(P^1_1, \ldots, P^1_{|\rho^1|}\big), \ldots, L_{|\varepsilon|}\big(P^{|\varepsilon|}_1, \ldots, P^{|\varepsilon|}_{|\rho^{|\varepsilon|}|}\big)\Big)$$

as the action of these two functors coincide on every object and morphism of $\mathbb{C}^{\mathop{+\!\!+}_{u=1}^{|\varepsilon|} \nu^u}$. By showing that $W_u = L_u\big(P^u_1, \ldots, P^u_{|\rho^u|}\big)$ for all $u \in \{1, \ldots, |\varepsilon|\}$, one proves that $\chi \overset{C_j}{*} \left(\psi \overset{B_i}{*} \varphi\right)$ and $\left(\chi \overset{C_j}{*} \psi\right) \overset{B_i}{*} \varphi$ have the same domain; an analogous procedure shows that they also share the same codomain.

Finally, we briefly analyse only the left hand sides of the types of $\chi \overset{C_j}{*} \left(\psi \overset{B_i}{*} \varphi\right)$ and $\left(\chi \overset{C_j}{*} \psi\right) \overset{B_i}{*} \varphi$ (that is, the half of the cospan that involves the variance of the domain functors); the right hand sides are handled analogously. For $\chi \overset{C_j}{*} \left(\psi \overset{B_i}{*} \varphi\right)$ we have

$$\sum_{u=1}^{|\varepsilon|} |\nu^u| \xrightarrow{[r_1, \ldots, r_{|\varepsilon|}]} (j-1) + [(i-1) + n + (m-i)] + (l-j)$$

with, calling $N = (j-1) + [(i-1) + n + (m-i)] + (l-j)$ for short:

$$r_u = \begin{cases} \iota^N_{(i-1)+n+(m-i)} \circ [a_1, \ldots, a_{|\gamma|}] & \pi u = j \wedge \varepsilon_u = + \\ \iota^N_{(i-1)+n+(m-i)} \circ [b_1, \ldots, b_{|\delta|}] & \pi u = j \wedge \varepsilon_u = - \\ \iota^N_l K_{\pi u} & \pi u \neq j \end{cases}$$

where

$$\begin{array}{ccc} (i-1) + n + (m-i) & \xrightarrow{\iota^N_{(i-1)+n+(m-i)}} & N \\ x & \longmapsto & x + j - 1 \end{array} \qquad \begin{array}{ccc} l & \xrightarrow{\iota^N_l} & N \\ x & \longmapsto & \begin{cases} x & x \leq j \\ x + (i-1) + n + (m-i) - 1 & x > j \end{cases} \end{array}$$

For $\left(\chi \overset{C_j}{*} \psi\right) \overset{B_i}{*} \varphi$, which is the same as $\left(\chi \overset{j}{*} \psi\right) \overset{j-1+i}{*} \varphi$, we have

$$\sum_{u=1}^{|\varepsilon|} \sum_{v=1}^{|\rho^u|} |w^u_v| \xrightarrow{[s^1_1, \ldots, s^1_{|\rho^1|}, \ldots, s^{|\varepsilon|}_1, \ldots, s^{|\varepsilon|}_{|\rho^{|\varepsilon|}|}]} M$$

where $M = [(j-1+i)-1] + n + [((j-1)+m+(l-j)) - (j-1+i)]$ and

$$s^u_v = \begin{cases} \iota^M_n \circ \sigma & c_u(v) = j-1+i \wedge \rho^u_v = + \\ \iota^M_n \circ \tau & c_u(v) = j-1+i \wedge \rho^u_v = - \\ \iota^M_{(j-1)+m+(l-j)} K_{c_u(v)} & c_u(v) \neq j-1+i \end{cases}$$

with

$$\begin{aligned} n &\xrightarrow{\iota^M_n} M \\ x &\longmapsto x + [(j-1+i)-1] \end{aligned}$$

and

$$\begin{aligned} (j-1)+m+(l-j) &\xrightarrow{\iota^M_{(j-1)+m+(l-j)}} M \\ x &\longmapsto \begin{cases} x & x \leq j-1+i \\ x+n-1 & x > j-1+i \end{cases} \end{aligned}$$

(remember that $c_u(v) \in (j-1)+m+(l-j)$, so $K_{c_u(v)} \colon 1 \to (j-1)+m+(l-j)$). It is immediate to see that $N = M$ as natural numbers, hence they define the same set. Checking that $r_u = [s^u_1, \dots, s^u_{|\rho^u|}]$ and noticing that functions $[\dots r_u \dots]$ and $[\dots s^u_v \dots]$ coincide on every elements of their domain, we conclude. **Qed**

Now that we know that the two sides of (2.19) share the same signature, we can focus on proving that they coincide component-wise. The strategy will be to show that we can reduce ourselves to the classical case of Theorem (2.17). We first need a technical lemma that will allow us to do that.

(2.21) Lemma. *Let $\Phi = (\Phi_{V_1,\dots,V_p})$ and $\Psi = (\Psi_{W_1,\dots,W_q})$ be transformations such that Ψ is dinatural in W_s, for $s \in \{1,\dots,q\}$. Let $V_1,\dots,V_{r-1}, V_{r+1},\dots,V_p, W_1,\dots,W_{s-1}, W_{s+1},\dots,W_q$ be objects of $\mathbb{C}$, and let $\overline{\Phi}^{V_r}$ and $\overline{\Psi}^{W_s}$ be the focalisation of Φ and Ψ in its r-th and s-th variable respectively using the fixed objects above. Let also X be an object of $\mathbb{C}$. Then*

(i) $\left(\overline{\Psi}^{W_s} * \overline{\Phi}^{V_r}\right)_X = \left(\Psi \overset{W_s}{*} \Phi\right)_{W_1,\dots,W_{s-1},V_1,\dots,V_{r-1},X,V_{r+1},\dots,V_p,W_{s+1},\dots,W_q} = \left(\overline{\Psi \overset{W_s}{*} \Phi}^{V_r}\right)_X$

(ii) $(co)dom\left(\overline{\Psi \overset{W_s}{*} \Phi}^{V_r}\right)(x,y) = (co)dom\left(\overline{\Psi}^{W_s} * \overline{\Phi}^{V_r}\right)(x,y,y,x)$ *for any morphisms x and y.*

Proof. Part (i) asserts Remark (2.13) for arbitrary transformations, and it is a direct consequence of the definitions of horizontal composition and $\overline{(-)}^{W_s}, \overline{(-)}^{V_r}$ constructions. Regarding (ii), it is enough to repeat the argument we discussed in Lemma (2.14). In there, we computed $dom\left(\overline{\psi}^i * \overline{\varphi}^j\right)(id_X, f, f, id_X)$ (the top-left leg of (2.15)) and we showed it is equal to $dom\left(\psi \overset{i}{*} \varphi\right)(\dots, r_v^u, \dots)$. By definition, the latter is the same as $dom\left(\overline{\psi \overset{i}{*} \varphi}^{j}\right)(f, id_X)$. Claim (ii) in the present Lemma is proved in the same way *mutatis mutandis.* **Qed**

(2.22) Remark. Part (i) asserts an equality between *morphisms* and not *transformations*, as $\overline{\Psi}^{W_s} * \overline{\Phi}^{V_r}$ and $\Psi \overset{W_s}{*} \Phi$ have different types and even different domain and codomain functors.

We now finally have all the tools to prove associativity of horizontal composition in the general case.

Proof of Theorem (2.18). By Lemma (2.20), only equality between the single components has to be shown. Let us fix then $C_1, \dots, C_{j-1}, B_1, \dots, B_{i-1}, A_1, \dots, A_{k-1}, X, A_{k+1}, \dots, A_n, B_{i+1}, \dots, B_m, C_{j+1}, \dots, C_l$ objects in $\mathbb{C}$. Writing just V for this long list of objects, we have, by Lemma (2.21), that

$$\left(\left(\chi \overset{C_j}{*} \psi\right) \overset{B_i}{*} \varphi\right)_V = \left(\overline{\chi \overset{C_j}{*} \psi}^{B_i} * \overline{\varphi}^{A_k}\right)_X$$

Now, we cannot apply again Lemma (2.21) to $\overline{\chi \overset{C_j}{*} \psi}^{B_i}$ because of what we said in Remark (2.22), but we can use the definition of horizontal composition to write down explicitly the right-hand side of the equation above: it is the morphism

$$codom\left(\overline{\chi \overset{C_j}{*} \psi}^{B_i}\right)(id_{\overline{F}(X,X)}, (\overline{\varphi}^{A_k})_X) \circ \left(\overline{\chi \overset{C_j}{*} \psi}^{B_i}\right)_{\overline{F}(X,X)} \circ dom\left(\overline{\chi \overset{C_j}{*} \psi}^{B_i}\right)((\overline{\varphi}^{A_k})_X, id_{\overline{F}(X,X)})$$

(Remember that $\overline{\varphi}^{A_k} \colon \overline{F}^{A_k} \to \overline{G}^{A_k}$, here we wrote $\overline{F}(X,X)$ instead of $\overline{F}^{A_k}(X,X)$ to save space.) Now we *can* use Lemma (2.21) to "split the bar", as it were:

$$\begin{aligned} codom\left(\overline{\chi}^{C_j} * \overline{\psi}^{B_i}\right)&((\overline{\varphi}^{A_k})_X, id_{\overline{F}(X,X)}, id_{\overline{F}(X,X)}, (\overline{\varphi}^{A_k})_X) \circ \\ &\left(\overline{\chi}^{C_j} * \overline{\psi}^{B_i}\right)_{\overline{F}(X,X)} \circ \\ &dom\left(\overline{\chi}^{C_j} * \overline{\psi}^{B_i}\right)(id_{\overline{F}(X,X)}, (\overline{\varphi}^{A_k})_X, (\overline{\varphi}^{A_k})_X, id_{\overline{F}(X,X)}) \end{aligned}$$

This morphism is equal, by definition of horizontal composition, to

$$\left(\left(\overline{\chi}^{C_j} * \overline{\psi}^{B_i}\right) * \overline{\varphi}^{A_k}\right)_X$$

which, by Theorem (2.17), is the same as

$$\left(\overline{\chi}^{C_j} * \left(\overline{\psi}^{B_i} * \overline{\varphi}^{A_k}\right)\right)_X .$$

An analogous series of steps shows how this is equal to $\left(\chi \overset{C_j}{*} \left(\psi \overset{B_i}{*} \varphi\right)\right)_V$, thus concluding the proof. **Qed**

§2.4 (In?)Compatibility with vertical composition

Looking at the classical natural case, there is one last property to analyse: the *interchange law* [Mac78]. In the following situation,

$$\begin{tikzcd} \mathbb{A} \arrow[r, bend left=60, ""{name=U, below}] \arrow[r, bend right=60, ""{name=D, above}] \arrow[r, ""{name=M}] & \mathbb{B} \arrow[r, bend left=60, ""{name=U2, below}] \arrow[r, bend right=60, ""{name=D2, above}] \arrow[r, ""{name=M2}] & \mathbb{C} \arrow[from=U, to=M, phantom, "\Downarrow\varphi"] \arrow[from=M, to=D, phantom, "\Downarrow\psi"] \arrow[from=U2, to=M2, phantom, "\Downarrow\varphi'"] \arrow[from=M2, to=D2, phantom, "\Downarrow\psi'"] \end{tikzcd}$$

with φ, φ', ψ and ψ' natural transformations, we have:

$$(\dagger) \qquad (\psi' \circ \varphi') * (\psi \circ \varphi) = (\psi' * \psi) \circ (\varphi' * \varphi).$$

The interchange law is the crucial property that makes $\mathbb{C}\mathrm{at}$ a 2-category and completes the Godement calculus for natural transformations. It is then certainly highly interesting to wonder whether a similar property holds for the more general notion of horizontal composition for dinatural transformations too.

As we know all too well, dinatural transformations are far from being as well-behaved as natural transformations, given that they do not, in general, vertically compose; on the other hand, their horizontal composition always works just fine. Are these two operations compatible, at least when vertical composition is defined? The answer, unfortunately, is *No*, at least if by "compatible" we mean "compatible as in the natural case (†)". Indeed, consider classical dinatural transformations

$$(2.23) \qquad \begin{tikzcd} \mathbb{A}^{\mathrm{op}} \times \mathbb{A} \arrow[r, bend left=60, "F", ""{name=U, below}] \arrow[r, bend right=60, "H"', ""{name=D, above}] \arrow[r, "G" description, ""{name=M}] & \mathbb{B} \arrow[from=U, to=M, phantom, "\Downarrow\varphi"] \arrow[from=M, to=D, phantom, "\Downarrow\psi"] \end{tikzcd} \qquad \begin{tikzcd} \mathbb{B}^{\mathrm{op}} \times \mathbb{B} \arrow[r, bend left=60, "J", ""{name=U, below}] \arrow[r, bend right=60, "L"', ""{name=D, above}] \arrow[r, "K" description, ""{name=M}] & \mathbb{C} \arrow[from=U, to=M, phantom, "\Downarrow\varphi'"] \arrow[from=M, to=D, phantom, "\Downarrow\psi'"] \end{tikzcd}$$

such that $\psi \circ \varphi$ and $\psi' \circ \varphi'$ are dinatural. Then

$$\varphi' * \varphi \colon J(G^{\mathrm{op}}, F) \to K(F^{\mathrm{op}}, G) \qquad \psi' * \psi \colon K(H^{\mathrm{op}}, G) \to L(G^{\mathrm{op}}, H)$$

which means that $\varphi' * \varphi$ and $\psi' * \psi$ are not even composable as families of morphisms, as the codomain of the former is not the domain of the latter. The problem stems from the fact that the codomain of the horizontal composition $\varphi' * \varphi$ depends on the codomain of φ' and also the domain *and* codomain of φ, which are not the same as the domain and codomain of ψ: indeed, in order to be vertically composable, φ and ψ must share only one functor, and not both. This does not happen in the natural case: the presence of mixed variance, which forces to consider the codomain of φ in $\varphi' * \varphi$ and so on, is the real culprit here.

The failure of (†) does not come completely unexpected: after all, our definition of horizontal composition is strictly more general than the classical one for natural transformations, as it extends the audience of functors and transformations it can be applied to quite considerably. Hence it is not surprising that this comes at the cost of losing one of its properties, albeit so desirable. Of course, one can wonder whether a different, "better", as it were, definition of horizontal composition exists for which (†) holds. Although I cannot exclude *a priori* this possibility, the fact that ours not only is a very natural generalisation of the classical definition for natural transformations (as it follows the same idea, see discussion after Definition (2.1)), but also enjoys associativity and unitarity, let me think that we *do* have the right definition at hand. (As a side point, behold Figure 2.1: its elegance cannot be the fruit of a wrong definition!)

What I suspect, instead, is that a different *interchange law* should be formulated, that can accommodate the hexagonal shape of the dinatural condition. Indeed, what proves (†) in the natural case is the naturality of either φ' or ψ'. For instance, the following diagrammatic proof uses the latter, for $\varphi \colon F \to G$, $\psi \colon G \to H$, $\varphi' \colon J \to K$, $\psi' \colon K \to L$ natural:

$$\begin{tikzcd}
JF(A) \arrow[r, "\varphi'_{F(A)}"] \arrow[dr, dashed, "(\varphi' * \varphi)_A"'] & KF(A) \arrow[r, "\psi'_{F(A)}"] \arrow[d, "K(\varphi_A)"] & LF(A) \arrow[d, "L(\varphi_A)"] \\
& KG(A) \arrow[r, "\psi'_{G(A)}"] \arrow[dr, dashed, "(\psi' * \psi)_A"'] & LG(A) \arrow[d, "L(\psi_A)"] \\
& & LH(A)
\end{tikzcd}$$

(The upper leg of the diagram is $(\psi' \circ \varphi') * (\psi \circ \varphi)$.) The naturality condition of ψ' is what causes φ and ψ' to swap places, allowing now φ and φ' to interact with each other via horizontal composition; same for ψ and ψ'.

However, for $\varphi, \psi, \varphi', \psi'$ dinatural as in (2.23), this does not happen:

$$
\begin{tikzcd}
 & & J(F,F) \arrow[r, "\varphi'"] & K(F,F) \arrow[r, "\psi'"] & L(F,F) \arrow[dr, "L(1,\varphi)"] & & \\
 & J(G,F) \arrow[ur, "J(\varphi,1)"] \arrow[rrrr, dashed, "(\psi' \circ \varphi') * \varphi"] & & & & L(F,G) \arrow[dr, "L(1,\psi)"] & \\
J(H,F) \arrow[ur, "J(\psi,1)"] & & & & & & L(F,H)
\end{tikzcd}
$$

Here, the upper leg of the diagram is again $(\psi' \circ \varphi') * (\psi \circ \varphi)$; we have dropped the lower-scripts of the transformations and we have written "$J(H,F)$" instead of "$J(H(A,A), F(A,A))$" to save space. The dinaturality conditions of φ' and ψ' do not allow a place-swap for φ and φ' or for φ and ψ'; in fact, they cannot be applied at all! The only thing we can notice is that we can isolate φ from φ', obtaining the following:

$$(\psi' \circ \varphi') * (\psi \circ \varphi) = L(1,\psi) \circ \Big((\psi' \circ \varphi') * \varphi \Big) \circ J(\psi, 1).$$

Notice that the right-hand side is *not* $\Big((\psi' \circ \varphi') * \varphi \Big) * \psi$, as one might suspect at first glance, simply because the domain of $(\psi' \circ \varphi') * \varphi$ is not J and its codomain is not L.

It is clear then that the only assumption of $\varphi' \circ \varphi$ and $\psi' \circ \psi$ being dinatural (for whatever reason) is not enough. One chance of success could come from involving the graph of our transformations; for example, if the composite graphs $\Gamma^*(\psi \circ \varphi)$ and $\Gamma^*(\psi' \circ \varphi')$ are acyclic—hence dinatural, yes, but for a "good" reason—then maybe we could be able to deduce a suitably more general, "hexagonal" version of (†) for dinatural transformations. It also may well be that there is simply no sort of interchange law, of course. This is still an open question, and the matter of further study in the future. In the conclusions §3.5 we shall make some additional comments in light of the calculus we will build in Chapter 3.

Chapter 3

Towards a Godement calculus

The Godement calculus for functors of a single variable and ordinary natural transformations is at the heart of category theory: it governs and describes the behaviour of vertical and horizontal composition of natural transformations, and it consists, ultimately, in the assertion "$\mathbb{C}$at is a 2-category" or, more strongly, "$\mathbb{C}$at is cartesian closed". In the previous chapters, we have seen a detailed analysis of the properties of generalised versions of such compositions, now for functors of mixed variance and dinatural transformations of many variables and of arbitrary types. Both have their virtues and flaws: vertical composition is only partially defined, but we have a sufficient and essentially necessary condition that ensures compositionality—acyclicity; on the other hand, horizontal composition is always defined, but it is still unclear how it interacts with vertical composition. This chapter is dedicated to setting down formally the first steps to build a complete Godement calculus for our generalised transformations. Such a calculus will be the overarching structure entailing both vertical and horizontal composition.

In §3.1, we will give an overview of Kelly's original approach that led him to generalise the classical Godement calculus for *covariant-only* functors of many variables and natural transformations. In §3.2, we will introduce the notion of *generalised graph* of a transformation to allow for internal places (unlike the graphs considered in Chapter 1), which will require us to prove a more general compositionality result corresponding to Theorem (1.38). This will be needed in §3.3 where we will define a generalised functor category $\{\mathbb{B},\mathbb{C}\}$. Finally, in §3.4 we will prove that the functor $\{\mathbb{B},-\}$ has a left adjoint $- \circ \mathbb{B}$. This brings us significantly closer to the formulation of a Godement calculus, although non-trivial work is left to do, as we shall see in §3.5.

§3.1 Kelly's fully covariant case

In 1972, Kelly [Kel72a] developed a full generalisation of the Godement calculus for functors of many arguments, but fully covariant, and generalised natural transformations of many variables. These transformations are described as in Chapter 1 of this thesis: they are families of morphisms equipped with a type. However, in Kelly's case they are particularly simple: their domain and codomain functors have the same arity and their arguments are linked *in pairs*. Hence why in [Kel72a] the type (or "graph", as Kelly called it) of his natural transformations are not cospans, but simply *permutations*. In this section we shall give an overview of his work, following [Kel72a, §2].

Notation. To keep notations consistent with [Kel72a], in this section we shall denote the components of transformations φ in k variables as $\varphi(A_1, \dots, A_k)$ instead of the usual $\varphi_{A_1,\dots,A_k}$.

As we mentioned, Kelly considered the category $\mathbb{P}$ of permutations: its objects are natural numbers (with our same convention whereby we ambiguously denote by n the natural number n or the finite set $\{1, \dots, n\}$), with no morphisms $n \to m$ for $n \neq m$, and with permutations of n as the morphisms $n \to n$. He then defined a "generalised functor category" $\{\mathbb{B}, \mathbb{C}\}$ as follows.

(3.1) Definition. Let $\mathbb{B}$ and $\mathbb{C}$ be categories. The category $\{\mathbb{B}, \mathbb{C}\}$ consists of the following data:

- Objects are pairs (n, T), where $n \in \mathbb{N}$ and $T \colon \mathbb{B}^n \to \mathbb{C}$ is a functor;
- There are no morphisms $(n, T) \to (m, S)$ unless $n = m$, that is, unless T and S have the same arity. In that case, a morphism $(n, T) \to (n, S)$ is a pair $(\xi, [\varphi])$, for $\xi \colon n \to n$ a permutation, and $[\varphi]$ the equivalence class of a natural transformation $\varphi \colon T \to S$ "of graph ξ": in our notations, φ is a natural transformation of type
$$n \xrightarrow{\xi} n \xleftarrow{id_n} n$$
hence it has components of the form
$$\varphi(B_1, \dots, B_n) \colon T(B_{\xi 1}, \dots, B_{\xi n}) \to S(B_1, \dots, B_n). \qquad \square$$

(3.2) Remark. A permutation $\xi \colon n \to n$ induces a functor

$$\begin{array}{ccc} \mathbb{B}^n & \xrightarrow{\quad \mathbb{B}^{\xi} \quad} & \mathbb{B}^n \\ (B_1, \dots, B_n) & \longmapsto & (B_{\xi 1}, \dots, B_{\xi n}) \end{array}$$

Hence a natural transformation $\varphi \colon T \to S \colon \mathbb{B}^n \to \mathbb{C}$ of graph ξ is a classical natural transformation (as in [Mac78]) $\varphi \colon T\mathbb{B}^{\xi} \to S$.

(3.3) Proposition. *Defining* $\Gamma(n, T) = n$ *and* $\Gamma(\xi, \varphi) = \xi$*, we have that* $\{\mathbb{B}, \mathbb{C}\}$ *is an object of* $\mathbb{C}\mathrm{at}/\mathbb{P}$*, the category of categories over* $\mathbb{P}$*, with augmentation* Γ.

Now, the assignment $\mathbb{B}, \mathbb{C} \mapsto \{\mathbb{B}, \mathbb{C}\}$ provides a functor $\mathbb{C}\mathrm{at}^{\mathrm{op}} \times \mathbb{C}\mathrm{at} \to \mathbb{C}\mathrm{at}/\mathbb{P}$ continuous in C (that is, preserving all limits). We then have the following preliminary result.

(3.4) Theorem. *The functor* $\{\mathbb{B}, -\}$ *has a left adjoint*

$$\begin{tikzcd} \mathbb{C}\mathrm{at}/\mathbb{P} \arrow[rr, bend left, "-\circ\mathbb{B}"] \arrow[rr, phantom, "\perp"] & & \mathbb{C}\mathrm{at} \arrow[ll, bend left, "\{\mathbb{B},-\}"] \end{tikzcd}$$

therefore there is a natural isomorphism

(3.5) $$\mathbb{C}\mathrm{at}\big(\mathbb{A} \circ \mathbb{B}, \mathbb{C}\big) \cong \mathbb{C}\mathrm{at}/\mathbb{P}\big(\mathbb{A}, \{\mathbb{B}, \mathbb{C}\}\big).$$

Moreover, $\circ\colon \mathbb{C}\mathrm{at}/\mathbb{P} \times \mathbb{C}\mathrm{at} \to \mathbb{C}\mathrm{at}$ *is a functor.*

In order to see what $\mathbb{A} \circ \mathbb{B}$ looks like, let us analyse the right side of (3.5). Write Γ for all augmentations over $\mathbb{P}$. An element Φ of $\mathbb{C}\mathrm{at}/\mathbb{P}\big(\mathbb{A}, \{\mathbb{B}, \mathbb{C}\}\big)$, that is a functor $\Phi\colon \mathbb{A} \to \{\mathbb{B}, \mathbb{C}\}$ over $\mathbb{P}$, consists of the following data:

1. for each $A \in \mathbb{A}$ with $\Gamma A = n$, a functor $\Phi A\colon \mathbb{B}^n \to \mathbb{C}$, which means:

   1.a) for each $B_1, \dots, B_n \in \mathbb{B}$, objects $\Phi A(B_1, \dots, B_n)$ in $\mathbb{C}$,

   1.b) for each $g_i\colon B_i \to B'_i$ in $\mathbb{B}$, morphisms

   $$\Phi A(g_1, \dots, g_n)\colon \Phi A(B_1, \dots, B_n) \to \Phi A(B'_1, \dots, B'_n) \text{ in } \mathbb{C},$$

2. for each $f\colon A \to A'$ in $\mathbb{A}$ with $\Gamma f = \xi\colon n \to n$, a natural transformation $\Phi f\colon \Phi A \to \Phi A'$ of graph ξ, that is a family of morphisms

   $$\Phi f(B_1, \dots, B_n)\colon \Phi A(B_{\xi 1}, \dots, B_{\xi n}) \to \Phi A'(B_1, \dots, B_n).$$

All such data subject to the conditions making Φ and ΦA functors and Φf natural. This means that $\mathbb{A} \circ \mathbb{B}$ consists of:

- objects of the form $A[B_1, \dots, B_n]$ with $A \in A$, $B_i \in \mathbb{B}$ and $\Gamma A = n$,

- morphisms to be generated by $A[g_1, \dots, g_n]\colon A[B_1, \dots, B_n] \to A[B'_1, \dots, B'_n]$ and $f[B_1, \dots, B_n]\colon A[B_{\xi 1}, \dots, B_{\xi n}] \to A'[B_1, \dots, B_n]$,

all this data is to satisfy conditions corresponding to the relations making Φ and ΦA functors and Φf natural above (in this way, Φ can indeed be seen as a functor from $\mathbb{A} \circ \mathbb{B}$ to $\mathbb{C}$ where $\Phi\big(A[B_1, \dots, B_n]\big) = \Phi A(B_1, \dots, B_n)$ and so on). One of these, the naturality of Φf, gives the following commutative square:

(3.6)
$$\begin{tikzcd}
A[B_{\xi 1},\dots,B_{\xi n}] \arrow[r, "{f[B_1,\dots,B_n]}"] \arrow[d, "{A[g_{\xi 1},\dots,g_{\xi n}]}"'] & A'[B_1,\dots,B_n] \arrow[d, "{A'[g_1,\dots,g_n]}"] \\
A[B'_{\xi 1},\dots,B'_{\xi n}] \arrow[r, "{f[B'_1,\dots,B'_n]}"] & A'[B'_1,\dots,B'_n]
\end{tikzcd}$$

Writing $f[g_1,\dots,g_n]$ for the diagonal of the above diagram, one can see that this is the most general morphism of $\mathbb{A}\circ\mathbb{B}$, that is, that every morphism in $\mathbb{A}\circ\mathbb{B}$ has its form; the edges of (3.6) are just the special cases in which A and B_i stand for id_A and id_{B_i}, as is usual.

The construction of $\mathbb{A}\circ\mathbb{B}$ as such is only the first step towards a full Godement calculus for natural transformations with permutations for types. The next one is extending $\circ\colon \mathbb{C}\mathrm{at}/\mathbb{P}\times\mathbb{C}\mathrm{at}\to\mathbb{C}\mathrm{at}$ to a functor

$$\circ\colon \mathbb{C}\mathrm{at}/\mathbb{P}\times\mathbb{C}\mathrm{at}/\mathbb{P}\to\mathbb{C}\mathrm{at}/\mathbb{P}.$$

One defines $\mathbb{A}\circ\mathbb{B}$ exactly as before, ignoring the fact that $\mathbb{B}$ is a category over $\mathbb{P}$, and then augment $\mathbb{A}\circ\mathbb{B}$ by setting

$$\Gamma\big(A[B_1,\dots,B_n]\big)=\Gamma B_1+\dots+\Gamma B_n$$

on objects, with an appropriate definition on morphisms (essentially, one has to permute the $\Gamma(g_i)$ according to Γf to get $\Gamma\big(f[g_1,\dots,g_n]\big)$). By verifying that the bifunctor $\circ$ on $\mathbb{C}\mathrm{at}/\mathbb{P}$ is coherently associative with a coherent identity J, given by

$$\begin{array}{ccc} \mathbb{I} & \xrightarrow{J} & \mathbb{P} \\ * & \longmapsto & 1 \end{array}$$

one proves that $\mathbb{C}\mathrm{at}/\mathbb{P}$ is a monoidal category. Finally, one shows that our functor $\{-,-\}\colon \mathbb{C}\mathrm{at}^{\mathrm{op}}\times\mathbb{C}\mathrm{at}\to\mathbb{C}\mathrm{at}/\mathbb{P}$ extends to

$$\{-,-\}\colon (\mathbb{C}\mathrm{at}/\mathbb{P})^{\mathrm{op}}\times(\mathbb{C}\mathrm{at}/\mathbb{P})\to\mathbb{C}\mathrm{at}/\mathbb{P}$$

and the natural isomorphism (3.5) to

(3.7)
$$\mathbb{C}\mathrm{at}/\mathbb{P}\big(\mathbb{A}\circ\mathbb{B},\mathbb{C}\big)\cong\mathbb{C}\mathrm{at}/\mathbb{P}\big(\mathbb{A},\{\mathbb{B},\mathbb{C}\}\big)$$

which proves $\mathbb{C}\mathrm{at}/\mathbb{P}$ is a monoidal *closed* category with $\circ$ as tensor.

From the closed structure of $\mathbb{C}\mathrm{at}/\mathbb{P}$, then, Kelly extracted the generalisation of the Godement calculus he sought. The objects and the morphisms of $\{\mathbb{B},\mathbb{C}\}$ replace the functors and the natural transformations of the classical calculus, and composition in

$\{\mathbb{B},\mathbb{C}\}$ plays the role of generalised vertical composition. By iterating the "evaluation map" $\varepsilon\colon \{\mathbb{B},\mathbb{C}\} \circ \mathbb{B} \to \mathbb{C}$, which is the counit of the adjunction (3.7), we obtain a functor

$$\{\mathbb{B},\mathbb{C}\} \circ \{\mathbb{A},\mathbb{B}\} \circ \mathbb{A} \xrightarrow{1\circ\varepsilon} \{\mathbb{B},\mathbb{C}\} \circ \mathbb{B} \xrightarrow{\varepsilon} \mathbb{C}$$

and hence by adjunction (3.7) a functor over $\mathbb{P}$

$$\mu\colon \{\mathbb{B},\mathbb{C}\} \circ \{\mathbb{A},\mathbb{B}\} \to \{\mathbb{A},\mathbb{C}\}.$$

The operation μ is what embodies substitution, which is a generalisation of the classical horizontal composition. If $T\colon \mathbb{B}^n \to \mathbb{C}$, $S_i\colon \mathbb{A}^{m_i} \to \mathbb{B}$ are functors for $i \in \{1,\dots,n\}$, then $\mu\big(T[S_1,\dots,S_n]\big)$ is the following ordinary composite:

$$\mathbb{A}^{m_1} \times \cdots \times \mathbb{A}^{m_n} \xrightarrow{S_1\times\cdots\times S_n} \mathbb{B}^n \xrightarrow{\quad T \quad} \mathbb{C}$$

Writing $\mu\big(T[S_1,\dots,S_n]\big) = T(S_1,\dots,S_n)$, its image on objects is

$$T(S_1,\dots,S_n)(A^1_1,\dots,A^1_{m_1},\dots,A^n_1,\dots,A^n_{m_n}) = T\big(S_1(A^1_1,\dots,A^1_{m_1}),\dots,S_n(A^n_1,\dots,A^n_{m_n})\big)$$

and similarly on morphisms. If $\varphi\colon T \to T'$ is a natural transformation of graph ξ, and $\psi_i\colon S_i \to S'_i$ are natural transformations of graph η_i for $i \in \{1,\dots,n\}$, then $\mu\big(\varphi[\psi_1,\dots,\psi_n]\big)$ is the classical horizontal composite $\varphi * (\psi_1 \times \cdots \times \psi_n)$:

$$\begin{tikzcd}
A^{m_1} \times A^{m_n} \arrow[rr, bend left, "S_1\mathbb{A}^{\eta_1}\times\cdots\times S_n\mathbb{A}^{\eta_n}"] \arrow[rr, bend right, "S'_1\times\cdots\times S'_n"'] \arrow[rr, phantom, "\Downarrow \psi_1\times\cdots\times\psi_n"] & & \mathbb{B}^n \arrow[rr, bend left, "T\mathbb{B}^{\xi}"] \arrow[rr, bend right, "T'"'] \arrow[rr, phantom, "\Downarrow \varphi"] & & \mathbb{C}
\end{tikzcd}$$

What we have done and what we have yet to do. Kelly's setting is perfectly in line with our definition of horizontal composition for dinatural transformations of arbitrary type. Take φ and ψ as they appear in Definition (2.6), assuming however that all the functors involved are fully covariant. The functors $H(X_1,\dots,X_{|\gamma|})$ and $K(Y_1,\dots,Y_{|\delta|})$ in there, domain and codomain of the horizontal composition, are defined exactly as $\mu\big(T[S_1,\dots,S_n]\big)$ above. The i-th horizontal composition $\psi \overset{i}{*} \varphi$ itself would then be $\mu\big(\psi[id_{id_\mathbb{C}},\dots,id_{id_\mathbb{C}},\varphi,id_{id_\mathbb{C}},\dots,id_{id_\mathbb{C}}]\big)$, where φ is in i-th position in the list. Moreover, the associativity of horizontal composition would be the reflection of the fact that $\circ$ is coherently associative.

This sheds a light of hope for the formalisation of a full Godement calculus for functors of mixed variance, as we do have a notion of substitution at hand that already shows promising signs of success. However, this task is far from being simple to realise, as we shall see. What we have to do is to follow Kelly's steps enlightened above as far as we possibly can, starting from the very first one: find the right "category of graphs", which we shall call $\mathbb{G}$, and define a generalised functor category *over* $\mathbb{G}$. The morphisms of this category will not be simply dinatural transformations in many variables, because these do not, in general, always vertically compose. We shall then have instead transformations that are dinatural only in *some* of their variables, and use the theory of Chapter 1 to handle the dinaturality properties of composite transformations.

§3.2 A compositionality result for general graphs

For Kelly's natural transformations whose graphs do nothing wilder than permuting the variables, the category $\mathbb{P}$ of permutations is the natural choice. We need, however, something more complex than that. Our transformations, as defined in Chapter 1, carry a *cospan* of functions between finite sets, what we called their *type*, to describe which arguments of their domain and codomain functors are to be equated when writing down their general component. Hence our category $\mathbb{G}$ of graphs has to contain this information.

In this section, we will build up the theory needed to define a category of functors and transformations $\{\mathbb{B},\mathbb{C}\}^*$ and a category of generalised graphs $\mathbb{G}^*$, both of which contain *extra* elements which we will not need, ultimately. However, for the sake of clarity of exposure, we believe it is convenient to first introduce these relatively "large" categories, and then define the desired $\{\mathbb{B},\mathbb{C}\}$ and $\mathbb{G}$ as specific (non-full) subcategories of them. In this way we will be able to use the full theory designed in this section to prove that $\{\mathbb{B},\mathbb{C}\}^*$ is indeed a category, whose too-general transformations have graphs in $\mathbb{G}^*$; only after this we shall "trim down" $\{\mathbb{B},\mathbb{C}\}^*$ to the desired, more *natural* $\{\mathbb{B},\mathbb{C}\}$ by restricting ourselves only to the transformations that can arise in nature.

A first attempt. Bearing in mind that our aim is to develop a generalised functor category $\{\mathbb{B},\mathbb{C}\}$ whose morphisms are transformations that are dinatural in *some* of their variables, and the category $\mathbb{G}$ we want to define has to take into account in which variables a given transformation is dinatural, our first attempt would be to define $\mathbb{G}$ in the following way.

- Objects: $\mathrm{List}\{+,-\}$.
- Morphisms: a morphism $f\colon \alpha \to \beta$ is an equivalence class of diagrams in $\mathbb{F}\mathrm{in}\mathbb{S}\mathrm{et}$

$$\begin{tikzcd} {|\alpha|} \arrow[r, "\sigma"] & k \arrow[d, "\Delta_f"] & {|\beta|} \arrow[l, "\tau"'] \\ & \{0,1\} & \end{tikzcd}$$

  Two diagrams being equivalent if they differ by a coherent permutation on k. Δ_f here is the "discriminant" function that tells us in which variables a transformation φ of graph f is dinatural: if $\Delta_f(i) = 1$, then φ would be dinatural in its i-th variable. The pair (σ, τ) defines a graph $\Gamma(\sigma, \tau)$ exactly as in Definition (1.16).

- Composition: given $f = (\sigma, \tau, \Delta_f) \colon \alpha \to \beta$ as above and $g = (\eta, \theta, \Delta_g)$ (equivalence classes of) diagrams in $\mathbb{F}\mathrm{in}\mathbb{S}\mathrm{et}$, their composite is given by (the equivalence class of) diagram $(\zeta\sigma, \xi\theta, \Delta_{gf})$ as in:

$$
\begin{tikzcd}
 & & {|\gamma|} \arrow[d, "\theta"] & \\
 & {|\beta|} \arrow[r, "\eta"] \arrow[d, "\tau"'] \arrow[dr, phantom, "\ulcorner", very near start] & p \arrow[d, "\xi"] & \\
{|\alpha|} \arrow[r, "\sigma"] & k \arrow[r, "\zeta"] & q \arrow[dr, "\Delta_{gf}"] & \\
 & & & \{0,1\}
\end{tikzcd}
$$

  where $\Delta_{gf}(x)$ is defined to be 1 if the x-th connected component of the composite graph $\Gamma^*((\eta, \theta) \circ (\sigma, \tau))$ (obtained by joining together $\Gamma(\sigma, \tau)$ and $\Gamma(\eta, \theta)$ along the common interface) is acyclic and for all $y \in \zeta^{-1}\{x\}$ and $z \in \xi^{-1}\{x\}$ we have that $\Delta_f(y) = 1 = \Delta_g(z)$.

At this point one would define the functor category $\{\mathbb{B}, \mathbb{C}\}$ to have as objects pairs $(\alpha, F \colon \mathbb{B}^\alpha \to \mathbb{C})$ and a morphism $(\alpha, F) \to (\beta, G)$ would be a tuple $(\sigma, \tau, \Delta, \varphi)$ of a transformation $\varphi \colon F \to G$ of type $|\alpha| \xrightarrow{\sigma} k \xleftarrow{\tau} \beta$ that is dinatural in all variables in $\Delta^{-1}\{1\}$. By Theorem (1.59), composition in $\{\mathbb{B}, \mathbb{C}\}$ would be always defined.

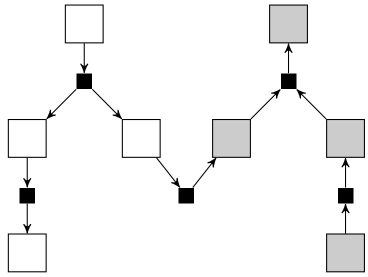
There is only one problem: $\mathbb{G}$ so defined is not a category, and neither is $\{\mathbb{B}, \mathbb{C}\}$! What fails here is associativity of composition. In the following example we show five "consecutive" transformations, whose composite is a family of morphisms with two different Δ discriminant functions depending on the bracketing we choose. (All the rest of the data does not cause any problems: composition of families of morphisms *is* associative, as is composition of cospans.)

(3.8) Example. Let $\mathbb{C}$ be a cartesian closed category, and B a fixed object of $\mathbb{C}$. Consider the following transformations:

$$
\begin{aligned}
\varphi^1 &= \big(\delta_A \times \delta_{A \Rightarrow B} \colon A \times (A \Rightarrow B) \to A \times A \times (A \Rightarrow B) \times (A \Rightarrow B)\big)_{A \in \mathbb{C}} \\
\varphi^2 &= \big(id_A \times eval_{A,B} \times id_{A \Rightarrow B} \colon A \times A \times (A \Rightarrow B) \times (A \Rightarrow B) \to A \times B \times (A \Rightarrow B)\big)_{A \in \mathbb{C}} \\
\varphi^3 &= \big(\sigma_{X,B} \times id_{Y \Rightarrow B} \colon X \times B \times (Y \Rightarrow B) \to B \times X \times (Y \Rightarrow B)\big)_{X,Y \in \mathbb{C}} \\
\varphi^4 &= (id_B \times \varphi^1_A)_{A \in \mathbb{C}} \\
\varphi^5 &= (id_B \times \varphi^2_A)_{A \in \mathbb{C}}
\end{aligned}
$$

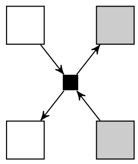
We have then that $\Gamma^*\big(\varphi^2 \circ \varphi^1\big)$ is the following graph:

(3.9)



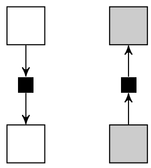
Hence, by Theorem (1.59), $\varphi^2 \circ \varphi^1$ is dinatural. $\Gamma^*\big(\varphi^5 \circ \varphi^4\big)$ looks exactly the same as (3.9), therefore

(3.10) $\Gamma\big(\varphi^2 \circ \varphi^1\big) = \Gamma\big(\varphi^5 \circ \varphi^4\big) =$



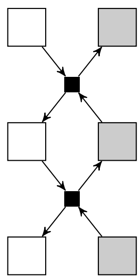
and since

$\Gamma\big(\varphi^3\big) =$



we have $\varphi^5 \circ \varphi^4$ and $(\varphi^5 \circ \varphi^4) \circ \varphi^3$ are both dinatural, with $\Gamma\big((\varphi^5 \circ \varphi^4) \circ \varphi^3\big) = \Gamma\big(\varphi^5 \circ \varphi^4\big)$. Hence, by composing with $\varphi^2 \circ \varphi^1$, we obtain

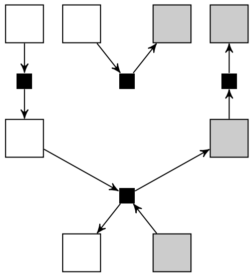
(3.11) $\Gamma^*\big((\varphi^5 \circ \varphi^4 \circ \varphi^3) \circ (\varphi^2 \circ \varphi^1)\big) =$



We have created a cycle: the discriminant function of the transformation $(\varphi^5 \circ \varphi^4 \circ \varphi^3) \circ (\varphi^2 \circ \varphi^1)$ is the function $\Delta\colon 1 \to \{0,1\}$ returning 0.

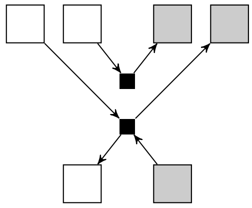
However, let us see what happens when we compose $\varphi^5 \circ \varphi^4 \circ \varphi^3$ with φ^2 first, and then φ^1 at a later time. We get

$$\Gamma^*\big((\varphi^5 \circ \varphi^4 \circ \varphi^3) \circ \varphi^2\big) =$$



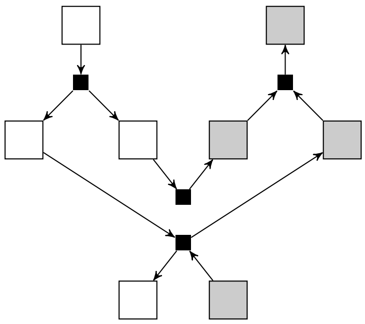
This means that $(\varphi^5 \circ \varphi^4 \circ \varphi^3) \circ \varphi^2$ is dinatural and, once we collapse the connected components, we obtain

$$\Gamma\big((\varphi^5 \circ \varphi^4 \circ \varphi^3) \circ \varphi^2\big) =$$



We then have that $\Gamma^*\big((\varphi^5 \circ \varphi^4 \circ \varphi^3 \circ \varphi^2) \circ \varphi^1\big)$ is

(3.12)

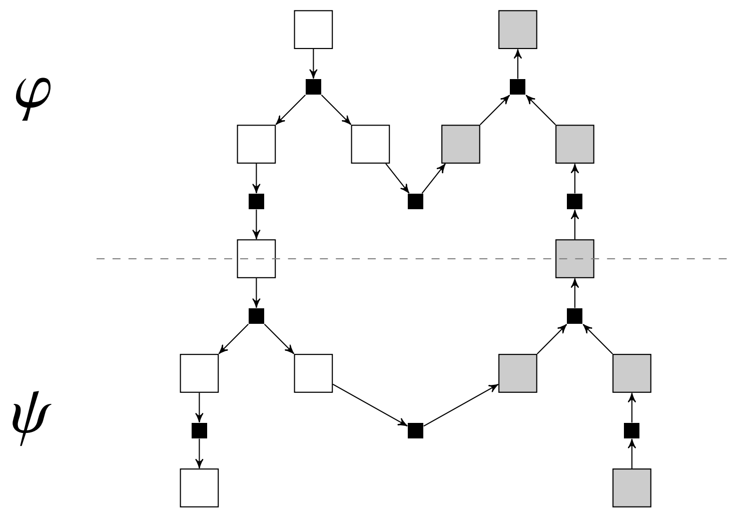


which is acyclic! Hence the discriminant function of the transformation $(\varphi^5 \circ \varphi^4 \circ \varphi^3 \circ \varphi^2) \circ \varphi^1$, which is no different in any aspect from $(\varphi^5 \circ \varphi^4 \circ \varphi^3) \circ (\varphi^2 \circ \varphi^1)$, is $\Delta' \colon 1 \to \{0,1\}$ returning 1. Therefore composition in $\mathbb{G}$ is not associative. $\square$

What went wrong? In the graph of $\varphi^2 \circ \varphi^1$, depicted in (3.10), there is a path from the bottom-right node to the bottom-left node, which then extends to a cycle once connected to $\Gamma\big(\varphi^5 \circ \varphi^4 \circ \varphi^3\big)$, as shown in (3.11). That path was created upon collapsing the composite graph $\Gamma^*\big(\varphi^2 \circ \varphi^1\big)$, pictured in (3.9), into a single connected component: but in (3.9) there was no path from the bottom-right node to the bottom-left one! And rightly so: to get a token moved to the bottom-left vertex of (3.9), we have no need to put one token in the bottom-right vertex. Therefore, once we have formed (3.10), we have lost a crucial information about which sources and sinks are *directly* connected with which others, because we have collapsed the entire connected component into a single internal transition, with no internal places. As it happens, by computing the composite graph in a different order, instead, no new paths have been created, hence no cycles appear where there should not be. After all, by Theorem (1.59) we know that $\varphi^5 \circ \cdots \circ \varphi^1$ is dinatural because it can be written as the composite of two dinatural transformations, namely $\varphi^5 \circ \varphi^4 \circ \varphi^3 \circ \varphi^2$ and φ^1, whose composite graph is acyclic.

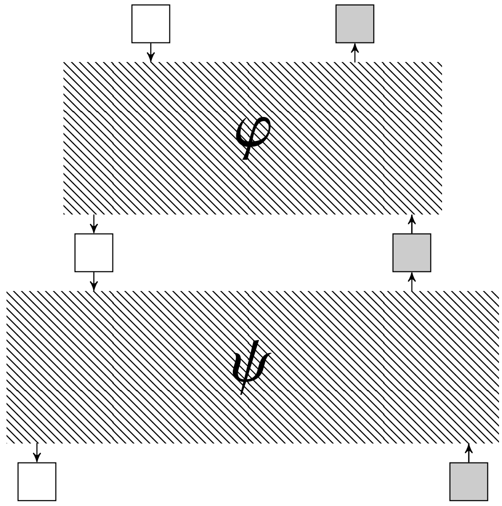
We should emphasise again the fact that composition of transformations and composition of types (that is, cospans of functions over finite sets) *are* associative. Indeed, $(\varphi^5 \circ \varphi^4 \circ \varphi^3 \circ \varphi^2) \circ \varphi^1$ and $(\varphi^5 \circ \varphi^4 \circ \varphi^3) \circ (\varphi^2 \circ \varphi^1)$ are the same family of morphisms, between the same functors, with the same type (hence, the same graph). More importantly, the previous example *does not contradict* our compositionality theorem (1.59): if we call $\varphi = \varphi^2 \circ \varphi^1$ and $\psi = \varphi^5 \circ \varphi^4 \circ \varphi^3$, since $\Gamma^*(\psi \circ \varphi)$ contains a cycle, we cannot conclude anything about the dinaturality of $\psi \circ \varphi$. Also, our "essentially necessary" result (1.63) has not been confuted: it is true that there is no way to prove the dinaturality of $\psi \circ \varphi$ by only using the dinaturality properties of φ and ψ themselves (and not also of their composing blocks φ^i!). This can be seen more clearly if we link together the graphs of all the φ^i's without collapsing anything (we only omit $\Gamma(\varphi^3)$ as it would add only a straight line):

(3.13)



To prove that $\psi \circ \varphi$ is dinatural, we do have to use the dinaturality properties of the

φ^i's: if we treat φ and ψ as "black boxes",



ignoring the fact that they actually are the composite of simpler transformations, we are not able to "move the f's" from the sources all the way to the sinks.

This tells us that the crucial reason for which associativity fails in our preliminary definition of the category $\mathbb{G}$ is that only keeping track of which connected component each of the arguments of the domain and codomain functors belongs to is not enough: we are forgetting too much information, namely the paths that directly connect the white and grey boxes. Hence our category of graphs will have to consist of more complicated Petri Nets that do contain internal places, and upon composition we shall simply link the graphs together along the common interface, without collapsing entire connected components into a single transition.

The category of FBCF Petri Nets. Recall from Definition (1.50) that a FBCF Petri Net is a net where all the places have at most one input and at most one output transition. We now introduce the category of FBCF Petri Nets, using the usual definition of morphism for bipartite graphs.

(3.14) Definition. The category $\mathbb{PN}$ consists of the following data:

- objects are FBCF Petri Nets $N = (P_N, T_N, \bullet(-), (-)\bullet)$ together with a fixed ordering of its connected components. Such an ordering will allow us to speak about the "i-th connected component" of N;
- a morphism $f : N \to M$ is a pair of functions (f_P, f_T), for $f_P : P_N \to P_M$ and $f_T : T_N \to T_M$, such that for all $t \in T_N$

$$\bullet f_T(t) = \{f_P(p) \mid p \in \bullet t\} \quad \text{and} \quad f_T(t)\bullet = \{f_P(p) \mid p \in t\bullet\}. \qquad \square$$

Note that if $f : N \to M$ is a morphism in $\mathbb{PN}$ then f preserves (undirected) paths, hence for C a c.c. of N we have that $f(C)$ is connected. In particular, if f is an isomorphism then $f(C)$ is a c.c. of M.

(3.15) Remark. We have a canonical inclusion $\mathbb{FinSet} \to \mathbb{PN}$ by seeing a set as a Petri Net with only places and no transitions.

For a function $x\colon A \to B$ of sets we call $\mathcal{P}(x)\colon \mathcal{P}(A) \to \mathcal{P}(B)$ the function such that $\mathcal{P}(x)(S) = \{x(a) \mid a \in S\}$ for $S \subseteq A$. We then have that if $f\colon N \to M$ is a morphism in $\mathbb{PN}$, then

$$\begin{tikzcd} T_N \arrow[r, "f_T"] \arrow[d, "\bullet(-)"'] & T_M \arrow[d, "\bullet(-)"] \\ \mathcal{P}(P_N) \arrow[r, "\mathcal{P}(f_P)"] & \mathcal{P}(P_M) \end{tikzcd} \quad \text{and} \quad \begin{tikzcd} T_N \arrow[r, "f_T"] \arrow[d, "(-)\bullet"'] & T_M \arrow[d, "(-)\bullet"] \\ \mathcal{P}(P_N) \arrow[r, "\mathcal{P}(f_P)"] & \mathcal{P}(P_M) \end{tikzcd}$$

commute by definition of the category $\mathbb{PN}$.

We now show that $\mathbb{PN}$ admits pushouts, with the aim then to define $\mathbb{G}$ using particular cospans in $\mathbb{PN}$.

(3.16) Proposition. *Let N, M, L be in $\mathbb{PN}$, and consider the following diagram in $\mathbb{PN}$:*

(3.17)
$$\begin{tikzcd} (P_N, T_N, \bullet_N(-), (-)\bullet_N) \arrow[r, "(g_P{,}g_T)"] \arrow[d, "(f_P{,}f_T)"'] & (P_L, T_L, \bullet_L(-), (-)\bullet_L) \arrow[d, "(k_P{,}k_T)"] \\ (P_M, T_M, \bullet_M(-), (-)\bullet_M) \arrow[r, "(h_P{,}h_T)"] & (P_Q, T_Q, \bullet_Q(-), (-)\bullet_Q) \end{tikzcd}$$

where

$$\begin{tikzcd} P_N \arrow[r, "g_P"] \arrow[d, "f_P"'] & P_L \arrow[d, "k_P"] \\ P_M \arrow[r, "h_P"] & P_Q \end{tikzcd} \quad \textit{and} \quad \begin{tikzcd} T_N \arrow[r, "g_T"] \arrow[d, "f_T"'] & T_L \arrow[d, "k_T"] \\ T_M \arrow[r, "h_T"] & T_Q \end{tikzcd}$$

are pushouts and $\bullet_Q(-)\colon T_Q \to \mathcal{P}(P_Q)$ is the unique map (the dashed one) that makes the following diagram commute:

$$\begin{tikzcd} \mathcal{P}(P_N) \arrow[rrrd, bend left, "\mathcal{P}(g_P)"] \arrow[dddr, bend right, "\mathcal{P}(f_P)"'] & & & \\ & T_N \arrow[ul, "\bullet_N(-)"'] \arrow[r, "g_T"] \arrow[d, "f_T"'] & T_L \arrow[r, "\bullet_L(-)"] \arrow[d, "k_T"] & \mathcal{P}(P_L) \arrow[dd, "\mathcal{P}(k_P)"] \\ & T_M \arrow[r, "h_T"] \arrow[d, "\bullet_M(-)"] & T_Q \arrow[dr, dashed] & \\ & \mathcal{P}(P_M) \arrow[rr, "\mathcal{P}(h_P)"] & & \mathcal{P}(P_Q) \end{tikzcd}$$

$(-)\bullet_Q \colon T_Q \to \mathcal{P}(P_Q)$ *is defined analogously. Then (3.17) is a pushout.*

Proof. We check that the definition of pushout is satisfied. Suppose then we have morphisms $u\colon M \to R$ and $v\colon L \to R$ such that $u \circ f = v \circ g$. Then there are unique functions $w_P\colon P_Q \to P_R$ and $w_T\colon T_Q \to T_R$ that make the following diagrams commute:

$$\begin{tikzcd} P_N \arrow[r, "g_P"] \arrow[d, "f_P"'] & P_L \arrow[d, "k_P"] \arrow[ddr, bend left, "v_P"] & \\ P_M \arrow[r, "h_P"] \arrow[drr, bend right, "u_P"'] & P_Q \arrow[dr, dashed, "w_P"] & \\ & & P_R \end{tikzcd} \quad \text{and} \quad \begin{tikzcd} T_N \arrow[r, "g_T"] \arrow[d, "f_T"'] & T_L \arrow[d, "k_T"] \arrow[ddr, bend left, "v_T"] & \\ T_M \arrow[r, "h_T"] \arrow[drr, bend right, "u_T"'] & T_Q \arrow[dr, dashed, "w_T"] & \\ & & T_R \end{tikzcd}$$

We claim that the pair $w = (w_P, w_T)$ is a morphism in $\mathbb{PN}$ from Q to R such that $w \circ h = u$ and $w \circ k = v$. We have shown just now that these two equalities hold, therefore we only have to check that w satisfies the definition of morphism in $\mathbb{PN}$, which is tantamount to the commutativity of the following squares:

$$\begin{tikzcd} T_Q \arrow[r, "w_T"] \arrow[d, "\bullet_Q(-)"'] & T_R \arrow[d, "\bullet_R(-)"] \\ \mathcal{P}(P_Q) \arrow[r, "\mathcal{P}(w_P)"] & \mathcal{P}(P_R) \end{tikzcd} \quad \text{and} \quad \begin{tikzcd} T_Q \arrow[r, "w_T"] \arrow[d, "(-)\bullet_Q"'] & T_R \arrow[d, "(-)\bullet_R"] \\ \mathcal{P}(P_Q) \arrow[r, "\mathcal{P}(w_P)"] & \mathcal{P}(P_R) \end{tikzcd}$$

To prove the commutativity of the first square, since h_T and k_T are jointly epi (because they are the result of a pushout), it is enough to prove that

$$\begin{cases} \bullet_R(-) \circ w_T \circ h_T = \mathcal{P}(w_P) \circ \bullet_Q(-) \circ h_T \colon T_M \to \mathcal{P}(P_Q) \\ \bullet_R(-) \circ w_T \circ k_T = \mathcal{P}(w_P) \circ \bullet_Q(-) \circ k_T \colon T_L \to \mathcal{P}(P_Q) \end{cases}$$

We only show the first equation, the other is analogous. We have:

$$\begin{aligned} \bullet_R(-) \circ w_T \circ h_T &= \bullet_R(-) \circ u_T \\ &= \mathcal{P}(u_P) \circ \bullet_M(-) \\ &= \mathcal{P}(w_P) \circ \mathcal{P}(h_P) \circ \bullet_M(-) \\ &= \mathcal{P}(w_P) \circ \bullet_Q(-) \circ h_T \end{aligned}$$

The second square is then proved to be commutative in a similar way. **Qed**

A "preliminary" category of graphs. Remember from Remark (3.15) that finite sets can be seen as places-only Petri Nets: if S is a set and N is an object in $\mathbb{PN}$, then a morphism $f\colon S \to N$ in $\mathbb{PN}$ is a pair of functions $f = (f_P, f_T)$ where f_T is the empty map $\varnothing\colon \varnothing \to T_N$. Hence, by little abuse of notation, we will refer to f_P simply as f.

Bearing in mind Example (3.8) and the following discussion, we begin our "journey" towards individuating the correct category of graphs $\mathbb{G}$ of transformations by considering the following category, consisting of particular cospans in $\mathbb{PN}$. Such cospans are essentially Petri Nets N in $\mathbb{PN}$ with "interfaces", that is specific places seen as "inputs" and "outputs" of N. Composition will then be computed by "glueing together" two consecutive nets along the common interface. $\mathbb{G}$ will be built up using only *some* of its morphisms, as we shall see.

(3.18) Definition. The category $\mathbb{H}$ consists of the following data:

- objects are lists in $\mathrm{List}\{+,-\}$;
- morphisms $f\colon \alpha \to \beta$ are (equivalence classes of) cospans in $\mathbb{PN}$ of the form

$$|\alpha| \xrightarrow{\sigma} N \xleftarrow{\tau} |\beta|$$

  where $\sigma\colon |\alpha| \to P_N$ and $\tau\colon |\beta| \to P_N$ are injective functions, hence we can see $|\alpha|$ and $|\beta|$ as subsets of P_N. Two such cospans are in the same class if and only if they differ by an isomorphism of Petri Nets on N coherent with σ, τ and the ordering of the connected components of N;
- composition is that of $\mathbb{C}\mathrm{o}\mathbb{S}\mathrm{pan}(\mathbb{PN})$. □

We now show in detail how composition in $\mathbb{H}$ works. Consider $|\alpha| \xrightarrow{\sigma} M \xleftarrow{\tau} |\beta|$ and $|\beta| \xrightarrow{\eta} L \xleftarrow{\theta} |\gamma|$ two morphisms in $\mathbb{H}$. By Proposition (3.16) then, their composite is given by computing the pushouts

$$\begin{tikzcd} |\beta| \arrow[r, "\eta"] \arrow[d, "\tau"'] & P_L \arrow[d, "k_P"] \\ P_M \arrow[r, "h_P"] & P_Q \end{tikzcd} \quad \text{and} \quad \begin{tikzcd} \varnothing \arrow[r, "\varnothing"] \arrow[d, "\varnothing"'] & T_L \arrow[d, "k_T"] \\ T_M \arrow[r, "h_T"] & T_Q \end{tikzcd}$$

Now, the injectivity of η and θ implies that k_P and h_P are also injective, as the pushout (in $\mathbb{S}\mathrm{et}$) of an injective map against another yields injective functions. P_Q, in particular, can be seen as the quotient of $P_M + P_L$ where the elements of P_M and P_L with a common pre-image in $|\beta|$ are identified. Next, the pushout of the empty map against itself yields as a result the coproduct, thus $T_Q = T_M + T_L$ where h_T and k_T are the injections. Hence, the input function of the composite is defined as follows:

$$\begin{aligned} T_M + T_L &\xrightarrow{\quad {}^\bullet(-) \quad} \mathcal{P}(P_Q) \\ t &\longmapsto \begin{cases} {}^\bullet{}_M(t) & t \in T_M \\ {}^\bullet{}_L(t) & t \in T_L \end{cases} \end{aligned}$$

and similarly for the output function. All in all, therefore, composition in $\mathbb{H}$ is computed by "glueing" together the Petri Nets M and L along the common $|\beta|$-places.

Generalised graphs of a transformation. We can now start working towards the definition of a category $\{\mathbb{B},\mathbb{C}\}$ of functors of mixed variance and transformations that are dinatural only on some of their variables; $\{\mathbb{B},\mathbb{C}\}$ will be a category over $\mathbb{G}$ in the sense that transformations in $\{\mathbb{B},\mathbb{C}\}$ will carry along, as part of their data, certain cospans in $\mathbb{PN}$. The category of graphs $\mathbb{G}$ will be built from $\{\mathbb{B},\mathbb{C}\}$ by "forgetting" the transformations. As such, $\mathbb{G}$ will be defined *after* $\{\mathbb{B},\mathbb{C}\}$.

It is clear how to define the objects of $\{\mathbb{B},\mathbb{C}\}$: they will be pairs $(\alpha, F\colon \mathbb{B}^\alpha \to \mathbb{C})$. Morphisms are less obvious to define, as we learnt in our "first attempt" on p. 100. A morphism $(\alpha,F) \to (\beta,G)$ will consist of a transformation $\varphi\colon F \to G$ of type $|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|$, together though with a morphism $|\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|$ in $\mathbb{H}$ "coherent with the type of φ", in the sense that the Petri Net N, under certain conditions, looks exactly like $\Gamma(\varphi)$ as defined in (1.16) except that it allows for internal places as well. For example, (3.13) would be a graph coherent with the type of $\varphi^5 \circ \cdots \circ \varphi^1$ as in Example (3.8). In other words, N will have n connected components, its sources (sinks) are exactly the places corresponding to the positive (negative) entries of α and the negative (positive) entries of β, and elements in $|\alpha|$ ($|\beta|$) mapped by σ (τ) into the same $i \in \{1,\dots,n\}$ will belong to the i-th connected component of N. A priori N can contain places with no inputs or outputs: this will be useful for the special case of $\varphi = id_F$ as we shall see in Theorem (3.36); however, if all sources and sinks in N are proper, then N plays the role of a generalised $\Gamma(\varphi)$.

(3.19) Definition. Let $\varphi\colon F \to G$ be a transformation of type $|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|$. A cospan in $\mathbb{PN}$, which is a representative of a morphism in $\mathbb{H}$ $|\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|$ (hence $\overline{\sigma}$ and $\overline{\tau}$ are injective), is said to be *coherent with the type of φ* if and only if the following conditions are satisfied:

- N has n connected components;
- for all $i \in |\alpha|$ and $j \in |\beta|$, $\overline{\sigma}(i)$ belongs to the $\sigma(i)$-th connected component of N and $\overline{\tau}(j)$ belongs to the $\tau(j)$-th connected component of N;
- $sources(N) = \{\overline{\sigma}(i) \mid \alpha_i = +\} \cup \{\overline{\tau}(i) \mid \beta_i = -\}$;
- $sinks(N) = \{\overline{\sigma}(i) \mid \alpha_i = -\} \cup \{\overline{\tau}(i) \mid \beta_i = +\}$.

In this case we say that N is a *generalised graph of φ*. □

(3.20) Example. For $\varphi\colon F \to G$ a transformation of type $|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|$, recall that the set of places of $\Gamma(\varphi)$ is $P = |\alpha| + |\beta|$. If we call $\iota_{|\alpha|}$ and $\iota_{|\beta|}$ the injections as in (1.16), then

$$|\alpha| \xrightarrow{\iota_{|\alpha|}} \Gamma(\varphi) \xleftarrow{\iota_{|\beta|}} |\beta|$$

is indeed coherent with the type of φ. Moreover, if σ and τ are jointly epi, then also $|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|$ itself, seen as a cospan in $\mathbb{PN}$, is coherent with itself. (If there is $i \in n$ that is not in the image of σ or τ, then the i-th place in n seen as a Petri Net would be a source and a sink that would falsify the last two conditions of the definition.) $\square$

(3.21) Remark. If N is a generalised graph of φ as in the notations of Definition (3.19) and does not have any place which is a source and a sink at once, then N has exactly $|\alpha| + |\beta|$ sources and sinks and their union coincides with the joint image of $\overline{\sigma}$ and $\overline{\tau}$. Moreover, $\overline{\sigma}$ and $\overline{\tau}$ have to make sure that they map elements of their domain into places belonging to the correct connected component: in this way, N reflects the type of φ in a Petri Net like $\Gamma(\varphi)$, with the possible addition of internal places.

We shall now show how composition in $\mathbb{H}$ preserves generalised graphs, in the following sense.

(3.22) Proposition. *Let $\varphi\colon F \to G$ and $\psi\colon G \to H$ be transformations of type, respectively, $|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|$ and $|\beta| \xrightarrow{\eta} m \xleftarrow{\theta} |\gamma|$; let also $u = |\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|$ and $v = |\beta| \xrightarrow{\overline{\eta}} N' \xleftarrow{\overline{\theta}} |\gamma|$ be cospans in $\mathbb{PN}$ coherent with the type of φ and ψ, respectively. Suppose the type of $\psi \circ \varphi$ is given by*

$$\begin{tikzcd}
 & & {|\gamma|} \arrow[d, "\theta"] \\
 & {|\beta|} \arrow[r, "\eta"] \arrow[d, "\tau"'] \arrow[dr, phantom, "\ulcorner", very near start] & m \arrow[d, "\xi"] \\
{|\alpha|} \arrow[r, "\sigma"] & n \arrow[r, "\zeta"] & l
\end{tikzcd}$$

and that the composite in $\mathbb{H}$ of u and v is given by

(3.23)
$$\begin{tikzcd}
 & & {|\gamma|} \arrow[d, "\overline{\theta}"] \\
 & {|\beta|} \arrow[r, "\overline{\eta}"] \arrow[d, "\overline{\tau}"'] \arrow[dr, phantom, "\ulcorner", very near start] & N' \arrow[d, "\overline{\xi}"] \\
{|\alpha|} \arrow[r, "\overline{\sigma}"] & N \arrow[r, "\overline{\zeta}"] & N' \circ N
\end{tikzcd}$$

Then $v \circ u$ is coherent with the type of $\psi \circ \varphi$.

PROOF. As we said in the discussion after Definition (3.18), $N' \circ N$ is obtained by glueing together N and N' along the $|\beta|$ places which they have in common. The number of connected components of $N' \circ N$ is indeed l by construction. The morphisms $\overline{\zeta}$ and $\overline{\xi}$ in $\mathbb{PN}$ are pairs of injections that map each place and transition of N and N'

to itself in the composite $N' \circ N$. This means that $\overline{\zeta\sigma}(i)$ does belong to the $\zeta\sigma(i)$-th connected component of $N' \circ N$, as the latter contains the $\sigma(i)$-th c.c. of N; similarly the $\overline{\xi\theta}(j)$ belongs to the $\xi\theta(j)$-th c.c. of $N' \circ N$. Finally, we have that the sources of $N' \circ N$ are the sources of N and N' except those which happen to be $|\beta|$ places, which upon composition become internal places. Indeed, for all $j \in |\beta|$, if $\beta_j = +$ then we have that $\overline{\tau}(j)$ is a source for N and a sink for N'; if $\beta_j = -$, then vice versa. In other words,

$$\begin{aligned} sources(N' \circ N) &= \big(sources(N) \setminus \tau(|\beta|)\big) \cup \big(sources(N') \setminus \eta(|\beta|)\big) \\ &= \{\overline{\sigma}(i) \mid \alpha_i = +\} \cup \{\overline{\theta}(i) \mid \gamma_i = -\} \end{aligned}$$

and similarly for $sinks(N' \circ N)$. **QED**

(3.24) Remark. In the previous proposition, if $N = \Gamma(\varphi)$ and $N' = \Gamma(\psi)$, then $N' \circ N = \Gamma^*(\psi \circ \varphi)$.

A generalised compositionality theorem. At this point we need a means to tell in which variables, if any, a composite transformation $\psi \circ \varphi$ is dinatural, given the dinaturality properties of φ and ψ, that looks not at the acyclicity of $\Gamma^*(\psi \circ \varphi)$, since as discussed in Example (3.8) this leads to an incorrect definition, but at the acyclicity of the composite cospan in $\mathbb{PN}$. We have therefore to adapt our compositionality result (1.38) (and consequently also (1.59)) to the case in which $\Gamma(\varphi)$ and $\Gamma(\psi)$ may have internal places as well.

(3.25) Remark. By considering transformations carrying, as part of their data, a Petri Net with possibly internal places "as long as it is coherent with their type", we will be considering *far more* transformations than those arising in nature such as those of Examples (1.9)-(1.13). Hence why we will end up with a category $\{\mathbb{B},\mathbb{C}\}^*$ which is larger than strictly necessary, but for which a general compositionality result holds. For such "atomic" transformations like the ones in the examples above, the natural thing to do would still be to consider, as their generalised graphs, simply their graphs as in Definition (1.16); only upon composition of these simple transformations (as in Example (3.8)) we would consider the more complicated Petri Nets obtained by pasting together the graphs of the components. In this spirit, only transformations which are *explicitly* recognisable as the composite of two or more families of morphisms ought to have an associated Net with internal places. Nonetheless, the general morphism of $\{\mathbb{B},\mathbb{C}\}^*$ has to admit an arbitrarily complicated FBCF Net, hence why we will work in such generality. We will then define the proper $\{\mathbb{B},\mathbb{C}\}$ as the subcategory of $\{\mathbb{B},\mathbb{C}\}^*$ generated by the atomic transformations with their no-internal-places graphs.

The whole spirit of Theorem (1.38) was to reduce the dinaturality problem of the composite transformation $\psi \circ \varphi$ to a reachability problem of the composite Petri Net $\Gamma^*(\psi \circ \varphi)$, by showing that the firing of an enabled transition yields an equality of morphisms. To do so, we isolated a specific class of markings, the *labelled markings*

(Definition (1.41)), and defined an associated morphism to each of them in Definition (1.43). This was possible because every place in $\Gamma^*(\psi \circ \varphi)$ corresponds to an argument of one of the domain or codomain functors of φ and ψ; however, this is not the case any more if we allow for $\Gamma(\varphi)$ and $\Gamma(\psi)$ to have internal places, which do not correspond to anything in particular, in general. (In light of Remark (3.25), such internal places would indeed correspond to arguments of functors involved by transformations whose composite are φ and ψ, if these are not atomic.) Hence we need that any transformation in $\{\mathbb{B},\mathbb{C}\}^*$ has, in addition to a type and a cospan in $\mathbb{PN}$ that gives its graph, also a *translating function* $\mathcal{T}$ that converts a labelled marking into an actual morphism of $\mathbb{C}$. For transformations φ and ψ whose graph contains no internal places, the translating function of the composite $\psi \circ \varphi$ will be defined exactly as μ in Definition (1.43).

(3.26) Definition. Let $F \colon \mathbb{B}^\alpha \to \mathbb{C}$, $G \colon \mathbb{B}^\beta \to \mathbb{C}$ be functors, $\varphi \colon F \to G$ be a transformation of type $|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|$, $|\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|$ be a cospan in $\mathbb{PN}$ coherent with the type of φ. Call $\mathcal{LM}(N)$ the set of labelled markings for N, which are defined in the same way as in Definition (1.41). Then a *translating function* for (φ, N) $\mathcal{T}_{\varphi,N} \colon \mathcal{LM}(N) \to \mathrm{Morph}(\mathbb{C})$ is a map such that for all labelled marking (M, L, f) for N, with $f \colon A \to B$ in $\mathbb{B}$, the following conditions are satisfied:

- $\mathcal{T}_{\varphi,N}(M,L,f) = F(a_1,\dots,a_{|\alpha|}); x_{(M,L)}; G(b_1,\dots,b_{|\beta|})$ where
$$a_i = \begin{cases} f & M(\overline{\sigma}(i)) = 1 \\ id_{L(t)} & M(\overline{\sigma}(i)) = 0 \wedge t \in {\bullet}\overline{\sigma}(i) \cup \overline{\sigma}(i){\bullet} \end{cases}$$
$$b_i = \begin{cases} f & M(\overline{\tau}(i)) = 1 \\ id_{L(t)} & M(\overline{\tau}(i)) = 0 \wedge t \in {\bullet}\overline{\tau}(i) \cup \overline{\tau}(i){\bullet} \end{cases}$$
for a certain morphism $x_{(M,L)}$ in $\mathbb{C}$;
- if (M_0, L_0, f) and (M_d, L_d, f) are defined as in (1.45), then $x_{(M_0,L_0)} = \varphi_{B,\dots,B}$ and $x_{M_d,L_d} = \varphi_{A,\dots,A}$;
- if φ is dinatural in its i-th variable, $t \in T_N$ is an enabled transition belonging to the i-th connected component of N such that $L(t) = B$ and (M', L', f) is a labelled marking defined as in (1.47), then $\mathcal{T}_{\varphi,N}(M,L,f) = \mathcal{T}_{\varphi,N}(M',L',f)$. □

We shall then assume that the morphisms of $\{\mathbb{B},\mathbb{C}\}^*$ will be transformations together with a generalised graph that admit the existence of a translating function, which provides the key to interpret labelled markings for the generalised graph of the transformation as distinct morphisms in $\mathbb{C}$ that have a special shape; moreover, this translating function "preserves firings" of enabled, B-labelled transitions by definition. Given an ordinary transformation φ, we can always find a canonical translating function for it, if we take as generalised graph the usual $\Gamma(\varphi)$.

(3.27) Proposition. *Let $\varphi \colon F \to G$ be a transformation of type $|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|$. Then $(\varphi, \Gamma(\varphi))$ (cf. Example (3.20)) admits a canonical translating function $\mathcal{T}_{\varphi,\Gamma(\varphi)}$ which, for (M, L, f) labelled marking of $\Gamma(\varphi)$, is defined as follows:*

$$\mathcal{T}_{\varphi,\Gamma(\varphi)} = F(a_1, \dots, a_{|\alpha|}); \varphi_{L(1),\dots,L(n)}; G(b_1, \dots, b_{|\beta|})$$

where

$$a_i = \begin{cases} f & M(\iota_{|\alpha|}(i)) = 1 \\ id_{L(\sigma i)} & M(\iota_{|\alpha|}(i)) = 0 \end{cases} \qquad b_i = \begin{cases} f & M(\iota_{|\beta|}(i)) = 1 \\ id_{L(\tau i)} & M(\iota_{|\beta|}(i)) = 0 \end{cases}$$

(3.28) Proposition. *Let $\varphi \colon F \to G$ and $\psi \colon G \to H$ be transformations, and let $|\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|$ and $|\beta| \xrightarrow{\overline{\eta}} N' \xleftarrow{\overline{\theta}} |\gamma|$ be cospans in $\mathbb{PN}$ coherent with the type of φ and ψ, respectively. If (φ, N) and (ψ, N') admit a translating function, then so does $(\psi \circ \varphi, N' \circ N)$.*

Proof. Suppose that the composite generalised graph $N' \circ N$, obtained by just glueing together N and N' along the common interface, is given as in (3.23):

$$\begin{tikzcd}
 & & {|\gamma|} \arrow[d, "\overline{\theta}"] \\
 & {|\beta|} \arrow[r, "\overline{\eta}"] \arrow[d, "\overline{\tau}"'] \arrow[dr, phantom, "\ulcorner"] & N' \arrow[d, "\overline{\xi}"] \\
{|\alpha|} \arrow[r, "\overline{\sigma}"] & N \arrow[r, "\overline{\zeta}"] & N' \circ N
\end{tikzcd}$$

In particular, both N and N' are subnets, via $\overline{\zeta}$ and $\overline{\xi}$ (whose components are injective) of $N' \circ N$: it is immediate to see that if $f \colon A \to B$ in $\mathbb{B}$ and (M, L, f) is a labelled marking for $N' \circ N$, then the restrictions $M_{\restriction P_N}$ and $L_{\restriction T_N}$ form a labelled marking $(M_{\restriction P_N}, L_{\restriction T_N}, f)$ for N. (More precisely, the marking $M_{\restriction P_N}$ is the function $M \circ \overline{\zeta}_P$.)

Let $\mathcal{T}_{\varphi,N}$ and $\mathcal{T}_{\psi,N}$ be translating functions for (φ, N) and (ψ, N) respectively. There is a natural way to endow $\psi \circ \varphi$ and $N' \circ N$ with a translating function, that is also obtained by "glueing together" $\mathcal{T}_{\varphi,N}$ and $\mathcal{T}_{\psi,N'}$: for $f \colon A \to B$ in $\mathbb{B}$ and (M, L, f) labelled marking for $N' \circ N$, say we have

$$\mathcal{T}_{\varphi,N}(M_{\restriction P_N}, L_{\restriction T_N}, f) = F(a_1, \dots, a_{|\alpha|}); x_{(M_{\restriction P_N}, L_{\restriction T_N})}; G(b_1, \dots, b_{|\beta|})$$
$$\mathcal{T}_{\psi,N'}(M_{\restriction P_{N'}}, L_{\restriction T_{N'}}, f) = G(b'_1, \dots, b'_{|\beta|}); y_{(M_{\restriction P_{N'}}, L_{\restriction T_{N'}})}; H(c_1, \dots, c_{|\gamma|})$$

where

$$a_i = \begin{cases} f & M_{\restriction P_N}(\overline{\sigma}(i)) = 1 \\ id_{L_{\restriction T_N}(t)} & M_{\restriction P_N}(\overline{\sigma}(i)) = 0 \wedge t \in {\bullet}\overline{\sigma}(i) \cup \overline{\sigma}(i){\bullet} \end{cases}$$

$$b_i = \begin{cases} f & M_{\restriction P_N}(\overline{\tau}(i)) = 1 \\ id_{L_{\restriction T_N}(t)} & M_{\restriction P_N}(\overline{\tau}(i)) = 0 \wedge t \in \bullet\overline{\tau}(i) \cup \overline{\tau}(i)\bullet \end{cases}$$
$$b'_i = \begin{cases} f & M_{\restriction P_{N'}}(\overline{\eta}(i)) = 1 \\ id_{L_{\restriction T_{N'}}(t)} & M_{\restriction P_{N'}}(\overline{\eta}(i)) = 0 \wedge t \in \bullet\overline{\eta}(i) \cup \overline{\eta}(i)\bullet \end{cases}$$
$$c_i = \begin{cases} f & M_{\restriction P_{N'}}(\overline{\theta}(i)) = 1 \\ id_{L_{\restriction T_{N'}}(t)} & M_{\restriction P_{N'}}(\overline{\theta}(i)) = 0 \wedge t \in \bullet\overline{\theta}(i) \cup \overline{\theta}(i)\bullet \end{cases}$$

Notice that, in fact, $b_i = b'_i$, because $M_{\restriction P_N}(\overline{\tau}(i)) = M(\overline{\zeta}_P\overline{\tau}(i)) = M(\overline{\xi}_P\overline{\eta}(i)) = M_{\restriction P_{N'}}(\overline{\eta}(i))$. Define then $\mathcal{T}_{\psi\circ\varphi,N'\circ N} \colon \mathcal{LM}(N' \circ N) \to \mathrm{Morph}(\mathbb{C})$ as

(3.29) $\mathcal{T}_{\psi\circ\varphi,N'\circ N}(M,L,f) =$

$$\underbrace{F(a_1,\dots,a_{|\alpha|}); x_{(M\overline{\zeta}_P,L\overline{\zeta}_T)}; \overbrace{G(b_1,\dots,b_{|\beta|})}}_{\mathcal{T}_{\varphi,N}(M\overline{\zeta}_P,L\overline{\zeta}_T,f)}\overbrace{; y_{(M\overline{\xi}_P,L\overline{\xi}_T)}; H(c_1,\dots,c_{|\gamma|})}^{\mathcal{T}_{\psi,N'}(M\overline{\xi}_P,L\overline{\xi}_T,f)}.$$

It is easy to see that $\mathcal{T}_{\psi\circ\varphi,N'\circ N}$ so defined is indeed a translating function. **QED**

(3.30) Remark. If φ and ψ are two consecutive transformations, equipped with $\Gamma(\varphi)$ and $\Gamma(\psi)$ respectively as generalised graphs and with the canonical translating functions $\mathcal{T}_{\varphi,\Gamma(\varphi)}$ and $\mathcal{T}_{\psi,\Gamma(\psi)}$ as in Proposition (3.28), then $\Gamma(\psi) \circ \Gamma(\varphi) = \Gamma^*(\psi \circ \varphi)$ and $(\psi \circ \varphi, \Gamma^*(\psi \circ \varphi))$ admits as translating function the map μ given in Definition (1.43).

We can now state a more general compositionality theorem for dinatural transformations with a generalised graph accompanying them. Remember that *every* transformation φ can be equipped with a generalised graph N coherent with its type by simply taking $N = \Gamma(\varphi)$: the following theorem reduces to Theorem (1.38) if we do this for φ and ψ.

(3.31) Theorem. *Let $F \colon \mathbb{B}^\alpha \to \mathbb{C}$, $G \colon \mathbb{B}^\beta \to \mathbb{C}$, $H \colon \mathbb{B}^\gamma \to \mathbb{C}$ be functors, $\varphi \colon F \to G$ and $\psi \colon G \to H$ transformations of type $|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|$ and $|\beta| \xrightarrow{\eta} m \xleftarrow{\theta} |\gamma|$, with generalised graphs given by $|\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|$ and $|\beta| \xrightarrow{\overline{\eta}} N' \xleftarrow{\overline{\theta}} |\gamma|$ and translating functions, respectively, $\mathcal{T}_{\varphi,N}$ and $\mathcal{T}_{\psi,N'}$. Suppose $N' \circ N$ is connected and φ and ψ are dinatural in all their variables. If $N' \circ N$ is acyclic, then $\psi \circ \varphi$ is dinatural.*

PROOF. Let $f \colon A \to B$ be a morphism in B. Consider the labelled markings (M_0, L_0, f) and (M_d, L_d, f) as in (1.45). By definition of $\mathcal{T}_{\psi\circ\varphi,N'\circ N}$, if the composite $N' \circ N$ is computed as in (3.23), we have

$$\mathcal{T}_{\psi\circ\varphi,N'\circ N}(M_0,L_0,f) = F(a_1,\dots,a_{|\alpha|}) \circ \varphi_{B,\dots,B}; G(id_B,\dots,id_B); \psi_{B,\dots,B}; H(b_1,\dots,b_{|\gamma|})$$

where

$$a_i = \begin{cases} f & \overline{\zeta}_P\overline{\sigma}(i) \text{ source} \\ id_B & \text{otherwise} \end{cases} = \begin{cases} f & \alpha^i = + \\ id_B & \alpha^i = - \end{cases}$$

$$b_i = \begin{cases} f & \overline{\xi}_P\overline{\theta}(i) \text{ source} \\ id_B & \text{otherwise} \end{cases} = \begin{cases} f & \gamma_i = - \\ id_B & \gamma i = + \end{cases}$$

(G is computed in id_B everywhere because the places corresponding to the arguments of G are internal, hence not marked by M_0.) This means that $\mathcal{T}_{\psi\circ\varphi,N'\circ N}(M_0, L_0, f)$ is effectively one of the legs of the dinaturality hexagon for $\psi \circ \varphi$; in a similar way one can see that $\mathcal{T}_{\psi\circ\varphi,N'\circ N}(M_d, L_d, f)$ is the other one.

Now, by definition of translating function, the firing of a single, B-labelled transition generates a labelled marking whose image along $\mathcal{T}_{\psi\circ\varphi,N'\circ N}$ is the same as the original marking's image. Hence, it is enough to show that M_d is reachable from M_0 by only firing B-labelled transitions, and indeed Theorem (1.57) applied to the FBCF Petri Net $N' \circ N$ ensures us that M_d is in fact reachable from M_0 by firing each transition exactly once. The Theorem is then proved. **Qed**

A straightforward generalisation of Theorem (3.31), that corresponds to Theorem (1.59) but for transformations of arbitrarily complicated graph, is the following.

(3.32) Theorem. *Let $F \colon \mathbb{B}^\alpha \to \mathbb{C}$, $G \colon \mathbb{B}^\beta \to \mathbb{C}$, $H \colon \mathbb{B}^\gamma \to \mathbb{C}$ be functors, $\varphi \colon F \to G$ and $\psi \colon G \to H$ transformations of type $|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|$ and $|\beta| \xrightarrow{\eta} m \xleftarrow{\theta} |\gamma|$, with generalised graphs N and N' respectively. Consider the composite transformation $\psi \circ \varphi$ whose type is given by the following pushout:*

$$\begin{tikzcd} & & {|\gamma|} \arrow[d, "\theta"] \\ & {|\beta|} \arrow[r, "\eta"] \arrow[d, "\tau"'] \arrow[dr, phantom, "\ulcorner"] & m \arrow[d, "\xi"] \\ {|\alpha|} \arrow[r, "\sigma"] & n \arrow[r, "\zeta"] & l \end{tikzcd}$$

Suppose φ and ψ are dinatural in all those variables in $\zeta^{-1}(i)$ and in $\xi^{-1}(i)$, for a fixed $i \in \{1, \dots, l\}$. If the i-th connected component of $N' \circ N$ is acyclic, then $\psi \circ \varphi$ is dinatural in its i-th variable.

§3.3 A generalised functor category

We are now ready to define a category of "too general" transformations in a precise way. Morphisms will be transformations equipped with a morphism in $\mathbb{H}$ coherent with their type and a discriminant function that tells us in which variables the transformation is dinatural. We will only consider transformations admitting the existence of a translating function; due to Propositions (3.27) and (3.28) all ordinary transformations appear in this category. Here we are not requiring that translating functions be part of the data of a morphism, as there is no need for it and by not carrying them around proofs of the following Theorems will be simpler. As we mentioned in (3.25), the generalised functor category $\{\mathbb{B},\mathbb{C}\}$ will be its subcategory generated by ordinary transformations with their graphs as defined in Chapter 1.

(3.33) Definition. Let $\mathbb{B}$ and $\mathbb{C}$ be categories. The category $\{\mathbb{B},\mathbb{C}\}^*$ consists of the following data:

- objects are pairs (α, F), for $\alpha \in \mathrm{List}\{+,-\}$ and $F \colon \mathbb{B}^\alpha \to \mathbb{C}$ a functor;
- morphisms $(\alpha, F) \to (\beta, G)$ are equivalence classes of tuples

$$\Phi = (\varphi, |\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|, |\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|, \Delta_\Phi)$$

  where:

  - $\Delta_\Phi \colon n \to \{0,1\}$ is called the *discriminant function*,
  - $\varphi \colon F \to G$ is a transformation of type $|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|$ dinatural in all variables in $\Delta_\Phi^{-1}\{1\}$,
  - $|\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|$ is a cospan in $\mathbb{PN}$ coherent with the type of φ, where for all $i \in \{1,\dots,n\}$ the i-th connected component of N is acyclic whenever $\Delta_\Phi(i) = 1$*,
  - (φ, N) admits a translating function.

  We say that $\Phi \sim \Phi'$, for $\Phi' = (\varphi', |\alpha| \xrightarrow{\sigma'} n \xleftarrow{\tau'} |\beta|, |\alpha| \xrightarrow{\overline{\sigma'}} N' \xleftarrow{\overline{\tau'}} |\beta|, \Delta_{\Phi'})$ if and only if the transformations differ only by a permutation of their variables (in a coherent way with the rest of the data) and their generalised graphs are coherently isomorphic: more precisely, when

  - there is a permutation $\pi \colon n \to n$ such that $\sigma' = \pi\sigma$, $\tau' = \pi\tau$, $\varphi'_{A_1,\dots,A_n} = \varphi_{A_{\pi 1},\dots,A_{\pi n}}$, $\Delta_\Phi = \Delta_{\Phi'}\pi$;
  - there is an isomorphism $f = (f_P, f_T) \colon N \to N'$ in $\mathbb{PN}$ such that the following diagram commutes:

$$\begin{tikzcd} {|\alpha|} \arrow[r, "\overline{\sigma}"] \arrow[dr, "\overline{\sigma'}"'] & N \arrow[d, "f"] & {|\beta|} \arrow[l, "\overline{\tau}"'] \arrow[dl, "\overline{\tau'}"] \\ & N' & \end{tikzcd}$$

*This condition is essential to ensure that composition is unitary.

mapping the i-th connected component of N to the $\pi(i)$-th connected component of N'.

- Composition of Φ as above and

$$\Psi = (\psi, |\beta| \xrightarrow{\eta} m \xleftarrow{\theta} |\gamma|, |\beta| \xrightarrow{\overline{\eta}} N' \xleftarrow{\overline{\theta}} |\gamma|, \Delta_\Psi)$$

is component-wise: it is the equivalence class of the tuple

$$\Psi \circ \Phi = (\psi \circ \varphi, |\alpha| \xrightarrow{\zeta\sigma} l \xleftarrow{\xi\theta} |\gamma|, |\alpha| \xrightarrow{\overline{\zeta\sigma}} N' \circ N \xleftarrow{\overline{\xi\theta}} |\gamma|, \Delta_{\Psi\circ\Phi}) \tag{3.34}$$

where $\psi \circ \varphi$ is the transformation of type given by the result of the pushout

$$\begin{tikzcd}
 & & |\gamma| \arrow[d, "\theta"] \\
 & |\beta| \arrow[r, "\eta"] \arrow[d, "\tau"'] \arrow[dr, phantom, "\ulcorner", very near end] & m \arrow[d, "\xi"] \\
|\alpha| \arrow[r, "\sigma"] & n \arrow[r, "\zeta"] & l
\end{tikzcd}$$

$N' \circ N$ is computed by the pushout (3.23) and the discriminant $\Delta_{\Psi\circ\Phi} \colon l \to \{0,1\}$ is obtained by setting $\Delta_{\Psi\circ\Phi}(x) = 1$ if and only if the x-th connected component of $N' \circ N$ is acyclic *and* for all $y \in \zeta^{-1}\{x\}$ and $z \in \xi^{-1}\{x\}$ we have that $\Delta_\Phi(y) = 1 = \Delta_\Psi(z)$. The latter condition is tantamount to asking that φ and ψ are dinatural in all the variables involved by the x-th connected component of the composite graph $N' \circ N$ of $\psi \circ \varphi$. □

We shall prove that $\{\mathbb{B}, \mathbb{C}\}^*$ is in fact a category, but first we need to show that composition does not depend on the choice of the representatives of the equivalence classes of Φ and Ψ.

(3.35) Lemma. *Composition as in (3.34) is well defined.*

Proof. Notice first of all that (3.34) is indeed a morphism $(\alpha, F) \to (\beta, G)$: by Proposition (3.22) we have that $N' \circ N$ is a generalised graph for $\psi \circ \varphi$; by Theorem (3.31) we have that $\psi \circ \varphi$ is dinatural in all those variables in $\Delta^{-1}_{\Psi\circ\Phi}\{1\}$.

Next, suppose we have

$$\Phi = (\varphi, |\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|, |\alpha| \xrightarrow{\overline{\sigma}} N_1 \xleftarrow{\overline{\tau}} |\beta|, \Delta_\Phi) \colon (\alpha, F) \to (\beta, G)$$

$$\Phi' = (\varphi', |\alpha| \xrightarrow{\sigma'} n \xleftarrow{\tau'} |\beta|, |\alpha| \xrightarrow{\overline{\sigma'}} N_2 \xleftarrow{\overline{\tau'}} |\beta|, \Delta_{\Phi'}) \colon (\alpha, F) \to (\beta, G)$$

$$\Psi = (\psi, |\beta| \xrightarrow{\eta} m \xleftarrow{\theta} |\gamma|, |\beta| \xrightarrow{\overline{\eta}} N' \xleftarrow{\overline{\theta}} |\gamma|, \Delta_\Psi) \colon (\beta, G) \to (\gamma, H)$$

with $\Phi \sim \Phi'$. We want to show that $\Psi \circ \Phi \sim \Psi \circ \Phi'$; the same argument would also show that for $\Psi' \sim \Psi$ we have $\Psi \circ \Phi \sim \Psi' \circ \Phi'$.

It is well known that composition of cospans via pushouts is well defined for $\sim$, hence we only have to prove that there exists a permutation $\tilde{\pi}\colon l \longrightarrow l$ (if l is the number of variables of $\psi \circ \varphi$) such that $\Delta_{\Psi\circ\Phi} = \Delta_{\Psi\circ\Phi'}\tilde{\pi}$ and that there is an isomorphism $\tilde{f} = (\tilde{f}_P, \tilde{f}_T)\colon N' \circ N_1 \longrightarrow N' \circ N_2$ mapping the i-th connected component of $N' \circ N_1$ to the $\tilde{\pi}(i)$-th connected component of $N' \circ N_2$.

By the assumption that $\Phi \sim \Phi'$, we know that there is a permutation $\pi\colon n \longrightarrow n$ such that $\sigma' = \pi\sigma$, $\tau' = \pi\tau$, $\Delta_\Phi = \Delta_{\Phi'}\pi$ and there is an isomorphism in $\mathbb{PN}$ $f\colon N_1 \longrightarrow N_2$ mapping the x-th c.c. of N_1 to the $\pi(x)$-th c.c. of N_2 and such that $\overline{\sigma'} = f_P\overline{\sigma}$, $\overline{\tau'} = f_P\overline{\tau}$. Suppose then that the types and generalised graphs of $\psi \circ \varphi$ and $\psi \circ \varphi'$ are computed as follows.

$$
\psi \circ \varphi : \quad
\begin{tikzcd}
& & {|\gamma|} \arrow[d, "\theta"] \\
& {|\beta|} \arrow[r, "\eta"] \arrow[d, "\tau"'] \arrow[dr, phantom, "\ulcorner", very near end] & m \arrow[d, "\xi"] \\
{|\alpha|} \arrow[r, "\sigma"] & n \arrow[r, "\zeta"] & l
\end{tikzcd}
\qquad
\begin{tikzcd}
& & {|\gamma|} \arrow[d, "\overline{\theta}"] \\
& {|\beta|} \arrow[r, "\overline{\eta}"] \arrow[d, "\overline{\tau}"'] \arrow[dr, phantom, "\ulcorner", very near end] & N' \arrow[d, "\overline{\xi}"] \\
{|\alpha|} \arrow[r, "\overline{\sigma}"] & N_1 \arrow[r, "\overline{\zeta}"] & N' \circ N_1
\end{tikzcd}
$$

$$
\psi \circ \varphi' : \quad
\begin{tikzcd}
& & {|\gamma|} \arrow[d, "\theta"] \\
& {|\beta|} \arrow[r, "\eta"] \arrow[d, "\tau'"'] \arrow[dr, phantom, "\ulcorner", very near end] & m \arrow[d, "\xi'"] \\
{|\alpha|} \arrow[r, "\sigma'"] & n \arrow[r, "\zeta'"] & l'
\end{tikzcd}
\qquad
\begin{tikzcd}
& & {|\gamma|} \arrow[d, "\overline{\theta}"] \\
& {|\beta|} \arrow[r, "\overline{\eta}"] \arrow[d, "\overline{\tau'}"'] \arrow[dr, phantom, "\ulcorner", very near end] & N' \arrow[d, "\overline{\xi'}"] \\
{|\alpha|} \arrow[r, "\overline{\sigma'}"] & N_2 \arrow[r, "\overline{\zeta'}"] & N' \circ N_2
\end{tikzcd}
$$

(In fact $l = l'$, but here we keep two different names to easily distinguish them.) The desired isomorphisms $\tilde{f}$ and $\tilde{\pi}$ are given by the universal property of the pushouts, as the unique maps making everything commute:

$$
\begin{tikzcd}
{|\beta|} \arrow[r, "\eta"] \arrow[d, "\tau"] \arrow[dd, bend right, "\tau'"'] & m \arrow[d, "\xi"] \arrow[ddr, bend left, "\xi'"] & \\
n \arrow[r, "\zeta"] \arrow[d, "\pi"] & l \arrow[dr, dashed, "\tilde{\pi}"] & \\
n \arrow[rr, "\zeta'"] & & l'
\end{tikzcd}
\qquad
\begin{tikzcd}
{|\beta|} \arrow[r, "\overline{\eta}"] \arrow[d, "\overline{\tau}"] \arrow[dd, bend right, "\overline{\tau'}"'] & N' \arrow[d, "\overline{\xi}"] \arrow[ddr, bend left, "\overline{\xi'}"] & \\
N_1 \arrow[r, "\overline{\zeta}"] \arrow[d, "f"] & N' \circ N_1 \arrow[dr, dashed, "\tilde{f}"] & \\
N_2 \arrow[rr, "\overline{\zeta'}"] & & N' \circ N_2
\end{tikzcd}
$$

We argue that $\tilde{f}$ maps the i-th c.c. of $N' \circ N_1$ to the $\tilde{\pi}(i)$-th c.c. of $N' \circ N_2$. By assumption, we know that f maps the x-th c.c. of N_1 to the $\pi(x)$-th c.c. of N_2. Consider

then $i \in l$.
Case $\zeta^{-1}\{i\} = \emptyset$. Since ζ and ξ are jointly epi, then there must be a $y \in m$ such that $\xi(y) = i$, in which case $\xi'(y) = \tilde{\pi}(i)$. This means that the y-th c.c. of N' is "contained" (from the graphical point of view, it makes part of) in the $\tilde{\pi}(i)$-th c.c. of $N' \circ N_2$: since $\tilde{f}$ preserves undirected paths (because it preserves all inputs and outputs of every transition), the entire i-th c.c. of $N' \circ N_1$ must be mapped by $\tilde{f}$ to the $\tilde{\pi}(i)$-th c.c. of $N' \circ N_2$.
Case $\zeta^{-1}\{i\} \neq \emptyset$. Let $x \in \zeta^{-1}\{i\}$. The x-th c.c. of N_1 is mapped along f to the $\pi(x)$-th c.c. of N_2, which is contained in the $\tilde{\pi}(i)$-th c.c. of $N' \circ N_2$. Since it contains the x-th c.c. of N_1, the whole i-th c.c. of $N' \circ N_1$ is mapped to the $\tilde{\pi}(i)$-th c.c. of $N' \circ N_2$.

Finally, we prove that $\Delta_{\Psi\circ\Phi} = \Delta_{\Psi\circ\Phi'} \circ \tilde{\pi}$. By definition, for $i \in l$, we have that $\Delta_{\Psi\circ\Phi}(i) = 1$ precisely when the i-th c.c. of $N' \circ N_1$ is acyclic and when for all $a \in \zeta^{-1}\{i\}$ and for all $b \in \xi^{-1}\{i\}$ we have $\Delta_\Phi(a) = 1 = \Delta_\Psi(b)$. On the other hand, we have that $\Delta_{\Psi\circ\Phi'}(\tilde{\pi}(i)) = 1$ when:

- the $\tilde{\pi}(i)$-th c.c. of $N' \circ N_2$ is acyclic,
- for all $x \in \zeta'^{-1}\{\tilde{\pi}(i)\}$ we have $\Delta'_\Phi(x) = 1$,
- for all $y \in \xi^{-1}\{\tilde{\pi}(i)\}$ we have $\Delta_\Psi(y) = 1$.

We proved that $\tilde{f}$ maps the i-th c.c. of $N' \circ N_1$ to the $\tilde{\pi}(i)$-th c.c. of $N' \circ N_2$: since $\tilde{f}$ is an isomorphism, it preserves and reflect cycles, hence the first condition is satisfied. Now, we have the following chain of equivalences:

$$\begin{aligned} x \in \zeta'^{-1}\{\tilde{\pi}(i)\} \iff \zeta'(x) = \tilde{\pi}(i) &\iff \tilde{\pi}^{-1}\big(\zeta'(x)\big) = i \iff \zeta\big(\pi^{-1}(x)\big) = i \\ &\iff \pi^{-1}(x) \in \zeta^{-1}\{i\} \end{aligned}$$

and we know that for $a \in \zeta^{-1}\{i\}$, $1 = \Delta_\Phi(a) = \Delta_{\Phi'}(\pi(a))$, because $\Phi \sim \Phi'$. Let $x \in \zeta'^{1}\{\tilde{\pi}(i)\}$: then $a = \pi^{-1}(x) \in \zeta^{-1}\{i\}$, hence $\Delta_{\Phi'}(\pi(a)) = \Delta_{\Phi'}(x) = 1$, as we wanted. A similar argument also shows the third condition, and the proof is complete. **Qed**

(3.36) Theorem. $\{\mathbb{B},\mathbb{C}\}^*$ *is indeed a category.*

Proof. For (α, F) object of $\{\mathbb{B},\mathbb{C}\}^*$, the identity morphism is given by the equivalence class of

$$(id_F, |\alpha| \xrightarrow{id} |\alpha| \xleftarrow{id} |\alpha|, |\alpha| \xrightarrow{id} |\alpha| \xleftarrow{id} |\alpha|, K_1)$$

where the discriminant function K_1 is the constant function equal to 1, as the identity transformation is indeed (di)natural in all its variables. (Notice that $id_{|\alpha|}$ is an epimorphism, hence as discussed in Example (3.20) we have that $|\alpha|$ is a generalised graph for id_F.)
Unitarity. Consider

$$\Phi = (\varphi, |\alpha| \xrightarrow{\sigma_1} n \xleftarrow{\tau_1} |\beta|, |\alpha| \xrightarrow{\overline{\sigma_1}} N_1 \xleftarrow{\overline{\tau_1}} |\beta|, \Delta_\Phi) \colon (\alpha, F) \to (\beta, G).$$

We prove that $\Phi \circ id_{(\alpha,F)} = \Phi$ and $id_{(\beta,G)} \circ \Phi = \Phi$ (by "Φ" here we mean its equivalence class). It is clear that $\Phi \circ id_{(\alpha,F)}$ consists of φ together with its type and generalised graph as specified in Φ. Also, $\Delta_{\Phi\circ id_{(\alpha,F)}}(x) = 1$ precisely when the x-th connected component of N is acyclic and $\Delta_\Phi(x) = 1$, by definition. Given that $\Delta_\Phi(x) = 1$ implies that the x-th c.c. of N is acyclic, we have that $\Delta_{\Phi\circ id_{(\alpha,F)}} = \Delta_\Phi$. One can prove in a similar way the other identity law.

ASSOCIATIVITY. Consider $\Phi_1 = \Phi$ as above and also

$$\Phi_2 = (\varphi_2, |\beta| \xrightarrow{\sigma_2} m \xleftarrow{\tau_2} |\gamma|, |\beta| \xrightarrow{\overline{\sigma_2}} N_2 \xleftarrow{\overline{\tau_2}} |\gamma|, \Delta_{\Phi_2})\colon (\beta, G) \to (\gamma, H),$$

$$\Phi_3 = (\varphi_3, |\gamma| \xrightarrow{\sigma_3} p \xleftarrow{\tau_3} |\delta|, |\gamma| \xrightarrow{\overline{\sigma_3}} N_3 \xleftarrow{\overline{\tau_3}} |\delta|, \Delta_{\Phi_3})\colon (\gamma, H) \to (\delta, K).$$

We know that composition of cospans via pushout is associative, as well as composition of transformations; suppose therefore that $\varphi_3 \circ \varphi_2 \circ \varphi_1$ has type given by:

$$\begin{tikzcd}
 & & & {|\delta|} \arrow[d, "\tau_3"] \\
 & & {|\gamma|} \arrow[r, "\sigma_3"] \arrow[d, "\tau_2"'] \arrow[dr, phantom, "\ulcorner"] & p \arrow[d, "\xi_2"] \\
 & {|\beta|} \arrow[r, "\sigma_2"] \arrow[d, "\tau_1"'] \arrow[dr, phantom, "\ulcorner"] & m \arrow[r, "\zeta_2"] \arrow[d, "\xi_1"'] \arrow[dr, phantom, "\ulcorner"] & q \arrow[d, "\xi_3"] \\
{|\alpha|} \arrow[r, "\sigma_1"] & n \arrow[r, "\zeta_1"] & l \arrow[r, "\zeta_3"] & r
\end{tikzcd}$$

and the generalised graph $N_3 \circ N_2 \circ N_1$ is obtained as the result of the following pushout-pasting:

$$\begin{tikzcd}
 & & & {|\delta|} \arrow[d, "\overline{\tau_3}"] \\
 & & {|\gamma|} \arrow[r, "\overline{\sigma_3}"] \arrow[d, "\overline{\tau_2}"'] \arrow[dr, phantom, "\ulcorner"] & N_3 \arrow[d, "\overline{\xi_2}"] \\
 & {|\beta|} \arrow[r, "\overline{\sigma_2}"] \arrow[d, "\overline{\tau_1}"'] \arrow[dr, phantom, "\ulcorner"] & N_2 \arrow[r, "\overline{\zeta_2}"] \arrow[d, "\overline{\xi_1}"'] \arrow[dr, phantom, "\ulcorner"] & N_3 \circ N_2 \arrow[d, "\overline{\xi_3}"] \\
{|\alpha|} \arrow[r, "\overline{\sigma_1}"] & N_1 \arrow[r, "\overline{\zeta_1}"] & N_2 \circ N_1 \arrow[r, "\overline{\zeta_3}"] & N_3 \circ N_2 \circ N_1
\end{tikzcd}$$

We prove that $\Delta_{\Phi_3\circ(\Phi_2\circ\Phi_1)} = \Delta_{(\Phi_3\circ\Phi_2)\circ\Phi_1}$. We have that $\Delta_{\Phi_3\circ(\Phi_2\circ\Phi_1)}(x) = 1$ if and only if, by definition:

(1) the x-th c.c. of $N_3 \circ N_2 \circ N_1$ is acyclic;

(2) $\forall y \in \zeta_3^{-1}\{x\}.\, \Delta_{\Phi_2 \circ \Phi_1}(y) = 1$;

(3) $\forall z \in (\xi_3 \circ \xi_2)^{-1}\{x\}.\, \Delta_{\Phi_3}(z) = 1$;

which is equivalent to say that:

(1) the x-th c.c. of $N_3 \circ N_2 \circ N_1$ is acyclic;

(2a) $\forall y \in l.\, \Big[\zeta_3(y) = x \Rightarrow y\text{-th c.c. of } N_2 \circ N_1 \text{ is acyclic}\Big]$;

(2b) $\forall y \in l.\, \Big[\zeta_3(y) = x \Rightarrow \forall a \in n.\, \Big(\zeta_1(a) = y \Rightarrow \Delta_{\Phi_1}(a) = 1\Big)\Big]$;

(2c) $\forall y \in l.\, \Big[\zeta_3(y) = x \Rightarrow \forall b \in m.\, \Big(\xi_1(b) = y \Rightarrow \Delta_{\Phi_2}(b) = 1\Big)\Big]$;

(3) $\forall z \in p.\, \Big[\xi_3\big(\xi_2(z)\big) = x \Rightarrow \Delta_{\Phi_3}(z) = 1\Big]$.

Call A the conjunction of the conditions above. Next, we have that $\Delta_{(\Phi_3 \circ \Phi_2) \circ \Phi_1}(x) = 1$ if and only if:

(i) the x-th c.c. of $N_3 \circ N_2 \circ N_1$ is acyclic;

(ii) $\forall a \in n.\, \Big[\zeta_3\big(\zeta_1(a)\big) = x \Rightarrow \Delta_{\Phi_1}(a) = 1\Big]$;

(iiia) $\forall w \in q.\, \Big[\xi_3(w) = x \Rightarrow\ w\text{-th c.c. of } N_3 \circ N_2 \text{ is acyclic}\ \Big]$;

(iiib) $\forall w \in q.\, \Big[\xi_3(w) = x \Rightarrow \forall b \in m.\, \Big(\zeta_2(b) = w \Rightarrow \Delta_{\Phi_2}(b) = 1\Big)\Big]$;

(iiic) $\forall w \in q.\, \Big[\xi_3(w) = x \Rightarrow \forall z \in p.\, \Big(\xi_2(z) = w \Rightarrow \Delta_{\Phi_3}(z) = 1\Big)\Big]$

Call B the conjunction of these last five conditions. We prove that A implies B; in a similar way one can prove the converse as well.

(ii) Let $a \in n$, suppose $\zeta_3\big(\zeta_1(a)\big) = x$. By (2b), with $y = \zeta_1(a)$, we have $\Delta_{\Phi_1}(a) = 1$.

(iiia) Let $w \in q$, suppose $\xi_3(w) = x$. Then the w-th c.c. of $N_3 \circ N_2$ must be acyclic as it is part of the x-th c.c. of $N_3 \circ N_2 \circ N_1$, which is acyclic.

(iiib) Let $w \in q$, suppose $\xi_3(w) = x$. Let also $b \in m$ and suppose $\zeta_2(b) = w$. Then $x = \xi_3\big(\zeta_2(b)\big) = \zeta_3\big(\xi_1(b)\big)$. By (2c), with $y = \xi_1(b)$, we have $\Delta_{\Phi_2}(b) = 1$.

(iiic) Let $w \in q$, suppose $\xi_3(w) = x$. Let $z \in p$ be such that $\xi_2(z) = w$. Then $\xi_3\big(\xi_2(z)\big) = x$: by (3), we have $\Delta_{\Phi_3}(z) = 1$. **Qed**

As anticipated in Remark (3.25), there is a natural way to interpret ordinary transformations as morphisms in $\{\mathbb{B}, \mathbb{C}\}^*$.

(3.37) Definition. Let $F\colon \mathbb{B}^\alpha \to \mathbb{C}$, $G\colon \mathbb{B}^\beta \to \mathbb{C}$ be functors and $\varphi\colon F \to G$ be a transformation of type $|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|$. φ can be seen as a morphism $(\alpha, F) \to (\beta, G)$ in $\{\mathbb{B},\mathbb{C}\}^*$ in a natural way by considering the (equivalence class of)

$$\Phi = (\varphi, |\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|, |\alpha| \xrightarrow{\iota_{|\alpha|}} \Gamma(\varphi) \xleftarrow{\iota_{|\beta|}} |\beta|, \Delta_\Phi)$$

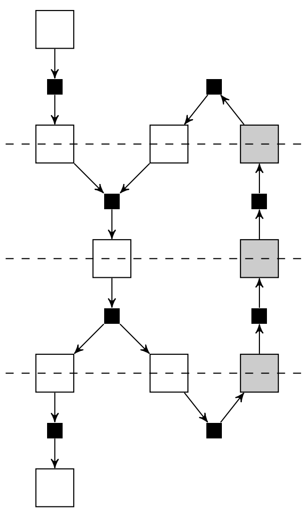
where we define $\Delta_\Phi(i) = 1$ if and only if φ is dinatural in its i-th variable. (Notice that, by construction, $\Gamma(\varphi)$ is acyclic.) We call (the equivalence class of) Φ *the standard representation of φ in $\{\mathbb{B},\mathbb{C}\}^*$*. □

Still in line with what we said in Remark (3.25), we would use the standard representation only for "atomic" transformations, that is transformations that we cannot (or do not want to) explicitly recognise as composite of smaller blocks.

Things start getting interesting upon composition. If we also have a $\psi\colon G \to H$, seen as a morphism Ψ in an analogous way, then $\Psi \circ \Phi$ consists of $\psi \circ \varphi$ with its type, equipped with $\Gamma^*(\psi \circ \varphi)$ as a generalised graph and μ as translating function, see (3.30). The discriminant $\Delta_{\Psi\circ\Phi}$ ends up mapping i to 1 precisely when $\psi \circ \varphi$ is dinatural in its i-th variable "for a good reason", i.e. because Theorem (1.59) applies.

(3.38) Example. Consider transformations $\varphi^1, \dots, \varphi^5$ as in Example (3.8). By composing their standard representations in $\{\mathbb{B},\mathbb{C}\}^*$, the generalised graph of the composite would be (3.13). Its acyclicity ensures the dinaturality of the composite. □

The condition "the i-th connected component of N is acyclic whenever $\Delta_\Phi(i) = 1$" in Definition (3.33) is designed to ignore dinaturality properties that happen to be satisfied "by accident", as it were, which could cause problems upon composition. Indeed, suppose that we have a transformation φ which is the composite of four transformations $\varphi_1, \dots, \varphi_4$, whose resulting generalised graph, obtained by pasting together $\Gamma(\varphi_1), \dots, \Gamma(\varphi_4)$, is as follows:

$N =$ 

Call Φ the tuple in $\{\mathbb{B},\mathbb{C}\}^*$ consisting of φ with its type $1 \longrightarrow 1 \longleftarrow 1$ and N as a generalised graph, as a composite of the standard representations of $\varphi_1,\dots,\varphi_4$. Suppose that φ happens to be dinatural in its only variable for some reason (extreme example: the category $\mathbb{C}$ is the terminal category). If in the definition of $\{\mathbb{B},\mathbb{C}\}^*$ the only condition on Δ were "φ is dinatural in every variable in $\Delta_\Phi^{-1}\{1\}$", without requiring that the i-th c.c. of N be acyclic if $\Delta_\Phi(i) = 1$, then equipping φ in Φ with a discriminant function Δ_Φ defined as

$$\begin{aligned} 1 &\xrightarrow{\Delta_\Phi} 1 \\ 1 &\longmapsto 1 \end{aligned}$$

would be legitimate. Compose now Φ with the identity morphism of $\{\mathbb{B},\mathbb{C}\}^*$: by definition we would obtain again Φ except for the discriminant function, which would be defined as $\Delta_{\Phi\circ id}(1) = 0$ because the composite graph, which is N, is not acyclic. Composition would not be unitary! The condition "the i-th connected component of N is acyclic whenever $\Delta_\Phi(i) = 1$" in Definition (3.33) is therefore not only sufficient, as we saw in the proof of unitarity of composition in $\{\mathbb{B},\mathbb{C}\}^*$, but also necessary.

The proper generalised functor category. Now we can "trim-down" the morphisms of $\{\mathbb{B},\mathbb{C}\}^*$ by only considering those which are either standard representations, or composites of them. In this way, we get a subcategory that consists *precisely* of transformations whose generalised graphs are either "simple" (they do not contain internal places) or a composite of simple graphs, in which case the transformation itself is a composite of simpler ones. The graph of a transformation φ in $\{\mathbb{B},\mathbb{C}\}$ contains only meaningful information: each place and transition really corresponds to an argument of a functor or a variable of a transformation used to build up φ, and the firing of an enabled transition really corresponds to applying a dinaturality condition. Such a φ, therefore, does admit a translating function that really works like μ in Definition (3.30).

(3.39) Definition. Let $\mathbb{B}$ and $\mathbb{C}$ be categories. The *generalised functor category* $\{\mathbb{B},\mathbb{C}\}$ is the wide subcategory of $\{\mathbb{B},\mathbb{C}\}^*$ (that is, it contains all the objects of $\{\mathbb{B},\mathbb{C}\}^*$) generated by the standard representations of transformations. Hence, a morphism in $\{\mathbb{B},\mathbb{C}\}$ is a morphism of $\{\mathbb{B},\mathbb{C}\}^*$ that is either:

- an identity $(id_F, |\alpha| \xrightarrow{id} |\alpha| \xleftarrow{id} |\alpha|, |\alpha| \xrightarrow{id} |\alpha| \xleftarrow{id} |\alpha|, K_1)$,
- a standard representation of a transformation φ of type $|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|$:

  $$\Phi = (\varphi, |\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|, |\alpha| \xrightarrow{\iota_{|\alpha|}} \Gamma(\varphi) \xleftarrow{\iota_{|\beta|}} |\beta|, \Delta_\Phi)$$

  with $\Delta_\Phi(i) = 1$ if and only if φ is dinatural in its i-th variable; we call these morphisms of $\{\mathbb{B},\mathbb{C}\}$ *atomic*,
- a finite composite of standard representations of transformations. □

(3.40) Remark. Although it is impossible, in general, to judge whether a transformation is or is not a composite of others by looking at its type, one can distinguish atomic morphisms of $\{\mathbb{B}, \mathbb{C}\}$ from composite morphisms by looking at the generalised graph N they come together with. Indeed, if a non-identity morphism of $\{\mathbb{B}, \mathbb{C}\}^*$

$$\Phi = (\varphi, |\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|, |\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|, \Delta_\Phi)$$

is actually a morphism in $\{\mathbb{B}, \mathbb{C}\}$ too, then Φ is atomic if and only if $N = \Gamma(\varphi)$. In case $N \neq \Gamma(\varphi)$, then N contains internal places as a result of composing together "atomic" graphs of transformations: that is, we have that $\varphi = \varphi_k \circ \cdots \circ \varphi_1$ for some transformations φ_i, and $N = \Gamma(\varphi_k) \circ \cdots \circ \Gamma(\varphi_1)$. This decomposition of φ and N is not necessarily unique.

The category of graphs. We can now finally individuate the category $\mathbb{G}$ of graphs of transformations. To do so, much like we did to find the proper functor category $\{\mathbb{B}, \mathbb{C}\}$, we will first build a "large" category of graphs $\mathbb{G}^*$, which will consist of those morphisms in $\mathbb{H}$ that are the generalised graph of a transformation in $\{\mathbb{B}, \mathbb{C}\}^*$, together with a discriminant function, and later define the "proper" $\mathbb{G}$ as a subcategory of it.

We begin by defining the notion of *skeleton* of a morphism in $\mathbb{H}$, as it will be useful later on.

(3.41) Definition. Let $f = |\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|$ be a morphism in $\mathbb{H}$, and let n be the number of connected components of N. The *skeleton* of the cospan f is an (equivalence class of) cospan(s) in $\mathbb{F}\mathrm{in}\mathbb{S}\mathrm{et}$

$$|\alpha| \xrightarrow{\quad\sigma\quad} n \xleftarrow{\quad\tau\quad} |\beta|$$

where $\sigma(i)$ is the number of the connected component of N to which $\overline{\sigma}(i)$ belongs to, and similarly is defined τ. ◻

(3.42) Remark. If φ is a transformation and N is a generalised graph of φ, then the type of φ is the skeleton of N.

The category $\mathbb{G}^*$ will then consist of only part of the data of $\{\mathbb{B}, \mathbb{C}\}^*$, obtained, as it were, by discarding functors and transformations, and only considering the graphs and the discriminant functions.

(3.43) Definition. The category $\mathbb{G}^*$ of graphs consists of the following data.

- Objects are lists in $\mathrm{List}\{+, -\}$.
- Morphisms $\alpha \longrightarrow \beta$ are equivalence classes of pairs

$$\left(\ |\alpha| \xrightarrow{\quad\overline{\sigma}\quad} N \xleftarrow{\quad\overline{\tau}\quad} |\beta|\ , \Delta_N\right)$$

where:

– $(\overline{\sigma}, \overline{\tau}, N)$ is a morphism in $\mathbb{H}$,

– *sources*$(N) = \{\overline{\sigma}(i) \mid \alpha_i = +\} \cup \{\overline{\tau}(i) \mid \beta_i = -\}$,

– *sinks*$(N) = \{\overline{\sigma}(i) \mid \alpha_i = -\} \cup \{\overline{\tau}(i) \mid \beta_i = +\}$,

– let n be the number of connected components of N: then $\Delta_N : n \longrightarrow \{0, 1\}$ is called *discriminant function* and it is such that $\Delta(i) = 1$ implies that the i-th connected component of N is acyclic.

A pair above is equivalent to another $((\overline{\sigma}', \overline{\tau}', N'), \Delta_{N'})$, where N' also has n connected components, if and only if there exists $f : N \longrightarrow N'$ an isomorphism in $\mathbb{PN}$ and $\pi : n \longrightarrow n$ a permutation such that

$$\begin{tikzcd} {|\alpha|} \arrow[r, "\overline{\sigma}"] \arrow[dr, "\overline{\sigma'}"'] & N \arrow[d, "f"] & {|\beta|} \arrow[l, "\overline{\tau}"'] \arrow[dl, "\overline{\tau'}"] \\ & N' & \end{tikzcd} \quad \text{and} \quad \begin{tikzcd} n \arrow[r, "\Delta_N"] \arrow[d, "\pi"'] & \{0,1\} \\ n \arrow[ur, "\Delta'_N"'] & \end{tikzcd}$$

commute and f maps the i-th c.c. of N to the $\pi(i)$-th c.c. of N'.

- Composition is defined exactly as in $\{\mathbb{B}, \mathbb{C}\}^*$. To wit, composition of

$$\left(|\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta| \ , \Delta_N \right) \quad \text{and} \quad \left(|\beta| \xrightarrow{\overline{\eta}} N \xleftarrow{\overline{\theta}} |\gamma| \ , \Delta_{N'} \right)$$

is the equivalence class of the pair

$$\left(|\alpha| \xrightarrow{\overline{\zeta\sigma}} N' \circ N \xleftarrow{\overline{\xi\theta}} |\gamma| \ , \Delta_{g \circ f} \right)$$

where $N' \circ N$ is the Petri Net given by the result of the pushout

$$\begin{tikzcd} & & {|\gamma|} \arrow[d, "\overline{\theta}"] \\ & {|\beta|} \arrow[r, "\overline{\eta}"] \arrow[d, "\overline{\tau}"'] \arrow[dr, phantom, "\ulcorner"] & N' \arrow[d, "\overline{\xi}"] \\ {|\alpha|} \arrow[r, "\overline{\sigma}"] & N \arrow[r, "\overline{\zeta}"] & N' \circ N \end{tikzcd}$$

and $\Delta_{N' \circ N}$ is defined as follows. If $|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|$ and $|\beta| \xrightarrow{\eta} m \xleftarrow{\theta} |\gamma|$ are the skeletons of $(\overline{\sigma}, \overline{\tau}, N)$ and $(\overline{\eta}, \overline{\theta}, N')$ respectively, then the skeleton of $(\overline{\zeta\sigma}, \overline{\xi\theta}, N' \circ N)$

is given by the pushout

$$\begin{tikzcd} & & {|\gamma|} \arrow[d, "\theta"] \\ & {|\beta|} \arrow[r, "\eta"] \arrow[d, "\tau"'] \arrow[dr, phantom, "\ulcorner"] & m \arrow[d, "\xi"] \\ {|\alpha|} \arrow[r, "\sigma"] & n \arrow[r, "\zeta"] & l \end{tikzcd}$$

(cf. Proposition (3.22)). Define therefore $\Delta_{N' \circ N}(x) = 1$ if and only if the x-th connected component of $N' \circ N$ is acyclic *and* for all $y \in \zeta^{-1}\{x\}$ and $z \in \xi^{-1}\{x\}$ we have that $\Delta_N(y) = 1 = \Delta_{N'}(z)$. □

(3.44) Definition. The category $\mathbb{G}$ of graphs is the wide subcategory of $\mathbb{G}^*$ generated by equivalence classes of pairs

$$\left(\ |\alpha| \xrightarrow{\ \overline{\sigma}\ } N \xleftarrow{\ \overline{\tau}\ } |\beta| \ , \Delta_N \right)$$

where $P_N = |\alpha| + |\beta|$, $\overline{\sigma} = \iota_{|\alpha|}$, $\overline{\tau} = \iota_{|\beta|}$ and for all p place, $|\bullet p| + |p \bullet| = 1$ (equivalently, N has no internal places and every place is either a proper source or a proper sink). Hence, the general morphism of $\mathbb{G}$ is either:

- an identity $\left(|\alpha| \xrightarrow{id} |\alpha| \xleftarrow{id} |\alpha|, K_1\right)$,
- a generator satisfying the conditions above; such morphisms are called *atomic*,
- a finite composite of atomic morphisms. □

The assignment $(\alpha, F) \mapsto \alpha$ and

$$\left[(\varphi, |\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|, |\alpha| \xrightarrow{\iota_{|\alpha|}} \Gamma(\varphi) \xleftarrow{\iota_{|\beta|}} |\beta|, \Delta_\Phi)\right] \mapsto \left[\left(|\alpha| \xrightarrow{\iota_{|\alpha|}} \Gamma(\varphi) \xleftarrow{\iota_{|\beta|}} |\beta|, \Delta_\Phi\right)\right]$$

mapping atomic morphisms of $\{\mathbb{B}, \mathbb{C}\}$ to atomic morphisms of $\mathbb{G}$ uniquely extends to a functor $\overline{\Gamma}\colon \{\mathbb{B}, \mathbb{C}\} \to \mathbb{G}$. Moreover, $\overline{\Gamma}$ has two special properties, by virtue of the "modularity" of our $\{\mathbb{B}, \mathbb{C}\}$ and $\mathbb{G}$ and the fact that all and only atoms in $\{\mathbb{B}, \mathbb{C}\}$ have atomic images: it reflects compositions and identities. By "reflects identities" we mean that if $\Phi\colon (\alpha, F) \to (\alpha, F)$ is such that $\overline{\Gamma}(\Phi) = id_{|\alpha|}$, then $\Phi = id_{(\alpha, F)}$. By "reflects compositions" we mean that if Φ is a morphism in $\{\mathbb{B}, \mathbb{C}\}$ and $\overline{\Gamma}(\Phi)$ is not atomic, i.e. $\overline{\Gamma}(\Phi) = (N_k, \Delta_k) \circ \cdots \circ (N_1, \Delta_1)$ with (N_i, Δ_i) atomic in $\mathbb{G}$, then there must exist $\Phi_1, \ldots, \Phi_k$ morphisms in $\{\mathbb{B}, \mathbb{C}\}$ such that:

- $\Phi = \Phi_k \circ \cdots \circ \Phi_1$,
- $\overline{\Gamma}(\Phi_i) = (N_i, \Delta_i)$.

Hence, say $\Phi = (\varphi, |\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|, |\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|, \Delta_\Phi)$: then there must exist transformations φ_i with graph $\Gamma(\varphi_i)$ (hence atomic), dinatural according to Δ_i, such that $\varphi = \varphi_k \circ \cdots \circ \varphi_1$, cf. (3.40). In other words, $\overline{\Gamma}$ satisfies the following definition.

(3.45) Definition. Let $\mathbb{D}, \mathbb{E}$ be any categories. A functor $P \colon \mathbb{D} \to \mathbb{E}$ is said to be a *weak Conduché fibration* (WCF) if, given $f \colon A \to B$ in $\mathbb{D}$:

- $P(f) = id$ implies $f = id$;
- given a decomposition $P(f) = u \circ v$ in $\mathbb{E}$, we have that there exist g, h in $\mathbb{D}$ such that $f = g \circ h$, $P(g) = u$, $P(h) = v$.

We define $\overline{\mathbb{C}\mathrm{at}/_{\mathbb{E}}}$ to be the full subcategory of $\mathbb{C}\mathrm{at}/_{\mathbb{E}}$ whose objects are the categories over $\mathbb{E}$ whose augmentation is a weak Conduché fibration. □

We have then proved the following theorem.

(3.46) Theorem. $\{\mathbb{B}, \mathbb{C}\}$ *is an object of* $\overline{\mathbb{C}\mathrm{at}/_{\mathbb{G}}}$.

Conduché fibrations were individuated in [Con72] as a re-discovery after the original work of Giraud [Gir64] on exponentiable functors in slice categories. They have to satisfy an additional property than our weak version, namely that the decomposition $f = g \circ h$ is unique up to equivalence, where we say that two factorisations $g \circ h$ and $g' \circ h'$ are equivalent if there exists a morphism $j \colon codom(h) \to dom(g')$ such that everything in sight commutes in the following diagram:

$$\begin{tikzcd}
& codom(h) \arrow[r, "g"] \arrow[d, "j"] & B \\
A \arrow[ur, "h"] \arrow[r, "h'"'] & dom(g') \arrow[ur, "g'"'] &
\end{tikzcd}$$

We will not, in fact, need such uniqueness; moreover, it is not evident whether our $\overline{\Gamma}$ is a Conduché fibration or not.

(3.47) Remark. The fact that $\{\mathbb{B}, \mathbb{C}\}$ is not just an object of $\mathbb{C}\mathrm{at}/_{\mathbb{G}}$, but even of $\overline{\mathbb{C}\mathrm{at}/_{\mathbb{G}}}$, will allow us to build the substitution category $\mathbb{A} \circ \mathbb{B}$ just for categories $\mathbb{A}$ over $\mathbb{G}$ whose augmentation is more than a mere functor: it is a weak Conduché fibration. Indeed, ultimately we will be interested in a functor $\mu \colon \{\mathbb{B}, \mathbb{C}\} \circ \{\mathbb{A}, \mathbb{B}\} \to \{\mathbb{A}, \mathbb{C}\}$, like Kelly, that will embody the substitution calculus: this means that as long as the domain of $\circ$ contains $\{\mathbb{B}, \mathbb{C}\}$, we will be content. The main advantage of restricting our attention to $\overline{\mathbb{C}\mathrm{at}/_{\mathbb{G}}}$ is that a category $\mathbb{A}$ in it inherits, in a sense, the modular structure of $\mathbb{G}$, as we shall see in the next Lemma.

(3.48) Definition. Let $P \colon \mathbb{D} \to \mathbb{G}$ be an object of $\overline{\mathbb{C}\mathrm{at}/_{\mathbb{G}}}$. A morphism d in $\mathbb{D}$ is said to be *atomic* if $P(d)$ is atomic. □

(3.49) Lemma. *Suppose that, in the following diagram, P is a weak Conduché fibrations and Q is an ordinary functor.*

$$\begin{tikzcd} \mathbb{D} \arrow[r, "Q"] \arrow[dr, "P"'] & \mathbb{F} \\ & \mathbb{G} \end{tikzcd}$$

Then Q is completely determined on morphisms by the image of atomic morphisms of $\mathbb{D}$.

Proof. Let $d\colon D \to D'$ be a morphism in $\mathbb{D}$ with $P(D) = \alpha$, $P(D') = \beta$ and $P(d) = \big[\big(|\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|, \Delta_d\big)\big]$. If $P(d)$ is not atomic, then either $P(d) = id$, in which case $d = id$ (because P is a weak Conduché fibration), or $P(d) = (N_k, \Delta_k) \circ \cdots \circ (N_1, \Delta_1)$ for some (not necessarily unique) atomic (N_i, Δ_i). Hence there must exist $d_1, \ldots, d_k$ in $\mathbb{D}$ such that $d = d_k \circ \cdots \circ d_1$ and $P(d_i) = (N_i, \Delta_i)$. Then $Q(d)$ will necessarily be defined as id in the first case, or as $Q(d_k) \circ \cdots \circ Q(d_1)$ in the second case, otherwise Q would not be a functor. **Qed**

§3.4 The category of formal substitutions

Come to this point, Kelly considers the functor $\{\mathbb{B}, -\}$ and claims that it is "evidently continuous", which leads to Theorem (3.4). Although far from being *evident*, it is true that the proof of its continuity is a classic exercise of Category Theory. Here we report a detailed proof for our case.

First, we give an explicit definition of the functor $\{\mathbb{B}, -\}\colon \mathbb{C}\mathrm{at} \to \overline{\mathbb{C}\mathrm{at}/_{\mathbb{G}}}$. Given a functor $K\colon \mathbb{C} \to \mathbb{C}'$, we define $\{\mathbb{B}, K\}\colon \{\mathbb{B}, \mathbb{C}\} \to \{\mathbb{B}, \mathbb{C}'\}$ to be the functor mapping $(\alpha, F\colon \mathbb{B}^\alpha \to \mathbb{C})$ to $(\alpha, KF\colon \mathbb{B}^\alpha \to \mathbb{C}')$; and if

$$\Phi = (\varphi, |\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|, |\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|, \Delta_\Phi)\colon (\alpha, F) \to (\beta, G)$$

is a morphism in $\{\mathbb{B}, \mathbb{C}\}$, then $\{\mathbb{B}, K\}(\Phi)$ is obtained by whiskering K with φ, obtaining therefore a transformation with the same type and generalised graph as before, with the same dinaturality properties:

$$\{\mathbb{B}, K\}(\Phi) = (K\varphi, |\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|, |\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|, \Delta_\Phi).$$

In particular, $\{\mathbb{B}, K\}$ is clearly a functor over $\mathbb{G}$.

We wish to prove that $\{\mathbb{B}, -\}$ is continuous, that is, preserves all small limits. We recall the definition of limit of a functor $X\colon \mathbb{S} \to \mathbb{C}\mathrm{at}$, which will set up the notation for the following Theorem.

(3.50) Definition. Let $\mathbb{S}$ be a (non-empty) small category, $X\colon \mathbb{S} \to \mathbb{C}\mathrm{at}$ a functor. Call I the set of objects of $\mathbb{S}$, $\mathbb{X}_i = X(i)$ for $i \in I$, $X_a = X(a)$ for a a morphism in $\mathbb{S}$.

A *cone* of X is a pair $(\mathbb{L}, (P_i)_{i\in I})$ where $\mathbb{L}$ is a category and for all $i \in I$, $P_i : \mathbb{L} \to \mathbb{X}_i$ is a functor such that

$$\forall a\colon i \to j \text{ in } \mathbb{S}, \qquad \begin{tikzcd} \mathbb{L} \arrow[r, "P_i"] \arrow[dr, "P_j"'] & \mathbb{X}_i \arrow[d, "X_a"] \\ & \mathbb{X}_j \end{tikzcd} \quad \text{commutes.}$$

A *limit* of X is a universal cone, that is, is a cone $(\mathbb{L}, (P_i)_{i\in I})$ such that for any cone $(\mathbb{A}, (F_i : \mathbb{A} \to \mathbb{X}_i)_{i\in I})$ there exists a unique functor $F : \mathbb{A} \to \mathbb{L}$ such that

$$\begin{tikzcd} \mathbb{L} \arrow[r, "P_i"] & \mathbb{X}_i \\ \mathbb{A} \arrow[u, "F"] \arrow[ur, "F_i"'] & \end{tikzcd}$$

commutes.

A functor $T : \mathbb{C}\mathrm{at} \to \mathbb{E}$ is said to be *continuous* if and only if for all $X : \mathbb{S} \to \mathbb{C}\mathrm{at}$ functor and $(\mathbb{L}, (P_i)_{i\in I})$ limit of X (if it exists), the pair $(T(\mathbb{L}), (T(P_i))_{i\in I})$ is a limit in $\mathbb{E}$ for the composite $\mathbb{S} \xrightarrow{X} \mathbb{C}\mathrm{at} \xrightarrow{T} \mathbb{E}$. ◻

(3.51) Remark. The uniqueness condition in the notion of limit is equivalent to requiring that the family $(F_i)_{i\in I}$ be *jointly mono*, which in our case means that if u and v are objects (or morphisms) in $\mathbb{L}$ such that $P_i(u) = P_i(v)$ for all $i \in I$, then $u = v$.

(3.52) Theorem. $\{\mathbb{B}, -\}$ *is continuous.*

Proof. In the same notations of the previous definition, suppose that $(\mathbb{L}, (P_i)_{i\in I})$ is a limit in $\mathbb{C}\mathrm{at}$ of $X : \mathbb{S} \to \mathbb{C}\mathrm{at}$. We have to prove that the pair

$$\big(\{\mathbb{B}, \mathbb{L}\}, (\{\mathbb{B}, P_i\})_{i\in I}\big)$$

is a limit in $\overline{\mathbb{C}\mathrm{at}/\mathbb{G}}$ of $\mathbb{S} \xrightarrow{X} \mathbb{C}\mathrm{at} \xrightarrow{\{\mathbb{B},-\}} \overline{\mathbb{C}\mathrm{at}/\mathbb{G}}$. In this proof, when we talk about categories or functors "over $\mathbb{G}$", we mean objects or morphisms of $\overline{\mathbb{C}\mathrm{at}/\mathbb{G}}$.

Any functor transforms cones into cones, so we have to prove that it is universal. Call Γ all the weak Conduché fibrations that categories in $\overline{\mathbb{C}\mathrm{at}/\mathbb{G}}$ come along with. Let then D be a category over $\mathbb{G}$, and let, for all $i \in I$, $G_i : \mathbb{D} \to \{\mathbb{B}, \mathbb{X}_i\}$ be a functor over $\mathbb{G}$ such that $(\mathbb{D}, (G_i)_{i\in I})$ is a cone of $\{\mathbb{B}, -\} \circ X$, which means that for all $a : i \to j$ in $\mathbb{S}$, the following triangle in $\overline{\mathbb{C}\mathrm{at}/\mathbb{G}}$

$$(\dagger) \qquad \begin{tikzcd} \mathbb{D} \arrow[r, "G_i"] \arrow[dr, "G_j"'] & \{\mathbb{B}, \mathbb{X}_i\} \arrow[d, "\{\mathbb{B}, X_a\}"] \\ & \{\mathbb{B}, \mathbb{X}_j\} \end{tikzcd}$$

commutes. To conclude, we have to define a functor $G \colon \mathbb{D} \to \{\mathbb{B}, \mathbb{L}\}$ over $\mathbb{G}$, which means that

$$\begin{tikzcd} \mathbb{D} \arrow[r, "G"] \arrow[dr, "\Gamma"'] & \{\mathbb{B}, \mathbb{L}\} \arrow[d, "\Gamma"] \\ & \mathbb{G} \end{tikzcd}$$

has to commute, such that for all $i \in I$ also the following triangle commutes:

$$\begin{tikzcd} \{\mathbb{B}, \mathbb{L}\} \arrow[r, "\{\mathbb{B}, P_i\}"] & \{\mathbb{B}, \mathbb{X}_i\} \\ \mathbb{D} \arrow[u, "G"] \arrow[ur, "G_i"'] & \end{tikzcd}$$

We define the action of G on objects first. Given an object $D \in \mathbb{D}$ with $\Gamma(D) = \alpha$, we have to provide a pair $G(D) = (\alpha, T_D \colon \mathbb{B}^\alpha \to \mathbb{L})$ such that $\{\mathbb{B}, P_i\}\big(G(D)\big) = G_i(D)$ as objects of the generalised functor category $\{\mathbb{B}, \mathbb{X}_i\}$ for all $i \in I$. Now, for all $i \in I$ we do have pairs

$$G_i(D) = (\alpha, F_i^D \colon \mathbb{B}^\alpha \to \mathbb{X}_i).$$

(The functors F_i^D have all the same variance α because G_i is a functor over $\mathbb{G}$, hence $\Gamma\big(G_i(D)\big) = \Gamma(D) = \alpha$ for all $i \in I$.) Consider then the pair

$$\big(\mathbb{B}^\alpha, (F_i^D)_{i \in I}\big).$$

Is it a cone of X in $\mathbb{C}\mathrm{at}$? It is if and only if for all $a \colon i \to j$ in $\mathbb{S}$ the following diagram commutes:

$$\begin{tikzcd} \mathbb{B}^\alpha \arrow[r, "F_i^D"] \arrow[dr, "F_j^D"'] & \mathbb{X}_i \arrow[d, "X_a"] \\ & \mathbb{X}_j \end{tikzcd}$$

and indeed it does because of (†), which says that for any D object of $\mathbb{D}$, $X_a \circ F_i^D = F_j(D)$ by definition of $\{\mathbb{B}, X_a\}$. Hence, by universality of $\big(\mathbb{L}, (P_i)_{i \in I}\big)$, there exists a unique functor $T_D \colon \mathbb{B}^\alpha \to \mathbb{L}$ such that $P_i \circ T_D = F_i^D$. Define then

$$G(D) = (\alpha, T_D).$$

Then $(\{\mathbb{B}, P_i\} \circ G)(D) = (\alpha, P_i \circ T_D) = (\alpha, F_i^D) = G_i(D)$, as required.

We now define G on morphisms as follows. Let $d \colon D \to D'$ be a morphism in $\mathbb{D}$ with $\Gamma(D) = \alpha$, $\Gamma(D') = \beta$ and $\Gamma(d) = \big[\big(|\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|, \Delta_d\big)\big]$. Fix a representative N and suppose that the Petri Net N has n ordered connected components. (A different representative N' of the same class still has n connected components, possibly ordered in a different way.) By Lemma (3.49) we can assume, without loss of generality, that

$\Gamma(d)$ is atomic. Hence, suppose that $P_N = |\alpha| + |\beta|$, $\overline{\sigma} = \iota_{|\alpha|}$, $\overline{\tau} = \iota_{|\beta|}$ and every place in N is either a proper source or a proper sink. Then for all $i \in I$ we have that $G_i(d)$ is an equivalence class of tuples as the following one:

$$G_i(d) = \Big[\big(\varphi^{i,d}, |\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|, |\alpha| \xrightarrow{\iota_{|\alpha|}} N \xleftarrow{\iota_{|\beta|}} |\beta|, \Delta_d\big)\Big].$$

Once an ordering of the connected components of N has been fixed, the functions σ and τ are uniquely determined by $\overline{\sigma}$ and $\overline{\tau}$ (in fact, (σ, τ, n) is the skeleton of $(\iota_{|\alpha|}, \iota_{|\beta|}, N)$); different orderings yield equivalent tuples and hence the same morphism in $\{\mathbb{B}, \mathbb{X}_i\}$. Notice in particular that N is none other than the graph of $\varphi^{i,d}$ in the sense of Definition (1.16).

This means that we have transformations $\varphi^{i,d} \colon T_i^D \to T_i^{D'}$ with components

$$\varphi^{i,d}_{B_1,\dots,B_n} \colon T_i^D(B_{\sigma 1}, \dots, B_{\sigma|\alpha|}) \to T_i^{D'}(B_{\tau 1}, \dots, B_{\tau|\beta|}),$$

all of the same graph N, each such $\varphi^{i,d}$ being dinatural in all variables B_k such that $\Delta_d(k) = 1$. Moreover, because of (†) and by definition of $\{\mathbb{B}, X_a\}$ we have that for all $a \colon i \to j$:

$$X_a(\varphi^{i,d}) = \varphi^j_d.$$

We aim to define a morphism $G(d)$ in $\{\mathbb{B}, \mathbb{L}\}$, which means we have to find a transformation $\varphi^d \colon T_D \to T_{D'}$ of type $|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|$ (hence its graph is automatically N) and Δ_d as discriminant function, in such a way that $(\{\mathbb{B}, P_i\} \circ G)(d) = G_i(d)$ for all $i \in I$.

We shall, of course, construct φ^d by building a cone of X in $\mathbb{C}\mathrm{at}$ and then using the universality of $(\mathbb{L}, (P_i))$, as we did with the definition of $G(D)$. However, cones are made of functors $\mathbb{A} \to \mathbb{X}_i$, while we would like to build the cone of all the $\varphi^{i,d}_{B_1,\dots,B_n}$, which are actual morphisms in $\mathbb{X}_i$. The trick is to consider the "arrow category" $\mathbb{A}\mathrm{rr}$, which consists of two objects, called *dom* and *codom*, and only one non-identity arrow *dom* $\to$ *codom*. Then a functor from $\mathbb{A}\mathrm{rr}$ to any category $\mathbb{C}$ is precisely a morphism of $\mathbb{C}$. If $f \colon A \to B$ is in $\mathbb{C}$, call $\ulcorner f \urcorner \colon \mathbb{A}\mathrm{rr} \to \mathbb{C}$ the corresponding functor.

For $B_1, \dots, B_n$ objects of $\mathbb{B}$, we then have that the pair

$$\big(\mathbb{A}\mathrm{rr}, (\ulcorner \varphi^{i,d}_{B_1,\dots,B_n} \urcorner \colon \mathbb{A}\mathrm{rr} \to \mathbb{X}_i)_{i \in I}\big)$$

is indeed a cone of X in $\mathbb{C}\mathrm{at}$: there exists then a unique functor $\mathbb{A}\mathrm{rr} \to \mathbb{L}$, i.e. a unique morphism $\varphi^d_{B_1,\dots,B_m}$ of $\mathbb{L}$, such that $P_i(\varphi^d_{B_1,\dots,B_n}) = \varphi^{i,d}_{B_1,\dots,B_n}$ for all $i \in I$. We have therefore a family of morphisms $(\varphi^d_{B_1,\dots,B_n})$, but is it actually a transformation $T_D \to T_{D'}$ of type $|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|$? To answer this question, we have to calculate the domain and codomain of $\varphi^d_{B_1,\dots,B_n}$ and prove that the former is precisely $T_D(B_{\sigma 1}, \dots, B_{\sigma|\alpha|})$, the latter $T_{D'}(B_{\tau 1}, \dots, B_{\tau|\beta|})$.

Remember that $\mathbb{I}$ is the category with one object and one morphism: a functor $\mathbb{I} \to \mathbb{C}$ is precisely an object of $\mathbb{C}$. If we write $\ulcorner C \urcorner$ for the functor $\mathbb{I} \to \mathbb{C}$ that "indicates" the object C of $\mathbb{C}$, consider the following composite:

$$\mathbb{I} \xrightarrow{\ulcorner dom \urcorner} \mathbb{A}\mathrm{rr} \xrightarrow{\ulcorner \varphi^{i,d}_{B_1,\dots,B_n} \urcorner} \mathbb{X}_i$$

As a family in i it makes a cone of X, hence there exists a unique object L of $\mathbb{L}$ (functor $\mathbb{I} \to \mathbb{L}$) such that $P_i(L) = dom\left(\varphi^{i,d}_{B_1,\dots,B_n}\right) = F^D_i(B_{\sigma 1}, \dots, B_{\sigma|\alpha|})$. We show that both $dom\left(\varphi^{d}_{B_1,\dots,B_n}\right)$ and $T_D(B_{\sigma 1}, \dots, B_{\sigma|\alpha|})$ satisfy the same property of L, hence they must be equal. Indeed,

$$P_i\left(dom\left(\varphi^{d}_{B_1,\dots,B_n}\right)\right) = dom\left(P_i\left(\varphi^{d}_{B_1,\dots,B_n}\right)\right) = dom\left(\varphi^{i,d}_{B_1,\dots,B_n}\right) = F^D_i(B_{\sigma 1}, \dots, B_{\sigma|\alpha|})$$

(the first equation is due, of course, to the functoriality of P_i), and also

$$P_i\big(T_D(B_{\sigma 1}, \dots, B_{\sigma|\alpha|})\big) = F^D_i(B_{\sigma 1}, \dots, B_{\sigma|\alpha|})$$

by construction of T_D as the unique functor that, once post-composed with P_i, is equal to F^D_i. Hence the domain of $\varphi^{d}_{B_1,\dots,B_n}$ is indeed $T_D(B_{\sigma 1}, \dots, B_{\sigma|\alpha|})$; in a completely analogous way one checks that its codomain is $T_{D'}(B_{\tau 1}, \dots, B_{\tau|\beta|})$. We therefore have a transformation $\varphi^d \colon T_D \to T_{D'}$ of type $|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|$.

Finally, we have to prove that φ^d so defined is dinatural in all variables B_k with $\Delta_d(k) = 1$. We show how to see this in the special case of $\alpha = \beta = [-,+]$ and $n = 1$, but the argument holds for any α, β and n, as will be evident.

We are wondering whether φ^d is dinatural in its only variable, that is if it is true that for all $f \colon A \to B$ in $\mathbb{B}$ the following hexagon commutes:

(3.53)
$$\begin{tikzcd}
 & T_D(A,A) \arrow[r, "\varphi^d_A"] & T_{D'}(A,A) \arrow[dr, "T_{D'}(1,f)"] & \\
T_D(B,A) \arrow[ur, "T_D(f,1)"] \arrow[dr, "T_D(1,f)"'] & & & T_{D'}(A,B) \\
 & T_D(B,B) \arrow[r, "\varphi^d_B"'] & T_{D'}(B,B) \arrow[ur, "T_{D'}(f,1)"'] &
\end{tikzcd}$$

The image along P_i of the diagram is, by functoriality of P_i and by definition of T_D,

$T_{D'}$ and φ^d, none other than

$$\begin{tikzcd}
 & F_i^D(A,A) \arrow[r, "\varphi_A^{i,d}"] & F_i^{D'}(A,A) \arrow[dr, "F_i^{D'}(1,f)"] & \\
F_i^D(B,A) \arrow[ur, "F_i^D(f,1)"] \arrow[dr, "F_i^D(1,f)"'] & & & F_i^{D'}(A,B) \\
 & F_i^D(B,B) \arrow[r, "\varphi_B^{i,d}"'] & F_i^{D'}(B,B) \arrow[ur, "F_i^{D'}(f,1)"'] &
\end{tikzcd}$$

which is indeed commutative because $\varphi^{i,d}$ is dinatural in its only variable. So the two legs of (3.53) are morphisms u and v such that $P_i(u) = P_i(v)$ for all $i \in I$: by joint-monicity of the family $(P_i)_{i\in I}$, we conclude that $u = v$. Now apply this argument to the general case: the dinaturality of φ^d in its k-th variable, with $\Delta_d(k) = 1$, is tantamount to proving that two morphisms in $\mathbb{L}$ are equal. We know that $\varphi^{i,d}$ is dinatural in its k-th variable for all $i \in I$, hence the image along P_i of the two legs of the dinaturality hexagon are equal morphisms in $\mathbb{X}_i$ for every i. Since the P_i's are jointly mono, we conclude.

Define therefore

$$G(d) = \left[(\varphi^d, |\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|, |\alpha| \xrightarrow{\iota_{|\alpha|}} N \xleftarrow{\iota_{|\beta|}} |\beta|, \Delta_d)\right].$$

This extends to a functor $G\colon \mathbb{D} \to \{\mathbb{B}, \mathbb{L}\}$, as we have seen before. Moreover, it is the only possible such functor satisfying the condition $\{\mathbb{B}, P_i\} \circ G = G_i$ for all $i \in I$ by construction. **Qed**

The category $\mathbb{A} \circ \mathbb{B}$. The continuity of $\{\mathbb{B}, -\}$ gives us hope for the existence of a left adjoint

$$- \circ \mathbb{B} \colon \overline{\mathbb{C}\mathrm{at}/\mathbb{G}} \to \mathbb{C}\mathrm{at}.$$

We shall prove so by first constructing the category $\mathbb{A} \circ \mathbb{B}$ explicitly, and then showing the existence of a universal arrow $(\mathbb{A} \circ \mathbb{B}, F_{\mathbb{A}} \colon \mathbb{A} \to \{\mathbb{B}, \mathbb{A} \circ \mathbb{B}\})$ from $\mathbb{A}$ to $\{\mathbb{B}, -\}$.

To see what $\mathbb{A} \circ \mathbb{B}$ looks like, we follow Kelly's strategy: we aim to prove that there is a natural isomorphism

$$\mathbb{C}\mathrm{at}(\mathbb{A} \circ \mathbb{B}, \mathbb{C}) \cong \overline{\mathbb{C}\mathrm{at}/\mathbb{G}}(\mathbb{A}, \{\mathbb{B}, \mathbb{C}\})$$

and we use this to infer how $\mathbb{A} \circ \mathbb{B}$ must be. Write Γ for all augmentations (as weak Conduché fibrations) over $\mathbb{G}$, and let Φ be an element of $\overline{\mathbb{C}\mathrm{at}/\mathbb{G}}(\mathbb{A}, \{\mathbb{B}, \mathbb{C}\})$. We now spell out all we can infer from this fact. To facilitate reading, and to comply with Kelly's notation in [Kel72a] as in §3.1, we shall now refer to the $(A_1, \ldots, A_m)$-th component of a transformation φ as $\varphi(A_1, \ldots, A_m)$ instead of $\varphi_{A_1,\ldots,A_m}$.

(a) For all $A \in \mathbb{A}$, $\Gamma(A) = \alpha$ we have $\Phi A \colon \mathbb{B}^\alpha \to \mathbb{C}$ is a functor, hence

(a.i) for all $B_1, \dots, B_{|\alpha|}$ objects of $\mathbb{B}$, $\Phi A(B_1, \dots, B_{|\alpha|})$ is an object of $\mathbb{C}$,

(a.ii) for all $g_1, \dots, g_{|\alpha|}$, with $g_i \colon B_i \to B'_i$ a morphism in $\mathbb{B}$, we have

$$\Phi(A)(g_1, \dots, g_{|\alpha|}) \colon \Phi A(C_1, \dots, C_{|\alpha|}) \to \Phi A(D_1, \dots, D_{|\alpha|})$$

is a morphism in $\mathbb{C}$, where

$$C_i = \begin{cases} B_i & \alpha_i = + \\ B'_i & \alpha_i = - \end{cases} \qquad D_i = \begin{cases} B'_i & \alpha_i = + \\ B_i & \alpha_i = - \end{cases}$$

This data is subject to functoriality of ΦA, that is:

(1) $\Phi A(id_{B_1}, \dots, id_{B_{|\alpha|}}) = id_{\Phi A(B_1, \dots, B_{|\alpha|})}$

(2) For $h_1, \dots, h_{|\alpha|}$, with $h_i \colon B'_i \to B''_i$ morphism of $\mathbb{B}$,

$$\Phi A(x_1 \circ_{\mathbb{B}^{\alpha_1}} y_1, \dots, x_{|\alpha|} \circ_{\mathbb{B}^{\alpha_{|\alpha|}}} y_{|\alpha|}) = \Phi A(x_1, \dots, x_{|\alpha|}) \circ \Phi A(y_1, \dots, y_{|\alpha|})$$

where

$$x_i = \begin{cases} h_i & \alpha_i = + \\ g_i & \alpha_i = - \end{cases} \qquad y_i = \begin{cases} g_i & \alpha_i = + \\ h_i & \alpha_i = - \end{cases}$$

(b) For all $f \colon A \to A'$ in $\mathbb{A}$ with $\Gamma(f) = \left[\left(|\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|, \Delta_f\right)\right]$, we have that Φf is an equivalence class of transformations whose graphs are representatives of $\Gamma(f)$, such transformations being dinatural in some variables according to Δ_f. Hence for all $\xi = \big((\overline{\sigma}, \overline{\tau}, N), \Delta_\xi\big) \in \Gamma(f)$ we have a transformation $\Phi f_\xi \colon \Phi A \to \Phi A'$ whose type $|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|$ is the skeleton of $(\overline{\sigma}, \overline{\tau}, N)$ and with discriminant function Δ_ξ that tells us in which variables Φf_ξ is dinatural. Therefore to give Φf one has to provide, for all $\xi = \big((\overline{\sigma}, \overline{\tau}, N), \Delta_\xi\big) \in \Gamma(f)$, for all $B_1, \dots, B_n$ objects of $\mathbb{B}$, a morphism in $\mathbb{C}$

$$\Phi f_\xi(B_1, \dots, B_n) \colon \Phi A(B_{\sigma 1}, \dots, B_{\sigma|\alpha|}) \to \Phi A'(B_{\tau 1}, \dots, B_{\tau|\beta|})$$

such that:

(3) for all $\pi \colon n \to n$ permutation, $\Phi f_{\pi\xi}(B_1, \dots, B_n) = \Phi f_\xi(B_{\pi 1}, \dots, B_{\pi n})$,

(4) for $g_1, \dots, g_n$ morphisms in $\mathbb{B}$, with $g_i \colon B_i \to B'_i$ if $\Delta_\xi(i) = 1$, otherwise

$g_i = id_{B_i}$, the following hexagon commutes:

$$\begin{tikzcd}
& \Phi A(B_{\sigma 1}, \ldots, B_{\sigma|\alpha|}) \arrow[r, "\Phi f_\xi(B_1,\ldots,B_n)"] & \Phi A'(B_{\tau 1}, \ldots, B_{\tau|\beta|}) \arrow[dr, "\Phi A'(y_1,\ldots,y_{|\beta|})"] & \\
\Phi A(C_1, \ldots, C_{|\alpha|}) \arrow[ur, "\Phi A(x_1,\ldots,x_{|\alpha|})"] \arrow[dr, "\Phi A(x'_1,\ldots,x'_{|\alpha|})"'] & & & \Phi A'(D_1, \ldots, D_{|\beta|}) \\
& \Phi A(B'_{\sigma 1}, \ldots, B'_{\sigma|\alpha|}) \arrow[r, "\Phi f_\xi(B'_1,\ldots,B'_n)"'] & \Phi A'(B'_{\tau 1}, \ldots, B'_{\tau|\beta|}) \arrow[ur, "\Phi A'(y'_1,\ldots,y'_{|\beta|})"'] &
\end{tikzcd}$$

where

$$C_i = \begin{cases} B_{\sigma i} & \alpha_i = + \\ B'_{\sigma i} & \alpha_i = - \end{cases} \qquad x_i = \begin{cases} B_{\sigma i} & \alpha_i = + \\ g_{\sigma i} & \alpha_i = - \end{cases} \qquad y_i = \begin{cases} g_{\tau i} & \beta_i = + \\ B_{\tau i} & \beta_i = - \end{cases}$$

$$D_i = \begin{cases} B'_{\tau i} & \beta_i = + \\ B_{\tau i} & \beta_i = - \end{cases} \qquad x'_i = \begin{cases} g_{\sigma i} & \alpha_i = + \\ B_{\sigma i} & \alpha_i = - \end{cases} \qquad y'_i = \begin{cases} B_{\tau i} & \beta_i = + \\ g_{\tau i} & \beta_i = - \end{cases}$$

(c) The data provided in (a) and (b) is subject to the functoriality of Φ itself, hence:

(5) $\Phi(id_A) = id_{\Phi A}$,

(6) for $f\colon A \longrightarrow A'$ and $f'\colon A' \longrightarrow A''$, $\Phi(f' \circ_{\mathbb{A}} f) = \Phi f' \circ_{\{\mathbb{B},\mathbb{C}\}} \Phi f$.

We now mirror all the data and properties of a functor $\Phi\colon \mathbb{A} \longrightarrow \{\mathbb{B}, \mathbb{C}\}$ over $\mathbb{G}$ to define the category $\mathbb{A} \circ \mathbb{B}$.

(3.54) Definition. Let $\mathbb{A}$ be a category over $\mathbb{G}$ via a weak Conduché fibration $\Gamma\colon \mathbb{A} \longrightarrow \mathbb{G}$, and let $\mathbb{B}$ be any category. The category $\mathbb{A} \circ \mathbb{B}$ of *formal substitutions* of elements of $\mathbb{B}$ into those of $\mathbb{A}$ is the free category generated by the following data. We use the same enumeration as above to enlighten the correspondence between each piece of information.

(a.i) Objects are of the form $A[B_1, \ldots, B_{|\alpha|}]$, for A an object of $\mathbb{A}$, $\Gamma(A) = \alpha$, and for objects $B_1, \ldots, B_{|\alpha|}$ in $\mathbb{B}$.

(a.ii),(b) Morphisms are to be generated by

$$A[g_1, \ldots, g_{|\alpha|}]\colon A[C_1, \ldots, C_{|\alpha|}] \longrightarrow A[D_1, \ldots, D_{|\alpha|}]$$

for A in $\mathbb{A}$ with $\Gamma(A) = \alpha$, and $g_i\colon B_i \longrightarrow B'_i$ in $\mathbb{B}$, where

$$C_i = \begin{cases} B_i & \alpha_i = + \\ B'_i & \alpha_i = - \end{cases} \qquad D_i = \begin{cases} B'_i & \alpha_i = + \\ B_i & \alpha_i = - \end{cases}$$

and by
$$f_\xi[B_1,\dots,B_n]\colon A[B_{\sigma 1},\dots,B_{\sigma|\alpha|}] \to A'[B_{\tau 1},\dots,B_{\tau|\beta|}]$$
for $f\colon A \to A'$ in $\mathbb{A}$, $\xi = \big(|\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|, \Delta_\xi\big)$ a representative of $\Gamma(f)$, (σ,τ,n) the skeleton of $(\overline{\sigma},\overline{\tau},N)$, $B_1,\dots,B_n$ objects of $\mathbb{B}$.

Such data is subject to the following conditions:

(3) For all $\pi\colon n \to n$ permutation, for all $B_1,\dots,B_n$ objects of $\mathbb{B}$,
$$f_{\pi\xi}[B_1,\dots,B_n] = f_\xi[B_{\pi 1},\dots,B_{\pi n}],$$

(1),(5) For all $A \in \mathbb{A}$, $\Gamma(A) = \alpha$, $B_1,\dots,B_{|\alpha|}$ objects on $\mathbb{B}$,
$$A[id_{B_1},\dots,id_{B_{|\alpha|}}] = id_{A[B_1,\dots,B_{|\alpha|}]} = id_A[B_1,\dots,B_{|\alpha|}],$$

(2) For all $A \in \mathbb{A}$, $\Gamma(A) = \alpha$, for all $g_i\colon B_i \to B_i'$ and $h_i\colon B_i' \to B_i''$ in $\mathbb{B}$, $i \in \{1,\dots,|\alpha|\}$,
$$A[x_1 \circ y_1,\dots,x_{|\alpha|} \circ y_{|\alpha|}] = A[x_1,\dots,x_{|\alpha|}] \circ A[y_1,\dots,y_{|\alpha|}]$$
where
$$x_i = \begin{cases} h_i & \alpha_i = + \\ g_i & \alpha_i = - \end{cases} \qquad y_i = \begin{cases} g_i & \alpha_i = + \\ h_i & \alpha_i = - \end{cases}$$

(6) For all $f\colon A \to A'$ and $f'\colon A' \to A''$ in $\mathbb{A}$, for all
$$\big(|\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|, \Delta\big) \in \Gamma(f) \quad \text{and} \quad \big(|\beta| \xrightarrow{\overline{\eta}} M \xleftarrow{\overline{\theta}} |\gamma|, \Delta'\big) \in \Gamma(f'),$$
with (σ,τ,n) and (η,θ,m) the skeletons of, respectively, $(\overline{\sigma},\overline{\tau},N)$ and $(\overline{\eta},\overline{\theta},M)$, and for all choices of a pushout
$$\begin{tikzcd} & & {|\gamma|} \arrow[d, "\theta"] \\ & {|\beta|} \arrow[r, "\eta"] \arrow[d, "\tau"'] \arrow[dr, phantom, "\ulcorner"] & m \arrow[d, "\xi"] \\ {|\alpha|} \arrow[r, "\sigma"] & n \arrow[r, "\zeta"] & l \end{tikzcd}$$
each choice determining the skeleton of (the first projection of) a representative of $\Gamma(f' \circ f)$,
$$f'_{(\eta,\theta)}[B_{\xi 1},\dots,B_{\xi m}] \circ f_{(\sigma,\tau)}[B_{\zeta 1},\dots,B_{\zeta n}] = (f' \circ f)_{(\zeta\sigma,\xi\theta)}[B_1,\dots,B_l],$$

(4) For all $f\colon A \to A'$, $\xi = \left(|\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|, \Delta_\xi\right) \in \Gamma(f)$, with (σ,τ,n) the skeleton of $(\overline{\sigma},\overline{\tau},N)$, for all $g_1,\dots,g_n$ in $\mathbb{B}$, with $g_i\colon B_i \to B'_i$ if $\Delta_\xi(i) = 1$, otherwise $g_i = id_{B_i}$, the following hexagon commutes:

$$\text{(3.55)}\qquad \begin{tikzcd}[column sep=small]
 & A[B_{\sigma 1},\dots,B_{\sigma|\alpha|}] \arrow[r, "{f_\xi[B_1,\dots,B_n]}"] & A'[B_{\tau 1},\dots,B_{\tau|\beta|}] \arrow[dr, "{A'[y_1,\dots,y_{|\beta|}]}"] & \\
A[C_1,\dots,C_{|\alpha|}] \arrow[ur, "{A[x_1,\dots,x_{|\alpha|}]}"] \arrow[dr, "{A[x'_1,\dots,x'_{|\alpha|}]}"'] & & & A'[D_1,\dots,D_{|\beta|}] \\
 & A[B'_{\sigma 1},\dots,B'_{\sigma|\alpha|}] \arrow[r, "{f_\xi[B'_1,\dots,B'_n]}"'] & A'[B'_{\tau 1},\dots,B'_{\tau|\beta|}] \arrow[ur, "{A'[y'_1,\dots,y'_{|\beta|}]}"'] &
\end{tikzcd}$$

where

$$C_i = \begin{cases} B_{\sigma i} & \alpha_i = + \\ B'_{\sigma i} & \alpha_i = - \end{cases} \qquad x_i = \begin{cases} B_{\sigma i} & \alpha_i = + \\ g_{\sigma i} & \alpha_i = - \end{cases} \qquad y_i = \begin{cases} g_{\tau i} & \beta_i = + \\ B_{\tau i} & \beta_i = - \end{cases}$$

$$D_i = \begin{cases} B'_{\tau i} & \beta_i = + \\ B_{\tau i} & \beta_i = - \end{cases} \qquad x'_i = \begin{cases} g_{\sigma i} & \alpha_i = + \\ B_{\sigma i} & \alpha_i = - \end{cases} \qquad y'_i = \begin{cases} B_{\tau i} & \beta_i = + \\ g_{\tau i} & \beta_i = - \end{cases}$$

We will denote the diagonal of (3.55) as $f[g_1,\dots,g_n]$. □

(3.56) Remark. By (5) and (2), we have

$$A[g_1,\dots,g_{|\alpha|}] = id_A[g_1,\dots,g_{|\alpha|}]$$

and by (1), we have

$$f[B_1,\dots,B_n] = f[id_{B_1},\dots,id_{B_n}]$$

which is coherent with the usual notation of A for id_A.

Note that $f[g_1,\dots,g_n]$ is *not* the most general morphism of $\mathbb{A} \circ \mathbb{B}$, as opposed to what happens in Kelly's covariant case (cf. discussion after (3.6)). Indeed, consider $f[g_1,\dots,g_n]$ given by (3.55), and take $h_1,\dots,h_{|\beta|}$ morphisms of $\mathbb{B}$, where

$$h_i\colon \begin{cases} B'_{\tau i} \to B''_i & \beta_i = + \\ B''_i \to B_{\tau i} & \beta_i = - \end{cases}$$

Then $A'[h_1,\dots,h_{|\beta|}] \circ f[g_1,\dots,g_n]$ is not, in general, of the form $f'[g'_1,\dots,g'_n]$.

Indeed, although two consecutive morphisms both of type (a.ii) or both of type (b) can be "merged" together into a single one by (2) and (6), we have no way, in general, to swap the order of a morphism of type $A[g_1,\dots,g_{|\alpha|}]$ followed by one of the form $f_\xi[B_1,\dots,B_n]$, because the only axiom that relates the two generators is (3.55). This is a *dinaturality* condition, that is not quite like Kelly's *naturality* equation (3.6) which does allow the "cross-over" of morphisms of different kind. Of course, if (3.6) happens to be a naturality square, that is if f_ξ is a natural transformation, then everything works as in Kelly's case. Therefore, all we can say about the general morphism of $\mathbb{A} \circ \mathbb{B}$ is that it is a "string" of compositions of alternate morphisms of type (a.ii) and (b), subject to the equations (1)-(6).

(3.57) Remark. If $\mathbb{A}$ is such that $|\Gamma(A)| = 1$ for all objects A in $\mathbb{A}$, then $\mathbb{A} \circ \mathbb{B}$ is highly reminiscent of the category $\mathbb{A} \otimes \mathbb{B}$ as described by Power and Robinson in [PR97]. The authors studied the *other* symmetric monoidal closed structure of $\mathbb{C}\mathrm{at}$, where the exponential $[\mathbb{B}, \mathbb{C}]$ is the category of functors from $\mathbb{B}$ to $\mathbb{C}$ and morphisms are simply transformations (not necessarily natural), and $\otimes\mathbb{B}$ is the tensor functor that is the left adjoint of $[\mathbb{B}, -]$. The category $\mathbb{A} \otimes \mathbb{B}$ has pairs (A, B) of objects of $\mathbb{A}$ and $\mathbb{B}$, and a morphism from (A, B) to (A', B') is a finite sequence of non-identity arrows consisting of alternate chains of consecutive morphisms of $\mathbb{A}$ and $\mathbb{B}$. Composition is given by concatenation followed by cancellation accorded by the composition in $\mathbb{A}$ and $\mathbb{B}$, much like our $\mathbb{A} \circ \mathbb{B}$. The only difference with their case is that we have the additional dinaturality equality (4). For an arbitrary category $\mathbb{A}$ over $\mathbb{G}$, our $\mathbb{A} \circ \mathbb{B}$ would be a sort of "generalised tensor product", where the number of objects of $\mathbb{B}$ we "pair up" with an object A of $\mathbb{A}$ depends on $\Gamma(A)$.

A left adjoint. We conclude with a last result, that corresponds to Kelly's Theorem (3.4). This is going to be a crucial step towards a complete Godement calculus for dinatural transformations; we shall discuss some ideas and conjectures about the following steps afterwards.

(3.58) Theorem. *The functor* $\{\mathbb{B}, -\}$ *has a left adjoint*

$$\begin{tikzcd} \overline{\mathbb{C}\mathrm{at}/\mathbb{G}} \arrow[r, bend left, "-\circ\mathbb{B}"] \arrow[r, phantom, "\perp"] & \mathbb{C}\mathrm{at} \arrow[l, bend left, "\{\mathbb{B},-\}"] \end{tikzcd}$$

therefore there is a natural isomorphism

$$\mathbb{C}\mathrm{at}\big(\mathbb{A} \circ \mathbb{B}, \mathbb{C}\big) \cong \overline{\mathbb{C}\mathrm{at}/\mathbb{G}}\big(\mathbb{A}, \{\mathbb{B}, \mathbb{C}\}\big). \tag{3.59}$$

Moreover, $\circ \colon \overline{\mathbb{C}\mathrm{at}/\mathbb{G}} \times \mathbb{C}\mathrm{at} \to \mathbb{C}\mathrm{at}$ *is a functor.*

PROOF. Recall that to give an adjunction $(- \circ \mathbb{B}) \dashv \{\mathbb{B}, -\}$ is equivalent to give, for all $\mathbb{A} \in \overline{\mathbb{C}\mathrm{at}/\mathbb{G}}$, a universal arrow $(\mathbb{A} \circ \mathbb{B}, F_\mathbb{A} \colon \mathbb{A} \to \{\mathbb{B}, \mathbb{A} \circ \mathbb{B}\})$ from $\mathbb{A}$ to the functor $\{\mathbb{B}, -\}$; $F_\mathbb{A}$ being a morphism of $\overline{\mathbb{C}\mathrm{at}/\mathbb{G}}$. This means that, for a fixed $\mathbb{A}$, we have to define a functor over $\mathbb{G}$ that makes the following triangle commute:

$$\begin{tikzcd} \mathbb{A} \arrow[r, "F_{\mathbb{A}}"] \arrow[dr, "\Gamma"'] & \{\mathbb{B}, \mathbb{A} \circ \mathbb{B}\} \arrow[d, "\overline{\Gamma}"] \\ & \mathbb{G} \end{tikzcd}$$

which is universal among all arrows from $\mathbb{A}$ to $\{\mathbb{B}, -\}$: for all arrows $(\mathbb{C}, \Phi \colon \mathbb{A} \to \{\mathbb{B}, \mathbb{C}\})$ from $\mathbb{A}$ to $\{\mathbb{B}, -\}$ (Φ being a functor over $\mathbb{G}$), there must exist a unique morphism in $\mathbb{C}\mathrm{at}$, that is a functor, $H \colon \mathbb{A} \circ \mathbb{B} \to \mathbb{C}$ such that

$$\begin{tikzcd} \mathbb{A} \arrow[r, "F_{\mathbb{A}}"] \arrow[dr, "\Phi"'] & \{\mathbb{B}, \mathbb{A} \circ \mathbb{B}\} \arrow[d, "\{\mathbb{B}, H\}"] \\ & \{\mathbb{B}, \mathbb{C}\} \end{tikzcd}$$

commutes. In the proof we will refer to properties (1)-(6) as given in the definition of $\mathbb{A} \circ \mathbb{B}$.

Let then $\mathbb{A}$ be a category over $\mathbb{G}$ with $\Gamma \colon \mathbb{A} \to \mathbb{G}$ a weak Conduché fibration. We define the action of $F_{\mathbb{A}}$ on objects first. If A is an object of $\mathbb{A}$ with $\Gamma(A) = \alpha$, then the assignment

$$\begin{array}{ccc} \mathbb{B}^{\alpha} & \xrightarrow{F_{\mathbb{A}}(A)} & \mathbb{A} \circ \mathbb{B} \\ (B_1, \ldots, B_{|\alpha|}) & \longmapsto & A[B_1, \ldots, B_{|\alpha|}] \\ {\scriptstyle (g_1,\ldots,g_{|\alpha|})} \downarrow & \longmapsto & \downarrow {\scriptstyle A[g_1,\ldots,g_{|\alpha|}]} \\ (B'_1, \ldots, B'_{|\alpha|}) & \longmapsto & A[B'_1, \ldots, B'_{|\alpha|}] \end{array}$$

(each $g_i \colon B_i \to B'_i$ in $\mathbb{B}^{\alpha_i}$) is a functor by virtue of (1) and (2). By little abuse of notation, call $F_{\mathbb{A}}(A)$ also the pair $(\alpha, F_{\mathbb{A}}(A))$, which is an object of $\{\mathbb{B}, \mathbb{A} \circ \mathbb{B}\}$.

To define $F_{\mathbb{A}}$ on morphisms, let $f \colon A \to A'$ a morphism in $\mathbb{A}$, with $\Gamma(A) = \alpha$, $\Gamma(A') = \beta$, let

$$\xi = \left(|\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|, \Delta_{\xi}\right) \in \Gamma(f),$$

and call $|\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|$ the skeleton of $(\overline{\sigma}, \overline{\tau}, N)$. We define $F_{\mathbb{A}}(f) \colon F_{\mathbb{A}}(A) \to F_{\mathbb{A}}(A')$ to be the equivalent class of the tuple

$$\left(F_{\mathbb{A}}(f)_{\xi}, |\alpha| \xrightarrow{\sigma} n \xleftarrow{\tau} |\beta|, |\alpha| \xrightarrow{\overline{\sigma}} N \xleftarrow{\overline{\tau}} |\beta|, \Delta_{\xi}\right)$$

where $F_{\mathbb{A}}(f)_\xi$ is a transformation whose general component is

$$\begin{tikzcd} F_{\mathbb{A}}(A)(B_{\sigma 1},\dots,B_{\sigma|\alpha|}) \arrow[r, "f_\xi{[B_1,\dots,B_n]}"] \arrow[d, phantom, "\shortparallel"] & F_{\mathbb{A}}(A')(B_{\tau 1},\dots,B_{\tau|\beta|}) \arrow[d, phantom, "\shortparallel"] \\ A[B_{\sigma 1},\dots,B_{\sigma|\alpha|}] & A'[B_{\tau 1},\dots,B_{\tau|\beta|}] \end{tikzcd}$$

Then $F_{\mathbb{A}}(f)_\xi$ is indeed dinatural in its i-th variable whenever $\Delta_\xi(i) = 1$ because of (4). Moreover, $F_{\mathbb{A}}$ is well-defined on morphisms because of (3) and is in fact a functor thanks to (5) and (6). Finally, $F_{\mathbb{A}}(f)$ so defined is indeed a morphism of $\{\mathbb{B}, \mathbb{A} \circ \mathbb{B}\}$: if f is such that $\Gamma(f)$ is atomic, then $F_{\mathbb{A}}(f)$ is the standard representation of the transformation $F_{\mathbb{A}}(f)_\xi$, hence an atomic morphism of $\{\mathbb{B}, \mathbb{A} \circ \mathbb{B}\}$; if instead $\Gamma(f) = (N_k, \Delta_k) \circ \cdots \circ (N_1, \Delta_1)$ where (N_i, Δ_i) is atomic, then there exists a factorisation $f = f_k \circ \cdots \circ f_1$ in $\mathbb{A}$ with $\Gamma(f_i) = (N_i, \Delta_i)$ because Γ is a weak Conduché fibration. By functoriality of $F_{\mathbb{A}}$, we have that $F_{\mathbb{A}}(f) = F_{\mathbb{A}}(f_k) \circ \cdots \circ F_{\mathbb{A}}(f_1)$, hence it is a composite of standard representations of transformations.

We now prove that $F_{\mathbb{A}}$ is universal. Let then $\Phi \colon \mathbb{A} \to \{\mathbb{B}, \mathbb{C}\}$ be a morphism in $\overline{\mathbb{C}\mathrm{at}}/_{\mathbb{G}}$, that is a functor over $\mathbb{G}$. We define $H \colon \mathbb{A} \circ \mathbb{B} \to \mathbb{C}$ as follows:

(a.i) For $A \in \mathbb{A}$ with $\Gamma(A) = \alpha$,

$$H\bigl(A[B_1,\dots,B_{|\alpha|}]\bigr) = \Phi(A)(B_1,\dots,B_{|\alpha|});$$

(a.ii) For $A \in \mathbb{A}$ with $\Gamma(A) = \alpha$, for $g_i \colon B_i \to B'_i$ in $\mathbb{B}^{\alpha_i}$, $i \in \{1,\dots,|\alpha|\}$,

$$H\bigl(A[g_1,\dots,g_{|\alpha|}]\bigr) = \Phi(A)(g_1,\dots,g_{|\alpha|});$$

(b) For $f \colon A \to A'$ in $\mathbb{A}$, $\xi = (N_\xi, \Delta_\xi) \in \Gamma(f)$ where N_ξ has n connected components, for $B_1,\dots,B_n \in \mathbb{B}$,

$$H\bigl(f_\xi[B_1,\dots,B_n]\bigr) = \Phi(f)_\xi(B_1,\dots,B_n),$$

where $\Phi(f)_\xi$ is the representative of $\Phi(f)$ whose type is given by the skeleton of N_ξ, cf. the discussion on the data entailed by a functor $\Phi \colon \mathbb{A} \to \{\mathbb{B}, \mathbb{C}\}$ over $\mathbb{G}$ preceding Definition (3.54).

H so defined on the generators of $\mathbb{A} \circ \mathbb{B}$ extends to a unique functor provided that H preserves the equalities (1)-(6) in $\mathbb{A} \circ \mathbb{B}$, which it does as they have been designed *precisely* to reflect all the properties of a functor $\Phi \colon \mathbb{A} \to \{\mathbb{B}, \mathbb{C}\}$, and H is defined using Φ accordingly. Finally, by construction

$$\begin{tikzcd}
\mathbb{A} \arrow[r, "F_{\mathbb{A}}"] \arrow[dr, "\Phi"'] & \{\mathbb{B}, \mathbb{A} \circ \mathbb{B}\} \arrow[d, "\{\mathbb{B}, H\}"] \\
& \{\mathbb{B}, \mathbb{C}\}
\end{tikzcd}$$

commutes. The uniqueness of H follows from the fact that the commutativity of the above triangle implies that $\Phi(A) = H(F_{\mathbb{A}}(A))$ for all $A \in \mathbb{A}$ and $\Phi(f) = H(F_{\mathbb{A}}(f))$, hence any such functor H *must* be defined as we did to make the triangle commutative.

With such a universal arrow $(\mathbb{A} \circ \mathbb{B}, F_{\mathbb{A}} \colon \mathbb{A} \to \{\mathbb{B}, \mathbb{A} \circ \mathbb{B}\})$ we can define a functor $- \circ \mathbb{B}$ which is the left adjoint of $\{\mathbb{B}, -\}$. Given $F \colon \mathbb{A} \to \mathbb{A}'$ a functor over $\mathbb{G}$, by universality of $F_{\mathbb{A}}$ there exists a unique functor $F \circ \mathbb{B} \colon \mathbb{A} \circ \mathbb{B} \to \mathbb{A}' \circ \mathbb{B}$ that makes the following square commute:

$$\begin{tikzcd}
\mathbb{A} \arrow[r, "F_{\mathbb{A}}"] \arrow[d, "F"'] & \{\mathbb{B}, \mathbb{A} \circ \mathbb{B}\} \arrow[d, "\{\mathbb{B}, F \circ \mathbb{B}\}"] \\
\mathbb{A}' \arrow[r, "F_{\mathbb{A}'}"'] & \{\mathbb{B}, \mathbb{A}' \circ \mathbb{B}\}
\end{tikzcd}$$

Such $F \circ \mathbb{B}$ is defined on objects as $F \circ \mathbb{B}\big(A[B_1, \ldots, B_{|\alpha|}]\big) = (F_{\mathbb{A}'} \circ F)(A)(B_1, \ldots, B_{|\alpha|}) = FA[B_1, \ldots, B_{|\alpha|}]$ and on morphisms as

$$F \circ \mathbb{B}\big(A[g_1, \ldots g_{|\alpha|}]\big) = FA[g_1, \ldots, g_{|\alpha|}], \quad F \circ \mathbb{B}\big(f[B_1, \ldots, B_n]\big) = Ff[B_1, \ldots, B_n].$$

Finally, $\circ$ extends to a functor

$$\begin{tikzcd}
\overline{\mathbb{C}\mathrm{at}/\mathbb{G}} \times \mathbb{C}\mathrm{at} \arrow[rr, "\circ"] & & \mathbb{C}\mathrm{at} \\
\mathbb{A} \arrow[d, "F"'] & \mathbb{B} \arrow[r, mapsto] \arrow[d, "G"] & \mathbb{A} \circ \mathbb{B} \arrow[d, "F \circ G"] \\
\mathbb{A}' & \mathbb{B}' \arrow[r, mapsto] & \mathbb{A}' \circ \mathbb{B}'
\end{tikzcd}$$

where $F \circ G$ is defined as follows on the generators:

- $F \circ G\big(A[B_1, \ldots, B_{|\alpha|}]\big) = FA[GB_1, \ldots, GB_{|\alpha|}]$,
- $F \circ G\big(A[g_1, \ldots, g_{|\alpha|}]\big) = FA[Gg_1, \ldots, Gg_{|\alpha|}]$,
- $F \circ G\big(f[B_1, \ldots, B_n]\big) = Ff[GB_1, \ldots, GB_n]$.

It is easy to see that $F \circ G$ is well defined (i.e. it preserves equalities in $\mathbb{A} \circ \mathbb{B}$), thanks to the functoriality of F and G. It is also immediate to verify that $\circ$ is indeed a functor; for example, here is the proof that for $\mathbb{A} \xrightarrow{F_1} \mathbb{A}' \xrightarrow{F_2} \mathbb{A}''$ and $\mathbb{B} \xrightarrow{G_1} \mathbb{B}' \xrightarrow{G_2} \mathbb{B}''$ in, respectively, $\overline{\mathbb{C}\mathrm{at}}_{/\mathbb{G}}$ and $\mathbb{C}\mathrm{at}$, the functors $(F_2F_1) \circ (G_2G_1)$ and $(F_2 \circ G_2)(F_1 \circ G_1)$ coincide on objects:

$$\begin{aligned}
(F_2F_1) \circ (G_2G_1)\big(A[B_1, \dots, B_{|\alpha|}]\big) &= (F_2F_1)A[(G_2G_1)B_1, \dots, (G_2G_1)B_{|\alpha|}] \\
&= F_2(F_1A)[G_2(G_1B_1), \dots, G_2(G_1B_{|\alpha|})] \\
&= (F_2 \circ G_2)\big(F_1A[G_1B_1, \dots, G_1B_{|\alpha|}]\big) \\
&= (F_2 \circ G_2)\Big((F_1 \circ G_1)\big(A[B_1, \dots, B_{|\alpha|}]\big)\Big) \\
&= (F_2 \circ G_2)(F_1 \circ G_1)\big(A[B_1, \dots, B_{|\alpha|}]\big). \qquad \textbf{QED}
\end{aligned}$$

§3.5 *Coda*: conclusions and next steps

The story so far. We have come a long way from [DS70], where dinatural transformations, just discovered, revealed themselves as far from being accommodating, since they fail to compose. We have seen in the Introduction a survey of the literature in Computer Science that involves them, despite their evident problem, and how researchers had to circumvent their lack of compositionality via ad hoc, partial solutions; ultimately, however, dinatural transformations have remained poorly understood. Although Eilenberg and Kelly's work on extranatural transformations [EK66] gave us a hint of the fact that acyclicity is the appropriate requirement for compositionality, there is no hope to use, *mutatis mutandis*, their proof for the case of dinatural transformations: it relies on the crucial hypothesis of absence of ramifications in the graphs.

We have seen how, perhaps surprisingly at first, *Petri Nets*, traditionally used to model computational processes, have provided us with the correct technical tool to connect a purely algebraic condition, the commutativity of a certain hexagon in a category, with a purely geometric one: the acyclicity of a certain graph. Yet, the correspondence dinatural transformations - (certain) Petri Nets is extremely natural: applying the dinaturality condition of a transformation in one of its variable is tantamount to firing the (enabled by construction) transition corresponding to that variable. Such simple observation gave us the key to prove Theorem (1.38), by translating the dinaturality condition of a composite $\psi \circ \varphi$ into a reachability problem between two specific markings. An analysis of the latter revealed that, indeed under the hypothesis of acyclicity, the required reachability condition is always satisfied. The long-standing problem of compositionality of dinatural transformations is, at last, solved in its complete generality.

On a parallel road, we have studied also how dinatural transformations compose *horizontally*. A working definition of horizontal composition exists and is based on the same idea behind the well-known version for natural transformations. Such operation is, as it is proper, associative and unitary. The "classical" interchange law is not satisfied, that is true, but we are confident that a dinatural version of it can be found. This will be the object of further studies.

The two theories of compositionality of dinatural transformations are intertwined in the context of a Godement calculus that generalises the one for ordinary functors and natural transformations. The work towards such a calculus was started, as we saw, by Kelly [Kel72a] for purely covariant functors and generalised natural transformations. Our work in this final chapter was to replicate, as faithfully as possible, Kelly's steps. Once again, the simultaneous presence of both ramifications and U-turns (which are typical of extranaturality conditions) made things more complicated than Kelly's situation. Our notion of *graph* of a transformation is not just a permutation, and is not just a cospan in $\mathbb{F}\mathrm{in}\mathbb{S}\mathrm{et}$ either: it is a whole Petri Net with specified "domain" and "codomain" places along which to compose them. A generalisation of the compositionality result for transformations with (appropriate) "complicated" graphs, that is Theorem (3.31), yields a category $\{\mathbb{B},\mathbb{C}\}$ of functors of mixed variance from $\mathbb{B}$ to $\mathbb{C}$ and partially dinatural transformations between them. $\{-,-\}$ embodies the theory of vertical composition, and its left adjoint $\circ$ will, we believe, entail the theory of horizontal composition instead as indeed happens in Kelly's case.

A look into the future. The ultimate goal to achieve a complete Godement calculus of dinatural transformations is to obtain an appropriate functor over $\mathbb{G}$

$$\mu\colon \{\mathbb{B},\mathbb{C}\} \circ \{\mathbb{A},\mathbb{B}\} \to \{\mathbb{A},\mathbb{C}\}$$

which, *de facto*, realises a *formal* substitution of functors into functors and transformations into transformations as an *actual* new functor or transformation. As in Kelly's case, horizontal composition of dinatural transformations will be at the core, we believe, of the desired functor; the rules of vertical composition are, instead, already embodied into the definition of $\{\mathbb{B},\mathbb{C}\}$.

Such μ will arise as a consequence of proving that $\overline{\mathbb{C}\mathrm{at}/_{\mathbb{G}}}$ is a monoidal closed category, much like Kelly did, by showing that the natural isomorphism (3.59) extends to

$$\overline{\mathbb{C}\mathrm{at}/_{\mathbb{G}}}(\mathbb{A}\circ\mathbb{B},\mathbb{C}) \cong \overline{\mathbb{C}\mathrm{at}/_{\mathbb{G}}}(\mathbb{A},\{\mathbb{B},\mathbb{C}\}).$$

Necessarily then, we will first have to show that the substitution category $\mathbb{A}\circ\mathbb{B}$ is itself an object of $\overline{\mathbb{C}\mathrm{at}/_{\mathbb{G}}}$. Following Kelly's steps, this will be done by extending our functor $\circ\colon \overline{\mathbb{C}\mathrm{at}/_{\mathbb{G}}} \times \mathbb{C}\mathrm{at} \to \mathbb{C}\mathrm{at}$ to a functor

$$\circ\colon \overline{\mathbb{C}\mathrm{at}/_{\mathbb{G}}} \times \overline{\mathbb{C}\mathrm{at}/_{\mathbb{G}}} \to \overline{\mathbb{C}\mathrm{at}/_{\mathbb{G}}},$$

exhibiting $\overline{\mathbb{C}\mathrm{at}/_{\mathbb{G}}}$ as a monoidal category, with tensor $\circ$. To do so in his case, Kelly defined $\mathbb{A}\circ\mathbb{B}$ just as before, ignoring the augmentation on $\mathbb{B}$, and then augmented $\mathbb{A}\circ\mathbb{B}$ using the augmentations of $\mathbb{A}$ and $\mathbb{B}$. In fact, what he did, using the category

$\mathbb{P}$ of permutations, was to regard $\mathbb{P}$ as a category over itself in the obvious way and then to define a functor $P \colon \mathbb{P} \circ \mathbb{P} \to \mathbb{P}$ that computes substitution of permutations into permutations. That done, he set $\Gamma \colon \mathbb{A} \circ \mathbb{B} \to \mathbb{P}$ as a composite

$$\begin{tikzcd} \mathbb{A} \circ \mathbb{B} \arrow[r] \arrow[d, "\Gamma_{\mathbb{A}} \circ \Gamma_{\mathbb{B}}"'] & \mathbb{P} \\ \mathbb{P} \circ \mathbb{P} \arrow[ur, "P"'] & \end{tikzcd}$$

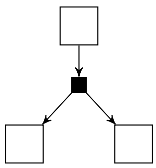
This suggests, as usual, to do the same in our case. Hence, the next step will be to come up with a "substitution" functor

$$S \colon \mathbb{G} \circ \mathbb{G} \to \mathbb{G},$$

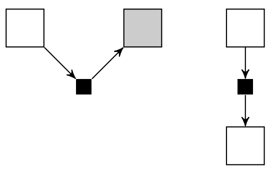
which is tantamount to define an operation of substitution of graphs, and then define $\Gamma \colon \mathbb{A} \circ \mathbb{B} \to \mathbb{G}$ as

(3.60)
$$\begin{tikzcd} \mathbb{A} \circ \mathbb{B} \arrow[r] \arrow[d, "\Gamma_{\mathbb{A}} \circ \Gamma_{\mathbb{B}}"'] & \mathbb{G} \\ \mathbb{G} \circ \mathbb{G} \arrow[ur, "S"'] & \end{tikzcd}$$

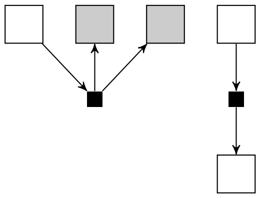
A possible hint to how to do this is given by how we defined the horizontal composition of dinatural transformations in Chapter 2, and what happened to the graphs of the transformations (that is, we look at the special case of $\mathbb{A} = \mathbb{B} = \{\mathbb{C}, \mathbb{C}\}$). Let us look back at Example (2.7). In there, we had the transformations $\delta \colon id_{\mathbb{C}} \to \times$ and $eval \colon H \to id_{\mathbb{C}}$, where $H \colon \mathbb{C}^{[+,-,+]} \to \mathbb{C}$ is defined as $H(X,Y,Z) = X \times (Y \Rightarrow Z)$. Then (the standard representations of) δ and $eval$ constitute elements of $\{\mathbb{C}, \mathbb{C}\}$

$(\delta, 1 \longrightarrow 1 \longleftarrow 2,$  $, K_1) \colon ([+], id_{\mathbb{C}}) \to ([+,+], \times)$

and

$$\left(eval,\ \begin{array}{ccccc} 3 & \longrightarrow & 2 & \longleftarrow & 1 \\ 1 & \longmapsto & 1 & & 1 \mapsto 2 \\ 2 & \longmapsto & 2 & & \\ 3 & \longmapsto & 2 & & \end{array},\right.$$  $, K_1) \colon ([+,-,+], H) \to ([+], id_{\mathbb{C}}).$

When we computed the first horizontal composition of δ and $(eval_{A,B})_{A,B}$, in fact we considered the formal substitution $eval\big[\delta, ([+], id_{\mathbb{C}})\big]$ in $\{\mathbb{C}, \mathbb{C}\} \circ \{\mathbb{C}, \mathbb{C}\}$, which we then realised into the transformation $eval \overset{1}{*} \delta$. The "realisation" part is what the desired functor μ will do, once properly defined. Now, consider, in $\mathbb{G} \circ \mathbb{G}$, the formal substitution $\Gamma(\mathit{eval})\,\big[\Gamma(\delta),[+]\big]$, which is the image of $\mathit{eval}\big[\delta,([+],\mathit{id}_{\mathbb{C}})\big]$ along the functor $\overline{\Gamma} \circ \overline{\Gamma} \colon \{\mathbb{C},\mathbb{C}\} \circ \{\mathbb{C},\mathbb{C}\} \to \mathbb{G} \circ \mathbb{G}$. Since $\mu \colon \{\mathbb{C},\mathbb{C}\} \circ \{\mathbb{C},\mathbb{C}\}$ ought to be a functor over $\mathbb{G}$, we have that $S\big(\Gamma(\mathit{eval})\,\big[\Gamma(\delta),[+]\big]\big)$ should be the graph that $\mathit{eval} \overset{1}{*} \delta$ has, which is



The intuition for it was that we "bent" $\Gamma(\delta)$ into the U-turn that is the first connected component of $\Gamma(\mathit{eval})$. The intuitive idea I intend to pursue, for a general definition of substitution of graphs into graphs, is the following: given two connected graphs N_1, N_2 in $\mathbb{G}$, the graph $S\big(N_1[N_2]\big)$ is the result of subjecting N_2 to all the ramifications and U-turns of N_1. Slightly more in detail, one would have to substitute a copy of N_2 in every *directed path* of N_1. This idea is not original, as it was suggested by Guglielmi, Gundersen and Parigot [GGP] in private communications to implement substitution of *atomic flows*, which are graphs extracted from certain proofs in *Deep Inference* and they look very much like a morphism in $\mathbb{G}$. For an excellent introduction to Deep Inference and atomic flows, we refer the reader to Gundersen's thesis [Gun09].

At the time of writing, I have not looked yet in detail at how to put into a formal, working definition such an intuitive idea, but I am confident it is indeed possible, although far from being trivial. Once that is done, the rest should follow relatively easily, and I would expect that the correct compatibility law for horizontal and vertical composition sought in §2.4 will become apparent, once the substitution functor μ above will be found as part of a monoidal closed structure. The task of defining the notion of substitution of graphs remains, however, the first and foremost obstacle towards a Godement calculus of dinatural transformations; if I am not able to solve this problem, to use Kelly's final words in [Kel72a], *perhaps some colleague will supply my lack of wit.*

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