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A Reduction Paradigm for Multivariate Laws

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Preface

This new research project at IIASA is concerned with modeling technological and organisational change; the broader economic developments that are associated with technological change, both as cause and effect; the processes by which economic agents – first of all, business firms – acquire and develop the capabilities to generate, imitate and adopt technological and organisational innovations; and the aggregate dynamics – at the levels of single industries and whole economies – engendered by the interactions among agents which are heterogeneous in their innovative abilities, behavioural rules and expectations. The central purpose is to develop stronger theory and better modeling techniques. However, the basic philosophy is that such theoretical and modeling work is most fruitful when attention is paid to the known empirical details of the phenomena the work aims to address: therefore, a considerable effort is put into a better understanding of the ‘stylized facts’ concerning corporate organisation routines and strategy; industrial evolution and the ‘demography’ of firms; patterns of macroeconomic growth and trade.

From a modeling perspective, over the last decade considerable progress has been made on various techniques of dynamic modeling. Some of this work has employed ordinary differential and difference equations, and some of it stochastic equations. A number of efforts have taken advantage of the growing power of simulation techniques. Others have employed more traditional mathematics. As a result of this theoretical work, the toolkit for modeling technological and economic dynamics is significantly richer than it was a decade ago.

During the same period, there have been major advances in the empirical understanding. There are now many more detailed technological histories available. Much more is known about the similarities and differences of technical advance in different fields and industries and there is some understanding of the key variables that lie behind those differences. A number of studies have provided rich information about how industry structure co-evolves with technology. In addition to empirical work at the technology or sector level, the last decade has also seen a great deal of empirical research on productivity growth and measured technical advance at the level of whole economies. A considerable body of empirical research now exists on the facts that seem associated with different rates of productivity growth across the range of nations, with the dynamics of convergence and divergence in the levels and rates of growth of income in different countries, with the diverse national institutional arrangements in which technological change is embedded.

As a result of this recent empirical work, the questions that successful theory and useful modeling techniques ought to address now are much more clearly defined. The theoretical work described above often has been undertaken in appreciation of certain stylized facts that needed to be explained. The list of these ‘facts’ is indeed very long, ranging from the microeconomic evidence concerning for example dynamic increasing returns in learning activities or the persistence of particular sets of problem-solving routines within business firms; the industry-level evidence on entry, exit and size-distributions – approximately log-normal; all the way to the evidence regarding the time-series properties of major economic aggregates. However, the connection between the theoretical work and the empirical phenomena has so far not been very close. The philosophy of this project is that the chances of developing powerful new theory and useful new analytical techniques

can be greatly enhanced by performing the work in an environment where scholars who understand the empirical phenomena provide questions and challenges for the theorists and their work.

In particular, the project is meant to pursue an ‘evolutionary’ interpretation of technological and economic dynamics modeling, first, the processes by which individual agents and organisations learn, search, adapt; second, the economic analogues of ‘natural selection’ by which interactive environments – often markets – winnow out a population whose members have different attributes and behavioural traits; and, third, the collective emergence of statistical patterns, regularities and higher-level structures as the aggregate outcomes of the two former processes.

Together with a group of researchers located permanently at IIASA, the project coordinates multiple research efforts undertaken in several institutions around the world, organises workshops and provides a venue of scientific discussion among scholars working on evolutionary modeling, computer simulation and non-linear dynamical systems.

The research will focus upon the following three major areas:

1. Learning Processes and Organisational Competence.
2. Technological and Industrial Dynamics
3. Innovation, Competition and Macrodynamics

Abstract

A *reduction paradigm* is a theoretical framework which provides a definition of structure for multivariate laws, and allows to simplify their representation and statistical analysis. The main idea is to decompose a law as the superposition of a *structural term* and a *noise*, so that the latter can be neglected *without loss of information on the structure*. When the structural term is supported by a lower-dimensional affine subspace, an *exhaustive dimension reduction* is achieved. We describe the reduction paradigm that results from selecting white noises, and convolution as superposition mechanism.

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A Reduction Paradigm for Multivariate Laws

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Introduction

A k -variate law is a complex object whose structure embodies both marginal and joint features. All those features can be translated, to some extent, into geometric characterizations of an iid sample from the law, meant as a cloud of points in \mathbb{R}^k . Dimension does not affect the analysis of marginal features, but as k increases it becomes progressively harder to conceive and articulate the joint ones. For example, how does one conceive and articulate the interdependencies among, say, 10 or 100 coordinate components? One is often forced to neglect high-order interactions, and/or to assume hierarchies among them¹. At the same time, for $k > 3$, the data cannot be visualized as a whole; while graphical tools can still be used to investigate low-dimensional marginals, a *direct* graphical investigation of the joint features is impossible.

Producing inferences in high-dimensional settings can then become complicated and challenging. A large variety of inference methods is available once strong assumptions on the nature of the law are imposed; that is, once a model for the law is chosen (see, among others, M.L. Eaton, 1983, R.J. Muirhead, 1982, and G.A.F. Seber, 1984). But the intuition based on graphical preliminary exploration that should precede the utilization of model-based methods is impaired by the conceptual and practical difficulties mentioned above.

These considerations, among others, justify the quest for simplified representations of multivariate laws, especially ones allowing a *reduction in dimension*. Simplified representations are often developed targeting some (more or less restricted) features of interest. *Exhaustiveness* becomes then an issue; once a *target* has been chosen, the information concerning it ought to be preserved by simplification. More generally, it ought to be clear in what relation the proposed simplified representation is to the target. If exhaustiveness is not always guaranteed, it should be possible to state under what assumptions on the nature of the law it is, and/or to establish to what extent the target is preserved (with or without assumptions).

These issues are very relevant in practice; the last thirty years have witnessed the development of a large number of graphical exploration procedures for high-dimensional data sets. Think for example of Principal Component Analysis, Factor Analysis (see G.A.F. Seber, 1984, and references therein), Projection Pursuit (H.J. Friedman and J.W. Tuckey, 1974, H.J. Friedman, 1987, and D. Cook, A. Buja, J. Cabrera and C. Hurley, 1995), or Grand Tours (D. Asimov, 1985, and A. Buja and D. Asimov, 1986). The theoretical rationale underlying any of these procedures can be interpreted as a simplified representation of the multivariate law from which the data are drawn; targets range anywhere

¹Conditional independence (see A.P. Dawid, 1979) provides a key to articulate interdependencies; a very interesting representation of them through *conditional independence graphs* is given by J. Whittaker, 1990.

from “variability”, to “linear interdependence structure” (correlation among the coordinate components), to “non-linear structure” (defined as departure from normality), to “structure” according to some other definition. Correspondingly, many of the critiques to these procedures can be interpreted in terms of choice of targets, and relations between simplified representations and targets. As we proceed, it will become clear that the simplified representation underlying Factor Analysis is the closest in spirit to the one we will propose. In fact, Factor Analysis differs from the other procedures mentioned above by its reference to a *latent factor* entirely embodying the correlation target.

Our focus will not be on techniques to make inference on simplified representations (“population” objects) based on data from a multivariate law, but on the theoretical premises for these techniques; that is, on how to define targets, and how to develop simplified representations guaranteed to embody them exhaustively.

In Sections 1 and 2, we introduce the concept of *reduction paradigm* and provide definitions and some key results. Section 3 concerns dimension reduction. We conclude with a brief summary and some remarks on inference in Section 4. More details can be found in F. Chiaromonte, 1996.

1 The reduction paradigm

Our analysis will be conducted at the level of laws on \mathbb{R}^k , and we will not distinguish among random vectors with the same distribution. The main idea behind a reduction paradigm is to decompose a law L on \mathbb{R}^k into two terms, one of which does not contribute to the structure (the target) and can therefore be neglected. In other words, the aim is to represent a law as the superposition of a *structural term* and a *noise*, or *no-structure term*. Hence, the specification of a reduction paradigm relies upon

- a definition of absence of structure; that is, a choice of noises
- a choice of superposition mechanism

which, conversely, determine a definition of structure. We have selected *white noises* $N_k(0, \beta I_k)$, $\beta \in \mathbb{R}_+^1$, and *convolution*. Hence, we write

$$L = \Lambda_\beta(L) * N_k(0, \beta I_k) \tag{1}$$

or, in terms of characteristic functions

$$\phi_L(u) = \phi_{\Lambda_\beta(L)}(u) e^{-\frac{\beta}{2}\|u\|^2}, \quad u \in \mathbb{R}^k \tag{2}$$

This is by no means the only possibility, but it is in line with much of the statistical tradition and thus constitutes a very natural first step. In fact, it expresses a situation in which an independent normal error is additively superimposed to the object of interest. One can envision reproducing the whole analysis we are about to develop with different noises and/or superposition mechanisms, though. As far as noises are concerned, one could take, for example, uniforms on hyper-spheres of radius $\rho \in \mathbb{R}_+^1$, or normals with independent components $N_k(0, \text{Diag}(\sigma_i))$, $\sigma \in \mathbb{R}_+^k$. In the first case one maintains the weakly spherical nature of white noises and loses independence of the coordinate components, while in the second case one loses weak sphericity and maintains independence. Regarding superposition, one could explore, for example, multiplicative (instead of additive) schemes.

Before proceeding let us remark that the reduction paradigm we have selected, as well as any other conceivable one, while certainly constituting a *model for decomposing a law*,

does not require strong assumptions on the nature of the law itself. A reduction paradigm can be applied without fixing at the outset a *model for the law*; that is, without assuming at the outset that the law belongs to a given (and possibly finally parameterized) class. Furthermore, our reduction paradigm corresponds to the inverse problem for heat-type diffusion of probability measures (for an easy introduction, see G.M. Wing, 1991, and A. Friedman and W. Littman, 1994). Paradigms resulting from a different choice of noises would correspond to inverse problems for processes with different kernels.

Indexing the structural term by β serves to stress the fact that the decomposition in (1) and (2) is not unique, unless it holds only with $\beta = 0$, and therefore $\Lambda_\beta(L) = L$ itself. Let

$$\mathcal{B}(L) = \left\{ \beta \in \mathbb{R}_+^I \text{ s.t. } \phi_L(\cdot) e^{\frac{\beta}{2}\|\cdot\|^2} \text{ is a ch. fct.} \right\}$$

This subset of \mathbb{R}_+^I is always non-empty, as it must contain 0, and is easily shown to be $\mathcal{B}(L) = [0, \beta_o(L)]$, where $\beta_o(L) = \sup \mathcal{B}(L) = \max \mathcal{B}(L)$. We call the corresponding structural terms

$$\Lambda_\beta(L) \leftrightarrow \phi_L(\cdot) e^{\frac{\beta}{2}\|\cdot\|^2}, \quad \beta \in \mathcal{B}(L)$$

sources, $\beta_o(L)$ *reduction coefficient*, and

$$\Lambda_o(L) \leftrightarrow \phi_L(\cdot) e^{\frac{\beta_o(L)}{2}\|\cdot\|^2}$$

primary source of L . Notice that reduction coefficient and primary source are unique by construction. If $\beta_o(L) = 0$, so that the only (and thus primary) source of L is L itself, we say that the law is *irreducible*. We call it *reducible* otherwise.

All sources share the structure of L , and can be equivalently taken as exhaustive “simplified” representations of the law. The primary source is the one in which no error is superimposed to the structure; that is, the one in which we have pushed simplification as far as possible. Hence, we will select $\Lambda_o(L)$ as simplified representation of L , and write

$$L = \Lambda_o(L) * N_k(0, \beta_o(L)I_k)$$

Let us fix ideas using the normal case as an example:

$$L = N_k \left(\mu, \sum_{j=1}^p \eta_j P_{V_j} + \eta P_V \right)$$

where $\sum_{j=1}^p \eta_j P_{V_j} + \eta P_V$ is the spectral decomposition of the covariance with (distinct) eigenvalues $\eta_1, \dots, \eta_p, \eta$ in decreasing order, and corresponding eigenspaces V_1, \dots, V_p, V . It is easy to show that

$$\phi_L(u) e^{\frac{\beta}{2}\|u\|^2} = \exp \left\{ iu'\mu - \frac{1}{2}u' \left(\sum_{j=1}^p (\eta_j - \beta) P_{V_j} + (\eta - \beta) P_V \right) u \right\}$$

is a characteristic function if and only if $\sum_{j=1}^p (\eta_j - \beta) P_{V_j} + (\eta - \beta) P_V$ is non-negative definite; that is, if and only if $\beta \leq \eta$. Hence, $\beta_o(L) = \eta$ and correspondingly

$$\Lambda_o(L) = N_k \left(\mu, \sum_{j=1}^p (\eta_j - \eta) P_{V_j} \right)$$

It is then clear that a normal is irreducible if and only if the smallest eigenvalue of its covariance is 0; the irreducible k -variate normals are all and only the ones supported by lower dimensional affine subspaces, and they constitute the primary sources of non-singular normals.

Primary sources are irreducible by construction. The class of all irreducible laws on \mathbb{R}^k represents the repertoire of possible structures. The following proposition provides a *sufficient condition for irreducibility*, thereby characterizing part of such repertoire.

Proposition 1.1 *If there exists a measurable set $B \subseteq \mathbb{R}^k$ such that $\text{Leb}(B) > 0$, but $L(B) = 0$, then L is irreducible.*

Proof: Suppose $\beta_o(L) > 0$. Then, for any choice of $v \in \mathbb{R}^k$, $N_k(v, \beta_o(L)I_k)$ is mutually absolutely continuous with respect to Leb . So $\text{Leb}(B) > 0$ implies

$$N_k(v, \beta_o(L)I_k)(B) > 0, \forall v \in \mathbb{R}^k$$

and thus

$$L(B) = \int_{\mathbb{R}^k} N_k(v, \beta_o(L)I_k)(B) \Lambda_o(L)(dv) > 0$$

contradicting our assumption. We can conclude that $\beta_o(L) = 0$, and therefore that L is irreducible. \square

Since we have selected white noises as no-structure terms, reducible laws must be mutually absolutely continuous with respect to the Lebesgue measure, because they “contain” a term that is. As a consequence, all laws having “thick” holes with respect to the Lebesgue measure are irreducible in \mathbb{R}^k . In particular, laws whose affine support $\text{As}(L)$ has dimension $< k$ are irreducible in \mathbb{R}^k ; we saw an instance of this with irreducible normals. So are laws whose closed support $\text{Cs}(L)$ is bounded, regardless of whether the latter is full-dimensional or embedded in a subspace or affine subspace of dimension $< k$.

Notice that existence of an everywhere positive density is *not* enough to guarantee reducibility; again because of our choice of no-structure terms, reducible laws’ densities must have “thick enough” tails. It is easy to show that a law with an everywhere positive density whose tails vanish too fast, at least along some directions, will still be irreducible (see F. Chiaromonte, 1996).

2 Some affine actions, and marginalizations

We will now explore the effects on reduction of some affine actions and of marginalizations.

Proposition 2.1 *Let $\mathcal{T}_{v,r,R}[L]$ be the law of $rRX - v$, where $X \in \mathbb{R}^k$ is any random vector distributed according to L , $v \in \mathbb{R}^k$, $r \in \mathbb{R}^1$, and R is a rotation of \mathbb{R}^k . Then $\beta_o(\mathcal{T}_{v,r,R}[L]) = \beta_o(L)$ and $\Lambda_o(\mathcal{T}_{v,r,R}[L]) = \mathcal{T}_{v,r,R}[\Lambda_o(L)]$.*

Proof: For $r = 0$, the transformation yields a point-mass at $-v$, and the statement is trivially true. Otherwise, using characteristic functions, one has

$$\begin{aligned} \phi_{\mathcal{T}_{v,r,R}[L]}(u) &= e^{-iu'v} \phi_L(rR'u) \\ &= e^{-iu'v} \phi_{\Lambda_o(L)}(rR'u) e^{-\frac{\beta_o(L)}{2} \|rR'u\|^2} \\ &= \phi_{\mathcal{T}_{v,r,R}[\Lambda_o(L)]}(u) e^{-\frac{r^2 \beta_o(L)}{2} \|u\|^2} \end{aligned}$$

so $\beta_o(\mathcal{T}_{v,r,R}[L]) \geq r^2\beta_o(L)$, and $\mathcal{T}_{v,r,R}[\Lambda_o(L)]$ is a source of $\mathcal{T}_{v,r,R}[L]$. But for $r \neq 0$ our transformation is invertible: $\mathcal{T}_{v,r,R}^{-1}[\cdot] = \mathcal{T}_{-v,1/r,R'}[\cdot]$. Hence

$$\begin{aligned}\phi_L(u) &= \phi_{\mathcal{T}_{-v,1/r,R'}\mathcal{T}_{v,r,R}[L]}(u) \\ &= \phi_{\mathcal{T}_{-v,1/r,R'}[\Lambda_o(\mathcal{T}_{v,r,R}[L])]}(u) e^{-\frac{(1/r)^2\beta_o(\mathcal{T}_{v,r,R}[L])}{2}\|u\|^2}\end{aligned}$$

and $\beta_o(L) \geq (1/r)^2\beta_o(\mathcal{T}_{v,r,R}[L])$. We can conclude that $\beta_o(\mathcal{T}_{v,r,R}[L]) = r^2\beta_o(L)$, and therefore that $\mathcal{T}_{v,r,R}[\Lambda_o(L)]$ is indeed the primary source of $\mathcal{T}_{v,r,R}[L]$. \square

The reduction coefficient is not affected by rotations and translations, and is multiplied by the square of a rescaling factor. Thus, rescalings, rotations and translations of L result into corresponding rescalings, rotations and translations of the primary source. In the following, we will use interchangeably the terms *marginalization* and *projection*. Besides the intuitive correspondence, “invariance” under rotations makes this rigorous; the choice of orthonormal basis does not matter.

In our discussion so far, we have considered the reduction of a law L on \mathbb{R}^k in \mathbb{R}^k . The reference to the space is important; laws on \mathbb{R}^k that are entirely concentrated on some subspace can also be meant as laws on such subspace, and reducing them *within the subspace* can produce a different set of sources, a different reduction coefficient and a different primary source. Laws that are entirely concentrated on a subspace of dimension $< k$ are irreducible in \mathbb{R}^k , but they might still be reducible within the subspace.

The noises within a given subspace $S \subseteq \mathbb{R}^k$ are represented by $N_k(0, \beta P_S)$, $\beta \in \mathbb{R}_+^1$. Notation-wise, when considering the reduction of a law \tilde{L} (entirely concentrated on S) within S , we will write $\beta_o(\tilde{L}, S)$, $\Lambda_o(\tilde{L}, S)$, etc.

Proposition 2.2 *Let $\mathcal{M}_S[L]$ be the law of $P_S X$, where $X \in \mathbb{R}^k$ is any random vector distributed according to L , and $S \subseteq \mathbb{R}^k$ is a non-degenerate subspace. Then $\beta_o(\mathcal{M}_S[L], S) \geq \beta_o(L)$ and*

$$\Lambda_o(\mathcal{M}_S[L], S) * N_k(0, \alpha P_S) = \mathcal{M}_S[\Lambda_o(L)]$$

where $\alpha = \beta_o(\mathcal{M}_S[L], S) - \beta_o(L)$. In particular, if $Cs(\Lambda_o(L))$ is bounded, $\beta_o(\mathcal{M}_S[L], S) = \beta_o(L)$ and $\Lambda_o(\mathcal{M}_S[L], S) = \mathcal{M}_S[\Lambda_o(L)]$.

Proof: Using characteristic functions, one has

$$\begin{aligned}\phi_{\mathcal{M}_S[L]}(u) &= \phi_L(P_S u) \\ &= \phi_{\Lambda_o(L)}(P_S u) e^{-\frac{\beta_o(L)}{2}\|P_S u\|^2} \\ &= \phi_{\mathcal{M}_S[\Lambda_o(L)]}(u) e^{-\frac{\beta_o(L)}{2}\|P_S u\|^2}\end{aligned}$$

so $\beta_o(\mathcal{M}_S[L], S) \geq \beta_o(L)$, and $\mathcal{M}_S[\Lambda_o(L)]$ is a source of $\mathcal{M}_S[L]$ within S . Equating the right hand side above with the right hand side of

$$\phi_{\mathcal{M}_S[L]}(u) = \phi_{\Lambda_o(\mathcal{M}_S[L], S)}(u) e^{-\frac{\beta_o(\mathcal{M}_S[L], S)}{2}\|P_S u\|^2}$$

we obtain

$$\phi_{\Lambda_o(\mathcal{M}_S[L], S)}(u) e^{-\frac{\alpha}{2}\|P_S u\|^2} = \phi_{\mathcal{M}_S[\Lambda_o(L)]}(u)$$

where $\alpha = \beta_o(\mathcal{M}_S[L], S) - \beta_o(L)$; that is

$$\Lambda_o(\mathcal{M}_S[L], S) * N_k(0, \alpha P_S) = \mathcal{M}_S[\Lambda_o(L)]$$

Now, assume that $\text{Cs}(\Lambda_o(L))$ is bounded. We need to show that this implies $\alpha = 0$. Suppose $\alpha > 0$. Then, because of the normal term

$$\text{Cs}(\mathcal{M}_S[\Lambda_o(L)]) = \text{Cs}(\Lambda_o(\mathcal{M}_S[L], S) * N_k(0, \alpha P_S)) = S$$

But if $\text{Cs}(\mathcal{M}_S[\Lambda_o(L)])$ is unbounded $\text{Cs}(\Lambda_o(L))$ must be unbounded, too, contradicting our assumption. We can conclude that $\beta_o(\mathcal{M}_S[L], S) = \beta_o(L)$, and therefore that $\Lambda_o(\mathcal{M}_S[L], S) = \mathcal{M}_S[\Lambda_o(L)]$. \square

The reduction coefficient (within S) of the marginal of L , must be greater than or equal to $\beta_o(L)$. Correspondingly, the marginal of $\Lambda_o(L)$ is a source (within S) of the marginal of L , even though not necessarily the primary one. Under the assumption that $\text{Cs}(\Lambda_o(L))$ is bounded, the reduction coefficients coincide. Thus, the marginal of $\Lambda_o(L)$ is indeed the primary source (within S) of the marginal of L . In other words, under the boundedness assumption the reduction coefficient is not affected by marginalizations (projections), and therefore marginalizations of L result into corresponding marginalizations of the primary source.

3 The structural subspace, and exhaustive dimension reduction

The affine support of $\Lambda_o(L)$ represents the smallest affine subspace supporting the structure of L , as defined by our reduction paradigm. We call the subspace underlying it the *structural subspace* of the law

$$S_o(L) = \text{As}(\mathcal{T}_v[\Lambda_o(L)])$$

where v is any element of $\text{Cs}(\Lambda_o(L))$, and \mathcal{T}_v stands for $\mathcal{T}_{v,1,I_k}$. Correspondingly, we call

$$d_o(L) = \dim(S_o(L))$$

the *structural dimension*. Whenever $d_o(L) < k$, our (exhaustive) simplified representation of L implies a drop in dimension.

This allows us to define an *exhaustive dimension reduction*. Let us see how. Suppose we know $v \in \text{Cs}(\Lambda_o(L))$. Then, the exercise of identifying $\Lambda_o(L)$ is equivalent to that of identifying $\Lambda_o(\mathcal{T}_v[L])$. In fact, by Proposition 2.1

$$\Lambda_o(L) = \mathcal{T}_{-v} \mathcal{T}_v[\Lambda_o(L)] = \mathcal{T}_{-v}[\Lambda_o(\mathcal{T}_v[L])]$$

Now, suppose $S_o(L)$ is known, too. Then, we can marginalize $\mathcal{T}_v[L]$ to $S_o(L)$ preserving all the information relative to the structure, as defined by our reduction paradigm. In fact, again by Proposition 2.1

$$S_o(L) = \text{As}(\mathcal{T}_v[\Lambda_o(L)]) = \text{As}(\Lambda_o(\mathcal{T}_v[L]))$$

so that indeed $\Lambda_o(\mathcal{T}_v[L])$ is supported by the structural subspace², and

$$\Lambda_o(\mathcal{T}_v[L]) = \mathcal{M}_{S_o(L)}[\Lambda_o(\mathcal{T}_v[L])]$$

²Notice that, by Proposition 2.1, the structural subspace is invariant under translations of L : $S_o(\mathcal{T}_v[L]) = S_o(L)$. When translating by an element of $\text{Cs}(\Lambda_o(L))$ we obtain a law which is actually supported by the subspace itself, instead of an affine subspace parallel to it.

But then, by Proposition 2.2

$$\Lambda_o(\mathcal{T}_v[L]) = \Lambda_o(\mathcal{M}_{S_o(L)} \mathcal{T}_v[L], S_o(L)) * N_k(0, \alpha P_{S_o(L)})$$

$\Lambda_o(\mathcal{T}_v[L])$ is a source for $\mathcal{M}_{S_o(L)} \mathcal{T}_v[L]$ within $S_o(L)$. Furthermore, if we can assume $\text{Cs}(\Lambda_o(L))$, and therefore of $\text{Cs}(\Lambda_o(\mathcal{T}_v[L]))$, to be bounded

$$\Lambda_o(\mathcal{T}_v[L]) = \Lambda_o(\mathcal{M}_{S_o(L)} \mathcal{T}_v[L], S_o(L))$$

that is, $\Lambda_o(\mathcal{T}_v[L])$ is the primary source of $\mathcal{M}_{S_o(L)} \mathcal{T}_v[L]$ within $S_o(L)$. This gives an even stronger meaning to the exhaustiveness of our marginalization; not only no structural information is lost marginalizing $\mathcal{T}_v[L]$, but the exercise of identifying $\Lambda_o(\mathcal{T}_v[L])$ (to be performed in k dimensions) would actually correspond to that of identifying $\Lambda_o(\mathcal{M}_{S_o(L)} \mathcal{T}_v[L], S_o(L))$ (to be performed in –possibly– smaller dimension).

The question becomes then how to identify translation term and structural subspace. Clearly, existence of finite moments of a certain order for L implies that of the corresponding moments for $\Lambda_o(L)$. If L admits finite first order moments $\text{E}(\Lambda_o(L)) = \text{E}(L)$, and one can take as translation term $v = \text{E}(L) \in \text{Cs}(\Lambda_o(L))$. Furthermore, if L admits finite second order moments, structural subspace and structural dimension can be related to the spectral decomposition of the covariance. $\text{Ind}(\cdot)$ is the indicator function of the argument condition.

Proposition 3.1 *Suppose L admits finite second order moments. Let $\eta(L)$ be the smallest eigenvalue of $\text{Cov}(L)$, and $V(L)$ the corresponding eigenspace. Then $\beta_o(L) \leq \eta(L)$ and*

$$S_o(L) = V(L)^\perp \oplus \text{Ind}(\eta(L) - \beta_o(L) > 0)V(L)$$

with $d_o(L) = k - \text{Ind}(\eta(L) - \beta_o(L) > 0)\dim(V(L))$.

Proof: Writing $\text{Cov}(L) = \sum_{j=1}^p \eta_j(L) P_{V_j(L)} + \eta(L) P_{V(L)}$ one has

$$\begin{aligned} \text{Cov}(\Lambda_o(L)) &= \text{Cov}(L) - \beta_o(L) I_k \\ &= \sum_{j=1}^p (\eta_j(L) - \beta_o(L)) P_{V_j(L)} + (\eta(L) - \beta_o(L)) P_{V(L)} \end{aligned}$$

$\beta_o(L) \leq \eta(L)$ is implied by non-negative definiteness of $\text{Cov}(\Lambda_o(L))$. The expression for the structural subspace derives from the fact that for any law with finite second order moments $\text{Span}(\text{Cov}(\cdot))$ gives the subspace underlying $\text{As}(\cdot)$. A drop in dimension occurs if and only if $\beta_o(L) = \eta(L)$, and when it occurs $d_o(L) = k - \dim(V(L))$, where $\dim(V(L))$ represents the multiplicity of $\eta(L)$. \square

Given the spectral decomposition of $\text{Cov}(L)$, the above proposition provides an upper bound for the reduction coefficient and a lower bound for the structural subspace; namely, the smallest eigenvalue of $\text{Cov}(L)$ and the orthogonal complement of its eigenspace. The spectral decomposition of $\text{Cov}(L)$ is not enough to identify the structural subspace, though; we still need to know whether the reduction coefficient is strictly smaller than, or equal to, the smallest eigenvalue.

Remember that for a normal law $\beta_o(L) = \eta$. Thus, under normality the drop in dimension always occurs, and one has $S_o(L) = V^\perp$ with $d_o(L) = k - \dim(V) \leq k - 1$. It is important to remark that coincidence of $\beta_o(L)$ with $\eta(L)$ (and therefore the drop in

dimension) is not guaranteed in general. Identifying the reduction coefficient with the smallest eigenvalue of the covariance can actually be very misleading. Take for example a “noisy” uniform on a hyper-cube $L = Un([-θ, θ]^k) * N_k(0, τI_k)$, $θ, τ ∈ ℝ_+^1 \setminus \{0\}$. For such a law one has $β_o(L) = τ < \frac{θ^2}{2} + τ = η(L)$ and $S_o(L) = ℝ^k \supset \{0\} = V(L)^\perp$, as the multiplicity of $\frac{θ^2}{2} + τ$ is k .

4 A brief summary with some remarks on inference

The ultimate aim within the framework defined by a reduction paradigm is that of making inference about the (unobservable) $Λ_o(L)$, which constitutes our simplified and yet exhaustive representation of the original law. As we have seen, if we can assume that L is normal, $β_o(L) = η$ and

$$Λ_o(L) = N_k \left(\mu, \sum_{j=1}^p (\eta_j - \eta) P_{V_j} \right)$$

which is entirely identified through the mean vector and the spectral decomposition of the covariance. Hence, if the data are consistent with normality, we could estimate the primary source based on estimates of those. Also, if the data can be transformed to approximate normality, the primary source could be estimated on the transformed scale. What can we do when the data contradicts normality on the original scale, and fails to approximate it also after applying normalizing transformations?

An intermediate aim is constituted by estimating a $v ∈ Cs(Λ_o(L))$ and $S_o(L)$. Besides the intrinsic interest, if indeed our simplified representation implied a drop in dimension, having such estimates would allow us to perform an exhaustive dimension reduction.

Given the results in the previous sections, we are clearly at an advantage if we are willing to assume boundedness of $Cs(Λ_o(L))$. Since the latter implies existence and finiteness for all the moments of L , we would have $E(L) ∈ Cs(Λ_o(L))$ and (Proposition 3.1)

$$S_o(L) = V(L)^\perp \oplus \text{Ind}(\eta(L) - \beta_o(L) > 0)V(L)$$

Furthermore, we could restrict inference on the reduction coefficient to any arbitrarily small non-degenerate subspace. In fact, by Proposition 2.2

$$\beta_o(L) = \beta_o(\mathcal{M}_t[L], t)$$

where t is any line in $ℝ^k$. Thus, we could take $\hat{E}(L)$ as translation term, and produce an estimate of the structural subspace based on $\hat{\eta}(L)$, $\hat{V}(L)$ and $\hat{\beta}_o(\mathcal{M}_t[L], t)$. Methods to estimate $E(L)$, and, less trivially, $\eta(L)$ and $V(L)$, exist in the literature and are not affected by how large k is (see M.L. Eaton and D. Tyler, 1994, and E. Bura, 1996).

As a matter of fact, in order to produce an estimate of the structural subspace we would only have to assess, selecting for example $t \subseteq \hat{V}$, whether $\beta_o(\mathcal{M}_t[L], t)$ is strictly smaller than, or coincides with $\text{var}(\mathcal{M}_t[L]) = \eta(L)$. This, in turn, is equivalent to assessing whether $\mathcal{M}_t[L]$ is a 1-dimensional normal.

Under the assumption that $Cs(Λ_o(L))$ is bounded, we also have that

$$Λ_o(L) = \mathcal{T}_{-v}[\Lambda_o(\mathcal{M}_{S_o(L)} \mathcal{T}_v[L], S_o(L))]$$

Hence, we could center the data cloud translating it by $\hat{E}(L)$, and restrict any further analysis to the projection of the centered cloud onto $\hat{S}_o(L)$; all the structural features (except for location, which is captured by $\hat{E}(L)$) would be preserved. If indeed $\hat{d}_o(L) = \dim(\hat{S}_o(L)) < k$, we would have achieved an exhaustive dimension reduction.

References

- Asimov D. (1985). The Grand Tour: a tool for viewing multidimensional data. *SIAM Journal of Scientific and Statistical Computing* **6**, 128–143.
- Buja A., Asimov D. (1986). Grand Tour methods: an outline. *Computing Science and Statistics* **17**, 63–67.
- Bura E. (1996). *Dimension Reduction via Inverse Regression*. Ph.D. Dissertation, School of Statistics, University of Minnesota.
- Chiaromonte F. (1996). *A Reduction Paradigm for Multivariate Laws*. Ph.D. Dissertation, School of Statistics, University of Minnesota.
- Cook D., Buja A., Cabrera J., Hurley C. (1995). Grand Tour and Projection Pursuit. *Journal of Computational and Graphical Statistics* **v.4, n.3**, 155–172.
- Dawid A.P. (1979). Conditional independence in statistical theory. *Journal of the Royal Statistical Society ser.B*, **41**, 1–31.
- Eaton M.L. (1983). *Multivariate Statistics*. Wiley & Sons, New York.
- Eaton M.L., Tyler D. (1994). The asymptotic distribution of singular values, with applications to canonical correlations and correspondence analysis. *Journal of Multivariate Analysis* **v.50, n.2**.
- Friedman A., Littman W. (1994). *Industrial Mathematics: a course in solving real world problems*. SIAM, Philadelphia.
- Friedman H.J. (1987). Exploratory Projection Pursuit. *Journal of the American Statistical Association* **82**, 249–266.
- Friedman H.J., Tuckey J.W. (1974). A Projection Pursuit algorithm for exploratory data analysis. *IEEE Transactions on Computers ser.C*, **23**, 881–889.
- Muirhead R.J. (1982). *Aspects of Multivariate Statistical Theory*. Wiley & Sons, New York.
- Posse C. (1995). Tools for two-dimensional exploratory Projection Pursuit. *Journal of Computational and Graphical Statistics* **v.4, n.2**, 83–100.
- Seber G.A.F. (1984). *Multivariate Observations*. Wiley & Sons, New York.
- Whittaker J. (1990). *Graphical Models in Applied Multivariate Statistics*. Wiley & Sons, New York.
- Wing G.M. (1991). *A Primer on Integral Equations of the First Kind: the Problem of Deconvolution and Unfolding*. SIAM, Port City Press.