

# DIPLOMARBEIT

Titel der Diplomarbeit

## CRITICAL PHENOMENA AND DYNAMICAL PHASE TRANSITIONS IN BOOLEAN NETWORKS

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Verfasser: Lukas GEYRHOFER Studienrichtung: A 411 Diplomstudium Physik UniStG Betreuer: Doz. Dr. Karl E. KÜRTEN

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*Hofstadter's Law: It always takes you longer than expected, even when you take into account Hofstadter's Law.*

Douglas Hofstadter, GEB

#### **Abstract**

Boolean Networks have been used as highly non-linear dynamical models in biology, sociology and economics. Together with the introduction as gene regulatory networks in the late 1960s, Stuart Kauffman established two different phases of the dynamics in Boolean Networks: the ordered phase, where eventual perturbations vanish rather quickly, and the disordered phase, where a small perturbation might spread over the whole network. In the 1980s statistical considerations by Bernard Derrida and coworkers yielded analytical results for the dynamical behavior of those networks, especially a statistical characterization of the critical condition for this phase transition was obtained. In this work, recent developments have been compiled and presented in a rather formal way, with special emphasis on this critical condition, which is important, because many networks in nature are believed to be close to this dynamical phase transition. An approach for the derivation of coupled iteration equations of the macroscopic parameters magnetization and Hamming distance is explained for arbitrary mixtures of Boolean functions and distribution of in-degrees. From these iteration equations the critical condition is derived, showing that this condition only depends on the average sensitivity of the mixture of Boolean functions. Furthermore, the equivalence of using higher sensitivities in the construction of the polynomial for the Hamming distance is established to be a restriction to the magnetization, which cannot be maintained over time, and therefore fails to predict the fixed point in the Hamming distance observed in computer simulations.

In the second part of this work, this formalism has been applied to Linear Threshold functions. They are a subclass of all possible Boolean functions and an explicit projection to Boolean functions is given. Complete phase diagrams have been calculated for several different Boolean Networks with all functions being Linear Threshold functions, where an two parameters have been included, the threshold  $h$  and the asymmetry  $p$  in the distribution of weights, which is an additional degree of freedom compared to several earlier publications. Finally, it has been proven for a simple mixture of Linear Threshold functions, that the parameter region corresponding to the ordered phase actually grows with increased connectivity  $K$ , and the parameter region of the disordered phase shrinks to a single value in the limit  $K \to \infty$ . This is contrary to the Kauffman model, where the opposite behavior is observed: the parameter region of the disordered phase spans the complete interval in the limit  $K \to \infty$ . This is an interesting result, because biological networks usually have a connectivity larger than the critical value  $K_c = 2$  in the (unbiased) Kauffman model, so that a more realistic topology could be imposed on the BN, where also nodes with a higher in-degree occur, without being restricted to extreme values of the external parameters.

#### Zusammenfassung

Boole'sche Netzwerke werden als hoch nicht-lineare dynamische Modelle in der Biologie, Soziologie und Wirtschaftwissenschaften verwendet. Schon bei der Einfuhrung als ¨ genetische Regelnetzwerke in den späten 1960ern durch Stuart Kauffman wurden zwei Phasen in der Dynamik unterschieden: eine geordnete Phase, wo mögliche Störungen rasch verschwinden, und die ungeordnete Phase, wo sich anfänglich kleine Störungen auf das ganze Netzwerk ausbreiten können. In den 1980ern führten statistische Überlegungen von Bernard Derrida und Kollegen zu einigen analytischen Ergebnissen für das dynamische Verhalten dieser Netzwerke, im Speziellen wurde eine statistische Charakterisierung der Kritischen Bedingung für den Phasenübergang abgeleitet. In dieser Arbeit wurden einige neuere Ergebnisse und Entwicklungen gesammelt und formal prasen- ¨ tiert, wobei ein Hauptaugenmerk auf die Kritische Bedingung gelegt wurde. Diese ist für viele Netzwerke in der Natur von Bedeutung, da deren Dynamik oft in der Nähe des Phasenübergangs liegt. Die Ableitung der gekoppelten Iterationsgleichungen für die beiden makroskopischen Parameter Magnetisierung und Hammingdistanz wird erklärt für beliebige Mischungen von Boole'schen Funktionen und Verteilungen von Verknüpfungsgraden. Aus diesen Iterationsgleichungen wird die Kritische Bedingung berechnet, und gezeigt, dass diese nur von der gemittelten "Empfindlichkeit" der Verteilung der Funktionen abhängt. Weiters wird gezeigt, dass das Verwenden von "Höheren Empfindlichkeiten" in der Iterationsgleichung der Hammingdistanz äquivalent ist zu einer Beschränkung der Magnetisierung, die aber nicht uber die Zeit aufrecht erhalten werden kann, und daher ¨ einen falschen Fixpunkt in der Hammingdistanz voraussagt.

Im zweiten Teil der Arbeit wird dieser Formalismus auf Lineare Schwellwertfunktionen angewendet. Lineare Schwellwertfunktionen sind eine kleine Untermenge aller moglichen ¨ Boole'schen Funktionen und eine explizite Projektionsgleichung auf diese allgemeinen Funktionen ist in dieser Arbeit angegeben. Fur verschiedene Boole'sche Netzwerke wurden ¨ Phasendiagramme berechnet, wobei zwei verschiedene Parameter verwendet wurden, der Schwellwert  $h$  und die Asymmetrie  $p$  in der Verteilung der Gewichte, was ein zusätzlicher Parameter im Vergleich mit einigen fruheren Arbeiten ist. Zum Schluss wird bewiesen, ¨ dass für eine einfache Mischung aus Linearen Schwellwertfunktionen der Parameterbereich der geordnete Phase mit steigender Konnektivität  $K$  wächst, und der Parameterbereich der ungeordnete Phase auf einen einzigen Wert zusammenschrumpft im Grenzübergang  $K \to \infty$ . Dieses Verhalten ist konträr zum Kauffman-Modell, wo das gegenteilige Verhalten beobachtet wird: der Parameterbereich der ungeordneten Phase nimmt das ganze Intervall im Grenzübergang  $K \to \infty$  ein. Das ist ein interessantes Ergebnis, weil biologische Netzwerke normalerweise eine höhere Verknüpfungsrate als den kritischen Wert  $K_c = 2$ im ursprünglichen Kauffman-Modell haben, so dass eine realistischere Topologie für das Boole'sche Netzwerk verwendet werden kann. In diesen realistischeren Topologien können dann auch höhere Verknüpfungsraten auftreten, ohne Extremwerte der Modellparameter annehmen zu müssen

## **Contents**







## 0 Introduction

How can biological processes be modeled? Questions about the nature around us have driven scientists for centuries. However, only in the last decades (maybe already starting with the discovery of the structure of the DNA molecule in 1953) it has become feasible to model a few biological processes from first principles with the aid of computers, because the information load in biological systems is in most cases just overwhelming. Most biological systems exhibit highly non-linear interactions, where an analytical treatment if often almost impossible. However, there are a few systems where this can actually be done. In his seminal paper, Stuart Kauffman proposed Boolean Networks as a simple model for gene regulatory processes [Kauffman, 1969], which is just an example for the wealth of biological and complex models emerging lately.

A brief synopsis of gene regulation might be appropriate here. The process of gene expression and regulation described here is vastly simplified, a more detailed explanation can be found in almost any textbook on molecular biology, e.g. [Alberts et al., 2002]. DNA is a double helical molecule, with two backbone strands, consisting of phosphate and sugar. On each of the sugars a base is attached. There are four different bases (adenine, thymine, guanine and cytosine), where two are complementary to each other (A-T, G-C). Only those two can be paired up on opposite positions on the two strands. The backbone winds tightly around the bases in the center, protecting them from unwanted chemical reactions. Between those windings, a major and minor groove exists, where each of the pairings of bases can still be distinguished, due to the chemical nature of parts exposed.

The basic unit of information is a single base pair, which are grouped to bigger units, genes, which constitute logically coherent units. Often such genes encode a single protein. To read out the information stored on the DNA, the helix is locally unfolded, the two strands separated and one of them is complemented by a RNA molecule, which is synthesized base by base using the complementarity of the 4 different bases. The RNA polymerase is the protein complex catalyzing this synthesis. The new RNA molecule is separated from the DNA and in most cases it attaches to a ribosome. There it is read in triplets of bases, where each triplet is translated into a single aminoacid. The aminoacids from consecutive triplets are covalently bonded to each other, forming a (long) chain. This aminoacid sequence folds itself (or with help of other proteins) into its final structure, then called a protein. Proteins constitute the tools for (almost) every task within a cell. These tasks include of course metabolism, motility, structural functions and several others, but also a large part is involved in inter- and intracellular signaling. Some of those signaling proteins, the "transcription factors" (TF), have a special folded structure, which not only fits exactly into the major or minor groove on the DNA, but also binds only to a specific sequence of bases on the DNA. TF binding affects genes in the vicinity of the binding site.

The activity of the RNA polymerase complex could probably increase, when a TF induces a structural change, which then exposes certain important parts of the DNA. However, the binding of a TF could also sterically circumvent a coupling of the transcription complex, and therefore the proteins encoded on this section of DNA are not expressed. Each TF could also be affected by direct or indirect interaction with other proteins, which might be needed for the TF to work. Any interaction of certain proteins with one of the complexes involved in either transcription or translation, as well as any intermediate process, could be possible and have an effect on the amount of protein expressed.

In Boolean Networks this rather complicated processes are abstracted to a bare minimum. Only parts of the genome, which are important for the regulation of other genes are considered. Furthermore, all elements are then just modeled by a simple yes/no choice. So a gene is either expressed or not, without accounting for the actual amount of the protein, encoded by the gene, present in the cell. The specific process (transcription, translation, etc.) where the actual interaction occurs, is not considered, only a combination of all genes having an effect determine the gene to be either expressed or not. This interdependency induces a non-linear dynamic on the regulatory network.

A big part of the real system is missing in a Boolean Network. In a Boolean Network no interactions with any signals from outside the modeled (small) network are considered. They are modeled to form self-consistent dynamical systems, going on infinitely. Each of the stable dynamical states, the "attractors", in the Boolean Network is thought to be a (cyclic) gene expression pattern in a cell. These patterns can be interpreted as different cell types, as each cell has the complete information (DNA) inside, however, only parts of the genome are actually expressed. The interaction with the environment is introduced, when looking at the stability of such a dynamical state. Two different phases of behavior can be distinguished if small, random perturbations are imposed on the states of the genes. Either the dynamic behaves completely chaotically and the stable state is left, or after a short transient time the original state is reached again. For biological systems both extremes are unfavorable. When the slightest perturbation drives the cell to behave completely erratically, this is clearly not very competitive. On the other hand, if the dynamical state never changes, no matter how strong the signals from outside, this might also cause problems in a changing environment, because it cannot adapt to meet current conditions better. Hence the ideal behavior would be something intermediate, close to the transition between the two phases. The main aim of this work is to mathematically characterize this phase transition.

However, the methods used in this work are still quite limited. It should be clear, that a statistical treatment, which is used here, does not allow to calculate specific features of the regulatory networks of single organisms, it just enables the general understanding of such systems on a more global scale.

Besides this biological viewpoint, Boolean Networks have been used lately to model any complex dynamical system, e.g. in economics and social sciences. But they are also of pure mathematical interest, especially since a few properties can be derived analytically.

This work is organized as follows. The first chapter explains the basic concepts of Boolean Networks, including the phase transition between the ordered and disordered dynamics. In chapter 2 a statistical approach, the Mean Field approximation, is developed, where several quantities in the dynamics could be derived analytically. Furthermore the explicit condition for the phase transition is stated and linked to other concepts. These methods are applied to Linear Threshold functions, a special subclass of all possible functions, in chapter 3.

## 1 Boolean Networks

## 1.1 Preliminary definitions

To introduce the concepts of Boolean Networks (BN) it is convenient to do so via a graph theoretical framework. A few definitions should suffice to explain the basic concepts. A more elaborate introduction to Graph theory can be found e.g. in the textbook of Bollobás [Bollobás, 1998], where the following definition of a graph is taken from:

**Definition 1.1.** A **graph** G is an ordered pair of disjoint, discrete sets  $G = (V, E)$  such that E is a subset of the set of unordered pairs of V,  $E \subseteq V \times V$ . The set V is the set of **vertices** *and E is the set of edges. The size of the graph is the number of edges, the order of the graph is the number of vertices.*

In this thesis vertices are denoted by numbers. If any vertex is meant, it is denoted by a lower-case Latin letter, i.e. *i*, *j*, etc. Using this convention a simple example for a graph would be a triangle: three points (the set of vertices)  $\{1, 2, 3\}$  connected via the three edges  $\{12, 23, 32\}$ . In this case the edges are not directed, i.e. the edge 12 can be identified with 21. However, in the context of Boolean Networks, it is important to distinguish between an incoming and outgoing connection/edge on a vertex. This leads to the definition of a directed graph:

**Definition 1.2.** A directed graph is a graph  $G = (V, E)$ , where the set of edges E consists *of ordered pairs. For pairs*  $i, j \in V$  *ij and ji denote different edges in E. The edge ij is a connection from the vertex* i *to* j*, and* ji *is an edge from* j *to* i*.*

Furthermore the notion of the degree of a vertex should be defined to be able to classify them later:

**Definition 1.3.** In a graph  $G = (V, E)$ , the **degree**  $k_i$  of a vertex  $i \in V$  *is the number of other vertices connected to i by an edge*  $ij \in E$ *:*  $k_i = |\{ij : j \in V, ij \in E\}|$ *. If the graph is* directed, one can distinguish the in-degree  $k_i^{(in)}$  and the out-degree  $k_i^{(out)}$  of a vertex. This *are the edges connecting to a vertex* i*, or coming from* i*, respectively. The values are given*  $b$ *y*  $k_i^{(in)} = |\{ji : j \in V, ji \in E\}|$  *and*  $k_i^{(out)} = |\{ij : j \in V, ij \in E\}|$ 

In Boolean Networks particularly the in-degree is of interest for many purposes. Therefore, if the degree is mentioned, usually only the in-degree is meant and the convention is used to denote the in-degree of a vertex  $i$  like the degree:  $k_i^{(in)}\equiv k_i.$  If the distinction between in-degree and out-degree is to be made, it will be mentioned in the text and the more explicit symbols  $k_i^{(in)}$  and  $k_i^{(out)}$  will be used.

Moreover a few additional definitions are needed, which will be used later in explaining the structure of the state space.

**Definition 1.4.**  $A \cdot i$ -j-path in a graph  $G = (V, E)$  is a sequence of vertices  $(i = z_0, z_1, \ldots, z_n = j)$ ,  $z_k \in V$ ,  $k \in \{1, \ldots, n\}$  where all vertices in the sequence are connected with edges  $z_i z_{i+1} \in E$ .

Equipped with this definition the concept of a connected graph can be introduced.

**Definition 1.5.** *A graph*  $G = (V, E)$  *is called connected, if for each*  $i, j \in V$  *there exists a* i*-*j*-path between those vertices. A graph is disconnected if it is not connected.*

**Definition 1.6.** *A closed path is a path*  $(i = z_0, z_1, \ldots, z_n = j)$  *with*  $i = j$ *.* 

**Definition 1.7.** *A tree is a connected graph*  $G = (V, E)$  *where for each*  $i, j \in V$  *only a single* i*-*j*-path exists.*

As there is only one  $i-j$ -path, a tree can not have any closed paths in its structure, since a closed path has always two different paths between any vertices in it. When visualizing a tree, its name gets clear, as a single node can be chosen as the "root" of the tree, with all edges and vertices branching out from this root vertex.

These few definitions suffice to introduce the concept of Boolean Networks in the next section.

## 1.2 Boolean Networks

**Definition 1.8.** *A* **Boolean Network (BN)** is a directed graph  $G = (V, E)$  with exactly N *vertices (or in the context of BN often called "nodes"), where each node i has a variable*  $x_i$ *with values in a discrete set M (e.g. spin-like*  $M = \{-1,1\}$ *). A function*  $f_i : M^{k_i} \to M$  *is*  $\emph{defined on each node.}\emph{k}_{i}$  is here the in-degree of node  $i.$ 

*A time-discrete dynamic is given by evaluating the functions*  $f_i$  *on each node i and apply*ing this result to  $x_i$ :

$$
x'_{i} = f_{i}(x_{i_{1}}, \ldots, x_{i_{k}}), \quad i = 1, \ldots, N,
$$
\n(1.1)

 $where \{i_1, \ldots, i_k\} = \{j : ji \in E\}$ . Hence the function  $f_i$  depends only on the  $k_i$  variables  $x_{i_j}$  to  $\bm{w}$ hich node  $i$  is connected. The prime in  $x_i'$  denotes the following timestep.

Many publications use the notation of explicit time-dependence of each node  $x_i(t)$ , where the dynamics equations reads  $x_i(t + 1) = f_i(\mathbf{x}(t))$ . As the dynamics depends only on the previous timestep but not on any other past timesteps, the notation is held clean, and only the prime in  $x_i^\prime$  is used for distinguishing between two following timesteps, not accounting for the exact position in time of those two consecutive timesteps.

From this definition it should be clear, that the dynamics of a BN are a Markov chain (of first order), exhibiting a highly nonlinear dynamic. To simplify the notation following convention is introduced:

 $\bf{Definition~1.9.}$  The variables  $(x_{i_1},\ldots,x_{i_k})$  of a specific function  $f_i$  are called input or input *tuple and will henceforth be denoted by*

$$
\mathbf{x} = (x_{i_1}, \dots, x_{i_k}).\tag{1.2}
$$



Figure 1.1: Example of a Boolean Network. The directed graph has  $N = 100$  nodes, where each node has exactly 3 incoming edges, i.e.  $\forall i:~k_i^{(in)}=3.$ 

### *The size of this tuple* x *is* k<sup>i</sup> *and therefore dependent on the context in which it is used, as the in-degree can vary from node to node.*

The choice of the (two) elements in  $M$  is just convention. Depending on the application and the calculations, either  $M = \{-1, 1\}$ ,  $M = \{0, 1\}$  or even the abstract symbols  $M =$ {+, −} are used. Sometimes one results in simpler formulas, sometimes a different one and the choice mainly depends on the use and abuse of notation in these cases. For example sometimes those symbols in  $M$  are used as elements of the real numbers in certain coefficients, which will be seen in the following chapters. In the context of BN the choice  $M = \{0, 1\}$  is the most convenient, and it will be used when introducing BNs in this chapter. However, the main focus of the subsequent chapters is on Linear Threshold functions, so the more convenient choice (in this case)  $M = \{-1, 1\}$  will be used. In this work those different values in  $M$  should be identified, so

$$
-1 \equiv 0 \equiv -,\tag{1.3a}
$$

$$
+1 \equiv 1 \equiv +.\tag{1.3b}
$$

The set  $M$  can also be extended to include more than just two elements. Such extensions resemble the Potts model in statistical physics, where also spin-like variables with more than 2 values are considered. Most of the formulas in the second chapter extend straightforward in this case.

Definition 1.8 leaves a few issues open, so in the following pages this definition will be fleshed out, to obtain a working model. Two of the main points will be dealt with in separate sections, viz. the Boolean Functions  $f_i$  in section 1.4 and the topology of the graph, i.e. how the degrees  $k_i$  are distributed, in section 1.3.

Another important point is the update order of the nodes. It should be quite clear, that the dynamics of a BN is affected by the order of updating each node. Two main methods can be distinguished: simultaneous/synchronous or sequential/asynchronous update order. If a simultaneous update order is used, all functions on the nodes are iterated at the same time, i.e. each node is updated using the states of all neighboring nodes from the previous iteration. A timestep is then defined as one of those iteration cycles, with each node updated once. In the other method, sequential update order, the notion of a timestep is not defined as clear as in the latter. The function on each node is updated separately, i.e. using all the values of already updated nodes. If now each node to be updated is chosen randomly from some distribution on all nodes, its obvious that not each node might receive an update until a node is chosen a second time, so its hard to speak of an global timestep as before. This would be called a stochastic update scheme. However, if the constraint of so-called "epochs" is introduced, where each node in the network is updated once before the cycle starts anew, a timestep in the simultaneous update order is more or less the same as such an "epoch", at least in the Mean Field approximation introduced in the next chapter.

A classification of all possible update schemes is found in [Gershenson, 2003]. According to this classification, all BN considered here in this work are CRBN ("Classical Random Boolean Networks"), using a sequential update order. So every time the acronym BN is used, it should be replaced by CRBN.

#### 1.2.1 Global formulation of the dynamics

The dynamics on BNs introduced in definition 1.8 with equation (1.1) can also be viewed in a global fashion. Whereas (1.1) could be called local, because all functions are defined locally on each node, the global description defines the function on the complete BN. The advantage of this is an easier description of some of the properties and concepts in a BN linked to the order-disorder phase transition introduced later in this chapter, although the calculations done in later chapters are still in the local description.

In this global view, all N variables  $x_i$  on the nodes are taken together as a tuple X =  $(x_1, \ldots, x_N)$ , which is called the state of the BN. Generalizing the Boolean functions  $f_i$ depends on the update order. When using a synchronous update order, a global Boolean function  $\mathbf{F}: M^N \to M^N, F=(f_1,\ldots,f_N)$  can be defined straightforward. In the sequential update order one defines intermediate functions  $\mathbf{F_i}: M^N \rightarrow M^N$  acting only on node  $i$  and leaving all others invariant:  $\mathbf{F_i} = (id, \dots, f_i, \dots, id)$  with  $id$  being the identity. The global dynamics for a single epoch is now the composition of these functions:  $\mathbf{F} = \mathbf{F}_{\pi(1)} \circ \cdots \circ \mathbf{F}_{\pi(N)}$ , where  $\pi$  is the ordering of the updated nodes. The global version of equation (1.1) now

reads

$$
\mathbf{X}' = \mathbf{F}(\mathbf{X}).\tag{1.4}
$$

#### 1.2.2 Additional notation

Moreover a few definitions to simplify the notation for calculations in this work are defined.

**Definition 1.10.** *Two special states of*  $X \in M^N$  *are*  $1 = (1, \ldots, 1)$  *and*  $0 = (0, \ldots, 0)$ *, where*  $M = \{0, 1\}$ . If a different M is used, the symbols in 1 and 0 change accordingly. The size *of these tuples should be clear from context, as* 1 *and* 0 *are always associated either with*  $\mathbf{X} \in M^N$  or  $\mathbf{x} \in M^{k_i}$ , so the sizes would be  $N$  and  $k_i$ , respectively.

 $\textbf{Definition 1.11.}\ \textbf{e}_{\textbf{i}}\ \text{is the tuple}\ \textbf{e}_{\textbf{i}}=(0,\ldots,0,1,0,\ldots,0)\ \text{with the}\ 1\ \text{on the}\ i\text{-th position.}$ 

Furthermore an operation on those tuples is defined, which is used several times in calculations in the next chapter.

**Definition 1.12.** *The operation*  $\oplus : M^n \times M^n \to M^n$  *is defined as XOR operation on each element of the tuples*  $X, Y \in M^n$  *(with*  $n \in \mathbb{N}$  *arbitrary):* 

$$
\mathbf{X} \oplus \mathbf{Y} = (x_1, \dots, x_n) \oplus (y_1, \dots, y_n) = (x_1 \text{ XOR } y_1, \dots, x_n \text{ XOR } y_n), \tag{1.5}
$$

*where XOR is the standard binary operation.*

### 1.3 Network topology

The topology of the underlying graph in a BN has an important influence in the model. Although a specific structure might capture the nature of a modeled system better, this is in the majority of cases not mathematically treatable in a feasible way. So in most cases the topology is represented by a distribution of connections or degrees:

**Definition 1.13.** A Random Graph is a graph  $G = (V, E)$  where the nodes are connected *randomly according to some probability distributions. In the case of BN those distributions include the in-degrees*  $k_i$  *of all nodes i. They are normalized* 

$$
\sum_{k} \Pr\left[k|\rho_k\right] = 1,\tag{1.6}
$$

*with the given distribution*  $\rho_k$  *of degrees*  $k_i$ *.* 

As mentioned before, BN are directed graphs where the in-degree is of central importance, because it is the number of variables in the Boolean function, so usually only a distribution of in-degrees is imposed onto the graph. The nodes from which those connections are originating are usually drawn from a uniform distribution of all nodes. This results in a Poissionian distribution for the out-degree.

The most convenient random graph for calculations has only a single degree for each node, i.e.  $Pr[k|\rho_k] = \delta(k - K)$  where  $k_i = K$  for all i. As will be demonstrated in the next

chapter, in a Mean Field approximation a degree-distribution  $\rho_k$  embeds nicely into the model. In this case the whole topology is introduced via  $\rho_k$ .

In the last decade scale-free topologies have attracted much interest [Barabási and Albert, 1999]. In this case the degree distribution follows a power-law

$$
\Pr\left[k|\rho_k\right] = const \frac{1}{k^{\gamma}}.\tag{1.7}
$$

As a scale-free distribution is heavy-tailed, there should be some highly connected nodes, whereas the majority of nodes has only one or few incoming connections. This leads to the absence of a favored size or scale in the system, as the name scale-free already suggests. Compared to the exponential distribution, there is a non-vanishing probability for highly connected nodes, which induces some problems in modeling. Many degree distributions of networks observed in nature seem to have such a distribution  $\rho_k$ . However, in finite systems this absence of a scale can only extend over a few orders of magnitude as many new properties emerge with every step in the scale.

Scale-free distributions occur also in critical processes, as will be briefly mentioned in section 1.5.3.

Applied to BNs, such a degree distribution shows many interesting features. [Aldana, 2003] showed that the dynamics on scale-free BNs is particularly stable, compared to other networks with similar average degree  $k_{avg}$ .

Further distributions often found in nature and natural processes include the binomial distribution or an exponential distribution of degrees. However, the discovery of scale-free networks [Barabási and Albert, 1999] has started a hype on those networks, that often biased researchers to see such networks everywhere [Clauset et al., 2009].

The underlying graph could also have a more ordered structure. If it is a lattice, then the Boolean Network would be a Cellular Automaton (CA). In that sense BNs are some kind of generalization of a CA.

### 1.4 Boolean functions

Finally the concepts of one of the most influential factor in the dynamics of BN will be dealt with, the Boolean functions  $f_i$  on each node i. In the context of BN such a function is often also called "update rule" or just "rule". It determines how the connected nodes "interact" with each other by evaluating the values of the neighboring nodes of  $i$  and applying the result to  $x_i$ , as given in the dynamics equation (1.1). As the topology of the network needs not to be homogeneous, i.e. different nodes could have different in-degrees, so the functions  $f_i$  defined on those nodes might have a different number of variables. Therefore, in the general case, one deals with classes or distributions of functions, instead of a single function. One of the main tasks when modeling real interacting networks is finding a suitable class of functions.

**Definition 1.14.** *The distribution or class of functions on a BN is denoted by*  $\rho_F$ *.* 

This definition is already in preparation of the Mean Field approximation in the next

chapter. It could also be true that there are fixed choices of the functions on each node.

For graphs G where each node has exactly in-degree  $k_i = 2$  on all nodes, the Boolean functions are given by the well known bit operators AND, OR and XOR (and their negations) for interacting functions as well as the functions copying or inverting only one of the input variables and the two constant functions (yielding always the same value in  $M$ , not depending on the input). If  $k_i > 3$ , one can represent the functions in a truth table, described in the following section.

#### 1.4.1 Truth table representation of Boolean functions

There are only discrete values allowed for Boolean functions, therefore it is feasible to write all possible values of the input tuples x together with the corresponding function value  $f(x)$  in a table, which is called truth or look-up table. An example is given in table 1.1. The number of possible combinations of input values is  $2^K$ , as for each of the  $K$  variables  $x_i$  two values in M are possible. For each of those input tuples two values of  $f(\mathbf{x}) \in M$  are possible, therefore the number of Boolean functions is  $2^{2^K}.$  Later probabilistic functions will be introduced, where the value of  $f(x)$  has just some probability to be one of the values in  $M$  and is not fixed as in the truth table, therefore the following definition is needed:

#### **Definition 1.15.** *Boolean functions given by a truth table are denoted by* f*.*

These functions  $f$  can be identified by a single number. When taking all the outputs  $f(x)$  in a truth table and reading it from bottom to top a binary string is obtained. For the example given in table 1.1 this string would be "11101000". This string can be interpreted as a binary number, therefore it can be converted to the decimal system, which would be 232 in this example. However this number is not yet unique, as the string can start with zeros. So the string "0000000011101000" would also be a feasible function f (in this case with  $K = 4$ ) and have also the decimal representation 232. Therefore the number of variables, i.e. the degree of the node on which the function is defined, is denoted as subscript to uniquely determine the function. In the example of the Majority rule for  $K = 3$  (table 1.1) this would be  $(232)_3$ .

This representation of a "Boolean" function is also possible if  $|M|\neq 2.1~$  In such cases the number of elements in  $M$  is taken as a basis for the number system and converted to decimal. However, an additional subscript should denote  $|M|$  in this case.

In the remainder of this section and most of this work the notation  $f$  is used again for a Boolean function, allowing Probabilistic Boolean functions again, not only those given by a truth table. The distinction between  $f$  and  $f$  is used only to formalize a few statements in chapter 2.

#### 1.4.2 Probabilistic Boolean functions

In [Shmulevich et al., 2002] the concept of Boolean functions was further generalized. In this model the result of a Boolean function  $f_i$  on a specific input tuple x is not the defined

<sup>&</sup>lt;sup>1</sup>In a strict sense such functions are not "Boolean" anymore, as this term refers explicitly to a 2-state  $M$ .

	input	output	
	$\mathbf x$	$f(\mathbf{x})$	
0	O	0	0
$\overline{0}$	0	1	0
$\overline{0}$	1	0	0
$\overline{0}$	1	1	1
1	0	0	0
1	0	1	1
1	1	ი	1
1		1	

Table 1.1: Example of a Boolean function f represented in a truth table. Shown is the Majority rule for  $k_i = 3$  or rule  $(232)_3$  for  $M = \{0, 1\}$ . Reading the output of the function as string from bottom to top gives 11101000, which has the decimal representation 232.

value of  $x'_i \in M$ , each output could be possible according to some probability distribution. This means that there could be a non-zero probability such that  $f_i(\mathbf{x}) = 0$  as well as a nonzero probability such that  $f_i(x) = 1$ . Such functions are easily incorporated into the formalism, which will be presented in the next chapter. Even more so, in a Mean Field description of a mixture of several functions, such a Probabilistic Boolean function would be the natural way to describe the complete distribution of functions. Hence we can expand definition 1.14:

**Definition 1.16.** *The distribution of Boolean functions*  $\rho_F$  *can be seen as mixture of all possible Boolean functions* f*, given by truth table. The probability for a specific Boolean function is given by*  $Pr[f|\rho_F]$ *, which is a normalized* 

$$
\sum_{\mathfrak{f}} \Pr\left[\mathfrak{f}|\rho_{\mathbf{F}}\right] = 1. \tag{1.8}
$$

In the Mean Field description, no node has a specific Boolean function, only a probability for this function to be one in the mixture  $\rho_F$ . This probability for a function can be seen naturally as a probability of the Boolean function to assume a specific value on a given input tuple x.

#### 1.4.3 The Kauffman model

An ubiquitous model in the treatment of BNs is the Kauffman model. It has been introduced by Stuart Kauffman in his seminal paper [Kauffman, 1969], which can be seen as one of the founding publications in the science of network dynamics. In the beginning only treated by simulations, its nice properties allowed for some results to be derived analytically, see e.g. [Derrida and Pomeau, 1986] for one of the first analytical treatments.

**Definition 1.17.** *The underlying graph of the Kauffman model is a random graph, where each of the* N *nodes has exactly in-degree* K. The values of the nodes are  $x_i \in M = \{0, 1\}$ . *The*  $2^{2^K}$  possible Boolean functions are distributed uniformly and randomly on all  $N$  nodes.

*All nodes are updated simultaneously. This can be formalized by the following distributions:*

$$
Pr[k|\rho_k] = \delta(k - K), \qquad (1.9a)
$$

$$
\Pr\left[\mathfrak{f}|\rho_{\mathbf{F}}\right] = \frac{1}{2^{2^K}} \quad \text{for all } \mathfrak{f}. \tag{1.9b}
$$

The only two parameters in this model are  $N$  and  $K$  with this definition. An additional parameter can be introduced by rephrasing the concept of the uniformly distributed functions.

**Lemma 1.18.** *The uniform distribution of all Boolean functions* f *is equivalent to a binomial distribution on functions with* i 1*s in their truth table. Therefore the number of* 1*s is also binomially distributed with mean* <sup>1</sup> 2 *. There holds*

$$
\Pr[f(\mathbf{x}) = 1|\mathbf{x}] = \Pr[f(\mathbf{x}) = 0|\mathbf{x}] = \frac{1}{2}.
$$
 (1.10)

*Proof.* In short consider the sum over the uniform distribution of all Boolean functions and rewrite it as distribution over the 1s. Let  $F^{(i)}$  denote the number of functions having exactly *i* 1s in their truth table (and therefore  $k - i$  0s). Counting permutations,  $F^{(i)}$  =  $\sqrt{ }$ 2 k i  $\setminus$ . Writing the sum over the uniform distribution of functions:

$$
1 = \sum_{\mathfrak{f}} \Pr\left[\mathfrak{f}|\rho_{\mathbf{F}}\right] = \sum_{\mathfrak{f}} \frac{1}{2^{2^K}} = \frac{1}{2^{2^K}} \sum_{i=1}^{2^{2^K}} 1 = \frac{1}{2^{2^K}} \sum_{i=0}^{2^K} F^{(i)} = \sum_{i=0}^{2^K} F^{(i)} \left(\frac{1}{2}\right)^{2^K}
$$

$$
= \sum_{i=0}^{2^K} \binom{2^k}{i} \left(\frac{1}{2}\right)^i \left(\frac{1}{2}\right)^{2^K - i} = \sum_{i=0}^{2^K} \binom{2^k}{i} p^i (1-p)^{2^K - i},
$$

where  $p = \frac{1}{2}$  $\frac{1}{2}$  and therefore the variable which is summed over, the number of 1s in the truth table of a function, is binomially distributed with mean  $p$ , which concludes the proof.  $\Box$ 

The parameter  $p$  used in the proof can be seen as another parameter of the Kauffman model:

**Definition 1.19.** *The internal homogeneity* p *in the Kauffman model is defined as*

$$
p := \Pr[f(\mathbf{x}) = 1|\mathbf{x}],\tag{1.11}
$$

*and therefore "skewing" the distribution of all functions*  $ρ<sub>F</sub>$  *towards a bias of the dynamics.* 

The term internal homogeneity was coined by Walker [Kauffman, 1984]. Those three parameters  $(N, K, p)$  are encountered in most publications using this model.

## 1.5 Ordered and Chaotic Dynamics

Now lets reconsider what has been stated so far about BNs. They are a (vast, but finite) network of interacting variables, too complicated to describe analytically as a whole, because they are essentially nonlinear. Important influences on the dynamics come from the underlying topology and of course from the type of interaction between those variables, described by the function or class of functions on the BN. As the complete dynamics of such a BN is unfeasible to describe analytically, often only the long time behavior of the dynamics is considered. Again using the argument of finiteness (as there are only  $N$  nodes), it is clear, that the state space of a BN is finite too, consisting of all states of the global dynamics.

**Definition 1.20.** *The state space of a BN is the set of all possible global tuples* X

$$
\{\mathbf{X}\} = M^N = \{(00...0), (10...0), \dots, (11...1)\}.
$$
\n(1.12)

Therefore after at maximum  $|M|^N$  timesteps a state has to repeat itself. Each step in the dynamics depends only on the previous timestep and hence this sequence of repeating states is called an attractor of the dynamics, because once the state of the BN is on such an attractor, it cannot leave it anymore. Every initial state inevitably runs into an attractor, when the global function  $F$  is applied several times to it. The time before the dynamics reaches a state on the attractor is called transient time.

**Proposition 1.21.** *The structure imposed by the dynamics on the state space can be viewed as a directed graph. Each vertex is a state* X *of the dynamics. Edges are directed and defined by the global dynamics, i.e. two states*  $X_1$  *and*  $X_2$  *have an edge from*  $X_1$  *to*  $X_2$  *if and only if*  $X_2 = F(X_1)$ *. The attractors are either closed paths or self-connected vertices (in*) *which case the state* X *is a fixed point:*  $X' = F(X) = X$ *). The transient time is represented as trees with all edges pointing inward to a single node on one of the attractors.*

*Proof.* By construction of the state space its structure is clear.

 $\Box$ 

Note that this graph contains much more information in it, as the underlying graph of the BN. In addition to this underlying graph  $G$ , it also has the complete time evolution of the whole BN somehow encoded. The number of vertices in the underlying graph is only N, whereas in this state space graph the number of vertices is  $|M|^N$ . However, this construction works only in one direction. It is possible to construct the state space graph from a given underlying graph  $G$  and a global function  $F$ , but usually not feasible to reconstruct those from a given state space graph, e.g. see [Delgado-Eckert, 2009]. A recent study also tries to infer the structure and functions of small BNs from noisy data [Liu et al., 2008], using the additional constraint of criticality on the BN.

From the construction in proposition 1.21 it should be clear, that the resulting graph with vertices denoted by  $X \in M^N$  is usually not connected, as each vertex has only a single outgoing edge. The different connected sub-graphs are called basins of attraction, consisting of the transient phase leading to the attractor and the attractor cycle itself. In this graph-picture of the state space a few interesting properties can be seen directly. Using the global function F as equivalence relation, i.e. two points in  $M^N$  are equivalent if they are in the same basin of attraction. Therefore the set of these basins can be taken as a quotient:

$$
\mathcal{A} := \{A\} \cong M^N / \mathbf{F},\tag{1.13}
$$

with A being a basin of attraction (or equivalently an attractor itself).

Another, even more important consequence is

**Corollary 1.22.** *The dynamics on a BN is not invertible*

$$
\nexists \mathbf{F}^{-1}: M^N \to M^N, \text{ such that } \mathbf{X} = \mathbf{F}^{-1}(\mathbf{X}') \text{ holds for all } \mathbf{X} \in M^N \tag{1.14}
$$

*in the sense of equation* (1.4)*.*

*Proof.* This follows from the structure of the state space graph, given in the last proposition. The proof only works if the dynamics has a transient time for at least some initial states.

There are two reasons why a global inverse  $\mathbf{F}^{-1}$  :  $M^N$   $\rightarrow$   $M^N$  does not exist. First consider the ends of the trees representing the transient time. Such states are called "garden-of-eden"-states, as they can only occur as initial conditions and cannot be reached via the dynamics. Therefore  $\mathbf{F}^{-1}$  cannot exist on those states.

Furthermore there are states which can be reached from more than one state. Take a state in the attractor cycle. If a transient time tree reaches the attractor cycle in this state, than there must be another state in the cycle itself, leading to the chosen state. Therefore  $\mathbf{F}^{-1}$  cannot be unique on such states.  $\Box$ 

There are special cases where a invertible map  $\mathrm{F}^{-1}$  can exist, which are shown implicitly in the proof. If the dynamics has no transient time, then all states are on attractor cycles, and the two arguments used in the proof fail, because the states considered there do not exist.

#### Examples of small BNs

A simple example for visualizing proposition 1.21 is given by the following BN. Consider a graph G with just three vertices  $V = \{1, 2, 3\}$ . The variables are  $x_1, x_2, x_3 \in M = \{0, 1\}$  and each of the nodes is connected to the two others. The three functions are  $f_1 = OR$ ,  $f_2 = OR$ and  $f_3 = AND$ . This graph is depicted in figure 1.2(a). Looking at the truth tables (given in table 1.2) of the functions, the global function  $\bf{F}$  can be constructed and the whole state space, consisting of the 8 states  $M^N = \{000, 001, \ldots, 111\}$ , is shown in figure 1.2(b), with edges between two consecutive states in the dynamics. In this case there are three attractors, the first one 000 just a single state, which is a fixed point without a transient time. The second one is a period-2-cycle without a transient time, permanently switching between the states 001 and 010. Finally, the third attractor is again a fixed point 111, with 4 states in the transient time.

Formally those attractors can be written as  $A = \{000\}$ ,  $\{100, 010\}$ ,  $\{111\}$ . The states used in the proof of corollary 1.22 exist only in the third attractor. These are the three



Figure 1.2: Graph and phase space structure of the BN with  $N = 3$  and  $K = 2$ . The Boolean functions are  $f_1 = OR$ ,  $f_2 = OR$  and  $f_3 = AND$ .

	(a) $f_1 = OR$			(b) $f_2 = OR$			(c) $f_3 = AND$		
$x_2$	$x_3$			$x_1$	$x_3$	I2	$x_1$	$x_2$	

Table 1.2: Representation of the BN  $N = 3$ ,  $K = 2$  with truth tables.

states 001, 011 and 101, which are the garden-of-eden-states, only occurring as initial conditions, because they cannot be reached within the dynamics. The second type of states used in the last proof would be state 111, as it lies on the attractor (which is the fixed point in this case), but also a tree for the transient time enters the attractor cycle there, so 111 has two predecessors (110 and 111) in the dynamics. Note that 110 would also be a state with more than one predecessor, however, its existence is just by chance, whereas the other two types of states exists already with the existence of a transient time.

	x		$(\mathbf{x})$
0	0	0	0
$\overline{0}$	0	1	1
$\overline{0}$	1	0	1
$\overline{0}$	1	1	$\Omega$
1	0	0	1
1	$\overline{0}$	1	1
1	1	0	0
1	1	1	0

Table 1.3: Truth table representation of rule  $(54)_3$ .

Another, more sophisticated example is the state space graph depicted in figure 1.3. The underlying graph of the BN consists of 6 nodes and is depicted on the left side. Each node has the Boolean function  $f_i = (54)_3$ , explained in table 1.3. The structure imposed by the dynamics on the state space is shown on the right side of the figure. Although the number



Figure 1.3: Network structure and state space graph for a BN with  $N = 6$ ,  $K = 3$  and  $f_i = (54)_3, 1 \leq i \leq 6.$ 

of nodes only doubled from the previous example, the state space graph has a much more complex structure with its 4 attractors (shown in dark blue). The basins of attraction for those attractors are separated by the dashed red line. However, the number of attractors did not change much, it increased only from 3 to 4. The four attractors in this case are

> $\mathcal{A} = \{ \{111010, 000110, 101100 \}, \{011110, 000010, 101000 \}, \}$  $\{011100, 101011, 110100, 110111\}, \{000000\}\}.$

#### 1.5.1 The Hamming distance  $d$

To look at phase transitions in the dynamics of a BN, a concept of measurability or distance on the state space  $M^N$  is needed. One of the natural ways to do that is via the so-called Hamming distance:

**Definition 1.23.** *The Hamming distance* D *between two states*  $X, Y \in M^N$  *is the number of nodes, which are different in the two states*

$$
D(\mathbf{X}, \mathbf{Y}) := |\{x_i \neq y_i : \mathbf{X} = (x_1, \dots, x_N) \in M^N, \mathbf{Y} = (y_1, \dots, y_N) \in M^N\}|.
$$
 (1.15)

*In most of the following text a normalized Hamming distance* d ∈ [0, 1] *is used*

$$
d\left(\mathbf{X}, \mathbf{Y}\right) := \frac{1}{N} D\left(\mathbf{X}, \mathbf{Y}\right). \tag{1.16}
$$

*The special cases*  $d = 0$  *corresponds to*  $X = Y$  *and*  $d = 1$  *corresponds to two states which are the exact complements to each other, i.e.*  $X = Y \oplus 1$ *.* 

Note that this definition also extends to the limit  $N \to \infty$ , i.e. if the state space is infinite. Moreover, also a local tuple  $x \subseteq X$  could be used as argument, e.g. from the dynamics

equation (1.1). The size of the tuples should be identical for both arguments  $d(., .),$  which is the only restriction in this definition.

The importance of the Hamming distance in BNs was first discovered by Derrida in several of his works in the 1980s [Derrida and Pomeau, 1986, Derrida and Weisbuch, 1986] and is also used in Kauffman's book [Kauffman, 1993] as a crucial parameter for determining the stability of the dynamics in BNs.

#### 1.5.2 Phase transitions

An important characterization of the dynamics is its stableness. If small perturbations in the state force the dynamics to leave the current attractor, a BN is classified as unstable or "chaotic". A small perturbation in this context is, when only a few of the variables in the initial state are flipped, i.e.  $(x_i = 1) \mapsto (x_i = 0)$  or vice versa. The number n of such flipped nodes is assumed to be tiny against the size of the complete BN,  $n \ll N$ . The term "chaotic" might be misleading here, as real chaotic behavior could only occur in infinite BNs, when the dynamics is not constrained to reach an attractor cycle and can remain in the transient time forever. However, for finite BNs the dynamics could be on a very long periodic attractor, which is practically indistinguishable from chaos if the BN is large enough, as its state space grows exponentially with N.

The stableness crucially depends on the distributions of functions  $\rho_F$  and the distributions of degrees  $\rho_k$  in the BN, hence the following definition is needed.

**Definition 1.24.** All parameters in the distributions  $\rho_F$  and  $\rho_k$  are taken together in the *abstract symbol* γ*, denoting the set of external parameters. Hence*

$$
\rho_{\mathbf{F}} \quad := \quad \rho_{\mathbf{F}}(\gamma), \tag{1.17a}
$$

$$
\rho_k \quad := \quad \rho_k(\gamma). \tag{1.17b}
$$

*Therefore, incorporating those parameters in the global Boolean function*  $\mathbf{F}: M^N \to M^N$ , *it can be written as*

$$
\mathbf{F} = \mathbf{F}[\gamma]. \tag{1.18}
$$

The term stableness of a BN makes only sense in a long-time behavior, as the perturbation settles down after a transient time and either the same or a different attractor is reached. Formalizing this one looks at two identical BNs, one with initial state X, the other with an "almost identical" initial state Y.

**Definition 1.25.** *The dynamics of a BN is classified as stable if*

$$
\lim_{t \to \infty} d\left(\mathbf{F}[\gamma]^t(\mathbf{X}), \mathbf{F}[\gamma]^t(\mathbf{Y})\right) = 0,
$$
\n(1.19)

where **X** is "almost identical" with **Y**. "Almost identical" means  $0 < d$ ( $\mathbf{X}, \mathbf{Y}) = \mathcal{O}\left(\frac{1}{N}\right) \ll 1$ . *The exponent in the global Boolean function* F *is meant as composition, i.e. consecutive* *application of the function to the state:*

$$
\mathbf{F}[\gamma]^t = \underbrace{\mathbf{F}[\gamma] \circ \cdots \circ \mathbf{F}[\gamma]}_{t \text{ times}}.
$$
 (1.20)

It makes sense to refer to the analogy to statistical mechanics now. In statistical mechanics a continuous phase transition is characterized by several properties. First of all, a concise mathematical treatment of phase transitions is only possible in infinite systems. This point will be circumvented by the Mean Field approximation in the next chapter, as the completely statistical approach used there is more or less equivalent to such an infinite size of the BN.

Furthermore, each continuous phase transition is accompanied by a order parameter, which could be either a simple scalar, a vector, or even a tensor. In the case of BNs the Hamming distance d takes the place of this order parameter, or to be more precise the long time-behavior of  $d$ , e.g. the fixed point  $d^*$ . Such a continuous phase transition occurs at a critical point, which is in BNs often not only a single point, but a manifold. In the specific BNs studied in this work, where all nodes have a Linear Threshold function, the parameters are  $\gamma = \{p, h\}$  (see chapter 3). For these parameters, this critical "point" is in fact a one-dimensional line in the  $p-h$ -plane, depicted and explained in figure 3.8.

Another important feature at such critical points is, that several quantities of the system exhibit scaling behavior, i.e. they follow a power-law  $q \sim \tau^{\alpha_q}$  (here  $q$  stands for the observed quantity,  $\tau$  is the distance to the critical point, usually a normalized temperature, and  $\alpha_q$ is the so-called "critical exponent"). The values of those critical exponents  $\alpha_q$  for the quantities  $q$  are universal for several models exhibiting a continuous phase transition, leading to the definition of universality classes of models. However, in this thesis only the critical point in the parameters  $\gamma_{crit}$  itself is treated and calculated, not those critical exponents. This would be the topic of future work.

Now a concept of a dynamical phase transition can be defined for a BN, which is central for this work:

**Definition 1.26.** *A BN is said to be in an ordered phase if its dynamics is stable in the sense of definition 1.25 and in a disordered (or "chaotic") phase if it is unstable. When varying the external parameters* γ*, a change between ordered and disordered phase is called dynamical phase transition.*

It should be clear, that this definition is problematic with finite BNs. The Mean Field approximation introduced in the next chapter avoids this problem, by working just with probabilities, and is therefore more or less equivalent to an infinite system.

#### 1.5.3 Attractor basins structure  $\mathcal A$

The structure of simple BNs has already been shown in figures 1.2(b) and 1.3, where only small finite BNs were considered. In general they are defined through equation (1.13). One of the main goals is to derive properties of  $A = \{A\}$ , especially the number of attractors  $|A|$ and the distribution of lengths of attractors  $|A|$ . A few first attempts were made for simple

 $\rho_k$  and  $\rho_F$ , see e.g. [Kauffman, 1984], [Luque and Sole, 2000], [Greil and Bassler, 2009] or [Greil and Drossel, 2005] and references therein, however, a general theory is still missing. It can be conjectured (and is shown for this simple systems), that those quantities, the number and length of attractors, scales with a power-law at the critical point, as predicted by statistical mechanics.

A more graph theoretic approach was used by [Macauley and Mortveit, 2009], where the authors show the equivalence of the attractors of a BN under a few transformations on the update order.

It might be possible to find interesting results using Random Graph theory (RGT). RGT was introduced by Erdös in several publications the 1960s, see e.g. [Erdös and Rényi, 1960], and a treatment can be found in almost all modern textbooks on Graph theory, e.g. [Bollobás, 1998]. In RGT, Erdös also found a phase transition, when considering completely random graphs, where each possible edge between all vertices is formed with a given probability  $p$ . It should be clear, that for low  $p$ , the graph is usually not connected. However, by increasing this probability, at some point  $p_c$  almost all smaller components of the graph merge, making the graph (almost completely) connected $^2.$  This result is reminiscent of the phase transition described here in this work. When considering the graph imposed by the dynamics on the state space, above the critical point, a (infinitely) small perturbation of the dynamics forces it to leave the current attractor, i.e. the trajectory of the dynamics is now on another, not connected component of the state space graph. So above the critical point, the state space graph consists of mostly small, disconnected components. However, at the critical point and below, small perturbations of the dynamics do not change the attractor, i.e. almost the complete state space graph could be viewed as a single connected component. This analogy is immediate, however, the structure of the state space graph is much more than just those random wiring probability  $p$ , because each node has exactly out-degree  $k^{(out)}=1.$  A real mathematical treatment of these questions is not part of this work, and the problems remain open as part of possible future work.

<sup>&</sup>lt;sup>2</sup>The parameter value for this phase transition is found to be  $p_c = 0.5$ .

## 2 Mean Field Approximation

### 2.1 Preliminaries

The ideas in the last few sections were presented in a more global fashion. With the Mean Field (MF) approximation the original local description of the interaction of nodes is used again (given in definition 1.8 of BNs). In MF this local description consists only of the interactions of a single node and sets it in an averaged background of all other nodes, therefore linearizing the usually highly complex and nonlinear dynamics. Using a statistical approach it considers interactions of this whole background with the chosen node. As each node is assumed to be equivalent to all others, the average over all nodes is taken to be the background in the next timestep, resulting in a theory describing average interactions in the system.



Figure 2.1: Mean Field approximation explained graphically. The highly complex and nonlinear interactions between the nodes are linearized by just taking a single node in an averaged background. In the network on the left the states of the nodes are  $x_i \in M = \{\text{``blue''}, \text{``red''}\}\$ , on the right side only probabilities for a node (or the background) to be in a specific state is given. The mixed colors should indicate that fact. From this picture it should be clear, that MF is some kind of linearization over the "borders" of a node, shown as dashed line.

As seen in the last chapter, an analytical description of the number and length of attractors is still an open problem. A more subtle way to characterize the dynamics is looking how small perturbations affect it. From there, equations for the stability of the dynamics

can be derived, which are intimately coupled to the Hamming distance, described in the last chapter. This concept has been introduced by Derrida and Pomeau in their seminal paper [Derrida and Pomeau, 1986] under the name of "annealed approximation" and later refined in several works [Derrida and Weisbuch, 1986, Derrida and Flyvbjerg, 1987, Flyvbjerg, 1988]. More recent publications on this topic include [Moreira and Amaral, 2005] or [Kesseli et al., 2006]. This chapter is based mainly on the ideas proposed in those works.

The first timestep in such a BN with random initial conditions and randomly connected nodes can definitely treated by mere statistics, as the MF approximation is. For all consecutive timesteps an additional assumption has to be made to keep the validity of this approximation, because the time evolution of the complete BN might have local correlations, based on mutually connected nodes or on small cycles in the underlying graph. To overcome this problem, the number of nodes in the BN has to be assumed large enough compared to the connectivity. An estimation of this "large enough" can be found in [Derrida et al., 1987]:

**Lemma 2.1.** *The MF approximation is valid as long the average connectivity* K *of a node scales with*

$$
K \lesssim \log N. \tag{2.1}
$$

*Proof.* Construct an ancestor tree for a given node for the backward evolution in time. In the current timestep, only a single node has to be considered. In the previous timestep  $K$  different nodes are in the input of the given node. In the timestep before that, each of those K nodes had K input nodes, resulting in  $K^2$  nodes, etc. In the Tth timestep backwards  $K^T$  nodes have to be considered. This yields

$$
1 + K + K^{2} + \dots + K^{T} = \sum_{t=0}^{T} K^{t} = \frac{K^{T+1} - 1}{K - 1} \overset{T}{\approx} \frac{\text{large}}{\approx} K^{T}.
$$

If this number of nodes in the ancestor tree is small compared to the number of nodes  $N$ , it can be assumed, that they are actually all different nodes in the BN:  $K^T \ll N \Rightarrow K < N^{1/T}.$ As the  $T$ th root grows at a slower rate than the logarithm for large  $T$ , this can be bounded by  $\log N$ , resulting in the estimation above.  $\Box$ 

This restriction on the size of the underlying graph is primarily for computer simulations of different BN models. Usually another additional technique is used when doing such simulations. Because on a computer only finite systems can be treated, the topology of the BN is reshuffled at every timestep, i.e. the input nodes are drawn randomly for each evaluation of the Boolean functions. This further increases the apparent size of the BN, resulting in a better agreement and less noise when comparing those simulations and the calculations, which are presented in this chapter. When more than one Boolean function f is present in the mixture  $\rho_F$ , the assignment of Boolean functions could also be drawn randomly in every timestep. When either topology or Boolean functions is reshuffled in such a manner, it is called "annealed", otherwise it is said to be modeled "quenched" (kept constant for the complete simulation).

In the analytical calculations of the MF approximation such a reshuffling is more or less

inherent in the theory. As only probabilities are considered, which are real numbers, the MF approximation is again an exact description of an infinite system. So applying the MF approximation can be seen as nothing else than imposing the thermodynamic limit on the system, i.e.

$$
N \to \infty, \tag{2.2}
$$

for which the condition from lemma (2.1) is clearly true.

In the description of the dynamics different orders can be distinguished. Each order assumes an additional identical replica of the original BN to run in parallel, where the identity is only in the topology and the Boolean functions, whereas each replica has its own state X. In the first order, assuming a MF approximation, only the probabilities for a node to be in one of the states of  $M$  are taken into account for the description of the whole dynamics. Higher orders will be introduced and used later.

**Definition 2.2.** *Let*  $M = \{-1, +1\}$ *, then the symbols*  $z_{(+)}$  *and*  $z_{(-)}$  *denote the probabilities for a arbitrary node*  $x_i$  *to be in state*  $x_i = +1$  *or*  $x_i = -1$ *, respectively:* 

$$
z_{(+)} := \Pr[x_i = +1|i], \tag{2.3a}
$$

$$
z_{(-)} := \Pr[x_i = -1|i]. \tag{2.3b}
$$

Using the analogy to statistical physics, these probabilities can be used to define a "magnetization"  $m$ , as in many other spin- $\frac{1}{2}$ -models in statistical mechanics.

**Definition 2.3.** *The magnetization* m *is the average over the all states of the nodes*

$$
m := \langle x_i \rangle_{i \in \{1, \dots, N\}}. \tag{2.4}
$$

*In term of the probabilities the magnetization* m *is nothing else than*

$$
m = z_{(+)} - z_{(-)}.\tag{2.5}
$$

There is also another approach to the magnetization. There is only one independent variable in those probabilities  $z_{(\pm)}.$  Hence the magnetization  $m$  is just a transformation of variables. Explicitly the transformation is

$$
\begin{array}{rcl}\n1 & = & z_{(+)} + z_{(-)} \\
m & = & z_{(+)} - z_{(-)}\n\end{array}\n\right\} \Rightarrow\n\begin{cases}\nz_{(+)} & = & \frac{1}{2}(1+m) \\
z_{(-)} & = & \frac{1}{2}(1-m)\n\end{cases}.\n\tag{2.6}
$$

A different transformation would be

$$
\widetilde{m} = z_{(+)}. \tag{2.7}
$$

This would be the average of all the nodes when  $M = \{0, 1\}$ , which is given explicitly by

$$
\begin{array}{rcl}\n1 & = & z_{(+)} + z_{(-)} \\
\widetilde{m} & = & z_{(+)}\n\end{array}\n\right\} \Rightarrow\n\begin{cases}\nz_{(+)} & = & \widetilde{m} \\
z_{(-)} & = & 1 - \widetilde{m}\n\end{cases}.\n\tag{2.8}
$$

This distinction between m and  $\tilde{m}$  will be made throughout this work, so m corresponds

always to  $M = \{-1, 1\}$ , whereas  $\tilde{m}$  is the magnetization for  $M = \{0, 1\}$ .

Before starting with introducing the MF approximation, another symbol to simplify notation should be introduced:

**Definition 2.4.** Let  $M = \{-1, +1\}$ . The bracket  $\langle \cdot, \cdot \rangle : M^K \times M^K \to \mathbb{N}$  is the number of  $+1s$ *occurring at same positions in the two tuples as arguments:*

$$
\langle \mathbf{x}, \mathbf{y} \rangle := |\{i : x_i = +1, y_i = +1\}|. \tag{2.9}
$$

The number of  $-1$ s could also be represented with this bracket.  $x \oplus 1$  gives just the negative of x, i.e.  $x \oplus 1 = -x$ . Therefore

$$
\langle -\mathbf{x}, -\mathbf{x} \rangle = \langle \mathbf{x} \oplus \mathbb{1}, \mathbf{x} \oplus \mathbb{1} \rangle = K - \langle \mathbf{x}, \mathbf{x} \rangle.
$$

A simple example would be the following. Let  $x = (-1, +1, +1)$  and  $y = (+1, -1, +1)$ . Then  $\langle \mathbf{x}, \mathbf{y} \rangle = 1$  and  $\langle \mathbf{x}, \mathbf{x} \rangle = \langle \mathbf{y}, \mathbf{y} \rangle = 2$ .

One of the central lemmas the MF approximation is the following

**Lemma 2.5.** Let  $M = \{-1, +1\}$ . The probability of occurrence for a random tuple  $x =$  $(x_1, \ldots, x_K)$  *with given probabilities*  $z_{(+)}$  *and*  $z_{(-)}$  *is* 

$$
\Pr\left[\mathbf{x}|z_{(\pm)}\right] = z_{(+)}^{\langle\mathbf{x},\mathbf{x}\rangle} z_{(-)}^{\langle\mathbf{x}\oplus\mathbb{1},\mathbf{x}\oplus\mathbb{1}\rangle}.
$$
 (2.10)

*Proof.* In a random tuple x each position is independent. There are  $\langle x, x \rangle +1$ s in the whole tuple, and  $\langle x \oplus 1, x \oplus 1 \rangle$  −1s. Multiplying the independent probabilities for a single position  $(z_{(\pm)}$ ), yields exactly the expression in the lemma. Hence

$$
\Pr\left[\mathbf{x}|z_{(\pm)}\right] = z_{(+)}^{\langle \mathbf{x}, \mathbf{x} \rangle} z_{(-)}^{\langle \mathbf{x} \oplus \mathbb{1}, \mathbf{x} \oplus \mathbb{1} \rangle}.
$$

Using the transformations  $(2.6)$  and  $(2.8)$  above, the probability depends only on m or  $\tilde{m}$ , respectively, and can be written as

$$
\begin{array}{rcl} \Pr\left[\mathbf{x}|m\right] & = & \left(\frac{1+m}{2}\right)^{\langle\mathbf{x},\mathbf{x}\rangle}\left(\frac{1-m}{2}\right)^{\langle\mathbf{x}\oplus\mathbb{1},\mathbf{x}\oplus\mathbb{1}\rangle}, \\ \Pr\left[\mathbf{x}|\widetilde{m}\right] & = & \widetilde{m}^{\langle\mathbf{x},\mathbf{x}\rangle}\left(1-\widetilde{m}\right)^{\langle\mathbf{x}\oplus\mathbb{1},\mathbf{x}\oplus\mathbb{1}\rangle}. \end{array}
$$

At this point the second transformation (to  $\tilde{m}$ ) seems simpler. However, for the application to Linear Threshold functions in the next chapter, the first one is needed.

### 2.2 Dynamics or iteration equation

#### 2.2.1 Magnetization  $m$

The aim of a MF approximation is to start from Lemma 2.5 and obtain or construct the state of the next timestep. At the beginning the iteration equations for the probabilities  $z_{(+)}$  will be constructed, although at first this seems to introduce too much overhead in the equations. However, using those probabilities already from the beginning, the generalizations to higher orders of the dynamics will be obvious, as will be seen explicitly later in section 2.2.4. The transformation to  $m$ , given by either equation (2.6) or (2.8), will be applied to those iteration equations to arrive at the final expressions  $m'$  (or  $\widetilde{m}'$ ).

First only a simple distribution of degrees  $\rho_k$  is assumed. This is done via the following theorem:

**Theorem 2.6.** *Let*  $M = \{-1, +1\}$  *and*  $\Pr[k|\rho_k] = \delta(K - k)$ *, i.e. all nodes have the same degree* K*. Furthermore consider a synchronous update order of all nodes. Then the iteration equation for the probabilities* z(±) *in a MF approximation is given by*

$$
z'_{(\pm)} = \sum_{\mathbf{x}} \Pr\left[f(\mathbf{x}) = \pm 1|\mathbf{x}\right] \Pr\left[\mathbf{x}|z_{(\pm)}\right].
$$
 (2.11)

*The summation is taken over all possible* K-tuples  $x \in M^K$ .

*Proof.* In principle the idea behind this theorem is quite simple. The probability of a single node to be in either state ( $z_{(+)}'$  or  $z_{(-)}'$ ) in the new timestep is the sum over all probabilities of tuples, which lead to this state, when "plugged into"  $f$ .

From definitions 2.2 and 1.8 it is known that

$$
z'_{(\pm)} = \Pr\left[x'_i = \pm 1 | i\right] = \Pr\left[f\left(x_{i_1}, \ldots, x_{i_k}\right) = \pm 1 | i, \{i_j\}\right] = \ldots
$$

Applying the MF approximation, it is possible to assume that the node  $i$  is equivalent to each other node, therefore dropping the dependence on it. Additionally the concept of neighbors  $(x_{i_1}, \ldots, x_{i_K}) = \mathbf{x}$  of node  $i$  cannot be used anymore, because in MF the node  $i$ does not have any specific neighbors, only K connections to the averaged "background". Therefore a sum over all possible tuples  $x$  as neighbors can be introduced, weighting them according to their probability of occurrence, given by lemma 2.5:

$$
\cdots = \Pr\left[f\left(x_{i_1},\ldots,x_{i_k}\right) = \pm 1|i,\{i_j\}\right] \stackrel{MF}{=} \sum_{\mathbf{x}} \Pr\left[f\left(\mathbf{x}\right) = \pm 1|\mathbf{x}\right] \Pr\left[\mathbf{x}|z_{(\pm)}\right]
$$

When more than one different degree on the nodes occurs, the iteration equation has to be weighted accordingly.

**Corollary 2.7.** *For a more elaborate distribution of degrees*  $\rho_k$  *the iteration equation is* 

$$
z'_{(\pm)} = \sum_{k} \Pr\left[k|\rho_k\right] \left(\sum_{\mathbf{x} \in M^k} \Pr\left[f(\mathbf{x}) = \pm 1|\mathbf{x}\right] \Pr\left[\mathbf{x}|z_{(\pm)}\right]\right). \tag{2.12}
$$

*Proof.* Clear in a MF approximation, because the probability for a state in the next timestep  $z'_{(\pm)}$  is the average over all nodes, and hence weighted with the probability of a node having  $k$  neighbors.  $\Box$ 

 $\Box$ 

If the distribution of functions  $\rho_F$  is known explicitly, i.e. for every Boolean function f given by a truth table a positive frequency of occurrence is given

$$
\rho_{\mathbf{F}} \mapsto \Pr\left[\mathfrak{f}|\rho_{\mathbf{F}}\right],\tag{2.13}
$$

then this leads to a considerable simplification in the construction of the iteration equations.

**Corollary 2.8.** Let  $M = \{-1, +1\}$ . If the distribution of Boolean functions is given explicitly *by normalized and positive probabilities*  $Pr[f|\rho_F]$ *, the iteration equations can be written as* 

$$
z'_{(\pm)} = \sum_{k} \Pr\left[k|\rho_k\right] \left(\sum_{\mathfrak{f}} \sum_{\mathbf{x}} \Pr\left[\mathfrak{f}|\rho_{\mathbf{F}}\right] \Pr\left[\mathfrak{f}(\mathbf{x}) = \pm 1 | \mathbf{x}, \mathfrak{f}\right] \Pr\left[\mathbf{x} | z_{(\pm)}\right]\right). \tag{2.14}
$$

*Proof.* Follows immediately from the splitting

$$
\Pr\left[f(\mathbf{x}) = \pm 1|\mathbf{x}\right] = \sum_{\mathfrak{f}} \Pr\left[\mathfrak{f}|\rho_{\mathbf{F}}\right] \Pr\left[\mathfrak{f}(\mathbf{x}) = \pm 1|\mathbf{x}, \mathfrak{f}\right],\tag{2.15}
$$

which is clear in a MF description, because everything is treated only statistically. The simplification comes from the fact, that  $Pr[f(x) = \pm 1|x, f|]$  can only be either one or zero, which can be directly read from the truth table.  $\Box$ 

The last corollary also shows that each iteration equation can be seen as mixture of the iteration equations for a specific Boolean function f:

$$
z'_{(\pm)} = \sum_{k} \Pr\left[k|\rho_k\right] \sum_{\mathfrak{f}} \Pr\left[\mathfrak{f}|\rho_{\mathbf{F}}\right] z'_{(\pm)} \left[\mathfrak{f}\right]. \tag{2.16}
$$

The iteration equations  $z'_{(\pm)}[{\mathfrak f}]$  can be constructed by simple combinatorics using the truth table. An example will be given later in this section. An example for a Boolean function, which is not given by a truth table, would be a Linear Threshold function  $f(\mathbf{x}) = \text{sign}\left(\sum_{\{j\}} c_{ij} x_j + h\right)$ . This is still a function  $f : M^{k_i} \to M$ . However, if the coefficients  $c_{ij}$  are not given explicitly, but rather are drawn randomly from a distribution  $\rho_c$ , the explicit probabilities for a Boolean function  $\mathfrak f$  in  $\Pr\left[\mathfrak f|\rho_{\bf F}\right]$  are cumbersome to determine $^1.$ In this case it is easier to calculate  $Pr[f(x) = \pm 1|x]$ . However, the complete chapter 3 is devoted to this case, so it will be postponed until then.

Besides Linear Threshold functions there might be other classes of functions for which  $Pr[f|\rho_F]$  is not known explicitly, because they depend on some external parameters  $\gamma$ . In all those cases it is still possible to calculate  $Pr[f|\rho_F] \equiv Pr[f|\gamma]$  via

$$
\Pr\left[\mathfrak{f}|\gamma\right] = \int \mathcal{D}\gamma \left(\prod_{\mathbf{x}} \Pr\left[f(\gamma; \mathbf{x}) = \mathfrak{f}(\mathbf{x})\right]\right),\tag{2.17}
$$

with  $\mathcal{D}_{\gamma}$  an normalized measure over the external parameters  $\gamma$ . However, in most such cases it is way easier to go the direct route via  $Pr[f(x) = \pm 1|x]$ , than first calculate  $Pr[f|\rho_F]$ ,

<sup>1</sup>except for some special cases

calculate all  $z'_{(\pm)}$  for those Boolean functions  ${\mathfrak f}$  and weight them accordingly.

This should just illustrate, that  $Pr[f|\rho_F]$  is not always known explicitly to use in the sense of corollary 2.8.

The iteration equation for the magnetization is introduced with the following definition:

**Definition 2.9.** The iteration equation for the magnetization  $m'$  is denoted by M. If the *distributions of degrees*  $\rho_k$  *and functions*  $\rho_F$  *depend on the external parameters*  $\gamma$  *(as in*) *definition 1.24), it is given by*

$$
m' = \mathcal{M}\left(\gamma; m\right). \tag{2.18}
$$

Here  $\gamma$  could mean anything from the internal homogeneity p and the connectivity K in the Kauffman model ( $\gamma = \{p, K\}$ ), to the two parameters p and h in the distributions of weights and the connectivity  $K$  used in the Linear Threshold functions in next chapter  $(\gamma = \{p, h, K\})$  or even some other parameter in the distribution of degrees  $\rho_k$  or functions  $\rho_{\bf F}$ .

Hence we can state the "final" result for the magnetization:

**Corollary 2.10.** *The iteration equation for the magnetization*  $m' = \mathcal{M}(\gamma; m)$  *is a polynomial in m* of maximal order  $\mathcal{O}(m^K)$  with  $K = \max(\rho_k)$ .

*If only a single Boolean function* f *is used (and therefore also only a single degree on all nodes), the iteration polynomial reads for*  $M = \{-1, +1\}$ *:* 

$$
m' = \sum_{\mathbf{x}} f(\mathbf{x}) \left(\frac{1+m}{2}\right)^{\langle \mathbf{x}, \mathbf{x} \rangle} \left(\frac{1-m}{2}\right)^{K-\langle \mathbf{x}, \mathbf{x} \rangle},\tag{2.19}
$$

*where*  $f(x) \in M$  *is used as*  $f(x) \in \mathbb{R}$ *. For*  $M = \{0, 1\}$ *, the iteration equation is*  $\widetilde{m}' = \sum_{k=1}^{\infty} f(x) \widetilde{m}'$  $\sum_{\mathbf{x}} \widetilde{\mathfrak{f}}(\mathbf{x}) \widetilde{m}^{\langle \mathbf{x}, \mathbf{x} \rangle}$  (1 –  $\widetilde{m} \rangle^{K-\langle \mathbf{x}, \mathbf{x} \rangle}$ *. If the distributions of degrees*  $\rho_k$  *and Boolean functions*  $\rho_{\mathbf{F}}$  *is* x *more complicated, and parameters in those distributions are taken together in the external parameters* γ*, the iteration polynomial can be extended as*

$$
m' = \sum_{k} \Pr\left[k|\rho_k\right] \left(\sum_{\mathfrak{f}} \Pr\left[\mathfrak{f}|\rho_{\mathbf{F}}\right] m'\left[\mathfrak{f}\right]\right),\tag{2.20}
$$

where  $m'$  [f] *denotes the iteration polynomial from equation* (2.19) *above for a single Boolean function* f*.*

*Proof.* First recall the definition 2.3 of the magnetization m and the relation to the probabilities,  $m = z_{(+)} - z_{(-)}$ . This has to be valid also in the next timestep,  $m' = z'_{(+)} - z'_{(-)}$ . If assuming a single Boolean function f and inserting the iteration equations from theorem 2.6 yields

$$
m' \begin{bmatrix} \mathfrak{f} \end{bmatrix} = z'_{(+)} \begin{bmatrix} \mathfrak{f} \end{bmatrix} - z'_{(-)} \begin{bmatrix} \mathfrak{f} \end{bmatrix}
$$

$$
= \left( \sum_{\mathbf{x}} \Pr \begin{bmatrix} \mathfrak{f}(\mathbf{x}) = +1|\mathbf{x} \end{bmatrix} \Pr \begin{bmatrix} \mathbf{x}|z_{(\pm)} \end{bmatrix} \right) - \left( \sum_{\mathbf{x}} \Pr \begin{bmatrix} \mathfrak{f}(\mathbf{x}) = -1|\mathbf{x} \end{bmatrix} \Pr \begin{bmatrix} \mathbf{x}|z_{(\pm)} \end{bmatrix} \right)
$$

$$
\hspace{1.6cm} = \hspace{.4cm} \sum_{\mathbf{x}} \left( \Pr\left[ f(\mathbf{x}) = +1 | \mathbf{x} \right] - \Pr\left[ f(\mathbf{x}) = -1 | \mathbf{x} \right] \right) \Pr\left[ \mathbf{x} | z_{(\pm)} \right] = \ldots
$$

Now note that  $Pr[f(x) = +1|x]$  can only be either zero or one, because a single Boolean function f can assume only one value in the truth table, and analogously for Pr  $[f(x) = -1|x]$ . Hence for the complete term

$$
\underbrace{\Pr\left[f(\mathbf{x})=+1|\mathbf{x}\right]}_{\in\{0,1\}}-\underbrace{\Pr\left[f(\mathbf{x})=-1|\mathbf{x}\right]}_{\in\{0,1\}}=\underbrace{f(\mathbf{x})}_{\in\{-1,1\}},
$$

where  $f(x) \in M$  is now taken as  $f(x) \in \mathbb{R}$ . Note that this term consists only of Pr  $[f(x) = +1|x]$ , if the iteration equation for  $\widetilde{m}'$  is examined, which already yields the correct expression if  $\Pr\left[\widetilde{\mathfrak{f}}(\mathbf{x})=+1|\mathbf{x}\right]=:\widetilde{\mathfrak{f}}(\mathbf{x})\in\mathbb{R}$  is assumed. Hence the iteration equation for  $m'$  (or  $\widetilde{m}'$ ) has the correct form

$$
\dots = \sum_{\mathbf{x}} f(\mathbf{x}) \left( \frac{1+m}{2} \right)^{\langle \mathbf{x}, \mathbf{x} \rangle} \left( \frac{1-m}{2} \right)^{\langle \mathbf{x} \oplus \mathbb{1}, \mathbf{x} \oplus \mathbb{1} \rangle}
$$

.

As  $\langle \mathbf{x},\mathbf{x}\rangle+\langle \mathbf{x}\oplus \mathbb{1},\mathbf{x}\oplus \mathbb{1}\rangle=k_i,$  this is a polynomial of order  $\mathcal{O}\left(m^{k_i}\right).$  Using the mixture from corollary 2.8, the complete iteration equation is of order  $\mathcal{O}\left(m^{K}\right)$  with  $K=\max\left(\rho_{k}\right).$ 

 $\Box$ 

#### Example

A simple example for the construction of the iteration equation for  $m$  would be the Majority rule (or rule  $(232)_3$ ) for  $K = 3$ , see table 2.1.

input x			output $f(\mathbf{x})$	$\Pr[\mathbf{x} z_{(\pm)}]$
$-1$	$-1 -1$		$-1$	$z_{(-)}^3$
	$-1$ $-1$ $+1$		$-1$	$z_{(+)}z_{(-)}^2$
	$-1$ +1 $-1$		$-1$	$z_{(+)}z_{(-)}^2$
	$-1$ $+1$ $+1$		$+1$	$z_{(+)}^2z_{(-)}$
	$+1$ $-1$ $-1$		$-1$	$z_{(+)}z_{(-)}^2$
$+1$	$-1\,$	$+1$	$+1$	$z_{(+)}^2z_{(-)}$
$+1$	$+1$ $-1$		$+1$	$z_{(+)}^2z_{(-)}$
	$+1$ $+1$ $+1$		$+1$	$z_{(+)}^3$

Table 2.1: Majority rule or rule  $(232)_3$ 

There are four states x, leading to +1:  $(+, +, +)$ ,  $(-, +, +)$ ,  $(+, -, +)$  and  $(+, +, -)$ . These have the probabilities  $Pr[(+,+,+)|z_{(\pm)}] = z_{(+)}^3$  for the first one, and  $Pr[(-,+,+)|z_{(\pm)}] = z_{(+)}^3$  $Pr[(+, -, +)|z_{(\pm)}] = Pr[(+, +, -)|z_{(\pm)}] = z_{(+)}^2 z_{(-)}$  for the others to occur. These have the
"coefficients"  $Pr[f(x) = +1|x] = 1$ , for other input tuples this coefficient is  $Pr[f(x) = +1|x] =$  $0$ , so they do not have to be counted. Therefore the iteration equation for  $z'_{(+)}$  is given by the sum of these probabilities:

$$
z'_{(+)}=z^3_{(+)}+3z^2_{(+)}z_{(-)}.
$$

The iteration equation for  $z'_{(-)}$  can be obtained analogously:

$$
z'_{(-)}=z^3_{(-)}+3z^2_{(-)}z_{(+)}.
$$

Inserting this into  $m' = z'_{(+)}-z'_{(-)}$  and using the transformation given in equations (2.6) yields

$$
m' = \left[ \left( \frac{1+m}{2} \right)^3 + 3 \left( \frac{1+m}{2} \right)^2 \left( \frac{1-m}{2} \right) \right] - \left[ \left( \frac{1-m}{2} \right)^3 + 3 \left( \frac{1-m}{2} \right)^2 \left( \frac{1+m}{2} \right) \right]
$$
  
=  $\left[ \frac{1}{4} (2+3m-m^3) \right] - \left[ \frac{1}{4} (2-3m+m^3) \right]$   
=  $\frac{3}{2}m - \frac{1}{2}m^3$ .

A transformation  $m \mapsto \tilde{m}$  would yield

$$
\widetilde{m}' = 3\widetilde{m}^2 - 2\widetilde{m}^3.
$$

#### 2.2.2 Hamming distance  $d$  in MF

Similar to the magnetization  $m$ , an iteration equation for the Hamming distance  $d$  can be derived in the MF approximation. The idea behind this is taking two variables  $x_i$  and  $y_i$  on each node i, but keeping only a single function  $f_i$ . The dynamics **F** is applied independently on both states,  $\mathbf{X} = (x_1, \dots, x_N)$  and  $\mathbf{Y} = (y_1, \dots, y_N)$ :

$$
\mathbf{X}' = \mathbf{F}(\mathbf{X}), \tag{2.21a}
$$

$$
Y' = F(Y). \t(2.21b)
$$

The update order is assumed to be simultaneous in both BNs, so the last two equations can also be taken together as a single one

$$
(\mathbf{X}', \mathbf{Y}') = (\mathbf{F}(\mathbf{X}), \mathbf{F}(\mathbf{Y}) = \overline{\mathbf{F}}(\mathbf{X}, \mathbf{Y})
$$
\n(2.22)

with a new global function  $\overline{F}: M^{2N} \to M^{2N}$ . Therefore a state of a single node can be described by the tuple  $(x_i, y_i)$ , resulting in  $|M|^2 = 4$  possible states, instead of just two before. This so-called "4-state-model" has already been mentioned and used in [Kesseli et al., 2006].

With the knowledge of both states X and Y, the Hamming distance  $d$  can be calculated at every timestep in the dynamics. It is the aim of this section to take those coupled iteration equations and arrive at an iteration equation for  $d'$ . Recall the definition of stableness of

BNs from definition 1.25:

$$
\lim_{t \to \infty} d\left(\mathbf{F}[\gamma]^t(\mathbf{X}), \mathbf{F}[\gamma]^t(\mathbf{Y})\right) = 0.
$$
\n(2.23)

The MF approximation allows now for explicit calculation of the condition given by this definition, as will be seen in this and later sections.

Extending the results of the previous section, the Hamming distance  $d$  could be called a parameter of the second order of the dynamics, whereas the magnetization  $m$  is a parameter of the first order. To formalize this, the definition and lemma from the previous section have to be adjusted as follows:

 $\bf{Definition 2.11.}$   $\it Let\ M=\{-1,1\}$ , then the symbols  $z_{(++)},\,z_{(+-)},\,z_{(-+)}$  and  $z_{(--)}$  denote the  $p$ robabilities for a arbitrary node  $i$  with variables  $(x_i, y_i)$  to be in the states  $(x_i = +1, y_i = +1),$  $(x_i = +1, y_i = -1)$ ,  $(x_i = -1, y_i = +1)$  *or*  $(x_i = -1, y_i = -1)$ *, respectively:* 

$$
z_{(++)} = \Pr[x_i = +1, y_i = +1|i], \qquad (2.24a)
$$

$$
z_{(+-)} = \Pr[x_i = +1, y_i = -1|i], \tag{2.24b}
$$

$$
z_{(-+)} = \Pr[x_i = -1, y_i = +1|i], \tag{2.24c}
$$

$$
z_{(--)} = \Pr[x_i = -1, y_i = -1|i]. \tag{2.24d}
$$

*The first index always corresponds to states* X *in the first BN, whereas the second one on the second (identical) BN with the different state* Y*.*

**Lemma 2.12.** Let  $M = \{-1, +1\}$ . The probability for a tuple  $(x, y) = ((x_1, y_1), \ldots, (x_K, y_K))$ *with given probabilities* z(±±) *is*

$$
\Pr\left[\mathbf{x}, \mathbf{y}|z_{(\pm\pm)}\right] = z_{(++)}^{n_1} z_{(+-)}^{n_2} z_{(-+)}^{n_3} z_{(--)}^{n_4},\tag{2.25}
$$

*where the exponents*  $n_i$  ( $i \in \{1, 2, 3, 4\}$ ) are given by the following expressions

$$
n_1 = |\{i : x_i = +1, y_i = +1\}| = \langle \mathbf{x}, \mathbf{y} \rangle, \tag{2.26a}
$$

$$
n_2 = |\{i : x_i = +1, y_i = -1\}| = \langle \mathbf{x}, \mathbf{y} \oplus \mathbb{1} \rangle, \tag{2.26b}
$$

$$
n_3 = |\{i : x_i = -1, y_i = +1\}| = \langle \mathbf{x} \oplus \mathbb{1}, \mathbf{y} \rangle,
$$
 (2.26c)

$$
n_4 = |\{i : x_i = -1, y_i = -1\}| = \langle \mathbf{x} \oplus \mathbb{1}, \mathbf{y} \oplus \mathbb{1} \rangle, \qquad (2.26d)
$$

*using also the bracket*  $\langle ., . \rangle$  *from definition 2.4.* 

*Proof.* As before in lemma 2.5, each position  $(x_i, y_i)$  in the tuple  $(x, y)$  is independent, therefore the complete probability is just the product of these probabilities for a single position, yielding exactly the expression stated in the current lemma.  $\Box$ 

With this lemma the reason for the introduction of the bracket  $\langle ., . \rangle$  should be clear. However, it works only up to the second order of the dynamics, higher orders, as treated in section 2.2.4, need additional, heavier notation.

Similar to the first order of the dynamics  $(z'_{(\pm)} )$ , at the beginning only a simple distribution of degrees  $\rho_k$  is assumed in the iteration equations.

**Proposition 2.13.** *Let*  $M = \{-1, +1\}$  *and*  $\Pr[k|\rho_k] = \delta(k - K)$ *. The iteration equations for the MF dynamics of the probabilities* z(±±) *is given by*

$$
z'_{(\pm\pm)} = \sum_{\mathbf{x},\mathbf{y}} \Pr\left[f(\mathbf{x}) = \pm 1, f(\mathbf{y}) = \pm 1 | \mathbf{x}, \mathbf{y} \right] \Pr\left[\mathbf{x}, \mathbf{y} | z_{(\pm\pm)}\right].
$$
 (2.27)

*Proof.* By the same reasoning as in theorem 2.6 for the iteration equation of  $z'_{(\pm)}$  it follows, that

$$
z'_{(\pm \pm)} = \Pr[x'_i = \pm 1, y'_i = \pm 1 | i]
$$
  
=  $\Pr[f(x_{i_1},..., x_{i_K}) = \pm 1, f(y_{i_1},..., y_{i_K}) = \pm 1 | i, \{i_j\}]$   
 $\stackrel{MF}{=} \sum_{\mathbf{x}, \mathbf{y}} \Pr[f(\mathbf{x}) = \pm 1, f(\mathbf{y}) = \pm 1 | \mathbf{x}, \mathbf{y}] \Pr[\mathbf{x}, \mathbf{y} | z_{(\pm \pm)}].$ 

**Corollary 2.14.** *The extension for arbitrary*  $\rho_k$  *and known* Pr  $[f|\rho_F]$  *is* 

$$
z'_{(\pm\pm)} = \sum_{k} \Pr\left[k|\rho_k\right] \left(\sum_{\mathfrak{f}} \sum_{\mathbf{x},\mathbf{y}} \Pr\left[\mathfrak{f}|\rho_{\mathbf{F}}\right] \Pr\left[\mathfrak{f}(\mathbf{x}) = \pm 1, \mathfrak{f}(\mathbf{y}) = \pm 1 | \mathbf{x}, \mathbf{y} \right] \Pr\left[\mathbf{x}, \mathbf{y} | z_{(\pm\pm)}\right]\right). \tag{2.28}
$$

*Proof.* Follows immediately from proposition 2.13 and the arguments used in the proofs of the corollaries for the iteration equations in the first order of the dynamics (corollaries 2.7 and 2.8).  $\Box$ 

Note that in the case of a single Boolean functions f, the combined probability can actually be factorized into a product:

$$
\Pr\left[f(\mathbf{x}) = \pm 1, f(\mathbf{y}) = \pm 1 | \mathbf{x}, \mathbf{y}\right] = \Pr\left[f(\mathbf{x}) = \pm 1 | \mathbf{x}\right] \Pr\left[f(\mathbf{y}) = \pm 1 | \mathbf{y}\right].\tag{2.29}
$$

This is possible, because for such Boolean functions f the values at different input tuples x and y are independent from each other. However, if no explicit probabilities for single Boolean functions f is given by  $Pr[f|\rho_F]$ , this cannot be done and the complete term  $Pr[f(x) = \pm 1, f(y) = \pm 1 | x, y]$  has to be calculated at once.

After stating all those iteration equations for the probabilities  $z_{(\pm\pm)}$ , the Hamming distance d can be introduced:

**Definition 2.15.** *The Hamming distance* d *in the MF approximation is*

$$
d := z_{(+-)} + z_{(-+)}.
$$
\n(2.30)

Note that this is nothing else than the probability for the variables  $x_i$  and  $y_i$  to be different at the same node *i*. The magnetizations  $m^{(X)}$  and  $m^{(Y)}$  could also be expressed by  $z_{(\pm\pm)}$ :

$$
m^{(\mathbf{X})} = z_{(++)} + z_{(+-)} - z_{(-+)} - z_{(--)},
$$
  
\n
$$
m^{(\mathbf{Y})} = z_{(++)} + z_{(-+)} - z_{(+-)} - z_{(--)}.
$$

 $\Box$ 

The iteration equations for  $z_{(++)},\,z_{(+-)},\,z_{(-+)}$  and  $z_{(--)}$  have already redundant information in them. Another redundancy is introduced, when restricting both BNs to the same attractor, i.e. setting

$$
m^{(\mathbf{X})} \approx m^{(\mathbf{Y})} =: m.
$$
\n(2.31)

This is valid, because in subsequent sections and chapters only the fixed points of the iteration equations are considered. So when looking at the fixed point in the Hamming distance  $d^*$ , it is assumed, that both of the two BNs have already reached their respective fixed points  $m^{(\mathbf{X})*}$  and  $m^{(\mathbf{Y})*}$ , because the fixed point is reached in the infinite time limit. Furthermore, only small perturbations of the initial conditions are considered. Both fixed points  $m^{(X)*}$  and  $m^{(Y)*}$  are considered stable, so small perturbations should bring the dynamics of the BN back to it, so if taking a complete replica of the first BN and only perturbing a few nodes, i.e. the condition  $d(\mathbf{X}, \mathbf{Y}) = \mathcal{O}\left(\frac{1}{N}\right)$  from definition 1.25, the assumption  $m^{(\mathbf{X})*}=m^{(\mathbf{Y})*}$  is justified. Therefore the iteration equations should be seen as algebraic expression, from which only the fixed point is obtained. However, simulations indicate, that also the time evolution of the BNs can be expressed by those equations, as they agree to an almost perfect extent.

The following transformation uses this fact and rewrites the probabilities  $z_{(\pm\pm)}$  in terms of only the magnetization  $m$  and the Hamming distance  $d$ .

$$
\begin{array}{rcl}\n1 & = & z_{(++)} + z_{(+-)} + z_{(-+)} + z_{(--)} \\
m^{(x)} & = & z_{(++)} + z_{(+-)} - z_{(-+)} - z_{(--)} \\
m^{(x)} & = & z_{(++)} + z_{(-+)} - z_{(+-)} - z_{(--)} \\
d & = & z_{(-+)} + z_{(+-)} \\
\end{array}\n\right\} \Rightarrow\n\begin{cases}\nz_{(++)} & = & \frac{1}{2}(1+m-d) \\
z_{(+-)} & = & \frac{1}{2}d \\
z_{(--)} & = & \frac{1}{2}d \\
z_{(--)} & = & \frac{1}{2}(1-m-d)\n\end{cases}.\n\tag{2.32}
$$

The probability  $\Pr\left[{\bf x},{\bf y}|z_{(\pm\pm)}\right]$  for the tuple  $({\bf x},{\bf y})$  can be expressed in the new variables  $m$ and  $d$  (or  $\widetilde{m}$  and  $d$ , respectively):

$$
\begin{array}{rcl} \Pr\left[\mathbf{x},\mathbf{y}|m,d\right] & = & \displaystyle \left(\frac{1+m-d}{2}\right)^{\langle\mathbf{x},\mathbf{y}\rangle}\left(\frac{d}{2}\right)^{\langle\mathbf{x},\mathbf{y}\oplus\mathbb{1}\rangle+\langle\mathbf{x}\oplus\mathbb{1},\mathbf{y}\rangle}\left(\frac{1-m-d}{2}\right)^{\langle\mathbf{x}\oplus\mathbb{1},\mathbf{y}\oplus\mathbb{1}\rangle},\\ \Pr\left[\mathbf{x},\mathbf{y}|\widetilde{m},d\right] & = & \displaystyle \left(\widetilde{m}-\frac{d}{2}\right)^{\langle\mathbf{x},\mathbf{y}\rangle}\left(\frac{d}{2}\right)^{\langle\mathbf{x},\mathbf{y}\oplus\mathbb{1}\rangle+\langle\mathbf{x}\oplus\mathbb{1},\mathbf{y}\rangle}\left(1-\widetilde{m}-\frac{d}{2}\right)^{\langle\mathbf{x}\oplus\mathbb{1},\mathbf{y}\oplus\mathbb{1}\rangle}. \end{array}
$$

Note that because of setting  $m^{(\mathbf{X})} \approx m^{(\mathbf{Y})}$ , the magnetization is in fact given by  $m = z_{(++)}$  –  $z_{(-)}$ . The central two terms cancel each other out, because with this restriction the probabilities  $z_{(\pm\pm)}$  are symmetric with respect to exchange of indices.

Using this transformation, the iteration equation for the Hamming distance  $d'$  is a polynomial in  $d$  and  $m$ . Similar to corollary 2.9 the polynomial for  $d$  is defined.

**Definition 2.16.** *The function* D *is the iteration equation for the Hamming distance* d*. It is a*  $p$ olynomial in  $m$  and  $d$  and of order  $\mathcal{O}\left(m^i d^j\right)$  with  $i+j\leq K=\max\left(\rho_k\right)$  and therefore  $\mathcal{O}\left(d^K\right)$ :

$$
d' = \mathcal{D}\left(\gamma; m, d\right) \tag{2.33}
$$

*where*  $\gamma$  *are the parameters in*  $\rho_k$  *and*  $\rho_F$ *.* 

**Corollary 2.17.** In the case of  $M = \{0, 1\}$ , the iteration equation of the Hamming distance d *for a single Boolean function*  $\tilde{f}$  *assumes a simple form* 

$$
d' = \sum_{\mathbf{x}, \mathbf{y}} \widetilde{\mathfrak{f}}(\mathbf{x}) \oplus \widetilde{\mathfrak{f}}(\mathbf{y}) \Pr[\mathbf{x}, \mathbf{y} | \widetilde{m}, d], \qquad (2.34)
$$

*where again*  $\widetilde{f}(\mathbf{x}) \oplus \widetilde{f}(\mathbf{y}) \in \{0, 1\} \subset \mathbb{R}$ .

*Proof.* Recall  $d' = z'_{(+-)} + z'_{(-+)}$ . Inserting the expressions for  $z'_{(\pm\pm)}$  yields

$$
d' = \left(\sum_{\mathbf{x}, \mathbf{y}} \Pr\left[\tilde{\mathfrak{f}}(\mathbf{x}) = 1, \tilde{\mathfrak{f}}(\mathbf{y}) = 0 | \mathbf{x}, \mathbf{y}\right] \Pr\left[\mathbf{x}, \mathbf{y} | z_{(\pm \pm)}\right]\right) + \left(\sum_{\mathbf{x}, \mathbf{y}} \Pr\left[\tilde{\mathfrak{f}}(\mathbf{x}) = 0, \tilde{\mathfrak{f}}(\mathbf{y}) = 1 | \mathbf{x}, \mathbf{y}\right] \Pr\left[\mathbf{x}, \mathbf{y} | z_{(\pm \pm)}\right]\right) = \sum_{\mathbf{x}, \mathbf{y}} \left(\Pr\left[\tilde{\mathfrak{f}}(\mathbf{x}) = 1, \tilde{\mathfrak{f}}(\mathbf{y}) = 0 | \mathbf{x}, \mathbf{y}\right] + \Pr\left[\tilde{\mathfrak{f}}(\mathbf{x}) = 0, \tilde{\mathfrak{f}}(\mathbf{y}) = 1 | \mathbf{x}, \mathbf{y}\right]\right) \Pr\left[\mathbf{x}, \mathbf{y} | z_{(\pm \pm)}\right]
$$

Now we need to inspect the central term more closely:

$$
\Pr\left[\widetilde{\mathfrak{f}}(\mathbf{x})=1,\widetilde{\mathfrak{f}}(\mathbf{y})=0|\mathbf{x},\mathbf{y}\right]+\Pr\left[\widetilde{\mathfrak{f}}(\mathbf{x})=0,\widetilde{\mathfrak{f}}(\mathbf{y})=1|\mathbf{x},\mathbf{y}\right]=\left\{\begin{array}{ll} 1 & \text{if }\widetilde{\mathfrak{f}}(\mathbf{x})\neq \widetilde{\mathfrak{f}}(\mathbf{y})\\ 0 & \text{else} \end{array}\right. =\ldots
$$

Using now the definition of  $\oplus$  (definition 1.12), it immediately follows that

$$
\cdots = \left\{ \begin{array}{ll} 1 & \text{if } \widetilde{\mathfrak{f}}(\mathbf{x}) \neq \widetilde{\mathfrak{f}}(\mathbf{y}) \\ 0 & \text{else} \end{array} \right\} = \widetilde{\mathfrak{f}}(\mathbf{x}) \oplus \widetilde{\mathfrak{f}}(\mathbf{y})
$$

when assuming  $\tilde{f}(x) \oplus \tilde{f}(y) \in \mathbb{R}$ .

This form of the iteration equation for the Hamming distance will be needed later. It should also be quite obvious, because it is nothing else than adding up all the probabilities of input possibilities, which give a different output, when "plugged into" the function  $\tilde{f}$ .

#### Example

Continuing the example from the last section about the magnetization, the iteration equation of the Hamming distance  $d'$  for the Majority rule is derived. The truth table (see table 2.2) is now considerably bigger than in the example for the magnetization, however, it can still be analyzed using simple combinatorics.

The iteration equations for the probabilities  $z'_{(\pm\pm)}$  are given by

$$
z'_{(++)} = z_{(--)}z_{(++)}z_{(++)} + z_{(-+)}z_{(++)}z_{(++)} + z_{(-+)}z_{(++)}z_{(+-)} + z_{(-+)}z_{(++)}z_{(++)}
$$
  
+
$$
z_{(+-)}z_{(-+)}z_{(++)} + z_{(+)}z_{(--)}z_{(++)} + z_{(+)}z_{(-+)}z_{(+-)} + z_{(+)}z_{(-+)}z_{(++)}
$$
  
+
$$
z_{(+-)}z_{(++)}z_{(-+)} + z_{(+)}z_{(+-)}z_{(-+)} + z_{(+)}z_{(+)}z_{(--)} + z_{(+)}z_{(+)}z_{(-+)}
$$
  
+
$$
z_{(+-)}z_{(++)}z_{(+)} + z_{(+)}z_{(--)}z_{(+)} + z_{(+)}z_{(+)}z_{(-+)} + z_{(+)}z_{(+)}z_{(+)}
$$

 $\Box$ 

input						
input	output	$\Pr\left[\mathbf{x},\mathbf{y} z_{(\pm\pm)}\right]$			output	$\Pr\left[\mathbf{x},\mathbf{y} z_{(\pm\pm)}\right]$
x $\mathbf y$	$\mathfrak{f}(\mathbf{x}), \mathfrak{f}(\mathbf{y})$		$\bf x$	$\mathbf y$	$\mathfrak{f}(\mathbf{x}), \mathfrak{f}(\mathbf{y})$	
$- \, 1$ $-1$ $-1$ $-1$ $-1$ $-1$	$-1, -1$	$\overline{z_{(--)}^3}$	$-1$ $-1$ $- \, 1$	$+1$ $- \, 1$ $-1$	$-1, -1$	$\sqrt[2]{(x+1)^2(-1)}$
$-1 -1$ $+1$ $-1 -1$ $-1$	$-1, -1$	$z_{(--)}^2$ $(z_{(-)})$	$-1$ $+1$ $-1$	$+1$ $-1$ $-1$	$-1, -1$	$z^{(n+1)}$ $(-1)^{z}$ $(-1)^{z}$ $(+1)^{z}$
$-1$ +1 $-1$ $-1$ $-1$ $-1$	$-1, -1$	$z_{(--)}^2$ $(z_{(-)})$	$-1$ +1 $- \, 1$	$+1$ $-1$ $-1$	$-1, -1$	$z^{(n+1)}$ $(z+1)$ $z^{(n+1)}$
$-1$ $+1$ $-1$ $-1$ $-1$ $+1$	$+1, -1$	$z^{2}(-z)^{2}(-z)$	$-1$ $+1$ $+1$	$+1$ $-1$ $-1$	$+1, -1$	$z^{2}(-1)^{z^{2}}_{(+-)}$
$-1$ $-1$ $-1$ $+1$ $-1$ $-1$	$-1, -1$	$z_{(--)}^2$ $(z_{(-)})$	$+1$ $-1$ $-1$	$+1$ $-1$ $-1$	$-1, -1$	$z^{2}(+)z^{2}(---)$
$-1$ $-1$ $+1$ $-1$ $+1$ $-1$	$+1, -1$	$z^{2}(-z)^{2}(-z)$	$+1$ $-1$ $+1$	$+1$ $-1$ $-1$	$+1, -1$	$z^{(+)z^{(+)}}$
$+1$ $-1$ $- \, 1$ $+1$ $-1$ $-1$	$+1, -1$	$z^{2}(-z)^{2}(-z)$	$+1$ $+1$ $-1$	$+1$ $-1$ $-1$	$+1, -1$	$z^{(n+1)}(x+1)$ $(z-1)$
$+1$ $+1$ $-1$ $-1 - 1$ $+1$	$+1, -1$	$z_{(+-)}^3$	$+1$ $+1$ $+1$	$+1$ $-1$ $-1$	$+1, -1$	$^{z}(++)$ $^{z}(+-)$
$-1 - 1$ $-1$ $-1$ $-1$ $+1$	$-1, +1$	$\sqrt{z^2-1}$ $(z-1)$	$-1$ $-1$ $-1$	$+1$ $-1$ $+1$	$-1, +1$	$\sqrt{z^2-1}$ $(z^2-1)^2$
$-1 -1$ $+1$ $-1 - 1$ $+1$	$-1, +1$	$z^2_{(--)}z^{(+)}$	$-1$ $-1$ $+1$	$+1$ $-1$ $+1$	$-1, +1$	$z^{(n+1)}$ $(z^{(n+1)})$ $z^{(n+1)}$
$-1$ +1 $-1$ $-1$ $-1$ $+1$	$-1, +1$	$z^{(n)}(-1)^{n}$ (+-) <sup>2</sup> (-+)	$+1$ $-1$ $-1$	$+1$ $-1$ $+1$	$-1, +1$	$z^2_{(-+)}z^{(+-)}$
$-1$ +1 $-1$ $+1$ $-1$ $+1$	$+1, +1$	$z^{(n)}(-1)^{z}(+-)z^{(n)}(+)$	$-1$ $+1$ $+1$	$+1$ $-1$ $+1$	$+1, +1$	$z^{(n+1)}$ $z^{(n+1)}$ $z^{(n+1)}$
$+1$ $-1$ $-1$ $-1$ $-1$ $+1$	$-1, +1$	$z^{(+)z^{(+)}}$	$+1$ $-1$ $-1$	$+1$ $-1$ $+1$	$-1, +1$	$z^{(+)z^{(+)}}$
$+1$ $- \, 1$ $-1$ $+1$ $-1$ $+1$	$+1, +1$	$z^{(+)z^{(+)}}$	$+1$ $- \, 1$ $+1$	$+1$ $-1$ $+1$	$+1, +1$	$z^2_{(++)}z_{(--)}$
$+1$ $+1$ $-1$ $-1$ $-1$ $+1$	$+1, +1$	$z^2_{(+-)}z^{(-+)}$	$+1$ $+1$ $-1$	$+1$ $-1$ $+1$	$+1, +1$	$z^{2}(++)z^{2}(+-)z^{2}(-+)$
$+1$ $+1$ $+1$ $-1$ $-1$ $+1$	$+1, +1$	$z_{(+-)}^2$ $(z_{(++)}^2$	$+1$ $+1$ $+1$	$+1$ $-1$ $+1$	$+1, +1$	$\sqrt[2]{(1+i)^z(1-i)}$
$- \, 1$ $+1$ $-1$ $-1$ $-1$ $-1$	$-1, -1$	$z^2_{(--)}z^{(-+)}$	$-1$ $-1$ $-1$	$+1$ $+1$ $-1$	$-1, +1$	$z_{(-+)}^2$ $z_{(--)}$
$-\mathbf{1} \quad -\mathbf{1}$ $-1$ $+1$ $+1$ $-1$	$-1, -1$	$z^{(n-1)}(z+1)$ $(z+1)$	$-1 - 1$ $+1$	$+1$ $+1$ $-1$	$-1, +1$	$z^2(-+)$ $z^2(+-)$
$-\,1\quad+\,1$ $-1$ +1 $-1$ $-1$	$-1, -1$	$z^2_{(--)}z^{(+)}$	$-1$ $+1$ $-1$	$+1$ $+1$ $-1$	$-1, +1$	$z^{2}(-+)$ $z^{2}(++)$ $z^{2}(--)$
$+1$ $-1$ +1 $+1$ $-1$ $-1$	$+1, -1$	$z^{(n)}(-1)^{n}$ (++) $z^{(n)}(-1)^{n}$	$-1$ +1 $+1$	$+1$ $+1$ $-1$	$+1, +1$	$z(-+)$ $z(++)$ $z(+-)$
$+1$ $-1$ $+1$ $-1$ $-1$ $-1$	$-1, -1$	$z^{(+)z^{(+)}}$	$+1$ $-1$ $-1$	$+1$ $+1$ $-1$	$-1, +1$	$z^{(++) z^{(+)z^{(-+)}}$
$-1$ $+1$ $-1$ $+1$ $-1$ $+1$	$+1, -1$	$z_{(+-)}^2$ $(z_{(+)})$	$-1$ $+1$ $+1$	$+1$ $+1$ $-1$	$+1, +1$	$z^{(+)z^{(+)}}$
$+1$ $-1$ +1 $+1$ $-1$ $-1$	$+1, -1$	$z^{(+)z^{(+)z^{(+)z^{(+)z^{(+)z^{+}}}}$	$+1$ $+1$ $-1$	$+1$ $+1$ $-1$	$+1, +1$	$z^2_{(++)}z_{(--)}$
$+1$ $+1$ $+1$ $+1$ $-1$ $-1$	$+1, -1$	$z_{(+-)}^2$ $z_{(++)}$	$+1$ $+1$ $+1$	$+1$ $+1$ $-1$	$+1, +1$	$z_{(++)}^2$ $z_{(+-)}$
$-1$ $+1$ $-1$ $-1$ $-1$ $+1$	$-1, +1$	$z^{2}(-1)^{z^{2}}(-+)$	$-1\,$ $-1$ $-1$	$+1$ $+1$ $+1$	$-1, +1$	$z_{(-+)}^3$
$-1$ $-1$ $+1$ $-1$ $+1$ $+1$	$-1, +1$	$z^{(z)}(-1)^{z}(-1)^{z}(++)$	$-1$ $-1$ $+1$	$+1$ $+1$ $+1$	$-1, +1$	$z^2_{(-+)}z^{(++)}$
$-1$ +1 $+1$ $-1$ $-1$ $+1$	$-1, +1$	$z^{(n)}(x-1)$ $z^{(n)}(x+1)$ $z^{(n)}(x+1)$	$-1$ +1 $-1$	$+1$ $+1$ $+1$	$-1, +1$	$z^2_{(-+)}z(++)$
$+1$ $-1$ +1 $-1$ $+1$ $+1$	$+1, +1$	$z^{2}(-1)^{z^{2}}(++)$	$-1$ +1 $+1$	$+1$ $+1$ $+1$	$+1, +1$	$z^{2}(-1)^{z^{2}}(+1)$
$-1$ +1 $+1$ $-1$ $-1$ $+1$	$-1, +1$	$z^{2}(+-)z^{2}(-+)$	$+1$ $-1$ $-1$	$+1$ $+1$ $+1$	$-\,1,\,+1$	$^{z}(++)^{z}(-+)$
$+1$ $-1$ +1 $-1$ $+1$ $+1$	$+1, +1$	$z^{(+)z^{(+)}}$	$+1$ $-1$ $+1$	$+1$ $+1$ $+1$	$+1, +1$	$z^2_{(++)}z_{(-+)}$
$+1$ $+1$ $+1$ $-1$ $-1$ $+1$	$+1, +1$	$z^{(+)z^{(+)z^{(+)}}$	$+1$ $+1$ $-1$	$+1$ $+1$ $+1$	$+1, +1$	$z^2_{(++)}z_{(-+)}$
$-\,1\quad+\,1$ $+1$ $+1$ $+1$ $+1$	$+1, +1$	$^{z}(+-)$ $^{2}(++)$	$+\mathbf{1}$ $\hspace{0.1cm} +\mathbf{1}$ $+1$	$+1$ $+1$ $+1$	$+1, +1$	$z_{(++)}^3$

Table 2.2: Truth table for rule  $(232)_3$  in the second order of the dynamics

$$
\begin{array}{lcl} z'_{(+-)}&=&z_{(--)}z_{(+-)}+z_{(--)}z_{(+-)}z_{(++)}+z_{(--)}z_{(++)}+z_{(-+)}z_{(+-)}+z_{(-+)}z_{(+-)}z_{(+-)}\\&+z_{(+-)}z_{(--)}z_{(+-)}+z_{(+-)}z_{(--)}z_{(++)}+z_{(+-)}z_{(-+)}z_{(+-)}+z_{(++)}z_{(--)}z_{(+-)}\\&+z_{(+-)}z_{(-+)}z_{(--)}+z_{(+-)}z_{(-+)}+z_{(+-)}z_{(++)}z_{(--)}+z_{(++)}z_{(+-)}z_{(--)}\\&+z_{(+-)}z_{(+-)}z_{(+-)}+z_{(+-)}z_{(+-)}z_{(++)}+z_{(+-)}z_{(++)}+z_{(+-)}z_{(+-)}+z_{(++)}z_{(+-)}z_{(+-)},\\z'_{(-+)}&=&z_{(--)}z_{(-+)}z_{(-+)}+z_{(-+)}z_{(--)}z_{(-+)}+z_{(-+)}z_{(-+)}z_{(-+)}z_{(-+)}z_{(-+)}z_{(-+)}\\&+z_{(--)}z_{(-+)}z_{(++)}+z_{(-+)}z_{(--)}z_{(++)}+z_{(-+)}z_{(-+)}z_{(+-)}+z_{(-+)}z_{(++)}z_{(++)}\\ \end{array}
$$

$$
+z_{(--)}z_{(++)}z_{(-+)} + z_{(-+)}z_{(++)}z_{(-+)} + z_{(-+)}z_{(++)}z_{(--)} + z_{(-+)}z_{(++)}z_{(-+)}+z_{(+-)}z_{(-+)}z_{(-+)} + z_{(++)}z_{(--)}z_{(-+)} + z_{(++)}z_{(-+)}z_{(--)} + z_{(++)}z_{(-+)}z_{(-+)}z'_{(--)} = z_{(--)}z_{(--)} + z_{(--)}z_{(--)}z_{(-+)} + z_{(--)}z_{(-+)}z_{(--)} + z_{(-+)}z_{(--)}z_{(--)}
$$

$$
+z_{(--)}z_{(--)}z_{(+-)}+z_{(--)}z_{(--)}z_{(++)}+z_{(--)}z_{(++)}+z_{(-+)}z_{(--)}z_{(++)}-z_{(-+)}z_{(--)}z_{(+-)}
$$
  
+
$$
+z_{(-)}z_{(+)}z_{(--)}+z_{(-)}z_{(+-)}z_{(++)}+z_{(-)}z_{(++)}z_{(--)}+z_{(-+)}z_{(-)}z_{(--)}
$$
  
+
$$
+z_{(+-)}z_{(--)}z_{(--)}+z_{(+-)}z_{(--)}z_{(-+)}+z_{(+-)}z_{(-+)}z_{(--)}+z_{(+)}z_{(--)}z_{(--)}
$$

Again, this is just summing up all lines in table 2.2, which give the corresponding probability  $z_{(\pm\pm)}$  in the output, because  $\Pr\left[ f(\mathbf{x}) = \pm 1, f(\mathbf{y}) = \pm 1 | \mathbf{x}, \mathbf{y} \right] \in \{0,1\}.$  Inserting the transformation  $(z_{(\pm\pm)}) \mapsto (m, d)$  yields

$$
\begin{array}{rcl} z'_{(++)} & = & \frac{1}{2}-\frac{3}{4}d+\frac{3}{4}d^2-\frac{1}{2}d^3+\frac{3}{4}m+\frac{3}{4}dm^2-\frac{1}{4}m^3, \\ z'_{(+-)} & = & \frac{3}{4}d-\frac{3}{4}d^2+\frac{1}{2}d^3-\frac{3}{4}dm^2, \\ z'_{(-+)} & = & \frac{3}{4}d-\frac{3}{4}d^2+\frac{1}{2}d^3-\frac{3}{4}dm^2, \\ z'_{(--)} & = & \frac{1}{2}-\frac{3}{4}d+\frac{3}{4}d^2-\frac{1}{2}d^3-\frac{3}{4}m+\frac{3}{4}dm^2+\frac{1}{4}m^3. \end{array}
$$

This leads finally to the iteration equation for the Hamming distance d:

$$
d' = z'_{(+-)} + z'_{(-+)} = \left(\frac{3}{2} - \frac{3}{2}m^2\right)d - \frac{3}{2}d^2 + d^3.
$$

As a check, also the iteration equation for the magnetization  $m$  should coincide with the calculation in section 2.2.1:

$$
m'=z'_{(++)}-z'_{(--)}=\frac{3}{2}m-\frac{1}{2}m^3.
$$

In this case  $(K = 3)$  it is still feasible to calculate the iteration equations for a single Boolean function f by hand, however, for higher connectivities  $K \geq 4$  a scripted computer algebra system might be very beneficial, as there are  $\left(2^K\right)^2$  different input tuples to consider for the dynamics in the second order.

See appendix B for a list of iteration equations  $z'_{(\pm\pm)}$  for all Boolean functions  $\mathfrak f$  with  $K = 3$ .

## 2.2.3 Hamming distance  $d$  in the Kauffman model

The Kauffman model, introduced in section 1.4.3, was the first model for which the Hamming distance in BN was computed analytically [Derrida and Pomeau, 1986]. Therefore any model, which allows the calculation of  $d$ , should include this as special case. In the formalism explained in the last section, this can be done in the following way.

**Theorem 2.18.** *The Hamming distance* d *in the Kauffman model emerges naturally from the formalism introduced in the last section:*

$$
d' = 2p(1-p)\left(1 - (1-d)^K\right). \tag{2.35}
$$

*Proof.* Start with the iteration equation for the probabilities  $z'_{(\pm\pm)}$  and split the summation over x and y into two parts:

$$
z'_{(\pm \pm)} = \sum_{\mathbf{x}} \sum_{\mathbf{y}} \Pr[f(\mathbf{x}) = \pm 1, f(\mathbf{y}) = \pm 1 | \mathbf{x}, \mathbf{y}] \Pr[\mathbf{x}, \mathbf{y} | z_{(\pm \pm)}]
$$

$$
= \left(\sum_{\substack{\mathbf{x}, \mathbf{y} \\ \mathbf{x} = \mathbf{y}}} \Pr\left[f(\mathbf{x}) = \pm 1, f(\mathbf{y}) = \pm 1 | \mathbf{x}, \mathbf{y} \right] \Pr\left[\mathbf{x}, \mathbf{y} | z_{(\pm \pm)}\right] \right) + \left(\sum_{\substack{\mathbf{x}, \mathbf{y} \\ \mathbf{x} \neq \mathbf{y}}} \Pr\left[f(\mathbf{x}) = \pm 1, f(\mathbf{y}) = \pm 1 | \mathbf{x}, \mathbf{y} \right] \Pr\left[\mathbf{x}, \mathbf{y} | z_{(\pm \pm)}\right] \right) = \dots
$$

Recall the result of lemma 1.18. The distribution of Boolean functions  $\rho_F$  in the Kauffman model is such that the functions with a specific number of  $+1$ s in the truth table are distributed binomially with parameter  $p$ . Note that this is independent of the position in the truth table, and therefore independent of the input tuple  $x$  (or  $y$ , respectively). This means the dependence on x can be dropped in those probabilities:

$$
Pr[f(x) = \pm 1, f(y) = \pm 1 | x, y] = Pr[f(any) = \pm 1, f(any other) = \pm 1].
$$

Therefore those factors can be written in front of the sum

$$
\dots = \Pr[f(\text{any}) = \pm 1, f(\text{any}) = \pm 1] \left( \sum_{\substack{\mathbf{x}, \mathbf{y} \\ \mathbf{x} = \mathbf{y}}} \Pr\left[\mathbf{x}, \mathbf{y} | z_{(\pm \pm)}\right] \right)
$$

$$
+ \Pr\left[f(\text{any}) = \pm 1, f(\text{any other}) = \pm 1\right] \left( \sum_{\substack{\mathbf{x}, \mathbf{y} \\ \mathbf{x} \neq \mathbf{y}}} \Pr\left[\mathbf{x}, \mathbf{y} | z_{(\pm \pm)}\right] \right).
$$

Note that in the first term "any" means the same position in both functions, because  $x = y$ . In the second term "any" and "any other" are distinct positions in the truth table, as  $x \neq y$ .

Now the summation  $\sum$  can be calculated separately. First the term with the restriction x,y of equality  $x = y$  is derived:

$$
\sum_{\substack{\mathbf{x},\mathbf{y}\\ \mathbf{x}=\mathbf{y}}}\Pr\big[\mathbf{x},\mathbf{y}|z_{(\pm\pm)}\big]=\sum_{\substack{\mathbf{x},\mathbf{y}\\ \mathbf{x}=\mathbf{y}}}\text{z}_{(++)}^{\langle\mathbf{x},\mathbf{y}\rangle}\text{z}_{(+-)}^{\langle\mathbf{x},\mathbf{y}\oplus\mathbb{1}\rangle}\text{z}_{(-+)}^{\langle\mathbf{x}\oplus\mathbb{1},\mathbf{y}\rangle}\text{z}_{(--)}^{\langle\mathbf{x}\oplus\mathbb{1},\mathbf{y}\oplus\mathbb{1}\rangle}=\dots
$$

The central two exponents are  $\langle x, y \oplus 1 \rangle = \langle x \oplus 1, y \rangle = 0$ , because  $x = y$ . Furthermore  $x = y$ reduces the summation to just a single summation:

$$
\sum_{\substack{\mathbf{x},\mathbf{y}\\ \mathbf{x}=\mathbf{y}}}\mapsto \sum_{\mathbf{x}}\,.
$$

Using transformation (2.32) ( $z_{(\pm\pm)} \mapsto (m,d)$ ) the following result is obtained

$$
\dots = \sum_{\mathbf{x}} \left( \frac{1+m-d}{2} \right)^{\langle \mathbf{x}, \mathbf{x} \rangle} \left( \frac{1+m-d}{2} \right)^{\langle \mathbf{x} \oplus \mathbf{1}, \mathbf{x} \oplus \mathbf{1} \rangle} \n= \sum_{i=0}^{K} {K \choose i} \left( \frac{1+m-d}{2} \right)^i \left( \frac{1-m-d}{2} \right)^{K-i}
$$

$$
= \left[ \left( \frac{1+m-d}{2} \right) + \left( \frac{1-m-d}{2} \right) \right]^K
$$

$$
= (1-d)^K
$$

From the first to the second line it is used, that the number of  $+1s$  is distributed binomially. From the second to third line the binomial expansion  $(a + b)^K = \sum_i {K \choose i} a^i b^{K-i}$  is used.

The summation  $\sum\limits_{\mathbf{x},\mathbf{y}}$  with restriction to  $\mathbf{x} \neq \mathbf{y}$  could be calculated analogously. However, it has to be the counter-probability to before, therefore

$$
\sum_{\substack{\mathbf{x}, \mathbf{y} \\ \mathbf{x} \neq \mathbf{y}}} \Pr\left[\mathbf{x}, \mathbf{y} | z_{(\pm \pm)}\right] = 1 - \sum_{\substack{\mathbf{x}, \mathbf{y} \\ \mathbf{x} = \mathbf{y}}} \Pr\left[\mathbf{x}, \mathbf{y} | z_{(\pm \pm)}\right] = 1 - (1 - d)^K.
$$

Now the probabilities for the functions to have a specific value in their truth table have to be calculated. Again, the case  $x = y$  is treated first:

$$
Pr[f(any) = +1, f(any) = +1] = p,
$$
  
\n
$$
Pr[f(any) = +1, f(any) = -1] = 0,
$$
  
\n
$$
Pr[f(any) = -1, f(any) = +1] = 0,
$$
  
\n
$$
Pr[f(any) = -1, f(any) = -1] = 1 - p
$$

Here, the first and last line have the same condition twice, therefore it is reduced to a single condition, which are then just  $Pr[f($ any $) = \pm 1]$ . This is exactly definition 1.19. The two central lines require the function to assume different values on the same input, which is not possible, hence they are zero. Then the case  $x \neq y$  is treated:

Pr 
$$
[f(\text{any}) = +1, f(\text{any other}) = +1]
$$
 =  $p^2$ ,  
\nPr  $[f(\text{any}) = +1, f(\text{any other}) = -1]$  =  $p(1-p)$ ,  
\nPr  $[f(\text{any}) = -1, f(\text{any other}) = +1]$  =  $(1-p)p$ ,  
\nPr  $[f(\text{any}) = -1, f(\text{any other}) = -1]$  =  $(1-p)^2$ .

Inserting this in the iteration equations for  $z'_{(\pm\pm)}$  yields:

$$
z'_{(++)} = p(1-d)^{K} + p^{2} (1 - (1-d)^{K}),
$$
  
\n
$$
z'_{(+-)} = p(1-p) (1 - (1-d)^{K}),
$$
  
\n
$$
z'_{(-+)} = (1-p)p(1 - (1-d)^{K}),
$$
  
\n
$$
z'_{(--)} = (1-p) (1-d)^{K} + (1-p)^{2} (1 - (1-d)^{K})
$$

Taking all those terms together leads to the correct expression for the Hamming distance  $d$ :

$$
d' = z'_{(+-)} + z'_{(-+)}
$$

37

.

$$
= p(1-p)\left(1-(1-d)^{K}\right) + (1-p)p\left(1-(1-d)^{K}\right) \n= 2p(1-p)\left(1-(1-d)^{K}\right).
$$

 $\Box$ 

Note that in the original paper [Derrida and Pomeau, 1986] much more was shown. The equation from last theorem gives just a single value for the Hamming distance  $d$ . However, Derrida and coworkers derived an iteration equation for the complete probability distribution of possible Hamming distances  $d$ , which is just sharply peaked around the value reproduced here.

#### 2.2.4 Higher orders of the dynamics and multistate networks

Higher orders of the dynamics have been mentioned several times, but now they are introduced formally:

**Definition 2.19.** *The order*  $n \in \mathbb{N}$  *of the dynamics of a BN is the number of variables on each node* i *in otherwise identical BNs (the in-degree* k<sup>i</sup> *and all Boolean functions* f *on each* node are assumed to be the same). The iteration equations are given by  $z'_{(\pm \cdots \pm)}$  where the *index set*  $(\pm \cdots \pm)$  *has exactly n elements.* 

This is nothing else, than assuming  $n$  variables  $\left(x_i^{(1)},x_i^{(2)},\ldots,x_i^{(n)}\right)$  on each node  $i$ , instead of just one  $x_i\equiv x_i^{(1)}$  for the magnetization  $m$  or two  $(x_i,y_i)\equiv\left(x_i^{(1)},x_i^{(2)}\right)$  for the Hamming distance d. In [Derrida and Weisbuch, 1986] the authors derive relations between those orders in the constraint of constant magnetization, i.e.  $m^{(1)}=m^{(2)}=\cdots=m^{(n)}.$  They show that for  $|M| = 2$  all odd orders depend only on the even orders. This is somehow intuitively clear for  $n = 3$ , as the only possibilities are that all 3 variables on a node *i* are equal or one is different than the other two, leading again to four different states on a node. However, for higher orders this is not so obvious, but nevertheless true. This fact does not hold when  $|M|\geq 3,$  which corresponds to a Potts model, where each variable  $x_i^{(.)}$ can assume the values  $M = \{1, 2, \ldots, q\}.$ 

In their work the authors define the overlap  $o_n$  as follows<sup>2</sup>

$$
o_n := \sum_{a \in M} z_{(a...a)}, \qquad |(a...a)| = n.
$$

Note that the overlap is the fraction of nodes, which are the same in all  $n$  BNs. Therefore the Hamming distance could also be expressed by those overlaps:

$$
d=1-o_2.
$$

These overlaps can be seen as generalized distances in the BN.

Further work [Derrida and Flyvbjerg, 1987] shows that those higher orders can also be related to the moments of the distribution of the magnetization  $m$  in a single BN. As

 $^2$ In the original work the overlap was defined with the symbol  $x_n$ , however, here  $x_i$  denotes the variable on node i.

already indicated at the end of last section, all formulas in this work only treat single valued iteration equations, i.e. only the peak value of complete distributions on those parameters (e.g.  $m$  or  $d$ ). Regarding to the work of Derrida and coworkers, complete distributions could be calculated by those higher orders of the dynamics<sup>3</sup>. Furthermore they introduce in [Derrida and Flyvbjerg, 1987] the so-called "stable core", which is the fraction of nodes, which are the same in all BNs, independent of their initial condition and do not change anymore in the time-evolution:

$$
s := \lim_{n \to \infty} o_n
$$

In [Flyvbjerg, 1988] an iteration equation for the stable core s is derived independently. It is shown that the parameter  $s$  is another order parameter for a phase transition between a so-called "frozen" and a "non-frozen" phase. The frozen phase corresponds to  $s = 1$ , where all nodes are independent from their initial condition and do not change in time anymore.

All these higher orders could also be calculated in the formalism introduced so far in this chapter.

**Proposition 2.20.** *Let* M *be some set and* n *indices*  $(a_1a_2...a_n)$  *with*  $a_i \in M$ *. Then the iteration equation for* z(a1a2...an) *is given by*

$$
z'_{(a_1 a_2...a_n)} = \sum_{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, ..., \mathbf{x}^{(n)}} \Pr\left[f(\mathbf{x}^{(1)}) = a_1, f(\mathbf{x}^{(2)}) = a_2, ..., f(\mathbf{x}^{(n)}) = a_n | \mathbf{x}^{(1)}, \mathbf{x}^{(2)}, ..., \mathbf{x}^{(n)}\right] \times \Pr\left[\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, ..., \mathbf{x}^{(n)} | z_{(a_1 a_2...a_n)}\right].
$$
\n(2.36)

This is nothing else than the canonical extension of the theorems 2.6 and 2.13. However, calculating the stable core  $s$  with this formula is not that easy, rather impossible as the order n tends to infinity.

The extension to  $|M| > 2$  has been made by several authors so far. A recent study [Wittmann et al., 2010] looks at a generalized Kauffman model, deriving the critical condition for these networks. They also restrict their functions to a class, called single switch functions, which resemble Linear Threshold functions, dealt with in the next chapter, and also give the critical condition for this model.

Calculating higher orders of the dynamics could also be seen as just increasing the size of M by a factor of  $|M|$  for each order. This is already indicated by the term "4state-model", coined by [Kesseli et al., 2006]. However, not all possible functions on this multistate network are allowed in this case, because already a "sub"-tuple of the complete input tuple determines the (partial) output of the function, with no interactions at all between those "sub"-tuples. Furthermore the function is symmetric with respect to each of its "sub"-tuples. So higher orders of the dynamics are nothing else than a restricted form of the dynamics in a multistate network.

<sup>&</sup>lt;sup>3</sup>This is also reminiscent of statistical mechanics, where the partition sum could also be calculated in principle by knowing all derivations of it (the correlation functions) up to infinite order.

# 2.3 Attractors in the MF dynamics

In a MF approximation most of the information about attractors is lost, and usually only fixed points of the iteration equations are calculated. Those fixed points are defined as solutions of the equations

$$
m^* = \mathcal{M}(\gamma; m^*), \qquad (2.37a)
$$

$$
d^* = \mathcal{D}(\gamma; m^*, d^*). \tag{2.37b}
$$

However, as explained in the first chapter, the attractors in BNs (without the MF approximation) are often limit cycles. Those fixed points given by the last equations all have period 1, so are no real cycles. Therefore the magnetization  $m^*$  and Hamming distance d <sup>∗</sup> obtained by the MF approximation could be seen as the average values of those parameters in the actual limit cycle of a BN. However, attractors with higher periods could somehow be constructed, as shown in later sections, but they are rather cumbersome to derive explicitly.

Several solutions  $m^*$  and  $d^*$  of equations 2.37 could exist, up to a maximum of the order of the polynomials  $M$  and  $D$ . However, not all these solutions might be in the correct interval. For  $M = \{0, 1\}$  these correct intervals are  $\widetilde{m}^*, d^* \in [0, 1]$ , whereas for  $M = \{-1, +1\}$ they are  $m^* \in [-1,1]$  and  $d^* \in [0,1]$ . From the Brouwer fixed point theorem it is clear, that at least one of the solutions has to be in the corresponding interval, because both mappings  $m \mapsto m' = \mathcal{M}(\gamma; m)$  and  $d \mapsto d' = \mathcal{D}(\gamma; m, d)$  are smooth in their variables m and d for a given set of parameters  $\gamma$  (since they are finite polynomials).

However, although such fixed points always exist, the main issue with those solutions is their stability against small perturbations, i.e. if those fixed points are attractive or repulsive. This stability can be determined with Linear Stability analysis. This stability of the fixed points  $m^*$  and  $d^*$  could change when varying parameters  $\gamma$  in the distributions  $\rho_k$  and  $\rho_F$ . This might lead to phase transitions between ordered and disordered phases in the BN, when the fixed point  $d^* = 0$  changes from attractive to repulsive.

## 2.3.1 Linear Stability analysis

Determining the stability of a fixed point of the iteration equation can be done via a Linear Stability analysis (LSA). A treatment of this method can be found in most textbooks on dynamical systems, e.g. [Strogatz, 1994]. The main idea is to take the series expansion of the iteration equation around the fixed point and looking only at the linear term. The following proposition explains this method to classify the fixed point.

**Proposition 2.21.** Let  $x' = \mathcal{P}(x)$  be some iteration equation and let  $x^*$  be a fixed point of *this equation*  $(x^* = \mathcal{P}(x^*))$ *. Then the fixed point*  $x^*$  *is stable if* 

$$
\left|\frac{\partial \mathcal{P}(x)}{\partial x}\right|_{x=x^*} < 1\tag{2.38}
$$

*Proof.* As already mentioned, first expand the function  $P$  into a series around the fixed

point  $x^*$ 

$$
\mathcal{P}(x) = \mathcal{P}(x^*) + \left. \frac{\partial \mathcal{P}(x)}{\partial x} \right|_{x^*} (x - x^*) + \frac{1}{2} \left. \frac{\partial^2 \mathcal{P}(x)}{\partial x^2} \right|_{x^*} (x - x^*)^2 + \dots
$$

By definition, the first term in this series is equal to the fixed point itself  $x^* = \mathcal{P}(x^*)$ . Defining a variable  $\Delta x := x - x^*$  as the distance to the fixed point and subtracting  $x^*$  from both sides of the iteration equation and the series expansion, one arrives at the following equation for the distance  $\Delta x$ 

$$
\Delta x' = \frac{\partial \mathcal{P}(x)}{\partial x}\bigg|_{x^*} \Delta x + \mathcal{O}\left(\Delta x^2\right)
$$

Hence if starting with an infinitesimal distance to the fixed point, higher orders in  $\Delta x$  can be neglected, and only the linear term is of importance. This iteration converges to the fixed point ( $\Delta x = 0$ ) if the condition

$$
\left|\frac{\partial \mathcal{P}(x)}{\partial x}\right|_{x^*} < 1
$$

is met, because then a small distance  $\Delta x$  gets mapped to an even smaller one  $\Delta x'.$  $\Box$ 

If the first coefficient  $\frac{\partial \mathcal{P}}{\partial x}$  equals 1, then  $\Delta x' = \Delta x$  and in first order of the expansion, the distance stays at its original value. Higher orders have to be calculated to determine, whether the fixed point  $x^*$  is attractive or repulsive, but the convergence/divergence is at a much lower rate, see also [Kürten, 1988a]. On the other hand, if the first coefficient is negative (−1 <  $\frac{\partial \mathcal{P}}{\partial x}$  < 0), then the distance oscillates around the fixed point, but still converges. If the coefficient is −1 then a bifurcation into a period-2 solution of the iteration equation occurs.

## 2.3.2 Phase transition and critical condition

The phase transition between ordered and disordered dynamics occurs when the fixed point  $d^* = 0$  changes its stability. The parameter  $d^*$  could be seen as order parameter of this dynamical phase transition, as  $d^*=0$  "above" the critical point  $\gamma_c$  and this is the unique stable fixed point of D. "Below" the critical point  $\gamma_c$  another stable fixed point  $d^*$ emerges with  $d^* > 0$ , whereas the fixed point  $d^* = 0$  becomes repulsive. However, as the parameters approach their critical values  $\gamma \to \gamma_c$ , this fixed point "below" the critical point also approaches the value of the stable phase

$$
d^* \stackrel{\gamma \to \gamma_c}{\longrightarrow} 0. \tag{2.39}
$$

Therefore the comparison to a continuous phase transition in statistical physics is justified. At and below this critical point  $\gamma_c$  small perturbations in the BN do not settle down anymore, they propagate through the whole BN until a finite fraction of all nodes has a different value compared to the original unperturbed BN.

One of the advantages of the MF approximation is, that the value of the external parameters  $\gamma_c$  can be calculated analytically.

**Definition 2.22.** Let  $\mathcal{D}(\gamma; m, d)$  be the iteration equation for the Hamming distance, intro*duced in definition 2.16 and*  $K = \max(\rho_k)$ *. The coefficients in a binomial expansion in the*  $p$ owers of  $d$  are denoted by  $\lambda_k\,(\gamma;m).$  The plain coefficients of  $d^k$  are denoted by  $\mu_k\,(\gamma;m).$ 

$$
d' = \mathcal{D}(\gamma; m, d)
$$
  
= 
$$
\sum_{k=0}^{K} {K \choose k} \lambda_k (\gamma; m) d^k (1 - d)^{K - k}
$$
 (2.40a)

$$
= \sum_{k=0}^{K} \mu_k(\gamma; m) d^k.
$$
 (2.40b)

An expansion like in equation  $(2.40a)$  for the Hamming distance d has been first given by Derrida in [Derrida, 1987], because the term  $\binom{K}{n}d^n(1-d)^{K-n}$  has the interpretation of the probability of having exactly  $n$  different positions in the inputs x and y. In some cases, but not in all, the coefficients  $\lambda_n$  have also an interesting interpretation according to damage spreading. This relation will be investigated further in the next section.

An example where the coefficients  $\lambda_n$  can be computed directly, and are not obtained by constructing the complete iteration equation for the Hamming distance  $d$ , like in corollary 2.17, and then transforming the polynomial to the form of equation (2.40a) is given e.g. in [Kürten and Clark, 2008].

The two different representations of the coefficients,  $\lambda_k$  and  $\mu_k$ , can be transformed into each other. The direction  $\lambda_k \mapsto \mu_k$  is given by

$$
\mu_k(\gamma; m) = \sum_{n=0}^k {K \choose n} {K-n \choose k-n} (-1)^{k-n} \lambda_n(\gamma; m).
$$
 (2.41)

The other direction,  $\mu_k \mapsto \lambda_k$ , can not be written as simple as above for arbitrary K. However, it only involves inverting a lower triangular matrix. The entries in this matrix consist only of the two binomial factors and a sign, so it has no zeros on the diagonal, i.e. has full rank, and is therefore invertible. Therefore this direction of transformation exists and is unique.

Recall from the remark after corollary 2.8, that every distribution on the functions could be explicitly written in principle as probabilities  $Pr[f|\rho_F]$  for each Boolean function f. Although it is not always straightforward to calculate them, it can be done with the projection of a generic function  $f$  to Boolean functions  $f$  defined by truth tables. This is already given by equation 2.17. Hence in the following proofs only a single Boolean function f has to be treated, because all expressions can always be weighted accordingly with  $Pr[f|\rho_F]$ afterwards.

Note that just assuming single Boolean functions f is also valid for Probabilistic Boolean functions, introduced in section 1.4.2. As already mentioned earlier, even if there are multiple outputs of the function possible with different probabilities, this can always be treated as a mixture of several single Boolean functions f. In each of the replicas of the BN the choice of a function f has to be the same, because the BNs are identical, except **only** their state  $x_i$  or  $y_i$  could be different. Hence this could also be modeled by just a single

Boolean function f at first, and the mixture of those functions is then introduced with the explicit probabilities Pr  $\left[\frac{f}{\rho_F}\right]$  later on.

Now a few technicalities have to be stated in order to fully characterize the critical condition, and therefore the phase transition, in the dynamics of the BN. However, these lemmas are completely obvious from the interpretation, because they only show that  $d^* = 0$ is always a fixed point of the iteration equation. This is clear, because a perturbation cannot arise out of nothing, so if inserting  $d = 0$  into D, this should always yield  $d' = 0$ . Nevertheless this has to be proven for the abstract polynomial  $D$ , which has been defined above.

**Lemma 2.23.** *The zeroth coefficient in* D *vanishes:*

$$
\lambda_0(\gamma; m) = \mu_0(\gamma; m) = 0. \tag{2.42}
$$

*Proof.* Because of the remark made before the lemma, only a single Boolean function f can be treated. Recall  $d' = z_{(+ -)}' + z_{(- +)}'$  and the iteration equations for  $z_{(\pm\pm)}'$ :

$$
z'_{(\pm\pm)} = \sum_{\mathbf{x},\mathbf{y}} \Pr\left[\mathfrak{f}(\mathbf{x}) = \pm 1, \mathfrak{f}(\mathbf{y}) = \pm 1 | \mathbf{x}, \mathbf{y} \right] \Pr\left[\mathbf{x}, \mathbf{y} | z_{(\pm\pm)}\right].
$$

If  $x = y$  then it follows

$$
Pr[f(\mathbf{x}) = +1, f(\mathbf{y}) = -1 | \mathbf{x} = \mathbf{y}] = Pr[f(\mathbf{x}) = -1, f(\mathbf{y}) = +1 | \mathbf{x} = \mathbf{y}] = 0
$$

because the function f cannot have two different values for the same input. Hence the sum in the iteration equation for  $d$  given above is in effectively only over all x and y with  $\mathbf{x} \neq \mathbf{y}$ . Recall Pr  $[\mathbf{x}, \mathbf{y}|z_{(\pm\pm)}] = z_{(++)}^{\langle \mathbf{x}, \mathbf{y} \rangle} z_{(+-)}^{\langle \mathbf{x}, \mathbf{y} \oplus \mathbb{1} \rangle}$  $\langle \mathbf{x}, \mathbf{y} \oplus \mathbb{1} \rangle$   $\chi \langle \mathbf{x} \oplus \mathbb{1}, \mathbf{y} \rangle$   $\chi \langle \mathbf{x} \oplus \mathbb{1}, \mathbf{y} \oplus \mathbb{1} \rangle$ <br>(+-)  $z$  (-+)  $z$  (--)  $\mathbf{C}(\mathbf{x} \oplus \mathbb{I}, \mathbf{y} \oplus \mathbb{I})$ . With  $\mathbf{x} \neq \mathbf{y}$  it follows

$$
\langle \mathbf{x}, \mathbf{y} \rangle + \langle \mathbf{x} \oplus \mathbb{1}, \mathbf{y} \oplus \mathbb{1} \rangle \quad \langle \quad K,
$$
  

$$
\langle \mathbf{x}, \mathbf{y} \oplus \mathbb{1} \rangle + \langle \mathbf{x} \oplus \mathbb{1}, \mathbf{y} \rangle \quad \geq \quad 1.
$$

and so there is at least one  $z_{(-+)}$  or  $z_{(+-)}$  in each of those terms. Using the transformation from equations 2.32, which is (partially) given by  $z_{(+-)} = z_{(-+)} = \frac{d}{2}$ , it follows immediately that each term has at least a factor d in it and is therefore order  $O(d)$  or higher. Hence the absolute term  $\mu_0(\gamma; m)$  in an expansion in orders of d has to be zero. Inserting this into equation 2.41, it follows  $0 = \mu_0 = {K \choose 0} {K \choose 0} \lambda_0$  and the proof is completed.

 $\Box$ 

An immediate consequence of this lemma is the existence of at least one known fixed point in the iteration equation for  $d$ :

**Proposition 2.24.** *The iteration equation*  $d' = D(\gamma; m, d)$  *has the fixed point* 

$$
d^* = 0.\t\t(2.43)
$$

*Proof.* Inserting  $d = 0$  into D gives  $\mathcal{D}(\gamma; m, 0) = 0$ , because each term is at least of order  $\mathcal{O}(d)$ . As from  $d = 0$  it follows that  $d' = 0$ , this is a fixed point  $d^* = 0$ .  $\Box$ 

The last proposition should be clear, because it says nothing else, that a perturbation of the dynamics cannot come out of nothing, i.e. if the two BNs with states  $X$  and  $Y$  start with the same initial conditions  $(X = Y)$ , they will stay identical to each other forever.

**Proposition 2.25.** *The critical condition*  $\gamma_c$  *for the stability of the dynamics in the BN is given by the implicit equations*

$$
K\lambda_1(\gamma_c; m^*) = \mu_1(\gamma_c; m^*) = 1.
$$
 (2.44)

*Proof.* The critical condition follows immediately from the LSA of the fixed point  $d^* = 0$ :

$$
\left. \frac{\partial \mathcal{D} \left( \gamma ; m, d \right)}{\partial d} \right|_{m = m^*, d^* = 0} = \binom{K}{1} \lambda_1 \left( \gamma ; m^* \right).
$$

All other terms in D are at least of order  $O(d)$  after the derivation, hence vanish if the fixed point  $d^* = 0$  is inserted into the equation.

From LSA this first coefficient has to be less than 1 and larger than −1 for the fixed point to be attractive/stable. As  $K\lambda_1(\gamma;m^*)=-1$  is no realistic solution, because at  $-1$  the fixed point bifurcates into a symmetric period-2 solution. The symmetry is with respect to the original fixed point, oscillating above and below it with the same magnitude, at least infinitesimally close to the bifurcation point. However, a negative solution of  $d^*$  is not possible, and hence the period-2 solution with a negative and positive accumulation point is also not possible. Therefore the critical condition is

$$
K\lambda_1(\gamma_c;m^*) = \mu_1(\gamma_c;m^*) = 1.
$$

In fact, this first coefficient  $\lambda_1$  or  $\mu_1$  can never be negative, as it has an interpretation as probability, which is always positive. This relation to a probability will be investigated further in the following pages.

 $\Box$ 

The critical condition for stability of the dynamics is already well known. For the Kauffman model it was first derived in [Derrida and Pomeau, 1986].

## 2.3.3 Perturbation approach via Sensitivities  $S^{\left( n\right) }$

Another approach to derive the iteration equation for the Hamming distance has been explored in the literature, besides the construction of the probabilities  $z'_{(\pm\pm)}$  and then the transformation  $\big(z_{(\pm\pm)}\big)\mapsto(m,d),$  see e.g. [Moreira and Amaral, 2005], [Shmulevich and Kauffman, 2004] or [Greil and Drossel, 2005] among several others. The authors follow closely the arguments given in [Derrida, 1987], where this derivation is made first. In this publication non-symmetric spin-glass models are treated, that can be related to BNs with Linear Threshold functions and a symmetric Gaussian distribution of weights. It is mentioned that this can be generalized to any other distribution, however, this generalization is not as straightforward as expected and this specific approach is only valid because of this specific class of Boolean function with the symmetric distribution, which is not present in the aforementioned publications. This generalization is shown in the next chapter and will be made clear in theorem 3.4, when all the concepts related to Linear Threshold functions are introduced. In this theorem the equivalence of the formalism presented so far in this work to the integral formalism in [Kürten, 1988b], which also uses symmetric distributions of weights in Linear Threshold functions.

This approach uses the so-called sensitivities and tries to derive the Hamming distance directly from an analysis of how perturbations spread in the BN. So nodes are considered perturbed or unperturbed with respect to their original attractor in each timestep. The ansatz is an expression similar to equation (2.40a). Note that the term  $\binom{K}{n}d^n(1-d)^{K-n}$  is exactly the probability to have  $n$  "perturbed" nodes in the input, as mentioned before. If this is multiplied by the probability that  $n$  changes in the input (or  $n$  perturbed nodes in the input) results in a change of the output of the function, this yields exactly $^4\!$ :

$$
d'_{S} = \sum_{n=1} S^{(n)} {K \choose n} d^{n}_{S} (1 - d_{S})^{K - n},
$$
\n(2.45)

where  $S^{(n)}$  are the sensitivities, which are defined as follows:

**Definition 2.26.** *The sensitivity*  $S_j$  *of variable*  $x_j$  *in the Boolean function*  $f : M^K \to M$  *is defined as the probability, that a change in the variable*  $x_j \mapsto x_j \oplus 1$  *changes the output of the function:*

$$
S_j := \Pr\left[ (x_j \mapsto x_j \oplus 1) \Rightarrow (\mathfrak{f} \mapsto \mathfrak{f} \oplus 1) \right]. \tag{2.46}
$$

*For*  $M = \{0, 1\}$  *this statement can be written as*  $\tilde{f}(x) \oplus \tilde{f}(x \oplus e_i)$ *. Note that this expression equals one iff the output of the function changes when the variable*  $x_j$  *is flipped, and is zero otherwise.*

In MF the sensitivity  $S_i$  has to be weighted according to the state of the BN:

$$
S_j = \sum_{\mathbf{x}} \widetilde{f}(\mathbf{x}) \oplus \widetilde{f}(\mathbf{x} \oplus \mathbf{e}_j) \Pr\left[\mathbf{x}|z_{(\pm)}\right].
$$
 (2.47)

Note that this expression has also been called "activities" in [Shmulevich and Kauffman, 2004].

**Definition 2.27.** *The average sensitivity* S *is defined as*

$$
S := \frac{1}{K} \sum_{j=1}^{K} S_j = \frac{1}{K} \sum_{j=1}^{K} \sum_{\mathbf{x}} \widetilde{f}(\mathbf{x}) \oplus \widetilde{f}(\mathbf{x} \oplus \mathbf{e}_j) \Pr\left[\mathbf{x} | z_{(\pm)}\right].
$$
 (2.48)

*Higher sensitivities*  $S^{(n)}$  *are defined as the probabilities, that simultaneous change of more than one variable in the input tuple*  $\bf{x}$  *changes the output of the function. Note that*  $S^{(1)}\equiv S.$  $S^{(2)}$  is the probability that the change of  $2$  variables changes  $\mathfrak f,$  etc. This can be stated with

<sup>&</sup>lt;sup>4</sup>This quantity is labeled  $d_S$  instead of d to hint at the fact, that the construction method is different from the Hamming distance introduced earlier in this work.

*the expression*

$$
S^{(n)} = \frac{1}{\binom{K}{n}} \sum_{\substack{I \\ |I| = n}} \sum_{\mathbf{x}} \widetilde{f}(\mathbf{x}) \oplus \widetilde{f}(\mathbf{x} \oplus \mathbf{e}_{\mathbf{i}_1} \oplus \cdots \oplus \mathbf{e}_{\mathbf{i}_n}) \Pr\left[\mathbf{x} | z_{(\pm)}\right].
$$
 (2.49)

This definition of sensitivities is related to the concept of the Boolean derivative, explained in more detail in the next section.

However, this ansatz (equation (2.45)) brings some problems with it. When compared to the iteration equation of the Hamming distance obtained by the formalism explained in the last sections, this perturbation ansatz can be shown to neglect the actual dynamics of the BN by looking only at this perturbation and the second BN (with state Y) is not allowed to relax to its fixed point  $m^*$  in the magnetization, but is rather restricted to keep a certain distance to it (at least below the critical point with  $d^{\ast}>0$ ). Therefore this iteration equation yields a wrong fixed point in the Hamming distance. This fact will be proved in theorem 2.30.

However, this perturbation ansatz is still quite useful. It can be shown, the the first coefficients coincide, i.e.

$$
\lambda_1 = S^{(1)},\tag{2.50}
$$

so that the critical condition is actually the same, obtained by both methods. As in this perturbation ansatz, the expressions for the sensitivities are given explicitly, this yields a method to obtain the critical condition, without having to compute the complete iteration equations.

This calculation is rather technical, and it is easier to rewrite both,  $\lambda_1$  and  $S^{(1)}$ , to a different form. Hence the proof is splitted into two parts to enhance readability of the complete derivation. Note further, that this proof is actually written for  $M = \{0, 1\}$ , because with this choice of  $M$ , the iteration equation for  $d$  could be stated as described in corollary 2.17. However, the statement is still true for  $M = \{-1, +1\}$ , but the derivation itself is more complicated.

Note that these proofs only use a single Boolean function f, but due to the remark made in the last section, all those terms could be weighted with  $Pr[k|\rho_k]$  and  $Pr[f|\rho_F]$  afterwards, to obtain the correct expression.

 ${\bf Lemma~ 2.28.}$  Let  $M=\{0,1\}.$  The average sensitivity  $S^{(1)}$  can be rewritten as

$$
S^{(1)} = \frac{1}{2K} \sum_{\mathbf{x}} \sum_{j=1}^{K} \widetilde{\mathfrak{f}}(\mathbf{x}) \oplus \widetilde{\mathfrak{f}}(\mathbf{x} \oplus \mathbf{e_j}) \widetilde{m}^{\langle \mathbf{x}, \mathbf{x} \rangle + \langle \mathbf{e_j}, \mathbf{x} \oplus \mathbf{e_j} \rangle - 1} (1 - \widetilde{m})^{K - \langle \mathbf{x}, \mathbf{x} \rangle - \langle \mathbf{e_j}, \mathbf{x} \oplus \mathbf{e_j} \rangle}
$$
(2.51)

*Proof.* Begin with the expression given in definition 2.27:

$$
S^{(1)} = \frac{1}{K} \sum_{\mathbf{x}} \sum_{j=1}^{K} \tilde{\mathfrak{f}}(\mathbf{x}) \oplus \tilde{\mathfrak{f}}(\mathbf{x} \oplus \mathbf{e}_{\mathbf{j}}) \Pr[\mathbf{x}|z_{(\pm)}]
$$
  

$$
= \frac{1}{2K} \sum_{\mathbf{x}} \sum_{j=1}^{K} \tilde{\mathfrak{f}}(\mathbf{x}) \oplus \tilde{\mathfrak{f}}(\mathbf{x} \oplus \mathbf{e}_{\mathbf{j}}) \left( \Pr[\mathbf{x}|z_{(\pm)}] + \Pr[\mathbf{x}|z_{(\pm)}] \right)
$$

$$
= \frac{1}{2K} \left( \sum_{\mathbf{x}} \sum_{j=1}^K \widetilde{\mathfrak{f}}(\mathbf{x}) \oplus \widetilde{\mathfrak{f}}(\mathbf{x} \oplus \mathbf{e_j}) \Pr\left[\mathbf{x} | z_{(\pm)}\right] + \sum_{\mathbf{x}} \sum_{j=1}^K \widetilde{\mathfrak{f}}(\mathbf{x} \oplus \mathbf{e_j}) \oplus \widetilde{\mathfrak{f}}(\mathbf{x}) \Pr\left[\mathbf{x} | z_{(\pm)}\right] \right) = \dots
$$

Now define  $y = x \oplus e_i$ . Since  $x \oplus e_j \oplus e_j = x$  it follows that also  $x = y \oplus e_i$ . When inserting y in the second term above, the second sum is taken over  $y \oplus e_i$  and the second term reads  $\sum_{k=1}^{K}$  $j=1$  $\sum$  $\sum_{\mathbf{y}\oplus\mathbf{e_j}}\!\!\!\!\!\!\!\!\!j\left(\mathbf{y}\right)\oplus\!\!\!\!\!\!\!j\left(\mathbf{y}\oplus\mathbf{e_j}\right)\Pr\big[\mathbf{y}\oplus\mathbf{e_j}|z_{(\pm)}\big].$  As the sum goes over all tuples in  $M^K$ , the summation over  $y \oplus e_i$  is the same as a summation over y. Then both terms have a different summation variable x or y. However, they can be joined together again by just replacing the symbols  $y \mapsto x$  in the second term:

$$
\begin{split}\n\cdots &= \frac{1}{2K} \sum_{\mathbf{x}} \sum_{j=1}^{K} \widetilde{\mathfrak{f}}(\mathbf{x}) \oplus \widetilde{\mathfrak{f}}(\mathbf{x} \oplus \mathbf{e}_{\mathbf{j}}) \left( \Pr\left[\mathbf{x} | z_{(\pm)}\right] + \Pr\left[\mathbf{x} \oplus \mathbf{e}_{\mathbf{j}} | z_{(\pm)}\right] \right) \\
&= \frac{1}{2K} \sum_{\mathbf{x}} \sum_{j=1}^{K} \widetilde{\mathfrak{f}}(\mathbf{x}) \oplus \widetilde{\mathfrak{f}}(\mathbf{x} \oplus \mathbf{e}_{\mathbf{j}}) \left( z_{(+)}^{(\mathbf{x},\mathbf{x})} z_{(-)}^{K-(\mathbf{x},\mathbf{x})} + z_{(+)}^{(\mathbf{x} \oplus \mathbf{e}_{\mathbf{j}},\mathbf{x} \oplus \mathbf{e}_{\mathbf{j}})} z_{(-)}^{K-(\mathbf{x} \oplus \mathbf{e}_{\mathbf{j}},\mathbf{x} \oplus \mathbf{e}_{\mathbf{j}})} \right) = \dots\n\end{split}
$$

Now a closer look at the exponents of  $z_{(\pm)}$  is needed.  ${\bf x}\oplus {\bf e_j}$  changes exactly one variable in the tuple x, therefore  $\langle x \oplus e_j, x \oplus e_j \rangle = \langle x, x \rangle \pm 1$ . If the operation  $\oplus e_j$  flips  $1 \mapsto 0$ , then the bracket is 1 less, if  $0 \mapsto 1$  then the bracket increases by 1. Note that

$$
\langle \mathbf{e_j}, \mathbf{x} \oplus \mathbf{e_j} \rangle = 1 \Leftrightarrow x_j = 0 \Leftrightarrow \langle \mathbf{x} \oplus \mathbf{e_j}, \mathbf{x} \oplus \mathbf{e_j} \rangle = \langle \mathbf{x}, \mathbf{x} \rangle + 1,
$$
  
 $\langle \mathbf{e_j}, \mathbf{x} \oplus \mathbf{e_j} \rangle = 0 \Leftrightarrow x_j = 1 \Leftrightarrow \langle \mathbf{x} \oplus \mathbf{e_j}, \mathbf{x} \oplus \mathbf{e_j} \rangle = \langle \mathbf{x}, \mathbf{x} \rangle - 1.$ 

Using this, the term  $\langle x \oplus e_j, x \oplus e_j \rangle$  can be written in closed form:

$$
\langle \mathbf{x} \oplus \mathbf{e_j}, \mathbf{x} \oplus \mathbf{e_j} \rangle = \langle \mathbf{x}, \mathbf{x} \rangle + 2 \langle \mathbf{e_j}, \mathbf{x} \oplus \mathbf{e_j} \rangle - 1.
$$

Inserting this into  $S^{(1)}$  above

$$
\begin{split}\n&\dots = \frac{1}{2K} \sum_{\mathbf{x}} \sum_{j=1}^{K} \tilde{f}(\mathbf{x}) \oplus \tilde{f}(\mathbf{x} \oplus \mathbf{e}_{j}) \left( z_{(+)}^{(\mathbf{x},\mathbf{x})} z_{(-)}^{K-(\mathbf{x},\mathbf{x})} + z_{(+)}^{(\mathbf{x},\mathbf{x})+2(\mathbf{e}_{j},\mathbf{x} \oplus \mathbf{e}_{j})-1} z_{(-)}^{K-(\mathbf{x},\mathbf{x})-2(\mathbf{e}_{j},\mathbf{x} \oplus \mathbf{e}_{j})+1} \right) = \\
&= \frac{1}{2K} \sum_{\mathbf{x}} \sum_{j=1}^{K} \tilde{f}(\mathbf{x}) \oplus \tilde{f}(\mathbf{x} \oplus \mathbf{e}_{j}) z_{(+)}^{(\mathbf{x},\mathbf{x})+(\mathbf{e}_{j},\mathbf{x} \oplus \mathbf{e}_{j})-1} z_{(-)}^{K-(\mathbf{x},\mathbf{x})-(\mathbf{e}_{j},\mathbf{x} \oplus \mathbf{e}_{j})} \times \\
&\times \underbrace{\left( z_{(+)}^{1-(\mathbf{e}_{j},\mathbf{x} \oplus \mathbf{e}_{j})} z_{(-)}^{(\mathbf{e}_{j},\mathbf{x} \oplus \mathbf{e}_{j})} + z_{(+)}^{(\mathbf{e}_{j},\mathbf{x} \oplus \mathbf{e}_{j})} z_{(-)}^{1-(\mathbf{e}_{j},\mathbf{x} \oplus \mathbf{e}_{j})} \right)}_{=:A}\n\end{split}
$$

Now there are two cases to distinguish for the calculation of the last term  $A$ , which lead to the same result:

$$
\langle \mathbf{e_j}, \mathbf{x} \oplus \mathbf{e_j} \rangle = 0 \Rightarrow A = z_{(+)}^{1-0} z_{(-)}^0 + z_{(+)}^0 z_{(-)}^{1-0} = z_{(+)} + z_{(-)} = 1,
$$
  
 $\langle \mathbf{e_j}, \mathbf{x} \oplus \mathbf{e_j} \rangle = 1 \Rightarrow A = z_{(+)}^{1-1} z_{(-)}^1 + z_{(+)}^1 z_{(-)}^{1-1} = z_{(-)} + z_{(+)} = 1.$ 

As  $A = 1$  the last term vanishes in the product. By replacing  $z_{(+)} = \tilde{m}$  and  $z_{(-)} = 1 - \tilde{m}$ , the

proof is concluded.

The extension for arbitrary  $\rho_F$  and  $\rho_k$  is as follows

$$
S^{(1)} = \sum_{k} \Pr\left[k|\rho_{k}\right] \frac{1}{2k} \sum_{\tilde{\mathfrak{f}}} \Pr\left[\tilde{\mathfrak{f}}|\rho_{\mathbf{F}}\right] \sum_{\mathbf{x}} \sum_{j=1}^{k} \tilde{\mathfrak{f}}(\mathbf{x}) \oplus \tilde{\mathfrak{f}}(\mathbf{x} \oplus \mathbf{e}_{\mathbf{j}}) \widetilde{m}^{\langle\mathbf{x}, \mathbf{x}\rangle + \langle\mathbf{e}_{\mathbf{j}}, \mathbf{x} \oplus \mathbf{e}_{\mathbf{j}}\rangle - 1} (1 - \widetilde{m})^{k - \langle\mathbf{x}, \mathbf{x}\rangle - \langle\mathbf{e}_{\mathbf{j}}, \mathbf{x} \oplus \mathbf{e}_{\mathbf{j}}\rangle} \tag{2.52}
$$

The structure of the expression in the last lemma becomes quite clear with the introduction of the Boolean derivative in the next section. A Boolean derivative is more or less nothing else than a mapping from a Boolean function to another Boolean function with one fewer variable, and hence the order of m should be  $\mathcal{O}(m^{K-1})$  in this expression, as seen in the lemma. This order is also clear, when considering that every term in the expansion of the Hamming distance  $d$  is at maximum of order  $\mathcal{O}(m^i d^{K-i})$  with  $0 \geq i \geq K$ , and hence  $\lambda_1$  should be of order  $\mathcal{O}(m^{K-1})$ , too. This is now proved in the second part of the equivalence.

**Theorem 2.29.** *The first coefficient*  $\lambda_1(\gamma; m)$  *in the binomial expansion of*  $\mathcal{D}(\gamma; m, d)$  *is equal to the probability, that a single flip in the input changes the output:*

$$
S^{(1)} = \lambda_1 \left( \gamma; m \right). \tag{2.53}
$$

*Proof.* Recall from corollary 2.17

$$
d' = \sum_{\mathbf{x}, \mathbf{y}} \widetilde{f}(\mathbf{x}) \oplus \widetilde{f}(\mathbf{y}) \Pr[\mathbf{x}, \mathbf{y} | \widetilde{m}, d]
$$
  
= 
$$
\sum_{\mathbf{x}, \mathbf{y}} \widetilde{f}(\mathbf{x}) \oplus \widetilde{f}(\mathbf{y}) \left( \widetilde{m} + \frac{d}{2} \right)^{\langle \mathbf{x}, \mathbf{y} \rangle} \left( \frac{d}{2} \right)^{\langle \mathbf{x}, \mathbf{y} \oplus 1 \rangle + \langle \mathbf{x} \oplus 1, \mathbf{y} \rangle} \left( 1 - \widetilde{m} - \frac{d}{2} \right)^{\langle \mathbf{x} \oplus 1, \mathbf{y} \oplus 1 \rangle} = \dots
$$

As only the term of order  $O(d)$  is of importance, the central exponent can be fixed,  $\langle x, y \oplus 1 \rangle + \langle x \oplus 1, y \rangle = 1$ , ignoring higher orders in d. Note that it cannot be zero because of lemma 2.23. Both brackets can only be a natural number, therefore there are two different cases:  $\langle x, y \oplus 1 \rangle = 1$ ,  $\langle x \oplus 1, y \rangle = 0$  and  $\langle x, y \oplus 1 \rangle = 0$ ,  $\langle x \oplus 1, y \rangle = 1$ 

Consider  $\langle x, y \oplus 1 \rangle = 1$ ,  $\langle x \oplus 1, y \rangle = 0$  first. The first equation states that y has exactly a single  $0$  in a position, where x has none (x has a 1 in this position). The second equation states that y has no more 1s than x. Therefore the only possibility is  $y = x \oplus e_i$  with  $x_i = 1$ . The second case  $(\langle x, y \oplus 1 \rangle = 0, \langle x \oplus 1, y \rangle = 1)$  is analogous and results again in  $y = x \oplus e_j$ , but here  $x_j = 0$ . Hence the summation over all y can be reduced to a summation over those y such that  $y = x \oplus e_j$ . All other tuples y contribute only to higher orders  $O(d^2)$ . Therefore the summation variable can be changed to  $j = 1, \ldots, K$  and hence

$$
\cdots = \sum_{\mathbf{x}} \sum_{j=1}^K \widetilde{\mathfrak{f}}(\mathbf{x}) \oplus \widetilde{\mathfrak{f}}(\mathbf{x} \oplus \mathbf{e}_j) \left( \widetilde{m} - \frac{d}{2} \right)^{\langle \mathbf{x}, \mathbf{x} \oplus \mathbf{e}_j \rangle} \left( \frac{d}{2} \right)^1 \left( 1 - \widetilde{m} - \frac{d}{2} \right)^{\langle \mathbf{x} \oplus \mathbf{1}, \mathbf{x} \oplus \mathbf{e}_j \oplus \mathbf{1} \rangle} + \mathcal{O} \left( d^2 \right).
$$

This expression has still higher orders of  $d$  in the expansions of  $z_{(++)}$  and  $z_{(--)}.$  Therefore the exponents  $\langle x, x \oplus e_i \rangle$  and  $\langle x \oplus \mathbb{1}, x \oplus e_i \oplus \mathbb{1} \rangle$  have to be calculated.  $x \oplus e_i$  has either one more 1 or one less 1 in it, depending on  $x_i$ . Therefore

$$
x_i = 0 \Leftrightarrow \langle \mathbf{x}, \mathbf{x} \oplus \mathbf{e_i} \rangle = \langle \mathbf{x}, \mathbf{x} \rangle,
$$
  

$$
x_i = 1 \Leftrightarrow \langle \mathbf{x}, \mathbf{x} \oplus \mathbf{e_i} \rangle = \langle \mathbf{x}, \mathbf{x} \rangle - 1.
$$

Using again  $\langle {\bf e_i}, {\bf x}\oplus {\bf e_i}\rangle$  as in the last proof the two cases can be written in closed form:

$$
\langle \mathbf{x}, \mathbf{x} \oplus \mathbf{e_i} \rangle = \langle \mathbf{x}, \mathbf{x} \rangle + \langle \mathbf{e_i}, \mathbf{x} \oplus \mathbf{e_i} \rangle - 1.
$$

Note that the following identity holds:

$$
\forall \mathbf{x}, \mathbf{y} \in M^K : \qquad \underbrace{\langle \mathbf{x}, \mathbf{y} \rangle}_{= \langle \mathbf{x}, \mathbf{x} \oplus \mathbf{e}_\mathbf{j} \rangle} + \underbrace{\langle \mathbf{x} \oplus \mathbb{1}, \mathbf{y} \rangle + \langle \mathbf{x}, \mathbf{y} \oplus \mathbb{1} \rangle}_{=1} + \underbrace{\langle \mathbf{x} \oplus \mathbb{1}, \mathbf{y} \oplus \mathbb{1} \rangle}_{= \langle \mathbf{x} \oplus \mathbb{1}, \mathbf{x} \oplus \mathbf{e}_\mathbf{j} \oplus \mathbb{1} \rangle} = K
$$

From this the second exponent can be obtained:

$$
\langle \mathbf{x} \oplus \mathbb{1}, \mathbf{x} \oplus \mathbf{e}_j \oplus \mathbb{1} \rangle = K - \langle \mathbf{x}, \mathbf{x} \rangle - \langle \mathbf{e}_j, \mathbf{x} \oplus \mathbf{e}_j \rangle.
$$

Expanding the two terms with d in them, neglecting first and higher orders  $\mathcal{O}(d)$ , the expansion is

$$
\begin{array}{rcl} \displaystyle \left(\widetilde{m}-\frac{d}{2}\right)^{\langle \mathbf{x},\mathbf{x}\rangle+\langle \mathbf{e_j},\mathbf{x}\oplus \mathbf{e_j}\rangle-1} & = & \displaystyle \widetilde{m}^{\langle \mathbf{x},\mathbf{x}\rangle+\langle \mathbf{e_j},\mathbf{x}\oplus \mathbf{e_j}\rangle-1}+\mathcal{O}\left(d\right), \\ \\ \displaystyle \left(1-\widetilde{m}-\frac{d}{2}\right)^{k-\langle \mathbf{x},\mathbf{x}\rangle+\langle \mathbf{e_j},\mathbf{x}\oplus \mathbf{e_j}\rangle-1} & = & \displaystyle \left(1-\widetilde{m}\right)^{K-\langle \mathbf{x},\mathbf{x}\rangle+\langle \mathbf{e_j},\mathbf{x}\oplus \mathbf{e_j}\rangle-1}+\mathcal{O}\left(d\right). \end{array}
$$

Reinserting this into the equation for  $d'$ , the final form is obtained:

$$
d' = \left(\frac{1}{2}\sum_{\mathbf{x}}\sum_{j=1}^K \widetilde{\mathfrak{f}}(\mathbf{x})\oplus \widetilde{\mathfrak{f}}(\mathbf{x}\oplus \mathbf{e_j})\widetilde{m}^{\langle \mathbf{x},\mathbf{x}\rangle + \langle \mathbf{e_j}, \mathbf{x}\oplus \mathbf{e_j}\rangle - 1}(1-\widetilde{m})^{K - \langle \mathbf{x},\mathbf{x}\rangle - \langle \mathbf{e_j}, \mathbf{x}\oplus \mathbf{e_j}\rangle}\right)d + \mathcal{O}\left(d^2\right).
$$

The first order coefficient of d is  $\mu_1 = K\lambda_1$ , which is identical to the expression derived in lemma 2.28 for  $KS^{(1)}$ . Therefore the proof is completed.  $\Box$ 

A different version of this proof of equivalence is given in the appendix of [Kesseli et al., 2006].

This completes the fact, that the perturbation ansatz, e.g made by [Moreira and Amaral, 2005], is in fact an order parameter for the phase transition between the ordered and disordered phase of the dynamics of BNs, because it shows the same behavior above the critical point, where its stable fixed point is  $d^* = d_S^* = 0$ , and non-zero below the critical point. The critical condition is given by

$$
\mu_1 = K\lambda_1 = KS^{(1)} = 1. \tag{2.54}
$$

However, this order parameter obtained by the perturbation ansatz is in general **not** the Hamming distance.

**Theorem 2.30.** *The construction of the iteration equation for the Hamming distance by the perturbation ansatz,*

$$
d'_{S} = \sum_{n=1}^{K} S^{(n)} {K \choose n} d^{n}_{S} (1 - d_{S})^{K - n},
$$
\n(2.55)

*does not allow the second BN to relax to its fixed point* m(Y)<sup>∗</sup> *. It is kept at a magnetization of*

$$
m^{(\mathbf{Y})} = m(1 - 2d),\tag{2.56}
$$

.

*which is usually not a fixed point in the magnetization. Therefore the fixed points in the*  $H$ amming distances,  $d^*$  and  $d^*_S$ , are in general not identical.

*Proof.* Another detailed calculation of this lemma can be found in the appendix of [Kesseli et al., 2006], however, the calculation here is slightly different.

The derivation here is more or less made backwards, so a brief synopsis is given here. First the transformation from the probabilities  $\big(z_{(\pm\pm)}\big) \mapsto \big(d, m^{(\mathbf{X})}, m^{(\mathbf{Y})}\big)$  is given, which is a generalization of the transformation in equations (2.32), where the condition  $m^{(\mathbf{X})} =$  $m^{(\mathbf{Y})}=m$  is used. However, now the condition  $m^{(\mathbf{Y})}=m(1-2d)$  is imposed on the second magnetization. This is then inserted into the probabilities  $\Pr\left[\mathbf{x},\mathbf{y}|z_{(\pm\pm)}\right]$ , and after a short calculation it can be shown, that with this transformation to  $(d, m)$ , the coefficients  $\lambda_n$  in the iteration equation are exactly the sensitivities  $S^{(n)}$  defined in this section.

The general transformation of variables is given by

$$
\begin{array}{lcl} 1 & = & z_{(++)} + z_{(+-)} + z_{(-+)} + z_{(--)} \\ m^{(\mathbf{X})} & = & z_{(++)} + z_{(+-)} - z_{(-+)} - z_{(--)} \\ m^{(\mathbf{Y})} & = & z_{(++)} + z_{(+-)} - z_{(+-)} - z_{(--)} \\ d & = & z_{(-+)} + z_{(+-)} \end{array} \bigg\} \Rightarrow \begin{cases} z_{(++)} & = & \frac{1}{2} \left( 1 + \frac{m^{(\mathbf{X})}}{2} + \frac{m^{(\mathbf{Y})}}{2} - d \right) \\ z_{(+-)} & = & \frac{1}{2} \left( \frac{m^{(\mathbf{X})}}{2} - \frac{m^{(\mathbf{Y})}}{2} + d \right) \\ z_{(+-)} & = & \frac{1}{2} \left( 1 - \frac{m^{(\mathbf{X})}}{2} - \frac{m^{(\mathbf{Y})}}{2} - d \right) \\ z_{(--)} & = & \frac{1}{2} \left( 1 - \frac{m^{(\mathbf{X})}}{2} - \frac{m^{(\mathbf{Y})}}{2} - d \right) \end{cases}
$$

In the calculations before, both magnetizations are set equal to each other, because only small perturbations to a fixed point in the magnetization are considered. As it is assumed, that this fixed point  $m^*$  is stable, the iteration equations in the second order of the dynamics have this restriction ( $m^{(\mathbf{X})}=m^{(\mathbf{Y})}$ ), because for computing fixed points only the long time behavior is of interest. This long time behavior is clearly  $m^{(\mathbf{X})*}=m^{(\mathbf{Y})*}=m^*.$ 

However, the initial conditions to the perturbation amounts exactly to  $m^{(\mathbf{Y})} = m(1 - 2d)$ . This can be seen as follows: There are  $dz_{(+)}$  changes from  $(+) \mapsto (-)$  and  $dz_{(-)}$  changes from  $(-) \mapsto (+)$  in the perturbation of the second BN. Therefore

$$
\begin{array}{rcl}\nz_{(+)}^{(\mathbf{Y})} & = & z_{(+)} - dz_{(+)} + dz_{(-)}, \\
z_{(-)}^{(\mathbf{Y})} & = & z_{(-)} - dz_{(-)} + dz_{(+)},\n\end{array}
$$

and hence

$$
m^{(\mathbf{Y})} = (z_{(+)} - dz_{(+)} + dz_{(-)}) - (z_{(-)} - dz_{(-)} + dz_{(+)}) = m(1 - 2d).
$$

This restriction is here not used only as initial condition, but in the general transformation

above. Therefore the probabilities  $z_{(\pm\pm)}$  are

$$
z_{(++)} = \frac{1}{2}(1+m)(1-d),
$$
  
\n
$$
z_{(+-)} = \frac{1}{2}(1+m)d,
$$
  
\n
$$
z_{(-+)} = \frac{1}{2}(1-m)d,
$$
  
\n
$$
z_{(--)} = \frac{1}{2}(1-m)(1-d),
$$

where the two variables  $m$  and  $d$  clearly factorize. This transformation with the condition  $m(Y) = m(1-2d)$  accounts now for the fact, that the second BN is not allowed to relax to its fixed point  $m^*$ , because  $m^*(1-2d^*)$  is usually no fixed point in the magnetization, except for some special cases like  $m^* = 0$  or  $d^* = 0$ . But the latter is above the critical point, and it is clear, that in this parameter region the correct fixed point  $d_S^* = 0$  is obtained, because the last theorem already established  $d_S^*$  as an order parameter of the dynamical phase transition.

Now this transformation above can be inserted into the probabilities  $\Pr\left[\mathbf{x},\mathbf{y}|z_{(\pm\pm)}\right]$  in iteration equation for the Hamming distance obtained already before in corollary 2.17:

$$
d' = \sum_{\mathbf{x}, \mathbf{y}} \tilde{\mathfrak{f}}(\mathbf{x}) \oplus \tilde{\mathfrak{f}}(\mathbf{y}) \Pr[\mathbf{x}, \mathbf{y}|m, d]
$$
  
\n
$$
= \sum_{\mathbf{x}, \mathbf{y}} \tilde{\mathfrak{f}}(\mathbf{x}) \oplus \tilde{\mathfrak{f}}(\mathbf{y}) \left(\frac{1}{2}(1+m)(1-d)\right)^{\langle \mathbf{x}, \mathbf{y} \rangle} \left(\frac{1}{2}(1+m)d\right)^{\langle \mathbf{x}, \mathbf{y} \oplus 1 \rangle} \times
$$
  
\n
$$
\times \left(\frac{1}{2}(1-m)d\right)^{\langle \mathbf{x} \oplus 1, \mathbf{y} \rangle} \left(\frac{1}{2}(1-m)(1-d)\right)^{\langle \mathbf{x} \oplus 1, \mathbf{y} \oplus 1 \rangle}
$$
  
\n
$$
= \left(\frac{1}{2}\right)^K \sum_{\mathbf{x}, \mathbf{y}} \tilde{\mathfrak{f}}(\mathbf{x}) \oplus \tilde{\mathfrak{f}}(\mathbf{y}) \left((1+m)^{\langle \mathbf{x}, \mathbf{y} \rangle + \langle \mathbf{x}, \mathbf{y} \oplus 1 \rangle}(1-m)^{\langle \mathbf{x} \oplus 1, \mathbf{y} \rangle + \langle \mathbf{x} \oplus 1, \mathbf{y} \oplus 1 \rangle}\right) \times
$$
  
\n
$$
\times \left(d^{\langle \mathbf{x} \oplus 1, \mathbf{y} \rangle + \langle \mathbf{x} \oplus 1, \mathbf{y} \rangle}(1-d)^{\langle \mathbf{x}, \mathbf{y} \rangle + \langle \mathbf{x} \oplus 1, \mathbf{y} \oplus 1 \rangle}\right) = \dots
$$

Note that  $\langle x, y \rangle + \langle x, y \oplus 1 \rangle = \langle x, 1 \rangle = \langle x, x \rangle$  and also  $\langle x \oplus 1, y \rangle + \langle x \oplus 1, y \oplus 1 \rangle = K - \langle x, x \rangle$ . Therefore the exponents of the terms with the magnetization are independent of y. Hence the two terms including the magnetization equal the probability  $\Pr\left[\mathbf{x}|z_{(\pm)}\right]$  for the tuple  $\mathbf{x},$ see lemma 2.5.

$$
\dots = \sum_{\mathbf{x},\mathbf{y}} \widetilde{\mathfrak{f}}(\mathbf{x}) \oplus \widetilde{\mathfrak{f}}(\mathbf{y}) \Pr\left[\mathbf{x}|z_{(\pm)}\right] \left( d^{(\mathbf{x} \oplus \mathbb{1}, \mathbf{y}) + \langle \mathbf{x} \oplus \mathbb{1}, \mathbf{y} \rangle} (1-d)^{\langle \mathbf{x}, \mathbf{y} \rangle + \langle \mathbf{x} \oplus \mathbb{1}, \mathbf{y} \oplus \mathbb{1} \rangle} \right) = \dots
$$

Now a trick is used for calculating the exponents of the terms with  $d$ . When writing y as the difference to the tuple x, then

$$
\mathbf{y}=\mathbf{x}\oplus\mathbf{e_{i_1}}\oplus\cdots\oplus\mathbf{e_{i_n}}
$$

and denoting the index set  $I = \{i_1, \ldots, i_n\}$ . The summation over y can be written as a summation over all possible index sets I. Rewriting y in that way, allows to calculate the

exponents:  $\langle x, y \oplus 1 \rangle + \langle x \oplus 1, y \rangle = n$  where n is the size of the index set I, because this is nothing else than summing up the positions which are different in the tuples  $x$  and  $y$ . It immediately follows that  $\langle x, y \rangle + \langle x \oplus \mathbb{1}, y \oplus \mathbb{1} \rangle = K - n$ . Inserting this in the calculation yields:

$$
\dots = \sum_{I} \sum_{\mathbf{x}} \widetilde{f}(\mathbf{x}) \oplus \widetilde{f}(\mathbf{x} \oplus \mathbf{e}_{\mathbf{i}_1} \oplus \cdots \oplus \mathbf{e}_{\mathbf{i}_n}) \Pr\left[\mathbf{x} | z_{(\pm)}\right] \left(d^n (1-d)^{K-n}\right) = \dots
$$

Splitting the sum over all index sets  $I$  into equal-sized sets yields

$$
\begin{array}{lll}\n\ldots &=& \sum_{n=1}^{K} \sum_{\mathbf{x}} \sum_{|I|=n} \widetilde{\mathfrak{f}}(\mathbf{x}) \oplus \widetilde{\mathfrak{f}}(\mathbf{x} \oplus \mathbf{e}_{\mathbf{i}_1} \oplus \cdots \oplus \mathbf{e}_{\mathbf{i}_n}) \Pr\left[\mathbf{x}|z_{(\pm)}\right] d^n (1-d)^{K-n} \\
&=& \sum_{n=1}^{K} S^{(n)} \binom{K}{n} d^n (1-d)^{K-n},\n\end{array}
$$

where the sensitivity  $S^{(n)}$  is

$$
S^{(n)} = \frac{1}{\binom{K}{n}} \sum_{\substack{I \\ |I|=n}} \sum_{\mathbf{x}} \widetilde{f}(\mathbf{x}) \oplus \widetilde{f}(\mathbf{x} \oplus \mathbf{e}_{\mathbf{i}_1} \oplus \cdots \oplus \mathbf{e}_{\mathbf{i}_n}) \Pr\left[\mathbf{x} | z_{(\pm)}\right],
$$

which is exactly the expression for the sensitivities  $S^{(n)}$  from definition 2.27 and the proof is concluded.  $\Box$ 

However, as has been already noted in [Kesseli et al., 2006], the restriction  $m^{(\mathbf{Y})} =$  $m(1 - 2d)$  can only be imposed on the initial condition. In the time evolution of the second BN, the magnetization will not stay in this relation to the first BN, because the iteration equations are independent of the variable d:

$$
m^{(\mathbf{X})'} = \mathcal{M}(\gamma; m^{(\mathbf{X})}),
$$
  

$$
m^{(\mathbf{Y})'} = \mathcal{M}(\gamma; m^{(\mathbf{Y})}).
$$

From there is should be clear, that keeping the restriction  $m^{(\mathbf{Y})} = m(1-2d)$  artificially over the time, results in a usually wrong long time behavior of  $m^{(\mathbf{Y})*}$ , and inserting those fixed points  $m^{(\mathbf{X})*}$  and  $m^{(\mathbf{Y})*}$  into

$$
d^* = \mathcal{D}(\gamma; m^{(\mathbf{X})*}, m^{(\mathbf{Y})*}, d^*)
$$

will yield often a deviating fixed point in the Hamming distance below the critical point,  $\gamma < \gamma_c$ . However, there are some examples where the Hamming distances derived by the perturbation ansatz and by the formalism presented earlier coincide. This is the case, when all coefficients  $\lambda_n$  and the sensitivities  $S^{(n)}$  are actually the same (and not only  $\lambda_1 = S^{(1)}$ ). The trivial cases  $m^* = 0$  and  $d^* = 0$  have already been mentioned in the proof. Another example will be treated later in theorem 3.4, where a BN with Linear Threshold functions and a symmetric distribution of weights is used. This system has been investigated in detail in [Derrida, 1987] and [Kürten, 1988b], and theorem 3.4 shows the equivalence of the formalism presented therein. It should be noted, that this coinciding

order parameters  $d^*$  and  $d^*_S$  results in this case from the symmetry of the distribution of weights. There might be other classes of Boolean functions, for which the order parameters are the same, and giving detailed conditions on these classes might be part of future work.

#### Comparison of calculation methods for the Hamming distance  $d$  with simulations

Consider a mixture of the four different Boolean functions  $(14)_2$ ,  $(13)_2$ ,  $(11)_2$  and  $(7)_2$  with a mixture parameter p

$$
\rho_{\mathbf{F}} \sim p^2 (14)_2 + p(1-p)(13)_2 + (1-p)p(11)_2 + (1-p)^2 (7)_2.
$$

This mixture is equivalent to Linear Threshold functions with connectivity  $K = 2$  and threshold  $h = 0$ , where the weights are distributed according to

$$
\rho_c^{(\delta)} = p\delta(c-1) + (1-p)\delta(c+1).
$$

Hence it is clear, that the mixture parameter  $p$  corresponds to the fraction of positive weights in a Linear Threshold function. This connection between  $\rho_{\bf F}$  and  $\rho_c^{(\delta)}$  will be further clarified in an example at the end of section 3.1. More results on this mixture/Linear Threshold function can also be found in chapter 3. Moreover, this mixture has been used as the example in [Greil and Drossel, 2007], where different ranges of the mixture parameter  $p$  are investigated. However, the authors in [Greil and Drossel, 2007] use the ansatz  $\lambda_n = S^{(n)}$  for calculating their Hamming distance d. To show that this gives the correct critical condition, but not the correct value of the fixed point in the Hamming distance  $d^*$ , several simulations are compared with the two methods to calculate the iteration equation for d.

First of all, the iteration equation for the magnetization is needed. This is straightforward using the methods presented so far and yields

$$
m' = \frac{1}{2} + (2p - 1)m + \left(-\frac{1}{2} + 2p - 2p^2\right)m^2.
$$

This iteration equation can be solved analytically to obtain the fixed point  $m^*$ ,

$$
m^* = \frac{-2 + 2p + \sqrt{5 - 12p + 8p^2}}{1 - 4p + 4p^2}.
$$

This fixed point  $m^*$  gets unstable below  $p < p_c^{m^*} = \frac{1}{4} \left( 3 - \frac{1}{2} \right)$ √  $(7) \approx 0.0886$ , as can be shown by a Linear Stability analysis. Below that point  $p_c^{m^\ast}$ , the fixed point in  $m$  bifurcates into a period-2 solution.

As has been derived in [Greil and Drossel, 2007], the sensitivities  $S^{(1)}$  and  $S^{(2)}$  are $^{\scriptscriptstyle 5}$ 

$$
S^{(1)} = \frac{1}{2}(1-(2p-1)m),
$$

<sup>5</sup>Note that [Greil and Drossel, 2007] uses  $\widetilde{m} \in [0,1]$ . This has to be transformed to  $m \in [-1,+1]$  here:  $\widetilde{m} = \frac{m+1}{2}$ .

$$
S^{(2)} = \frac{1}{2} (1 + (2p - 1)^2 m^2).
$$

This yields the following iteration equation for the "Hamming distance":

$$
d'_{S} = (1 - (2p - 1)m)d_{S} + \frac{1}{2}(-1 + 2(2p - 1)m + (2p - 1)^{2}m^{2}) d_{S}^{2}.
$$

As explained before and will be seen later when compared to simulations, this is not the Hamming distance, so this quantity is denoted by  $d<sub>S</sub>$  to hint at the relation, that it is constructed using the sensitivities.

When using the construction explained earlier in this work, i.e. using the restriction  $m^{(\mathbf{X})} = m^{(\mathbf{Y})} = m$ , then the iteration equation for the Hamming distance d is

$$
d' = (1 - (2p - 1)m)d - \frac{1}{2}d^2,
$$

and hence the coefficients  $\lambda_n$  are:

$$
\lambda_1 = \frac{1}{2} (1 - (2p - 1)m),
$$
  

$$
\lambda_2 = \frac{1}{2} (1 - 2(2p - 1)m).
$$

Using the fixed point solution for the magnetization  $m^*$  from above, the fixed points  $d^*$ and  $d_S^*$  can be obtained analytically. Both have  $d^* = d_S^* = 0$  as expected. The second fixed point is given by

$$
d^* = -\frac{2\left(-2 + 2p + \sqrt{5 - 12p + 8p^2}\right)}{-1 + 2p},
$$
  

$$
d^*_S = \frac{1 - 2p}{3 - 4p},
$$

in the interval  $p \in [0.0886, 0.5]$ . Above that interval the only fixed point is  $d^* = d^*_S = 0$ , which is also stable in this range. Below the interval the expressions are more complicated, because they involve solving the period-2 iteration equations, and they are not explicitly reproduced here, although the results are depicted in figure 2.2.

To decide which solution is correct, several simulations at different values for the mixture parameter p are conducted (in the relevant range  $p \in [0.0; 0.6]$ . The code for the simulation can be found in appendix C, although in lines 118 and 120 the weights have to be set directly to  $\pm 1$  instead of a random value in the ranges  $[-1, 0]$  and  $[0, 1]$ , respectively. All simulations are done with  $N = 10000$  nodes. Neighbors and functions are drawn each timestep randomly from all possible values. A simulation is run for  $s = 500$  timesteps with 2 BNs in parallel, where the second BN is started with a distance  $d_{start} = 0.01$  from the first one. The values for the Hamming distance  $d$  in figure 2.2 are averaged over the last 200 steps.

As seen figure 2.2, the construction of the Hamming distance  $d$  from sensitivities clearly fails to predict the correct fixed point in simulations. The restriction  $m^{(\mathbf{Y})} = m(1 - 2d)$  to the magnetization in the second BN does not allow the dynamics to relax to its correct



Figure 2.2: Comparison of the two calculation methods for the Hamming distance  $d$  with simulations. The black line is the fixed point of the Hamming distance  $d^*$ , the grey line corresponds to the fixed point  $d^*_S$  obtained by the perturbation ansatz. Simulations are shown in orange, which agree with the first calculation. At  $p = 0.1$  the fixed point  $d_S^*$  is off by roughly 27%.

fixed point. Therefore, using  $m^{(\mathbf{X})} = m^{(\mathbf{Y})} = m$  in the transformations is clearly to favor.

## 2.3.4 Non-fixed-point attractors

Non-fixed-point attractors, which are attractors that would have a periodical behavior with a period  $> 1$ , could theoretically also be computed by the MF approximation. However, increasing the period length under investigation, exponentially increases the effort to obtain those solutions in most cases. This comes from the fact, that the iteration equations are inserted into each other, yielding a polynomial which has a doubled order in their variables  $m$  and  $d$ .

So for example, when calculating period-2 solutions of the magnetization  $m$  and the Hamming distance  $d$ , the following equations have to be considered:

$$
m'' = \mathcal{M}(\gamma; \mathcal{M}(\gamma; m)), \qquad (2.58a)
$$

$$
d'' = \mathcal{D}(\gamma; \mathcal{M}(\gamma; m), \mathcal{D}(\gamma; m, d)). \tag{2.58b}
$$

It is clear, that those equations have all the fixed points, which are already present before. All new fixed points of these equations usually occur in pairs. These pairs are either a period-2 solution or two stable fixed points, depending on the first coefficient of the LSA, whereas with  $\frac{\partial \mathcal{M}}{\partial m}=-1$  the first and at  $\frac{\partial \mathcal{M}}{\partial m}=1$  the latter appears (or respectively  $\frac{\partial \mathcal{D}}{\partial d}$  for the Hamming distance).

Repeated insertion of the iteration equation into itself gives all periodical solutions with higher periods (or similarly another bifurcation to twice the number of stable fixed points).

The definition of the polynomials is done recursively:

$$
m' = \mathcal{M}^{(n)}(\gamma; m) = \mathcal{M}\left(\gamma; \mathcal{M}^{(n-1)}(\gamma; m)\right),
$$
 (2.59a)

$$
d^{\prime \cdots} = \mathcal{D}^{(n)}\left(\gamma; \mathcal{M}^{(n-1)}(\gamma; m), \mathcal{D}^{(n-1)}(\gamma; m, d)\right), \tag{2.59b}
$$

with the initial polynomials  $\mathcal{M}^{(1)} = \mathcal{M}$  and  $\mathcal{D}^{(1)} = \mathcal{D}$ .

Although this gives in principle all possible solutions to the iteration equation, the polynomial is of order  $\mathcal{O}\left(m^{nK}\right)$  or  $\mathcal{O}\left(d^{nK}\right)$  after  $n$  insertions, making it rather impossible to solve for higher *n*. Even if  $n = 2$ , not many solutions can still be obtained analytically, also for low connectivities like  $K = 2$  or  $K = 3$ , and often only numerical solutions are available.

## 2.4 Boolean derivative

## 2.4.1 Definition and Properties

Several authors [Bazsó and Lábos, 2006, Luque and Sole, 2000, Kesseli et al., 2006] use the concept of a Boolean derivative, which naturally occurred already in several calculations in this chapter. See also [Shmulevich and Kauffman, 2004], where some methods presented here are already applied to BNs. An earlier treatment of those concepts in connection with Cellular Automata is given in e.g. [Vichniac, 1990].

To begin with, the definition of the derivative is given.

**Definition 2.31.** *The Boolean derivative of a Boolean function* f *with respect to its variable*  $x_i$  *is* 

$$
\frac{\partial \mathfrak{f}(\mathbf{x})}{\partial x_j} := \mathfrak{f}(\mathbf{x}) \oplus \mathfrak{f}(\mathbf{x} \oplus \mathbf{e}_j).
$$
 (2.60)

Note how this resembles the definition of the partial derivative of a function  $f : \mathbb{R}^n \to \mathbb{R}^n$ in the direction of the unit vector v:

$$
\frac{\partial f(\mathbf{x})}{\partial \mathbf{v}} = \lim_{h \to 0} \frac{f(\mathbf{x} - h\mathbf{v}) - f(\mathbf{x})}{h}.
$$

As the minimal step size h in the discrete Boolean case can only be  $h = 1$ , the resemblance to the equation above is immediate, because also the subtraction and addition operation are actually the same in  $\mathbb{F}_2$ .

A few properties of the Boolean derivative are as follows. It should be obvious, that the derivative of a Boolean function  $f$  is again a Boolean function  $g$ , since it can also be described by a truth table. Moreover, this new Boolean function is independent of its variable  $x_j$ , as this short calculation shows:

$$
\mathfrak{g}(\mathbf{x}) = \frac{\partial \mathfrak{f}(\mathbf{x})}{\partial x_j} = \mathfrak{f}(\mathbf{x}) \oplus \mathfrak{f}(\mathbf{x} \oplus \mathbf{e_j}) = \mathfrak{f}(\mathbf{x} \oplus \mathbf{e_j} \oplus \mathbf{e_j}) \oplus \mathfrak{f}(\mathbf{x} \oplus \mathbf{e_j}) = \frac{\partial \mathfrak{f}(\mathbf{x} \oplus \mathbf{e_j})}{\partial x_j} = \mathfrak{g}(\mathbf{x} \oplus \mathbf{e_j}).
$$

In the crucial step the identity  $x \oplus e_j \oplus e_j = x$  is used. As now the function g is the same on the inputs x and  $x \oplus e_j$ , it can not depend on the value of the variable  $x_j$  anymore. This

leads immediately to another property of the derivative: the derivation  $\frac{\partial}{\partial x_j}$  is a nilpotent operator:

$$
\frac{\partial^2 \mathfrak{f}}{\partial x_j^2} \equiv (0)_K. \tag{2.61}
$$

where  $(0)_K$  describes the Boolean function with decimal representation 0 (see section 1.4.1) about truth tables). This follows from

$$
\frac{\partial^2 \mathfrak{f}(\mathbf{x})}{\partial x_j^2} = \frac{\partial}{\partial x_j} \mathfrak{g}(\mathbf{x}) = \mathfrak{g}(\mathbf{x}) \oplus \underbrace{\mathfrak{g}(\mathbf{x} \oplus \mathbf{e_j})}_{=\mathfrak{g}(\mathbf{x})} = 0.
$$

With those two properties, the derivation operator  $\frac{\partial}{\partial x_j}$  gets an important new interpretation: It reduces the number of variables in a Boolean function, because the resulting function is independent of  $x_j$ . If the original function had K variables, the resulting function has only K – 1 variables (or is equal to the constant  $(0)_K$  function, if it was already independent of  $x_j$ ). Moreover, the resulting function g has a 1 in the position, where f depends on  $x_i$  (i.e. a change in  $x_i$  changes f) and  $g(x) = 0$  if f was already independent of the position of  $x_j$  in the input x.

Now the concepts of the last section can be revisited. With those definitions the sensitivity  $S_i$  of a function f can be rewritten. Recall from definition 2.26

$$
S_j = \sum_{\mathbf{x}} f(\mathbf{x}) \oplus f(\mathbf{x} \oplus \mathbf{e_j}) \Pr\left[\mathbf{x}|z_{(\pm)}\right] = \sum_{\mathbf{x}} \frac{\partial f(\mathbf{x})}{\partial x_j} \Pr\left[\mathbf{x}|z_{(\pm)}\right].
$$

In this new light, the sensitivity  $S_i$  is nothing else than the partial derivative of the Boolean function, weighted according to the actual state of the BN. The average sensitivity is then given by

$$
S^{(1)} = \frac{1}{K} \sum_{j=1}^{K} \sum_{\mathbf{x}} \frac{\partial f(\mathbf{x})}{\partial x_j} \Pr\left[\mathbf{x}|z_{(\pm)}\right].
$$
 (2.62)

Higher sensitivities  $S^{(n)}$  lead to the introduction of a so-called "sensitivity operator":

**Definition 2.32.** *The sensitivity operator*  $\sigma_I$  *with an index set*  $I = \{i_1, \ldots, i_n\}$  *is defined as* 

$$
\sigma_I f(\mathbf{x}) := f(\mathbf{x}) \oplus f(\mathbf{x} \oplus \mathbf{e}_{i_1} \oplus \cdots \oplus \mathbf{e}_{i_n}). \tag{2.63}
$$

*Hence the higher average sensitivities*  $S^{(n)}$  *can now be written as* 

$$
S^{(n)} = \frac{1}{\binom{K}{n}} \sum_{\mathbf{x}} \sum_{\substack{I \\ |I| = n}} \sigma_I f(\mathbf{x}) \Pr\left[\mathbf{x} | z_{(\pm)}\right].
$$
 (2.64)

The sensitivity operator represents exactly, what was stated in definition 2.27. The resulting function  $g(x) = \sigma_I f(x)$  is equal to one, if a change of all variables in the index set I changes the output of f, and zero otherwise. Therefore equation (2.64) is nothing else than the probability for a change in the function  $\frac{1}{2}$  when n variables are changed, because it is averaged over all possible index sets with size  $|I| = n$ .

Of special interest is of course the first sensitivity  $S^{(1)}$ , because it is directly linked to the

phase transition. However, first the connection of this sensitivity operator to the Boolean derivatives is shown:

**Lemma 2.33.** *The following identities hold for a transformation from higher partial derivatives to sensitivities. If*  $I = \{i_1, \ldots, i_n\}$  *is an index set with n elements, then* 

$$
\frac{\partial^n f(\mathbf{x})}{\partial x_{i_1} \dots \partial x_{i_n}} = \bigoplus_{J \subseteq \{i_1, \dots, i_n\}} \sigma_J f(\mathbf{x}),\tag{2.65}
$$

$$
\sigma_I f(\mathbf{x}) = \bigoplus_{k=1}^n \left( \bigoplus_{\{j_1,\ldots,j_k\} \subseteq I} \frac{\partial^k f(\mathbf{x})}{\partial x_{j_1} \ldots \partial x_{j_k}} \right).
$$
 (2.66)

*Proof.* First look at the transformation  $\left(\frac{\partial^n}{\partial x_i}\right)^n$  $\partial x_{i_1}...\partial x_{i_n}$  $\Big) \mapsto (\sigma_I)$ :

$$
\frac{\partial^n \mathfrak{f}(\mathbf{x})}{\partial x_{i_1} \dots \partial x_{i_n}} = \frac{\partial^{n-1}}{\partial x_{i_2} \dots \partial x_{i_n}} \left( \underbrace{\mathfrak{f}(\mathbf{x}) \oplus \mathfrak{f}(\mathbf{x} \oplus \mathbf{e}_{i_1})}_{=: \mathfrak{g}(\mathbf{x})} \right)
$$
\n
$$
= \frac{\partial^{n-2}}{\partial x_{i_3} \dots \partial x_{i_n}} \left( \underbrace{\mathfrak{g}(\mathbf{x}) \oplus \mathfrak{g}(\mathbf{x} \oplus \mathbf{e}_{i_2})}_{=: \mathfrak{h}(\mathbf{x})} \right)
$$
\n
$$
= \dots = \mathfrak{k}(\mathbf{x}) = \dots
$$

Now by reinserting the explicit expression for each of those defined functions  $(\ell, \ldots, \mathfrak{h}, \mathfrak{g})$ step by step, a binary tree is created, where one leg has the changed variable  $\oplus \mathbf{e_{i_k}}$ , the other one not. Finally, this results in the function f XOR-ed with itself, with each possible combination of inputs changed:

$$
\cdots = \mathfrak{f}(\mathbf{x}) \oplus \mathfrak{f}(\mathbf{x} \oplus \mathbf{e}_{i_1}) \oplus \cdots \oplus \mathfrak{f}(\mathbf{x} \oplus \mathbf{e}_{i_n}) \oplus \mathfrak{f}(\mathbf{x} \oplus \mathbf{e}_{i_1} \oplus \mathbf{e}_{i_2}) \oplus \cdots \oplus \mathfrak{f}(\mathbf{x} \oplus \mathbf{e}_{i_1} \oplus \cdots \oplus \mathbf{e}_{i_n}) = \ldots
$$

Note that there are  $\binom{K}{n}$  terms with exactly  $n$  changed variables, so the whole expression has  $\sum_{k=1}^{K} {K \choose k} = 2^{K}$  terms. By definition of ⊕, XOR-ing the same value twice is a neutral operation, i.e.  $\mathbf{x} \oplus \mathbf{y} \oplus \mathbf{y} = \mathbf{x}$ . Hence the expression above could be expanded by  $2^K$  times the original function  $f(x)$ .

$$
\cdots = \mathfrak{k}(\mathbf{x}) \oplus \underbrace{\mathfrak{f}(\mathbf{x}) \oplus \cdots \oplus \mathfrak{f}(\mathbf{x})}_{2^K \text{ times}} = \ldots
$$

As the operation ⊕ is also associative and commutative, those expressions could be rearranged, so that each term with a changed variable is preceded by a plain term  $(f(x))$ . Recalling the definition of the sensitivity operator  $\sigma_I$ , it is clear, that each of those tuples (a plain term followed by a term with changed variables) can be written by this operator. As there is each possible combination of changed variables, the transformation equation above follows:

$$
\cdots = \bigoplus_{I \subseteq \{i_1,\ldots,i_n\}} \sigma_I f(\mathbf{x}).
$$

The other direction of the transformation  $(\sigma_I) \mapsto \left(\frac{\partial^n}{\partial x_i}\right)$  $\partial x_{i_1}...\partial x_{i_n}$  can be obtained analogously by XOR-ing the expressions with an even number of similar functions and using the fact from the transformation above, that the higher partial derivative is nothing else than XOR-ing the functions with all possible combinations of changed variables with each other.

$$
\sigma_I f(\mathbf{x}) = f(\mathbf{x}) \oplus f(\mathbf{x} \oplus \mathbf{e}_{i_1} \oplus \cdots \oplus \mathbf{e}_{i_n}) =
$$
\n
$$
= \frac{\partial^n f(\mathbf{x})}{\partial x_{i_1} \dots \partial x_{i_n}} \oplus f(\mathbf{x} \oplus \mathbf{e}_{i_1}) \oplus \cdots \oplus f(\mathbf{x} \oplus \mathbf{e}_{i_n}) \oplus \cdots \oplus
$$
\n
$$
\oplus \cdots \oplus f(\mathbf{x} \oplus \mathbf{e}_{i_1} \oplus \cdots \oplus \mathbf{e}_{i_{n-1}}) \oplus \cdots \oplus f(\mathbf{x} \oplus \mathbf{e}_{i_2} \oplus \cdots \oplus \mathbf{e}_{i_n}) =
$$
\n
$$
= \bigoplus_{k=1}^n \left( \bigoplus_{\{j_1,\ldots,j_k\} \subseteq I} \frac{\partial^k f(\mathbf{x})}{\partial x_{j_1} \dots \partial x_{j_k}} \right).
$$

Thus both, higher derivatives and sensitivities, could be transformed into each other.  $\Box$ 

## 2.4.2 Continuity equation?

Now the focus is back on  $S^{(1)}$ , which is important for the critical condition. It is restated here:

$$
KS^{(1)} = 1 \tag{2.67}
$$

A closer look to the sensitivities  $S_j$  reveals another concept. A variable  $x_j$  could be called "fictitious" [Shmulevich and Kauffman, 2004], if the function does not depend on it, i.e.  $f(x) = f(x \oplus e_j)$ . On the other hand, a variable  $x_j$  could be called "effective" if the function depends on it. By inspecting the expression for  ${\cal S}_j$ 

$$
S_j = \sum_{\mathbf{x}} \frac{\partial \mathfrak{f}(\mathbf{x})}{\partial x_j} \Pr\left[\mathbf{x} | z_{(\pm)}\right]
$$

this is the probability that the variable has an influence on the outcome. Noting that

$$
S_1 + S_2 + \dots + S_K = KS^{(1)}
$$

the term  $KS^{(1)}$  could be seen as the "effective" number of variables in the BN. Comparing that to the critical condition above, allows for the statement, that if the effective number of variables is exactly 1, the BN is in its critical state. This could be seen as preserving the information in the flow of the critical perturbation, as one (effective) variable determines the output on a single node (on which the function is defined), so it is in fact a  $1:1$ mapping from the input to the output. The analogy to classical flow equations goes even further. Note that the divergence operator div is defined by

$$
\mathrm{div}\equiv\sum_j\frac{\partial}{\partial x_j}
$$

Inserting this into  $S^{(1)}$  and looking at the critical condition it follows

$$
KS^{(1)} = \sum_{\mathbf{x}} \sum_{j} \frac{\partial f(\mathbf{x})}{\partial x_j} \Pr\left[\mathbf{x}|z_{(\pm)}\right] = \sum_{\mathbf{x}} \text{div } f(\mathbf{x}) \Pr\left[\mathbf{x}|z_{(\pm)}\right] = \langle \text{div } f \rangle \stackrel{!}{=} 1 \tag{2.68}
$$

This can be rewritten as

$$
-1 + \langle \text{div } \mathfrak{f} \rangle = 0 \tag{2.69}
$$

which looks like a continuity equation for an incompressible fluid:

$$
\frac{\partial \rho}{\partial t} + \text{div}(\mathbf{v}\rho) = 0 \tag{2.70}
$$

However, it still remains to show, what this quantity is, which changes over time. A first naive guess might that it is somehow linked to the self-distance [Luque and Sole, 2000], i.e. the probability that a node  $x_i$  changes its value between two consecutive timesteps, however, this seems not to work in all cases. About this idea of critical information flow in BN has already been speculated in [Andrecut and Kauffman, 2010] and several other publications.

# 3 Linear Threshold Functions

Linear Threshold functions (LTF) are a special subset of all possible Boolean functions. They are given in a local description by

$$
x'_{i} = f_{i}\left(x_{j_{1}},\ldots,x_{j_{k_{i}}}\right) = \tag{3.1a}
$$

$$
= \text{sign}\left(c_{i1}x_{j_1} + \dots + c_{ik_i}x_{j_{k_i}} - h\right) = \qquad (3.1b)
$$

$$
= \quad \text{sign}\bigg(\sum_{\{j\}} c_{ij} x_{i_j} - h\bigg) \tag{3.1c}
$$

with  $x_i \in M = \{-1,1\}$  and  $c_{ij}$  are weights determined either by a fixed value or in most cases by some distribution of weights  $\rho_c$ :

$$
c_{ij} \sim \rho_c \tag{3.2}
$$

The sum over  $\{j\}$  is over all neighbors of node i. Note that for the sign of h different conventions exist. So depending on the publication or author,  $h$  is either added to or subtracted from the sum  $\sum c_{ij}x_{i_j}$ . Although  $x_i \in M$  are discrete, they are considered to be real numbers in this calculation, i.e. it is assumed that  $M \subset \mathbb{R}$ . Note that here the choice of  $M = \{-1, 1\}$  instead of  $M = \{0, 1\}$  has an impact on the model. With  $M =$  $\{0,1\}$  the two states could be interpreted as "has no effect"/"has an effect", whereas with  $M = \{-1, +1\}$  the two states correspond to "inhibiting"/" activating", which are two clearly distinct choices. However, the choice  $M = \{0, 1\}$  can be transformed into  $M = \{-1, +1\}$ , when another distribution is imposed on the threshold parameter, which involves the distribution of weights  $\rho_c$ . This leads to an unnecessary complication of the expressions later on, and the more symmetric case is chosen, where also the threshold  $h$  is only a simple parameter and not given by a distribution. Additionally, weights  $c_{ij}$  are called activating if  $c_{ij} > 0$  and inhibiting if  $c_{ij} < 0$ .

Compared to arbitrary distributions of function  $\rho_F$ , Linear Threshold functions exhibit a few interesting properties. First of all, they are a subset of all monotone functions (either monotone increasing or monotone decreasing in all variables), where a monotone increasing variable  $x_i$  is given by

$$
\forall \mathbf{x}: \quad \mathbf{x} \leq \mathbf{x} \oplus \mathbf{e_i} \quad \Rightarrow \quad f(\mathbf{x}) \leq f(\mathbf{x} \oplus \mathbf{e_i}), \tag{3.3}
$$

and a monotone decreasing variable  $x_i$  is given by

$$
\forall \mathbf{x}: \quad \mathbf{x} \leq \mathbf{x} \oplus \mathbf{e_i} \quad \Rightarrow \quad f(\mathbf{x}) \geq f(\mathbf{x} \oplus \mathbf{e_i}). \tag{3.4}
$$

Monotone increasing variables could then be called "activating", whereas monotone decreasing variables could be called "inhibiting". This gives an alternative defintion of these terms, without the need of a distribution of weights  $\rho_c$ , directly from the truth table. This class of functions is also called unate Boolean functions. However, as will be explained later, such a truth table cannot be obtained easily for every  $\rho_c$ . Up to connectivity  $K = 3$ all such monotone functions are Linear Threshold functions. However, from  $K \geq 4$  on, the class of monotone functions is actually bigger.

In [Raeymaekers, 2002] a certain class of Boolean functions with connectivity  $K = 3$  is investigated and called "biologically meaningful", which can be shown to be an equivalent definition of non-degenerate Linear Threshold functions $^{\rm l}$ . It is assumed, that in such biological systems only a single threshold exists, where the output switches once and even if the input signal is increased, no switching back occurs [Wittmann et al., 2010]. These so-called "single-switch-functions" are just another description of those monotone functions (and therefore partially also LTFs) above. However, this characterization can also be generalized for multistate networks, i.e.  $|M| > 2$ .

Another property of LTFs is, that because of the restriction to a certain class of functions, the stability of the dynamics actually increases with increasing connectivity. This depends crucially on a non-symmetric distribution of positive and negative weights  $c_{ij}$ , as will be shown at the end of this chapter in section 3.3. However, this characterization with positive and negative weights is not applicable anymore when considering the bigger class of monotone Boolean functions, as there also higher orders occur in the argument of the sign-function. Unate functions exhibit the same or similar characteristics of the dynamics [Kürten, 2010a]. A detailed study on the dynamical properties of such restrictions on the classes of Boolean functions is currently in preparation [Kürten and Raeymaekers, 2010]. The increased size of the stability region for this class of Boolean functions is contrary to the Kauffman model, where all Boolean functions are allowed, leading to a higher critical connectivity  $K_c$ . In the Kauffman model the stability region rapidly shrinks, since most of the function exhibit highly non-linear or chaotic interactions. The number of Linear Threshold functions for certain connectivities  $K$  is given in table 3.1. From this table it should be clear, that the fraction of LTFs of all Boolean functions decreases rather fast, so a restriction to LTFs takes only a small fraction of all possible Boolean functions. The size of the class of monotone functions decreases not as fast as that, allowing for more functions to be present in the mixture.

Before going into details a short remark on notation is made. To simplify the expressions, the first index  $i$  is omitted from the local function  $f$ :

$$
x_i' = \text{sign}\left(\sum_j c_j x_j - h\right) \tag{3.5}
$$

as in a Mean Field approximation the dependence on i and its specific neighbors  $i_j$  are not of importance anymore, because all calculations are treated only statistically.

<sup>&</sup>lt;sup>1</sup>Non-degenerate Boolean functions depend on all their variables  $x_j$ , so there is no index j, such that  $f(x)$  =  $f(x \oplus e_i)$  for all x.

	number of	number of	fraction
	Boolean functions f	<b>LTFs</b>	
			1.000
$\mathcal{D}_{\mathcal{L}}$	16	14	0.875
3	256	104	0.406
	65536	1882	0.029
5	$4.29 \cdot 10^{10}$	94572	$2.20 \cdot 10^{-5}$

Table 3.1: Number of Linear Threshold functions compared to all Boolean functions for connectivities up to  $K = 5$  [Franco et al., 2006]

# 3.1 Integral formalism

In chapter 2 a way to construct the iteration equations for the magnetization  $m$  and for the Hamming distance d was shown for general distributions  $\rho_F$  and  $\rho_k$ . Here a few ideas already proposed earlier will be formulated explicitly in the form of integrals to incorporate the distribution of weights  $\rho_c$  for Linear Threshold functions.

First recall the result of corollary 2.8 and the remark after it. In the iteration equations for the probabilities  $z_{(\pm)}$  (and also for all higher orders of the dynamics), the term including the Boolean function can be splitted to a weighted sum over all single Boolean function f:

$$
\Pr\left[f(\mathbf{x}^{(1)} = \pm 1, ..., f(\mathbf{x}^{(n)} = \pm 1 | \mathbf{x}^{(1)}, ..., \mathbf{x}^{(n)}]\right]
$$
\n
$$
= \sum_{\mathfrak{f}} \Pr\left[\mathfrak{f}|\rho_{\mathbf{F}}\right] \Pr\left[\mathfrak{f}(\mathbf{x}^{(1)}) = \pm 1 | \mathbf{x}^{(1)}, \mathfrak{f}\right] \dots \Pr\left[\mathfrak{f}(\mathbf{x}^{(n)}) = \pm 1 | \mathbf{x}^{(n)}, \mathfrak{f}\right],\tag{3.6}
$$

where each of the terms  $Pr[f(x^{(k)}) = \pm 1 | x^{(k)}, f]$  is only either zero or one. Even if the probabilities  $Pr[f|\rho_F]$  are not given explicitly in the model, they can be derived with the projection of the function  $f$  on the single Boolean function  $f$ :

$$
\Pr\left[\mathfrak{f}|\gamma\right] = \int \mathcal{D}\gamma \prod_{\mathbf{x}} \Pr\left[f(\gamma; \mathbf{x}) = \mathfrak{f}(\mathbf{x})\right],\tag{3.7}
$$

where  $\mathcal{D}_{\gamma}$  is a measure over the external parameters  $\gamma$  of the model. In the case of LTFs these external parameters would be the connectivity K, the distribution of weights  $\rho_c$  and the threshold h, i.e.  $\gamma = \{K, \rho_c, h\}$ . In the next lemma this measure will be shown explicitly, at least for LTFs.

Hence all results from the last chapter also apply to LTFs, although in most cases the projection (and hence the explicit probabilities  $Pr[f|\rho_F]$ ) will not be calculated. However, this establishes a mapping from the distribution of weights  $\rho_c$  to a distribution of functions  $\rho_{\bf F}$ :

$$
\rho_c \mapsto \rho_{\mathbf{F}}.\tag{3.8}
$$

So far only the existence and uniqueness of this mapping is made plausible. In the next lemma, the direct probabilities  $\Pr\left[f(\mathbf{x^{(1)}}=\pm1,\ldots,f(\mathbf{x^{(n)}}=\pm1|\mathbf{x^{(1)}},\ldots,\mathbf{x^{(n)}}]\right]$  for a LTF will be rewritten to another form in which they are finally computed explicitly.

**Lemma 3.1.** *For LTFs the probability for the function to have specific values at different input tuples* x *can be expressed as an integral over the distribution of weights*  $\rho_c$ *:* 

$$
\Pr\left[f(\mathbf{x}^{(1)}) = \pm 1, \dots, f(\mathbf{x}^{(n)}) = \pm 1 | \mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\right]
$$
\n
$$
= \int \cdots \int dc_1 \dots dc_K \rho_c(c_1) \dots \rho_c(c_K) \Theta\left(\pm \left(\sum_i c_i x_i^{(1)} - h\right)\right) \dots \Theta\left(\pm \left(\sum_i c_i x_i^{(n)} - h\right)\right)
$$
\n
$$
= \int \mathcal{D}^K \rho_c \Theta\left(\pm \left(\sum_i c_i x_i^{(1)} - h\right)\right) \dots \Theta\left(\pm \left(\sum_i c_i x_i^{(n)} - h\right)\right),
$$
\n(3.9)

*introducing a complete, normalized measure*  $\mathcal{D}^K \rho_c$  *over all* K *different weights*  $c_i$  *to simplify notation.*

*Proof.* First assume  $n = 1$ , which are the integrals when calculating the magnetization m. The probability for a function to have value  $\pm 1$ , given an input tuple x, is  $Pr[f(x) = \pm 1|x]$ . As the function has a special form, the following derivation can be made:

$$
\Pr[f(\mathbf{x}) = \pm 1 | \mathbf{x}] = \Pr\left[\text{sign}\left(\sum_{i} c_i x_i - h\right) = \pm 1 | \mathbf{x}\right] =
$$

$$
= \Pr\left[\sum_{i} c_i x_i - h \geq 0 | \mathbf{x}\right] = \dots
$$

When the weights  $c_i$  are distributed according to some distribution  $\rho_c$ , the probability is the integral over all possible values in the distribution, but only counting those, which give the correct output in the function f. Therefore a Heaviside-Theta-function  $\Theta(\ldots)$  can be introduced as a characteristic function:

$$
\begin{array}{rcl}\n\cdots & = & \int \cdots \int dc_1dc_2 \ldots dc_K \rho_c(c_1) \rho_c(c_2) \ldots \rho_c(c_K) \Theta\left(\pm \left(\sum_i c_i x_i - h\right)\right) = \\
& = & \int \mathcal{D}^K \rho_c \Theta\left(\pm \left(\sum_i c_i x_i - h\right)\right),\n\end{array}
$$

where the sign inside the Theta-function is + if the original condition is  $f(x) = +1$  and − if  $f(\mathbf{x}) = -1$ .

For  $n>1$  the joint probability  $\Pr\left[f(\mathbf{x^{(1)}})=\pm 1,\ldots,f(\mathbf{x^{(n)}})=\pm 1|\mathbf{x^{(1)}},\ldots,\mathbf{x^{(n)}})\right]$  has to be calculated. This term does not factorize into several single probabilities,  $\prod_i \Pr\big[ f(\mathbf{x^{(i)}}) = \pm 1 | \mathbf{x^{(i)}} \big],$ when the function incorporates a distribution on a parameter $^2$ , here on the weights  $c_j.$ For the joint probability, the integral over the parameters incorporates several Thetafunctions, as characteristic functions for each of the conditions

$$
\Pr\left[f(\mathbf{x}^{(1)}) = \pm 1, \dots, f(\mathbf{x}^{(n)}) = \pm 1 | \mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\right]
$$

$$
= \int \mathcal{D}^K \rho_c \Theta\left(\pm \left(\sum_i c_i x_i^{(1)} - h\right)\right) \dots \Theta\left(\pm \left(\sum_i c_i x_i^{(n)} - h\right)\right).
$$

<sup>&</sup>lt;sup>2</sup>Note that in the case of a Boolean function f, given by a truth table, the probability factorizes again.
This is exactly the statement of the lemma.

The calculations will be simplified by using another property of such LTFs:

**Definition 3.2.** *A totalistic Boolean function does not depend on the order of its variables. They can be switched without changing the output of the function:*

$$
\forall i, j: \quad f(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_K) = f(x_1, \ldots, x_j, \ldots, x_i, \ldots, x_K), \tag{3.10}
$$

*resulting in an equivalence class of Boolean functions, which are dynamically identical.*

*Therefore only the number of* +1*s or* −1*s is important for the output, and hence the only necessary argument of the function could be the number of* +1*s in the original input* x*:*

$$
f(\mathbf{x}) \mapsto f(\langle \mathbf{x}, \mathbf{x} \rangle). \tag{3.11}
$$

*However, this is still the same Boolean function, and it should be clear from context, whether the argument is an integer number or a tuple in*  $M^k$ *.* 

Since in LTFs the dependence on the variables  $x_1, \ldots, x_K$  is only in a sum  $\sum\limits_j c_j x_j$ , which is commutative, LTFs are totalistic functions. Therefore the calculation load can be greatly reduced, if all integrals from lemma 3.1 are grouped together, where the number of  $+1s$ in the input (or the number of the different states  $(++)$ ,  $(+-)$ ,  $(-+)$  or  $(--)$  in the second order) is identical.

**Lemma 3.3.** The number of terms to calculate in the iteration polynomial for d' can be *reduced, when the Boolean function is totalistic.*

$$
z'_{(\pm \pm)} = \sum_{\mathbf{x}} \sum_{\mathbf{y}} \Pr[f(\mathbf{x}) = \pm 1, f(\mathbf{y}) = \pm 1 | \mathbf{x}, \mathbf{y}] \Pr[\mathbf{x}, \mathbf{y} | z_{(\pm \pm)}] =
$$
(3.12)  

$$
= \sum_{\substack{n_i=0 \ n_i=N}}^{K} \frac{K!}{n_1! n_2! n_3! n_4!} \Pr[f(n_1 + n_2) = \pm 1, f(n_1 + n_3) = \pm 1 |n_i| \ z_{(++)}^{n_1} z_{(+-)}^{n_2} z_{(--)}^{n_3} z_{(--)}^{n_4},
$$

*where the exponents*  $n_i$  *are given in lemma 2.12, which characterize the input tuples* x and y completely. The expression  $\Pr\left[f(n_1+n_2)=\pm 1, f(n_1+n_3)=\pm 1 | n_i\right]$  is just rewriting the *original probability to suit the new variables*  $n_i$  *instead of the old ones*  $\bf{x}$  *and*  $\bf{y}$ *.* 

*Proof.* Follows immediately from the fact that there are  $\frac{K!}{n_1!n_2!n_3!n_4!}$  permutations of the 4 possible states  $(++)$ ,  $(+-)$ ,  $(-+)$  and  $(--)$ , as this is a multinomial distribution on the  $\Box$ numbers  $n_1$ ,  $n_2$ ,  $n_3$  and  $n_4$  of those states.

This is exactly what was described above, as only the numbers of all input combinations, which are  $(++), (+-), (-+)$  and  $(--),$  are important.

#### Example of a projection of Linear Threshold functions to single Boolean functions f

Suppose a BN with Linear Threshold functions is given, where the distribution of weights  $\rho_c$  is defined by

$$
\rho_c^{(\delta)} = p\delta(c-1) + (1-p)\delta(c+1).
$$

 $\Box$ 

This distribution will also be used later in more elaborate calculations (and has also been used in an example in last chapter). Furthermore assume the connectivity  $K = 2$  and the threshold  $h = 0.3$  This is exactly the mixture of functions already used in an earlier example and also in [Greil and Drossel, 2007].

Using equation (3.7), this LTF will be split up into several single Boolean functions f. In the current case (with the distribution  $\rho_c^{(\delta)}$  given above), this can be done in several ways. The generic way would be explicitly calculating this integral for each of the  $2^{2^K}$  Boolean functions f separately. Hence

$$
\Pr[f|\rho_c, K=2] = \int dc_1dc_2\rho_c(c_1)\rho_c(c_2) \prod_{\mathbf{x}} \Pr[\text{sign}(x_1c_1 + x_2c_2) = f(\mathbf{x})].
$$

Here the probability  $Pr[\text{sign}(x_1c_1 + x_2c_2) = f(x)]$  can only be  $\in \{0,1\}$ , because either the functions (LTF and  $\mathfrak f$ ) coincide on the input x or not. In this case this results in  $2^K=4$ conditions to be met.

However, if the distribution of weights  $\rho_c$  is as simple as above, the projection could also be calculated easier. As  $c_j$  can only assume the values  $c_j \in \{-1, +1\}$ , there are only 4 possible combinations of  $c_1$  and  $c_2$ , which have the following probabilities:

$$
\Pr\left[c_1 = +1, c_2 = +1 | \rho_c^{(\delta)}\right] = p^2,
$$
\n
$$
\Pr\left[c_1 = +1, c_2 = -1 | \rho_c^{(\delta)}\right] = p(1-p),
$$
\n
$$
\Pr\left[c_1 = -1, c_2 = +1 | \rho_c^{(\delta)}\right] = (1-p)p,
$$
\n
$$
\Pr\left[c_1 = -1, c_2 = -1 | \rho_c^{(\delta)}\right] = (1-p)^2.
$$

Inserting those combinations into the LTF, gives a single value at every possible input x, which are listed in table 3.2.

input		output					
$\mathbf x$				$c_1 = +1, c_2 = +1$ $c_1 = +1, c_2 = -1$ $c_1 = -1, c_2 = +1$ $c_1 = -1, c_2 = -1$			

Table 3.2: Inserting all 4 combinations of  $c_1$  and  $c_2$  into the LTF.

The 4 Boolean functions in this table are  $(14)_2$ ,  $(13)_2$ ,  $(11)_2$  and  $(7)_2$ , respectively. Hence the distribution of functions  $\rho_F$  could be written as

$$
\rho_{\mathbf{F}} \sim p^2 \left(14\right)_2 + p(1-p) \left(13\right)_2 + p(1-p) \left(11\right)_2 + (1-p)^2 \left(7\right)_2.
$$

This example should also show, that except for such examples of distributions, like  $\rho_c^{(\delta)}$ above, the route via calculating  $Pr[f(x) = \pm 1|x]$  directly with lemma 3.1 is the simpler one,

<sup>&</sup>lt;sup>3</sup>This requires that sign(0) is also defined and sign(0)  $\in M$ . In this example it is set to sign(0) = +1.

as then a smaller number of Θ-functions (which is the order of the dynamics) appears in the integrals, that have to be calculated. So for the Hamming distance only 2 such Θ-functions are present, whereas with the projection to single Boolean functions there are  $2^K$   $\Theta$ -functions in the integrals $^4$ .

#### 3.1.1 Equivalence to other formalisms

The integral formalism presented so far can be used to establish the equivalence to the formalism introduced in [Kürten, 1988b], where the sensitivities, which are already mentioned several times in the last chapter, are used to construct the iteration polynomial for the Hamming distance  $d$ . Note that this is exactly one of the cases where the iteration equation for the Hamming distance  $d$  can actually be constructed by the sensitivities  $S^{(n)}.$ The reason for this is a symmetrical distribution of weights:

$$
\rho_c(c) = \rho_c(-c). \tag{3.13}
$$

Recall that sensitivities  $S^{(n)}$  are the probabilities, that a change in exactly  $n$  variables in the input tuple x changes the output of the Boolean function  $f$ . In [Kürten, 1988b] the symbol  $I_{Kn}$  (which is denoted with  $S^{\perp (n)}$  in this work here) is used as the probability, that n changes in the input **do not** change the output of the function. Hence here those probabilities will be denoted  $S^{\perp(n)}$  to distinguish them from the sensitivities  $S^{(n)}$  before. However, they are connected through the obvious relation

$$
S^{(n)} = 1 - I_{Kn} = 1 - S^{\perp(n)}.
$$
\n(3.14)

**Theorem 3.4.** *The integral formalism, proposed first by [Kurten, 1988b], is equivalent with ¨ the Mean Field description of the Hamming distance* d*, formalized in the last chapter, when using the condition*

$$
\rho_c(c) = \rho_c(-c). \tag{3.15}
$$

*If the weights are distributed symmetric, the iteration equation for the magnetization* m *reduces to a constant, i.e. the fixed point* m<sup>∗</sup> *is reached after a single timestep and the Hamming distance* d *is given by:*

$$
d' = \sum_{k=1}^{K} (-1)^{k+1} {K \choose k} a(k) d^k,
$$
\n(3.16)

*where*  $a(k) = 1 + \sum_{k=1}^{k}$  $\sum_{n=1}^{\infty}(-1)^{s}\binom{k}{n}S^{\perp(n)}$  and  $S^{\perp(n)} = \int \cdots \int dc_1 \ldots dc_K \rho_c(c_1) \ldots \rho_c(c_K) \Theta\left((c_{n+1} + \cdots + c_K - h)^2 - (x_1 + \cdots + x_n)^2\right)$ . (3.17)

 $4$ and  $K + 1$  Θ-functions in the totalistic case.

*Proof.* First the iteration equation for the magnetization  $m'$  is derived. Recall

$$
m' = z'_{(+)} - z'_{(-)}
$$
  
=  $\left(\sum_{\mathbf{x}} \Pr[f(\mathbf{x}) = +1|\mathbf{x}] \Pr[\mathbf{x}|z_{(\pm)}]\right) - \left(\sum_{\mathbf{x}} \Pr[f(\mathbf{x}) = -1|\mathbf{x}] \Pr[\mathbf{x}|z_{(\pm)}]\right)$   
=  $\sum_{\mathbf{x}} \left[\int \mathcal{D}^{K} \rho_{c} \left(\Theta\left(\sum_{j} x_{j} c_{j} - h\right) - \Theta\left(-\sum_{j} x_{j} c_{j} + h\right)\right)\right] \Pr[\mathbf{x}|z_{(\pm)}] = ...$ 

Now the probabilities  $\Pr\left[\mathbf{x}|z_{(\pm)}\right]=\left(\frac{1+m}{2}\right)^{(\mathbf{x},\mathbf{x})}\left(\frac{1-m}{2}\right)^{K-(\mathbf{x},\mathbf{x})}$  from lemma 2.5 are inserted. By using the fact, that LTFs are totalistic, the summation over x can be changed into a simple summation taken over  $a=0,\ldots,K$  when using the binomial coefficient  ${K\choose a}$  and relabeling the  $c_j$  so that the first a coefficients have a positive sign:

... = 
$$
\sum_{a=0}^{K} {K \choose a} \left[ \int \mathcal{D}^{K} \rho_c (\Theta (c_1 + \dots + c_a - c_{a+1} - \dots - c_K - h) -\Theta (-c_1 - \dots - c_a + c_{a+1} + \dots + c_K + h)) \right] \left( \frac{1+m}{2} \right)^a \left( \frac{1-m}{2} \right)^{K-a} = \dots
$$

Using  $\Theta(-x) = 1 - \Theta(x)$  the expression above simplifies:

$$
\dots = \sum_{a=0}^{K} {K \choose a} \left[ \int \mathcal{D}^{K} \rho_c \left( 2\Theta(c_1 + \dots + c_a - c_{a+1} - \dots - c_K - h) - 1 \right) \right] \times \left( \frac{1+m}{2} \right)^a \left( \frac{1-m}{2} \right)^{K-a} = \dots
$$

Now the symmetry of  $\rho_c$  is used. Therefore the integral can be written as

$$
\int \mathcal{D}^K \rho_c \Theta (c_1 + \dots + c_a - c_{a+1} - \dots - c_K - h) = \int \mathcal{D}^K \rho_c \Theta (c_1 + \dots + c_K - h),
$$

and is independent of  $a.$  Furthermore using the normalization of the measure  $\int {\cal D}^K \rho_c = 1$ the following expression is obtained, by writing the integrals in front of the sum:

$$
\begin{split}\n\cdots &= \left[ -1 + 2 \int \mathcal{D}^K \rho_c \Theta \left( c_1 + \dots + c_K - h \right) \right] \sum_{a=0}^K \binom{K}{a} \left( \frac{1+m}{2} \right)^a \left( \frac{1-m}{2} \right)^{K-a} \\
&= \left[ -1 + 2 \int \mathcal{D}^K \rho_c \Theta \left( c_1 + \dots + c_K - h \right) \right] \underbrace{\left( \frac{1+m}{2} + \frac{1-m}{2} \right)^K}_{=1} \\
&= -1 + 2 \int \mathcal{D}^K \rho_c \Theta \left( c_1 + \dots + c_K - h \right).\n\end{split}
$$

Hence the complete iteration equation is independent of  $m$  and the fixed point  $m^*$  is reached after a single timestep.

Now the equivalence of the iteration equation for the Hamming distance  $d$  has to be

shown. Recall again

$$
d' = z'_{(+-)} + z'_{(-+)}
$$
  
\n
$$
= \sum_{\mathbf{x}} \sum_{\mathbf{y}} (\Pr[f(\mathbf{x}) = +1, f(\mathbf{y}) = -1 | \mathbf{x}, \mathbf{y}] + \Pr[f(\mathbf{x}) = -1, f(\mathbf{y}) = +1 | \mathbf{x}, \mathbf{y}] \Pr[\mathbf{x}, \mathbf{y} | z_{(\pm \pm)}]
$$
  
\n
$$
= \sum_{\mathbf{x}, \mathbf{y}} \left[ \int \cdots \int d c_1 \cdots d c_K \rho_c(c_1) \cdots \rho_c(c_K) \left( \Theta \left( \sum_i c_i x_i - h \right) \Theta \left( - \sum_i c_i y_i + h \right) \right) \right. \\ \left. + \Theta \left( - \sum_i c_i x_i + h \right) \Theta \left( \sum_i c_i y_i - h \right) \right) \right] \Pr[\mathbf{x}, \mathbf{y} | z_{(\pm \pm)}] = \dots
$$

Using  $\Theta(-A)\Theta(B) + \Theta(A)\Theta(-B) = \Theta(-AB)$  and further the totalistic property of LTFs

$$
\begin{split}\n\cdots &= \sum_{\mathbf{x},\mathbf{y}} \left[ \int \mathcal{D}^{K} \rho_{c} \Theta \left( - \left( \sum_{i} c_{i} x_{i} - h \right) \left( \sum_{i} c_{i} y_{i} - h \right) \right) \right] \Pr \left[ \mathbf{x}, \mathbf{y} | z_{(\pm \pm)} \right] \\
&= \sum_{\substack{n_{i} = K}} \frac{K!}{n_{1}! n_{2}! n_{3}! n_{4}!} \left[ \int \mathcal{D}^{K} \rho_{c} \Theta \left( - \left( c_{1} + \dots + c_{n_{1}+n_{2}} - c_{n_{1}+n_{2}+1} - \dots - c_{K} - h \right) \times \right. \\
&\times \left( c_{1} + \dots + c_{n_{1}} - c_{n_{1}+1} - \dots - c_{n_{1}+n_{2}} + c_{n_{1}+n_{2}+1} + \dots + c_{n_{1}+n_{2}+n_{3}} \right. \\
&\quad \left. - c_{n_{1}+n_{2}+n_{3}+1} - \dots - c_{K} - h \right) \right] z_{\binom{n_{1}+1}{n_{1}}}^{n_{1}} z_{\binom{n_{1}+1}{n_{1}}}^{n_{2}} z_{\binom{n_{2}+1}{n_{2}}}^{n_{3}} z_{\binom{n_{1}+1}{n_{1}}}^{n_{4}} z_{\bin
$$

New summation variables are introduced instead of the  $n_i$ :

$$
a = n_1 + n_4 \qquad a = 0, ..., K
$$
  
\n
$$
A = n_4 \qquad A = 0, ..., a
$$
  
\n
$$
B = n_2 \qquad B = 0, ..., K - a
$$
  
\n
$$
n_3 = K - a - B
$$

69

Therefore

$$
\cdots = \sum_{a=0}^{K} \sum_{A=0}^{a} \sum_{B=0}^{K-a} \left(\frac{1}{2}\right)^K \frac{K!}{(a-A)!A!B!(K-a-B)!} \left(1 - S^{\perp(K-a)}\right) \times \times d^{K-a}(1+m-d)^{a-A}(1-m-d)^A
$$
  
\n
$$
= \sum_{a=0}^{K} \underbrace{\left(\sum_{B=0}^{K-a} \frac{1}{B!(K-a-B)!}\right)}_{=\frac{2K-a}{(K-a)!}} \underbrace{\left(\sum_{A=0}^{a} \frac{1}{A!(a-A)!}(1-m-d)^A(1+m-d)^{A-a}\right)}_{=\frac{2a}{a!}(-d)^a} \times K! \left(\frac{1}{2}\right)^K \left(1 - S^{\perp(K-a)}\right) d^{K-a}
$$
  
\n
$$
= \sum_{a=0}^{K} \frac{K!}{a!(K-a)!} \left(1 - S^{\perp(K-a)}\right) d^{K-a}(1-d)^a
$$
  
\n
$$
= \sum_{a=0}^{K} \left(\frac{K}{a}\right) \left(1 - S^{\perp(K-a)}\right) d^{K-a} \left(\sum_{b=0}^{a} \binom{b}{a}(-1)^b d^b\right)
$$
  
\n
$$
= \sum_{a=0}^{K} \sum_{b=0}^{a} \binom{K}{a} \binom{a}{b} \left(1 - S^{\perp(K-a)}\right) (-1)^b d^{K-a+b} = \dots
$$

Now the summation variables are changed again

$$
k = K - a + b \qquad k = 0, ..., K
$$
  

$$
n = K - a \qquad n = 0, ..., k
$$

and hence

... = 
$$
\sum_{k=0}^{K} \sum_{n=0}^{k} {K \choose k-n} {K-n \choose k-n} (1 - S^{\perp(n)}) (-1)^{k-n} d^k = ...
$$

Using  $\binom{K}{K-n}\binom{K-n}{k}=\binom{K}{k}\binom{k}{n}$  and inserting this in the expression for  $d'$  gives

$$
\dots = \sum_{k=0}^{K} (-1)^{k+1} {K \choose k} \underbrace{\left( \sum_{n=0}^{k} (-1)^{-n-1} {k \choose n} \left( 1 - S^{\perp(n)} \right) \right)}_{=a(k)} d^{k},
$$

which is the final form in [Kürten, 1988b], except for the sum starting at  $k = 0$  instead of  $k = 1$  in the original version and the expressions for  $a(k)$  are not yet matched completely:

$$
a(k) = \sum_{n=0}^{k} (-1)^{-n-1} {k \choose n} \left( 1 - S^{\perp(n)} \right) =
$$
  
= 
$$
- \underbrace{\left( \sum_{n=0}^{k} (-1)^{n} {k \choose n} \right)}_{= \delta_{0k}} + \sum_{n=0}^{k} (-1)^{n} {k \choose n} S^{\perp(n)} = \dots
$$

Now the two cases  $a(k = 0)$  and  $a(k > 0)$  have to be distinguished. Before that we need an

explicit calculation of  $S^{\perp(0)}$ :

$$
S^{\perp(0)} = \int \mathcal{D}^K \rho_c \Theta\left(\underbrace{(c_1 + \dots + c_K + h)^2}_{\geq 0}\right) = \int \mathcal{D}^K \rho_c = 1,
$$

and hence

$$
a(0) = -\delta_{00} + {0 \choose 0} (-1)^0 S^{\perp(0)} = -1 + 1 = 0,
$$
  
\n
$$
a(k) = -\delta_{0k} + \sum_{n=0}^k (-1)^n {k \choose n} S^{\perp(n)} = {k \choose 0} (-1)^0 S^{\perp(0)} + \sum_{n=1}^k (-1)^n {k \choose n} S^{\perp(n)}
$$
  
\n
$$
= 1 + \sum_{n=1}^k (-1)^n {k \choose n} S^{\perp(n)}.
$$

Using  $a(0) = 0$  the summation in the main expression starts with  $k = 1$ . Therefore the equivalence of the formalisms under the condition  $\rho_c(c) = \rho_c(-c)$  is finally established.  $\Box$ 

The expressions proved in the last theorem are not used for calculations in this work, because later on the distributions of weights  $\rho_c$  have an additional asymmetry parameter  $p \in [0, 1]$ , whereas in the derivation above the symmetry was used several times in crucial steps. In this case the iteration equation for the magnetization  $m'$  depends on m again, and is not just a constant anymore. Moreover, the integrals do not simplify as above and they are of the form

$$
S_{pseudo}^{(n_1, n_2, n_3, n_4)} = \int \mathcal{D}^K \rho_c \Theta \left( \left( \sum_{i}^{n_2} c_i - \sum_{i}^{n_3} c_i \right)^2 - \left( \sum_{i}^{n_1} c_i - \sum_{i}^{n_4} c_i - h \right)^2 \right)
$$
(3.18)

where  $\sum^{n_j}c_i$  means adding  $n_j$  of the weights  $c_i.$  Since all weights have the same distribution, the index  $i$  of the  $c_i$  does not matter, because they can be relabeled. An important point here is, that those integrals are not sensitivities anymore, because sensitivities are the probability of a sign reversal when changing a number of signs in the input. They can depend on the magnetization  $m$ , as seen in the last chapter, section 2.4, whereas the integrals of equation (3.18) are just numbers (and possibly depending on some model parameters), and hence are somewhat just "pseudo-sensitivities"  $S_{pseudo}$ . Those pseudosensitivities are coefficients in an expansion of the iteration equation of Hamming distance  $d'$  in **both** variables, the Hamming distance  $d$  itself and the magnetization  $m$ . Sensitivities are the coefficients in an (binomial) expansion in d **only**, at least in the case of symmetric distribution of weights  $\rho_c(c) = \rho_c(-c)$ .

## 3.2 Results

One part in this work was the calculation of the iteration equations for Linear Threshold functions with specific distributions of weights  $\rho_c$ . Results are available for two different distributions and the connectivities  $K = 2$  and  $K = 3$ . As shown in the previous chapter,

the polynomials are of order of the connectivity in  $m$  and  $d$  in those cases

$$
\mathcal{M}(\gamma; m) = \mathcal{O}(m^{K}), \n\mathcal{D}(\gamma; m, d) = \mathcal{O}(d^{K}),
$$

and could still be solved analytically.

The two distributions, for which results are calculated in this work are as follows:

$$
\rho_c^{(\delta)} = p\delta(c-1) + (1-p)\delta(c+1), \tag{3.19}
$$

$$
\rho_c^{(cont)} = \begin{cases}\n p & c \in [0, 1] \\
 1 - p & c \in [-1, 0) \\
 0 & \text{else}\n\end{cases} .
$$
\n(3.20)

With  $h > K$  or  $h < -K$  the iteration equations for both distributions are are quite trivial, because no combination of weights  $c_j$  and inputs x can exceed this value of the threshold.Hence for  $h > K$  the iteration equation is  $m' = -1$  and for  $h < -K$  it is  $m' = 1$ . For intermediate values of  $h$  (−K < h < K), the iteration equations have different structures, which change at certain values  $h_J$  of the threshold. For the distribution of weights  $\rho_c^{(\delta)}$ these "jumps"  $h_J$  in the threshold occur at even integers for odd connectivity K and at odd integers for even  $K$ , since the sum of weights multiplied by the state (see equation 3.1a) is also an integer. So for this  $\rho_c^{(\delta)}$ , the iteration equations are not explicitly dependent on the threshold  $h^5.$  The iteration equations for  $\rho_c^{(cont)}$  contain an explicit dependence on the threshold h, but also change their structure at  $h_J$ , which are all integers between  $-K$  and  $K$  in this case. Although the terms change structurally, as will be seen in the following pages, the change in the structure in the iteration equations is still "continuous":

$$
\lim_{\epsilon \to 0} \mathcal{M}\left(\rho_c^{(cont)}, p, h = h_J - \epsilon; m\right) = \lim_{\epsilon \to 0} \mathcal{M}\left(\rho_c^{(cont)}, p, h = h_J + \epsilon; m\right),
$$
  

$$
\lim_{\epsilon \to 0} \mathcal{D}\left(\rho_c^{(cont)}, p, h = h_J - \epsilon; m, d\right) = \lim_{\epsilon \to 0} \mathcal{D}\left(\rho_c^{(cont)}, p, h = h_J + \epsilon; m, d\right).
$$

In the next few pages the iteration equations for the magnetization  $m$  and for the Hamming distance  $d$  and their fixed point solutions for the two distributions of weights  $\rho_c^{(\delta)}$  and  $\rho_c^{(cont)}$  are given. The value of the single integrals (for a specific choice of  $n_i$ ) is not shown, as those give not very much insight into the construction of the iteration equations and there would be too many of them to list them all.

Each possible combination of tuples x and y, which is  $4^K$ , combined with the fact, that each integral has to be evaluated in each  $h$ -interval between those jumps separately (which are  $2K-2$  intervals for  $\rho_c^{(cont)}$  and  $K$  intervals for  $\rho_c^{(\delta)}$ ) already introduces a quite high number of integrals. Furthermore there are four different iteration equations, one for each of  $z_{(\pm\pm)}.$  This leads to the following number of integrals to calculate:

$$
\rho_c^{(\delta)}: \qquad K4^{K+1} \text{ integrals}
$$

<sup>&</sup>lt;sup>5</sup>Because it does not change the sign of the term, when subtracting e.g.  $h = 1.4$  or  $h = 1.5$  from an integer.

 $\rho_c^{(cont)}: \hspace{0.5cm} (2K-2)4^{K+1}$  integrals

However, some symmetries could be used to reduce the number of integrals:

- The iteration equation for the magnetization  $m$  could be calculated from the probabilities of second order  $z_{(\pm\pm)}$ , however probabilities of first order  $z_{(\pm)}$  would suffice, which are much easier to calculate, since they have only a single Θ-function.
- Furthermore, as  $z_{(+-)} = z_{(-+)}$  in MF, this leaves only a single of the four iteration polynomials to be calculated in second order for the Hamming distance d.
- By using the fact that Linear Threshold functions are totalistic, lemma 3.3 reduces the number of integrals again. The number of possible combinations of  $n_1$ ,  $n_2$ ,  $n_3$ ,  $n_4$ satisfying  $\sum_i n_i = K$  is exactly  $\binom{K+4-1}{4-1} = \binom{K+3}{3} = \frac{(K+3)!}{K!3!}$ , hence the reduction is by a factor of  $\frac{(K+3)!}{K!3!}4^{-K}$ , which is about 0.63 for  $K = 2$  and about 0.31 for  $K = 3$ .
- If the distribution  $\rho_c$  has additional symmetries, the number of integrals to evaluate can be reduced further. However, the two distributions of weights used in this work,  $\rho_{c}^{(\delta)}$  and  $\rho_{c}^{(cont)}$ , are not of this type. Such a property, which has been used in previous work, would be  $\rho_c(c) = \rho_c(-c)$ , like in [Kürten, 1988b].

This reduction leaves the following numbers of integrals:

$$
\rho_c^{(\delta)}: \quad \frac{(K+3)!}{6(K-1)!} \text{ integrals} \quad \Rightarrow 20 \text{ for } K = 2, \ 60 \text{ for } K = 3
$$
\n
$$
\rho_c^{(cont)}: \quad \frac{(2K-2)(K+3)!}{6K!} \text{ integrals} \quad \Rightarrow 20 \text{ for } K = 2, \ 80 \text{ for } K = 3
$$

The integrals for  $\rho_c^{(\delta)}$  are trivially evaluated, since the measure  ${\cal D}^K\rho_c^{(\delta)}$  is a pure point measure, i.e. it is just a sum. However, the evaluation for  $\rho_c^{(cont)}$  involves more effort, but can be done analytically, too. This evaluation of the integrals can be done e.g. geometrically, because the weights  $c_i$  are bounded by  $\pm 1$ , and are therefore constrained to a K-dimensional hypercube, where the Θ-functions correspond to  $(K - 1)$ -dimensional hyperplanes.

Additionally to the iteration equations for  $m$  and  $d$ , the phase diagrams for the (stable) fixed points  $m^*$  and  $d^*$  are shown in the coming sections (figures 3.1 to 3.4). Although there might be more than one solution of the iteration equations  $m' = \mathcal{M}(p, h; m)$  and  $d' = \mathcal{D}(p, h; m, d)$ , only one of them is stable and in the range  $m \in [-1, 1]$  and  $d \in [0, 1]$ , except for the case where a white area is shown in those phase diagrams. These white areas are usually around the parameter point  $(p, h) = (1, 0)$ , where two stable fixed points  $m<sup>*</sup>$  occur, and around the parameter point  $(p, h) = (0, 0)$ , which corresponds to a period-2solution in the magnetization, i.e. no single stable fixed point  $m^*$  exists.

The fixed point solutions are obtained by varying the the parameters  $p$  and  $h$  in small step-sizes, and solving the equations  $m^* = \mathcal{M}(p, h; m^*)$  and  $d^* = \mathcal{D}(p, h; m^*, d^*)$  at those parameters numerically. Therefore the results are only semi-analytically derived, because no closed form for the surfaces  $m^*(p, h)$  and  $d^*(p, h)$  could be found, except for  $K = 2$  and  $\rho_c^{(\delta)}$ , where those solutions are already given partially in the example at the end of section 2.3.2.

This system, a BN with LTFs and the distribution of degrees  $\rho_c^{(\delta)}$ , has already been investigated by several other authors. Besides [Kürten and Clark, 2008] and [Greil and Drossel, 2005], which have been mentioned earlier, also [Rohlf and Bornholdt, 2002] treats this BN, and furthermore [Nakamura, 2003] and [Nakamura, 2004], which are based on the latter. In [Rohlf and Bornholdt, 2002] the sensitivity  $S^{(1)}$  is derived combinatorially. However, it is then combined with the original iteration equation for the Hamming distance from [Derrida and Pomeau, 1986], which is only valid for the Kauffman model, but not for this specific mixture of Boolean functions, which is a LTF. Furthermore, the authors do not calculate any higher sensitivities  $S^{(n)}$  or coefficients  $\lambda_n$  for their iteration equation, and by combining the original iteration equation with their sensitivity, they just set  $\mu_n = (-1)^{n+1} \binom{K}{n} S^{(1)}$ , where  $\mu_n$  are the plain coefficients in the Hamming distance, see definition 2.22. They still get the correct critical condition, as this only depends on  $S^{(1)},$ but the method does not yield the correct fixed point in the Hamming distance  $d^*$ , which is clearly seen in their figure 3, which is explained by slow convergence below the critical point. In [Nakamura, 2003] the latter approach is copied and a more complicated degree distribution  $Pr[k|\rho_k]$ , as well as a different mixture of Boolean functions, depending on a parameter T, is incorporated into the model. Again, a correct critical condition, and therefore the critical connectivity  $K_c$ , is obtained, but fails to predict the fixed point in the Hamming distance.

#### Delta-peaked distribution of weights  $\rho_c^{(\delta)}$  and  $K=2$



Figure 3.1: Fixed point-solutions of the iteration equations  $m^* = \mathcal{M}(p,h;m^*)$  and  $d^* =$  $\mathcal{D}(p,h;m^*,d^*)$  for  $K=2$  and  $\rho_c^{(\delta)}.$ 

Iteration equations for the magnetization  $m$  for  $K=2$  and  $\rho_c^{(\delta)}$ :

 $-\infty < h < -2$ :  $m' = 1$  $-2 < h < 0:$   $m' = \left[\frac{1}{2}\right] + \left[2p - 1\right]m + \left[-\frac{1}{2}\left(2p - 1\right)^2\right]m^2$  $0 < h < 2$ :  $m' = \left[-\frac{1}{2}\right] + \left[2p - 1\right]m + \left[\frac{1}{2}\left(2p - 1\right)^2\right]m^2$   $2 < h < \infty$ :  $m' = -1$ 

Iteration equations for the Hamming distance  $d$  for  $K=2$  and  $\rho_c^{(\delta)}$ :



Uniform distribution of weights  $\rho_{c}^{(cont)}$  and  $K=2$ 



Figure 3.2: Fixed point-solutions of the iteration equations  $m^* = \mathcal{M}(p,h;m^*)$  and  $d^* =$  $\mathcal{D}(p,h; m^*,d^*)$  for  $K=2$  and  $\rho_c^{(cont)}$ .

Iteration equations for the magnetization  $m$  for  $K=2$  and  $\rho_c^{(cont)}$ :



Iteration equations for the Hamming distance  $d$  for  $K=2$  and  $\rho_c^{(cont)}$ :





#### Delta-peaked distribution of weights  $\rho_c^{(\delta)}$  and  $K=3$



Figure 3.3: Fixed point-solutions of the iteration equations  $m^* = \mathcal{M}(p,h;m^*)$  and  $d^* =$  $\mathcal{D}(p,h;m^*,d^*)$  for  $K=3$  and  $\rho_c^{(\delta)}.$ 

Iteration equations for the magnetization  $m$  for  $K=3$  and  $\rho_c^{(\delta)}$ :

 $-\infty < h < -3$   $m' = 1$  $-3 < h < -1$   $m' = \left[\frac{3}{4}\right] + \left[\frac{3}{4}(2p-1)\right]m + \left[-\frac{3}{4}(2p-1)^2\right]m^2 + \left[\frac{1}{4}(2p-1)^3\right]m^3$  $-1 < h < 1$   $m' = \left[\frac{3}{2}(2p-1)\right]m + \left[-\frac{1}{2}(2p-1)^3\right]m^3$ 1 < h < 3  $m' = \left[-\frac{3}{4}\right] + \left[\frac{3}{4}(2p-1)\right]m + \left[\frac{3}{4}(2p-1)^2\right]m^2 + \left[\frac{1}{4}(2p-1)^3\right]m^3$  $3 < h < \infty$   $m' = -1$ 

Iteration equations for the Hamming distance  $d$  for  $K=3$  and  $\rho_c^{(\delta)}$ :

 $-\infty < h < -3$  $d' = 0$  $-3 < h < -1$  d' =  $\left[\frac{3}{4} - \frac{3}{2}(2p-1)m + \frac{3}{4}(2p-1)^2m^2\right]d + \left[-\frac{3}{4} + \frac{3}{4}(2p-1)m\right]d^2 + \left[\frac{1}{4}\right]d^3$  $-1 < h < 1$   $d' = \left[\frac{3}{2} - \frac{3}{2}(2p - 1)^2 m^2\right] d + \left[-\frac{3}{2}\right] d^2 + \left[1\right] d^3$ 1 < h < 3  $d' = \left[\frac{3}{4} + \frac{3}{2}(2p - 1)m + \frac{3}{4}(2p - 1)^2m^2\right]d + \left[-\frac{3}{4} - \frac{3}{4}(2p - 1)m\right]d^2 + \left[\frac{1}{4}\right]d^3$  $3 < h < \infty$  $d' = 0$ 

Uniform distribution of weights  $\rho_c^{(cont)}$  and  $K=3$ 

Iteration equations for the magnetization  $m$  for  $K=3$  and  $\rho_c^{(cont)}$ :



Figure 3.4: Fixed point-solutions of the iteration equations  $m^* = \mathcal{M}(p, h; m^*)$  and  $d^* =$  $\mathcal{D}(p,h;m^*,d^*)$  for  $K=3$  and  $\rho_c^{(cont)}$ .



Figure 3.5: Fixed points in the magnetization  $m^*$  and stability of this fixed point in the range of low p for  $K = 3$  and  $\rho_c^{(cont)}$ .



Figure 3.6: Fixed points in Hamming distance  $d^*$  and stability of this fixed point in the range of low p for  $K = 3$  and  $\rho_c^{(cont)}$ .



Figure 3.7: Fixed points in the magnetization  $m^*$  in the range of high p for  $K = 3$  and  $\rho_c^{(cont)}.$  The green line indicates the solutions on the line  $h=0,$  also depicted in figure 3.9(b).

$$
-\infty < h < -3 \qquad m' = 1
$$
  
\n
$$
-3 < h < -2 \qquad m' = \left[1 - \frac{1}{24}(h+3)^3\right] + \left[\frac{1}{8}(h+3)^3(2p-1)\right]m +
$$
\n
$$
+ \left[-\frac{1}{8}(h+3)^3(1-2p)^2\right]m^2 + \left[\frac{1}{24}(h+3)^3(2p-1)^3\right]m^3
$$
\n
$$
-2 < h < -1 \qquad m' = \left[1 - \frac{1}{24}(h+3)^3\right] + \left[-\frac{1}{8}(h^3+3h^2-3h-11)(2p-1)\right]m +
$$
\n
$$
+ \left[\frac{1}{8}(3h^3+15h^2+21h+5)(1-2p)^2\right]m^2 +
$$
\n
$$
+ \left[-\frac{1}{24}(5h^3+27h^2+45h+21)(2p-1)^3\right]m^3
$$
\n
$$
-1 < h < 0 \qquad m' = \left[\frac{1}{12}h\left(h^2-9\right)\right] + \left[-\frac{1}{4}\left(h^3+3h^2-5\right)(2p-1)\right]m +
$$
\n
$$
+ \left[-\frac{1}{4}h\left(h^2-3\right)(1-2p)^2\right]m^2 + \left[\frac{1}{12}(5h^3+9h^2-3)(2p-1)^3\right]m^3
$$
\n
$$
0 < h < 1 \qquad m' = \left[\frac{1}{12}h\left(h^2-9\right)\right] + \left[\frac{1}{4}\left(h^3-3h^2+5\right)(2p-1)\right]m +
$$
\n
$$
+ \left[-\frac{1}{4}h\left(h^2-3\right)(1-2p)^2\right]m^2 + \left[-\frac{1}{12}(5h^3-9h^2+3)(2p-1)^3\right]m^3
$$
\n
$$
1 < h < 2 \qquad m' = \left[1 - \frac{1}{24}(h-3)^3\right] + \left[\frac{1}{8}\left(h^3-3h^2-3h+11\right)(2p-1)\right]m +
$$
\n
$$
+ \left[\frac{1}{8}(3h^3-1
$$

Iteration equations for the Hamming distance  $d$  for  $K=3$  and  $\rho_c^{(cont)}$ :

$$
-\infty < h < -3 \qquad d' = 0
$$
  
\n
$$
-3 < h < -2 \qquad d' = \left[\frac{1}{8}(h+3)^3 - \frac{1}{4}(h+3)^3(2p-1)m + \frac{1}{8}(h+3)^3(1-2p)^2m^2\right]d +
$$
  
\n
$$
+ \left[-\frac{1}{8}(h+3)^3 + \frac{1}{8}(h+3)^3(2p-1)m\right]d^2 +
$$
  
\n
$$
+ \left[\frac{1}{24}(h+3)^3\right]d^3
$$
  
\n
$$
-2 < h < -1 \qquad d' = \left[\frac{1}{8}\left(-h^3 - 3h^2 + 3h + 11\right) + \frac{1}{4}\left(3h^3 + 15h^2 + 21h + 5\right)(2p-1)m -\right] - \frac{1}{8}\left(5h^3 + 27h^2 + 45h + 21\right)(1-2p)^2m^2\right]d +
$$
  
\n
$$
+ \left[\frac{1}{8}\left(3h^3 + 15h^2 + 21h + 5\right) - \frac{1}{8}\left(5h^3 + 27h^2 + 45h + 21\right)(2p-1)m\right]d^2 +
$$
  
\n
$$
+ \left[\frac{1}{24}\left(-5h^3 - 27h^2 - 45h - 21\right)\right]d^3
$$

$$
-1 < h < 0
$$
\n
$$
d' = \left[\frac{1}{4}\left(-h^3 - 3h^2 + 5\right) - \frac{1}{2}h\left(h^2 - 3\right)(2p - 1)m + \right.
$$
\n
$$
+ \frac{1}{4}\left(5h^3 + 9h^2 - 3\right)(1 - 2p)^2 m^2\right] d +
$$
\n
$$
+ \left[\frac{1}{4}\left(2h^3 + 3h^2 - 3\right) + \frac{1}{4}h\left(2h^2 + 6h + 3\right)(2p - 1)m\right] d^2 +
$$
\n
$$
+ \left[\frac{1}{12}\left(-4h^3 + 9h + 6\right)\right] d^3
$$
\n
$$
0 < h < 1
$$
\n
$$
d' = \left[\frac{1}{4}\left(h^3 - 3h^2 + 5\right) - \frac{1}{2}h\left(h^2 - 3\right)(2p - 1)m - \frac{1}{4}\left(5h^3 - 9h^2 + 3\right)(1 - 2p)^2 m^2\right] d +
$$
\n
$$
+ \left[\frac{1}{4}\left(-2h^3 + 3h^2 - 3\right) + \frac{1}{4}h\left(2h^2 - 6h + 3\right)(2p - 1)m\right] d^2 +
$$
\n
$$
+ \left[\frac{1}{12}\left(4h^3 - 9h + 6\right)\right] d^3
$$
\n
$$
1 < h < 2
$$
\n
$$
d' = \left[\frac{1}{8}\left(h^3 - 3h^2 - 3h + 11\right) + \frac{1}{4}\left(3h^3 - 15h^2 + 21h - 5\right)(2p - 1)m +
$$
\n
$$
+ \frac{1}{8}\left(5h^3 - 27h^2 + 45h - 21\right)(1 - 2p)^2 m^2\right] d +
$$
\n
$$
+ \left[\frac{1}{8}\left(-3h^3 + 15h^2 - 21h + 5\right) - \frac{1}{8}\left(5h^3 - 27h^2 + 45h - 21\right)(2p - 1)m\right] d^2 +
$$
\n
$$
+ \left[\frac{1}{24}\left(5h^3 -
$$

#### 3.2.1 Phase diagrams

As can be seen in figure 3.8 (and also figures 3.1 to 3.4), the dynamics of the different BNs exhibit several different phases: In the majority of the phase space  $(p, h)$  there exits a single stable fixed point  $m^*$  for the magnetization. Except for some area around the  $h = 0$ line, the dynamics is also stable against perturbations, i.e.  $d^*=0.$  At  $p\approx 1$  and  $h\approx 0$  there exist two different stable fixed points  $m<sup>*</sup>$  of the magnetization. The dynamics in this two fixed point range is mostly ordered, however, for  $\rho_c^{(cont)}$  at the borders (with  $h\neq 0$ ) to the single fixed point, one of those fixed points  $m^*$  is associated with a increasing Hamming distance  $d^* \neq 0$ , until this fixed point  $m^*$  vanishes and only a single fixed point is left $^6$ . In the area around  $(p, h) = (0, 0)$  a period-2 solution for m' exists. At the border to the stable single fixed point solutions the dynamics is disordered  $(d^* \neq 0)$ . However,  $d^* \to 0$  quickly in this area when  $(p, h) \rightarrow (0, 0)$  is approached.

In figure 3.8 the information from figures 3.1 to 3.4 is reduced and relevant parts presented again. Blue lines show the phase-transition from disordered dynamics ( $d^* \neq 0$ ) in the center to ordered dynamics  $(d^* = 0)$  outside. The red and brown lines indicate the already mentioned changes in  $m^*$ : in the top of the phase diagrams ( $p \approx 1$ ), the red line separates the parameter range with a single stable fixed point from the two stable fixed points in m. In the bottom the brown line shows the transition to the period-2 solution of the dynamics.

From these results especially the dynamical behavior of the BNs on the line  $h = 0$  is of interest, because it can be compared to several already published works, for instance [Kürten, 2008], [Kürten, 2010b] or [Galam, 2008]. As can be seen in figures  $3.1$ (a) to  $3.4$ (a), the fixed point of the magnetization is  $m^* = 0$  on this  $h = 0$  line in the central p-interval.

 $6$ This will also be explored with simulations later, see figures 3.14.



Figure 3.8: Phase diagrams of the four systems. The parameter range corresponding to the area within the blue curve is the disordered phase ( $d^* \neq 0$ ), outside is the ordered phase  $(d^* = 0)$ . Brown lines separate the single stable fixed point in the magnetization  $m^*$  from the period-2 solution at low  $p$ . The red points/lines indicate the area with two stable fixed points  $m_1^*$  and  $m_2^*$  at high  $p$ .

In fact this *p*-interval is symmetric with respect to  $p = \frac{1}{2}$ . Hence the stability of this fixed point changes at  $p_{c\pm}^{m^*}$  with  $p_{c+}^{m^*}=1-p_{c-}^{m^*}.$  Above this interval, i.e.  $p\in\left[p_{c+}^{m^*},1\right],$  there exist two stable solutions of the magnetization, and it depends on the initial condition, which one is ultimately reached after the transient time. Below this interval, i.e.  $\,p\,\in\,\left[0,p_{c-}^{m^\ast}\right],\,$ again a bifurcation occurs, however, here the two solutions are only accumulations points of a period-2 solution. A further property of this change of stability of the fixed point  $m^* = 0$  at  $p = p_{c\pm}^{m^*}$  is, that the two fixed points  $m_1^*$  and  $m_2^*$  above  $p_{c+}^{m^*}$  are the same as the accumulation points  $m_1^{(acc)}$  and  $m_2^{(acc)}$  below  $p_{c-}^{m^\ast}$  at the  $h=0$  line. Moreover those two points (fixed points or accumulation points) on each side of the stable p-interval are symmetric with respect to  $m = 0$ . As the fixed point is a function of the parameter p, i.e.  $m^* = m^*(p)$ , it follows

$$
m_1^*(p) = -m_2^*(p) \qquad p \ge p_{c+}^{m^*} \tag{3.21a}
$$

$$
m_1^{(acc)}(p) = -m_2^{(acc)}(p) \quad p \le p_{c-}^{m^*}
$$
 (3.21b)

$$
n_1^{(acc)}(p) = m_1^*(1-p)
$$
 (3.21c)

However, those symmetry properties are not valid anymore if h changes, i.e.  $h \neq 0$ .

 $\mathbf{r}$ 

Although it is hard to distinguish in the figures  $3.1(b)$  to  $3.4(b)$ , the fixed point  $d^*$  of Hamming distance is exactly  $d^* = \frac{1}{2}$  in the interval where  $m^* = 0$  is stable at the  $h = 0$ line, starting to decrease rapidly at the critical points  $p_{c\pm}^{m^*}$  for the magnetization, and reaching  $d^*=0$  shortly thereafter. This gives rise to another set of critical values  $p_{c\pm}^{d^*}$  for the parameter  $p$ :

$$
0 < p_{c-}^{d^*} < p_{c-}^{m^*} < \frac{1}{2} < p_{c+}^{m^*} < p_{c+}^{d^*} < 1 \tag{3.22}
$$

This critical condition  $p_{c\pm}^{d^*}$  indicates the order-disorder phase transition. Between these two critical values  $p_{c\pm}^{d^*},$  small perturbations percolate through the complete BN. The numerical values for all those critical points are listed in table 3.3.



Figure 3.9: Fixed points for the Magnetization  $m^*$  (red) and the Hamming distance  $d^*$ (green) for  $K = 3$  and  $h = 0$  compared with the binary mixture of the Majority and Minority rule used in [Kürten, 2008]

	$p_{c-}^{m^*}$	$p_{c+}^{m^*}$	$p_{c-}^{d^*}$	$p_{c+}^{d^*}$
$\rho_c^{(\delta)}$	$K = 3 \begin{array}{c c c c c} & \frac{1}{6} \approx 0.17 & \frac{5}{6} \approx 0.83 & \frac{1}{8} \approx 0.13 & \frac{7}{8} \approx 0.88 \end{array}$			
$\rho_c^{(cont)}$	$K = 3 \begin{array}{c c} 1 & \frac{1}{10} = 0.10 \\ 0 & \frac{9}{10} = 0.90 \end{array}$ $\frac{1}{14} \approx 0.07 \frac{13}{14} \approx 0.93$			
[Kürten, 2008]	$K = 3 \begin{array}{c c c c c} & \frac{1}{6} \approx 0.17 & \frac{5}{6} \approx 0.83 & \frac{1}{8} \approx 0.13 & \frac{7}{8} \approx 0.88 \end{array}$			
	$K = 5 \left  \frac{7}{30} \approx 0.23 \right  \frac{23}{30} \approx 0.77 \right $		$\approx 0.18$	$\approx 0.82$

Table 3.3: Critical points  $p_{c\pm}^{m^*,d^*}$  for the change of stability (i.e. phase transition) in the magnetization  $m^*$  and the Hamming distance  $d^*$  on the line  $h = 0$ .

Figure 3.9 compares the two distributions of weights  $\rho_c^{(\delta)}$  and  $\rho_c^{(cont)}$  with the binary mixture of the Minority and Majority rule [Kürten, 2008]. It depicts the same data as in figures 3.3(b) and 3.4(b), however, here only the part for  $h = 0$  is shown. All three of the figures are quite similar, with the stable  $m<sup>*</sup> = 0$  range in the center, the period-2 solution for small  $p$  and the two stable fixed points for high  $p$ . From there the structure of other distributions of weights and connectivity could be inferred. Every single-parameter distribution of weights, where a high value of the parameter  $p$  coincides with a majority of positive weights in the Boolean function, and a small value of  $p$  corresponds to a majority of negative weights, should have the same or a similar structure at the  $h = 0$  line. Moreover, a high threshold value biases the function into complete triviality, as already mentioned at the beginning of this section  $(M(h < -K, p; m) = 1$  and  $M(h > K, p; m) = -1$ . These two facts help to infer that all such BN with a generic class of Linear Threshold functions (and even monotone Boolean functions) might have a phase diagram similar to those presented in figure 3.8 for the distributions  $\rho_c^{(\delta)}$  and  $\rho_c^{(cont)}.$ 

Such systems with a central parameter region, where a "tie"-phenomenon occurs (the symmetric  $m<sup>*</sup> = 0$  case), which then bifurcates at the borders of this region, has been extensively investigated by Galam and coworkers in the context of sociophysics, see [Galam, 2008] for a review of this research.

### 3.3 Binary mixture of Minority and Majority rule

As has been argued in the last section, general LTFs can be approximated by a simple binary mixture of the Minority and Majority rule, at least for the threshold  $h = 0$ , because they show similar dynamical behavior. Those two rules can be seen as prototypes of LTFs with either all negative or all positive weights. The distribution of functions is in this case given by

$$
\rho_{\mathbf{F}} \sim p[f_{MAJ}] + (1 - p)[f_{MIN}], \qquad (3.23)
$$

where in the original description an asymmetry parameter  $p$  is linked to the fraction of positive weights in the distribution  $\rho_c$ .

Due to the simple nature of this mixture, several results can be obtained analytically. Special emphasis in this section is laid on the fact, that this BN actually exhibits a more ordered dynamics when the connectivity K is increased.

Most of the results of this section have also been treated in [Kürten, 2010b] or in the Galam models [Galam, 2008].

**Lemma 3.5.** *The iteration equation for the magnetization* m *in the Majority rule for odd* K *is*

$$
m'_{MAJ} = -1 + 2 \sum_{n=\frac{K+1}{2}}^{K} {K \choose n} z_{(+)}^{n} z_{(-)}^{K-n}
$$
  
= -1 + 2 \sum\_{n=\frac{K+1}{2}}^{K} {K \choose n} \left(\frac{1+m}{2}\right)^{n} \left(\frac{1-m}{2}\right)^{K-n} . \t(3.24)

As the Minority rule  $f_{MIN}$  is just the inverse of the function  $f_{MAX}$ , its iteration equation is *given by*

$$
m'_{MIN} = -m'_{MAJ}.\t\t(3.25)
$$

*Hence the final iteration equation for the mixture*  $\rho_F$  *is* 

$$
m' = (2p - 1) \left( -1 + 2 \sum_{n = \frac{K+1}{2}}^{K} {K \choose n} \left( \frac{1+m}{2} \right)^n \left( \frac{1-m}{2} \right)^{K-n} \right).
$$
 (3.26)

*Proof.* The iteration equation for the magnetization of the Majority rule follows immediately from the fact that  $\int_{MAJ}$  is a totalistic function, and  $\int_{MAJ}(x) = +1$  if  $\langle x, x \rangle \ge \frac{K+1}{2}$ . Using further  $m' = z'_{(+)} - z'_{(-)} = -1 + 2z'_{(+)}$ , the iteration equation in the lemma follows, when weighting this with the mixture of Boolean functions, given by equation (3.23).  $\Box$ 

**Lemma 3.6.** *The fixed point*  $m^* = 0$  *is stable in the range*  $p \in \left[p_{c-}^{m^*}, p_{c+}^{m^*}\right]$  *where* 

$$
p_{c\pm}^{m^*} = \frac{1}{2} \pm \left(\frac{2^K}{K\left(\frac{K-1}{2}\right)}\right) \tag{3.27}
$$

*For large* K *this reaches the asymptotic value*

$$
p_{c\pm}^{m^*} = \frac{1}{2} \pm \sqrt{\frac{\pi}{8K}} \stackrel{K \to \infty}{\longrightarrow} \frac{1}{2}
$$
 (3.28)

*Proof.* Recall the stability of the fixed point  $m^* = 0$ :

$$
\left. \frac{\partial m'}{\partial m} \right|_{m^*=0} \stackrel{!}{=} \pm 1
$$

Hence

$$
\frac{\partial m'}{\partial m}\Big|_{m^*=0} = (2p-1)\left(2\sum_{n=\frac{K+1}{2}}^{K} {K \choose n} \left[ \frac{n}{2} \left(\frac{1+m}{2}\right)^{n-1} \left(\frac{1-m}{2}\right)^{K-n} \right.\right.\left. - \frac{K-n}{2} \left(\frac{1+m}{2}\right)^n \left(\frac{1-m}{2}\right)^{K-n-1} \right]\Big)\Big|_{m^*=0}\n= (2p-1)\left(\frac{1}{2}\right)^{K-1} \sum_{n=\frac{K+1}{2}}^{K} {K \choose n} \left[n - (K-n)\right]\n= (2p-1)\left(\frac{1}{2}\right)^{K-1} \left(-K \sum_{\frac{n=\frac{K+1}{2}}{2K-1}}^{K} {K \choose n} + 2 \sum_{n=\frac{K+1}{2}}^{K} {K \choose n} n\right) = ...
$$

Here the fact  $\sum_n\binom{K}{n}=2^K$  is used. With the symmetry of the binomial coefficients and  $K$ odd, then the sum is exactly half of that, if it is started at  $n = \frac{K+1}{n}$ , i.e.  $\sum_{n=1}^{K}$  $n=\frac{K-1}{2}$  $\binom{K}{n} = 2^{K-1}.$ Therefore

$$
\dots = (2p - 1) \left( -K + \left( \frac{1}{2} \right)^{K-2} \sum_{n = \frac{K+1}{2}}^{K} \frac{K!n}{n!(K-n)!} \right)
$$

$$
= (2p-1)\left(-K + \left(\frac{1}{2}\right)^{K-2} K \sum_{n=\frac{K+1}{2}}^{K} \frac{(K-1)!}{(n-1)!(K-1-(n-1))!}\right) = \dots
$$

Rewriting the summation variable to  $j = n - 1$  yields

... = 
$$
(2p-1)\left(-K + \left(\frac{1}{2}\right)^{K-2} K \sum_{j=\frac{K-1}{2}}^{K-1} {K-1 \choose j} \right) = ...
$$

Solving this with respect to  $p$  gives the critical values  $p_{c\pm}^{m^*}$  between which the fixed point  $m^* = 0$  is stable:

$$
\begin{array}{rcl} \dots & = & (2p-1) \left( -K + \left( \frac{1}{2} \right)^{K-2} K \left( 2^{K-2} + \frac{1}{2} \left( \frac{K-1}{\frac{K-1}{2}} \right) \right) \right) \\ \\ & = & (2p-1) \left( -K + K + \left( \frac{1}{2} \right)^{K-1} K \left( \frac{K-1}{\frac{K-1}{2}} \right) \right) \\ \\ & = & (2p-1) \left( \frac{1}{2} \right)^{K-1} K \left( \frac{K-1}{\frac{K-1}{2}} \right) .\end{array}
$$

Inserting in the critical condition above, leads to the critical condition for the stability of the fixed point  $m^* = 0$ :

$$
p_{c\pm}^{m^*} = \frac{1}{2} \left( 1 \pm \frac{2^{K-1}}{K\left(\frac{K-1}{2}\right)} \right)
$$

If  $K$  is large enough, the binomial coefficient can be expanded using Stirling's formula, yielding:

$$
\binom{K-1}{\frac{K-1}{2}} \approx 2^{K-1} \sqrt{\frac{2}{\pi (K-1)}}.
$$

Therefore

$$
p_{c\pm}^{m^*} \approx \frac{1}{2} \left( 1 \pm \frac{2^{K-1}}{K \left( 2^{K-1} \sqrt{\frac{2}{\pi K}} \right)} \right)
$$

$$
= \frac{1}{2} \pm \sqrt{\frac{\pi}{8K}} \stackrel{K \to \infty}{\longrightarrow} \frac{1}{2}
$$

Which is finally the approximate expression above.

This is an important result, because it shows that the range of  $p$  actually decreases with increased connectivity. This is used further to prove, that the range of the ordered phase gets larger with growing  $K$ . This is done again via the concept of sensitivities. First the sensitivity for a general LTF is derived, which is a new result compared to the publications cited before, since it has not been treated in this generality there.

 $\Box$ 

**Lemma 3.7.** *The sensitivity* S (1) *of a Linear Threshold function is*

$$
KS^{(1)} = \sum_{n=0}^{K} {K \choose n} \left[ n \int \mathcal{D}^{K} \rho_{c} \Theta \left( -\left( \sum_{i=0}^{n} c_{j} - \sum_{j=0}^{K-n} c_{j} - h \right)^{2} + 2c_{1} \left( \sum_{i=0}^{n} c_{j} - \sum_{j=0}^{K-n} c_{j} - h \right) \right) \right]
$$
(3.29)  
+
$$
(K - n) \int \mathcal{D}^{K} \rho_{c} \Theta \left( -\left( \sum_{i=0}^{n} c_{j} - \sum_{j=0}^{K-n} c_{j} - h \right)^{2} - 2c_{1} \left( \sum_{i=0}^{n} c_{j} - \sum_{j=0}^{K-n} c_{j} - h \right) \right) z_{(+)}^{n} z_{(-)}^{K-n}.
$$

*Proof.* Recall the definition of the sensitivity  $S^{(1)}$ , already weighted with a distribution of Boolean functions  $\rho_F$ :

$$
KS^{(1)} = \sum_{\mathfrak{f}} \Pr\left[\mathfrak{f}|\rho_{\mathbf{F}}\right] \sum_{\mathbf{x}} \sum_{i=1}^{K} \frac{\partial \tilde{\mathfrak{f}}(\mathbf{x})}{\partial x_i} \Pr\left[\mathbf{x}|z_{(\pm)}\right]
$$

Now the Boolean derivative for a LTF has to be rewritten. Note that for LTFs a change in a variable  $x_i$  is nothing else than subtracting it twice:

$$
(x_j \mapsto x_j \oplus 1) \Rightarrow \left( \left( \sum_j c_j x_j - h \right) \mapsto \left( \sum_j c_j x_j - h - 2c_i x_i \right) \right).
$$

One of the sums has to be positive, the other negative for the derivative to be  $+1$ . Using again the relation  $\Theta(-A)\Theta(B) + \Theta(A)\Theta(-B) = \Theta(-AB)$ , it follows<sup>7</sup>

$$
\frac{\partial \tilde{f}(\mathbf{x})}{\partial x_i} = \Theta\left(-\left(\sum_j c_j x_j - h\right)\left(\sum_j c_j x_j - h - 2c_i x_i\right)\right).
$$

With the fact, that weighting all functions with  $Pr[f|\rho_F]$  is nothing else than integrating over all weights  $c_j$ , the final result is obtained after a few steps:

$$
KS^{(1)} = \sum_{\mathfrak{f}} \Pr\left[\mathfrak{f}|\rho_{\mathbf{F}}\right] \sum_{\mathbf{x}} \sum_{i=1}^{K} \frac{\partial \tilde{\mathfrak{f}}(\mathbf{x})}{\partial x_{i}} \Pr\left[\mathbf{x}|z_{(\pm)}\right]
$$
  
\n
$$
= \sum_{\mathbf{x}} \sum_{i=1}^{K} \left[ \int \mathcal{D}^{K} \rho_{c} \Theta\left(-\left(\sum_{j} c_{j} x_{j} - h\right)\left(\sum_{j} c_{j} x_{j} - h - 2 c_{i} x_{i}\right)\right) \right] \Pr\left[\mathbf{x}|z_{(\pm)}\right]
$$
  
\n
$$
= \sum_{n=0}^{K} {K \choose n} \left[ n \int \mathcal{D}^{K} \rho_{c} \Theta\left(-\left(\sum_{j}^{n} c_{j} - \sum_{j}^{K-n} c_{j} - h\right)^{2} + 2 c_{1} \left(\sum_{j}^{n} c_{j} - \sum_{j}^{K-n} c_{j} - h\right)\right) + (K - n) \int \mathcal{D}^{K} \rho_{c} \Theta\left(-\left(\sum_{j}^{n} c_{j} - \sum_{j}^{K-n} c_{j} - h\right)^{2} - 2 c_{1} \left(\sum_{j}^{n} c_{j} - \sum_{j}^{K-n} c_{j} - h\right)\right) \left[ z_{(\pm)}^{n} z_{(\pm)}^{K-n} - z_{(\pm)} z_{(\pm)} \right]
$$

where again the totalistic property of LTFs is used:  $x \mapsto \langle x, x \rangle = n$ .

 $\Box$ 

This general result can be used to derive the sensitivity  $S^{(1)}$  of the mixture of Minority and Majority rule for arbitrary connectivity  $K$ :

<sup>&</sup>lt;sup>7</sup>Note that the expression for the sensitivity stated above is only valid for  $M = \{0, 1\}$ , whereas LTFs are usually defined with  $M = \{-1, +1\}$ . Hence the switch from sign  $\mapsto \Theta$ .

**Theorem 3.8.** Let  $\rho_F$  be a mixture of Minority and Majority rule with mixing parameter p, like in equation (3.23). The sensitivity  $S^{(1)}$  of this  $\rho_{\bf F}$  for arbitrary (but odd) connectivity  $K$  is

$$
KS^{(1)} = \left(\frac{1}{2}\right)^{K-1} K\left(\frac{K-1}{\frac{K-1}{2}}\right) \left(1 - m^2\right)^{\frac{K-1}{2}}.
$$
 (3.30)

 $\emph{Therefore the BN is in its disordered phase as long as $p\in\left[p_{c-}^{m^*},p_{c+}^{m^*}\right]$, where the $p_{c\pm}^{m^*}$ are $p_{c+}^{m^*}$, where $p_{c+}^{m^*}$ are $p_{c+}^{m^*$ *given by lemma 3.6, because with*  $m = 0 \Rightarrow KS^{(1)} > 1$ , but reaches its ordered phase soon *outside this interval at*  $p = p_{c\pm}^{d^*}.$  *These critical values*  $p_{c\pm}^{d^*}$  *are given by solving the critical condition*  $KS^{(1)} = 1$  *with respect to* m *and inserting this required fixed point*  $m^*$  *into the*  ${\it iteration~equation~}~m^{*''}=\mathcal{M}\left(p_{c\pm}^{d^*};\mathcal{M}\left(p_{c\pm}^{d^*};m^*\right)\right),~{\it since~outside~the~interval}~p\in\left[p_{c-}^{m^*},p_{c+}^{m^*}\right]~the~\left[1\right]$ *BN has either a period-2 solution or two stable fixed points.*

*For increasing connectivity K* this interval shrinks to the point  $p_{c\pm}^{d*} = \frac{1}{2}$ :

$$
\left[p_{c-}^{d^*}, p_{c+}^{d*}\right] \stackrel{K \to \infty}{\to} \left[\frac{1}{2}, \frac{1}{2}\right],\tag{3.31}
$$

*leading to increased stability of the dynamics with increasing* K*.*

*Proof.* Note that the Majority rule is also a LTF, where  $\rho_c(c) = \delta(c-1)$ , i.e. all weights are positive and  $c_j = 1$ , and the threshold  $h = 0$ . Inserting this into the expression for the sensitivity  $S^{(1)}$  for general LTFs from lemma 3.7 yields:

$$
KS^{(1)} = \sum_{n=0}^{K} {K \choose n} \left[ n \int \mathcal{D}^{K} \rho_{c} \Theta \left( -\left( \sum_{i=1}^{n} c_{j} - \sum_{j=1}^{K-n} c_{j} - h \right)^{2} + 2c_{1} \left( \sum_{i=1}^{n} c_{j} - \sum_{j=1}^{K-n} c_{j} - h \right) \right) \right]
$$
  
+ 
$$
(K - n) \int \mathcal{D}^{K} \rho_{c} \Theta \left( -\left( \sum_{i=1}^{n} c_{j} - \sum_{j=1}^{K-n} c_{j} - h \right) - 2c_{1} \left( \sum_{i=1}^{n} c_{j} - \sum_{j=1}^{K-n} c_{j} - h \right) \right) \left[ z_{(+)}^{n} z_{(-)}^{K-n} \right]
$$
  
= 
$$
\sum_{n=0}^{K} {K \choose n} \left[ n \Theta \left( -(n - (K - n))^{2} + 2(n - (K - n)) \right) + (K - n) \Theta \left( -(n - (K - n))^{2} - 2(n - (K - n)) \right) \right] z_{(+)}^{n} z_{(-)}^{K-n} = \dots
$$

A closer look to the arguments of the Θ-functions reveals that  $\Theta(\dots) = 1$  is obtained only for a single argument. For the first this is:

$$
\Theta\left(-(2n-K)^2 + 2(2n-K)\right) = 1 \quad \Longleftrightarrow \quad (2n-K)^2 \le 2(2n-K).
$$

This condition is only fulfilled if  $2n - K = 1$ , because  $2n - K$  can only be an odd number if K is odd, and therefore  $n = \frac{K+1}{2}$ . The second Θ-function leads analogously to  $n = \frac{K-1}{2}$ , as it requires  $2n - K = -1$ . Hence the sensitivity reduces to a sum of this two terms:

$$
\dots = \left(\frac{K}{\frac{K+1}{2}}\right) \left(\frac{K+1}{2}\right) z_{(+)}^{\frac{K+1}{2}} z_{(-)}^{K-\frac{K+1}{2}} + \left(\frac{K}{\frac{K-1}{2}}\right) \left(K - \frac{K-1}{2}\right) z_{(+)}^{\frac{K-1}{2}} z_{(-)}^{K-\frac{K-1}{2}}
$$

$$
= \left(\frac{K}{\frac{K+1}{2}}\right) \left(\frac{K+1}{2}\right) z_{(+)}^{\frac{K-1}{2}} z_{(-)}^{\frac{K-1}{2}} \underbrace{(z_{(+)} + z_{(-)})}_{=1}
$$
\n
$$
= \frac{K!}{\left(\frac{K+1}{2}\right)!\left(K - \frac{K+1}{2}\right)!} \frac{K+1}{2} \underbrace{(z_{(+)}z_{(-)})^{\frac{K-1}{2}}}_{=K \frac{(K-1)!}{\left(\frac{K-1}{2}\right)!\left(\frac{K-1}{2}\right)!} \left(z_{(+)}z_{(-)}\right)^{\frac{K-1}{2}}}
$$
\n
$$
= K \left(\frac{K-1}{\frac{K-1}{2}}\right) \left(\left(\frac{1+m}{2}\right) \left(\frac{1-m}{2}\right)\right)^{\frac{K-1}{2}}
$$
\n
$$
= \left(\frac{1}{2}\right)^{K-1} K \left(\frac{K-1}{\frac{K-1}{2}}\right) \left(1-m^2\right)^{\frac{K-1}{2}}.
$$

Similar to the Majority rule, the Minority rule could also be computed this way. Here the distribution of weights would be  $\rho_c(c) = \delta(c+1)$ , i.e. all  $c_j = -1$  and again  $h = 0$ . However, this calculation is not necessary, as the Boolean derivative of a function is the same as the derivative of its inverse function

$$
\frac{\partial}{\partial x_i} \mathfrak{f} = \frac{\partial}{\partial x_i} \big( \mathfrak{f} \oplus 1 \big),
$$

and hence the sensitivity of the Minority rule is the same as the sensitivity of the Majority rule and therefore the mixing parameter  $p$  cancels out.

As the dynamics of a BN are disordered if  $KS^{(1)} > 1$ , the interval  $p \in \left[p_{c-}^{m^*}, p_{c+}^{m^*}\right]$  where the fixed point  $m^* = 0$  is the only stable fixed point is always disordered, because inserting  $m^* = 0$  into the expression above yields always a value for  $KS^{(1)}$  larger than 1 for any K. However, above this interval, i.e.  $p > p_{c+}^{m*}$ , a bifurcation into two stable fixed points occurs, leading ultimately to the two fixed points  $m^* = \pm 1$  of the pure Majority rule for  $p=1.$  Below this interval, i.e.  $p < p_{c-}^{m^*},$  the BN starts oscillating between two accumulation points, which are also symmetric with respect to the solution  $m^* = 0$ , as has already been explained earlier. Hence, if the deviation from  $m^* = 0$  is large enough, which actually is quite close to this solution if  $K$  is increased, the term  $(1-m^{*2})^{\frac{K-1}{2}}$  in the sensitivity damps the other term,  $\left(\frac{1}{2}\right)^K\left(K-1\right)\left(\frac{K}{2-1}\right)$ , so that the average sensitivity  $KS^{(1)}$  is equal or below the critical value = 1 for only small deviations from  $m^* = 0$ .

Formally this can be shown as follows. Expanding the binomial coefficient again with Stirling's formula yields

$$
\begin{aligned}\n\left(\frac{1}{2}\right)^{K-1} K\left(\frac{K-1}{\frac{K-1}{2}}\right) &= \left(\frac{1}{2}\right)^{K-1} K \frac{\sqrt{2\pi (K-1)} \left(\frac{K-1}{e}\right)^{K-1}}{2\pi \left(\frac{K-1}{2}\right) \left(\frac{K-1}{2e}\right)^{K-1}} \\
&= \left(\frac{1}{2}\right)^{K-1} K \sqrt{\frac{2}{\pi (K-1)}} 2^{K-1} \\
&\approx \sqrt{\frac{2K}{\pi}}.\n\end{aligned}
$$

And hence the approximated critical condition is

$$
\sqrt{\frac{2K}{\pi}} \left( 1 - m^{*2} \right)^{\frac{K-1}{2}} = 1.
$$

Solving the original expression with respect to  $m^*$  and inserting the approximation for large  $K$  yields

$$
m^* = \pm \sqrt{1 - \frac{4}{\left(K\left(\frac{K-1}{2}\right)\right)^{\frac{2}{K-1}}}}
$$

$$
\approx \pm \sqrt{1 - \left(\frac{\pi}{2K}\right)^{\frac{1}{K-1}} \xrightarrow{K \to \infty} 0}
$$

As the interval where  $m^* = 0$  is stable is shrinking from  $\left[p_{c-}^{m^*}, p_{c+}^{m^*}\right]$  to  $\left[\frac{1}{2},\frac{1}{2}\right]$  if K tends to infinity, as given by lemma 3.6. For  $K$  large enough, the critical condition is already fulfilled for infinitesimal deviations from  $m^* = 0$ , and in the limit  $K \to \infty$  the dynamics of the BN is in its ordered phase for the whole range of the mixing parameter  $p$ , except for the central point  $p = \frac{1}{2}$ , albeit this value is approached very slowly. Therefore the stable range of the dynamics gets actually larger with increasing  $K$ , which is contrary to the Kauffman model, where the inverse behavior is observed.

The actual value of  $p_{c\pm}^{d^*}$  can be obtained, when inserting this expression for  $m^*$  above as fixed point into the iteration equation for  $m$  and solving with respect to  $p$ . Note that the iteration equation has to be inserted into itself first

$$
m'' = \mathcal{M}(p; \mathcal{M}(p; m)),
$$

because in the range  $p \notin \left[p_{c-}^{m^*}, p_{c+}^{m^*}\right]$ , either a period-2 solution (below this interval) or two different stable fixed points (above this interval) occurs, and the "fixed point" in the magnetization  $m^*$  (which deviates from  $m^* = 0$ ) is of that type outside this central pinterval.  $\Box$ 

Figure 3.10 shows a comparison of the phase diagrams of the model derived here (a binary mixture of the Minority and Majority rule with mixing parameter  $p$  as a prototype model of LTFs) and the Kauffman model, with its internal homogeneity  $p$ . Recall that the critical condition in the Kauffman model is  $2Kp(1-p) = 1$ , resulting in

$$
p_{c\pm}^{(Kauffman)} = \frac{1}{2} \left( 1 \pm \sqrt{\frac{K-2}{K}} \right). \tag{3.32}
$$

Therefore in the Kauffman model, the parameter region of the disordered phase grows with increasing connectivity  $K$ , spanning the complete range of the parameter  $p$  in the limit  $K \to \infty$ .

This feature of the binary mixture of Minority and Majority rule, and also LTFs in general, is quite interesting. Many biological networks have been modeled to exhibit a dynamic like the Kauffman network, i.e. allowing all possible combinations of Boolean



Figure 3.10: Comparison of the phase diagrams of the two BNs, Kauffman model and LTFs (approximated by a simple mixture of Minority and Majority rule. The blue line indicates the phase transition from ordered to disordered dynamics. In the right figure, the red line shows the bifurcation from the single fixed point  $m^* = 0$  to two stable fixed points, whereas the brown line shows the bifurcation into the period-2 solution of the iteration equation. Grey areas correspond to the ordered phase. Note that the external parameter  $p$  has different interpretations in the two models.

functions, only with a single control parameter  $p$ , the internal homogeneity (see definition 1.19). The problem with this approach is that for non-extreme values of  $p$ , the phase transition to the disordered phase occurs already at quite low  $K_c$ , whereas in biological systems a higher connectivity is observed. Since in the Kauffman model only the average connectivity is of importance, this problem could be solved by special degree distributions, where a few highly connected nodes a majority of nodes with a low number of connections appear. One of these distributions would be a scale-free distribution [Aldana, 2003], as already hinted at in section 1.3. A combination of these ideas, LTFs and a scale-free degree distribution has been investigated in [Kürten, 2010a].

However, just recently a study of so-called "single switch functions", which are a generalization of LTFs to allow more that just the 2 states  $M = \{-1, +1\}$  has been made [Wittmann] et al., 2010]. The authors also describe this interesting property of these functions, where the stable parameter range gets actually larger when the connectivity is increased.

The crucial point is, however, that the BN with LTFs has to be biased towards either state, and is not in its equilibrium  $z_{(+)} = z_{(-)} = \frac{1}{2}$ . This point has been missed in several publications so far, especially in the treatments of the sensitivity, see e.g. [Shmulevich and Kauffman, 2004] or [Liu et al., 2008].

## 3.4 Simulations

To verify the calculation results, several simulation runs were done. In all 4 cases ( $\rho_c^{(\delta)}$  and  $\rho_c^{(cont)}$ ,  $K=2$  and  $K=3$ ) the simulation results coincide quite well with the calculations, although only the most complex case with  $K=3$  and  $\rho_c^{(cont)}$  is shown here.

Simulations are done with a small self-written C-program. The code is attached in appendix C. Each simulation run had  $N = 10000$  nodes with two possible states in  $M =$  ${-1, 1}$ . In each timestep the coefficients  $c_{ij}$  were drawn randomly from the distribution  $\rho_c^{(cont)}$  for each of the nodes, i.e. the Boolean functions are annealed. The neighbors were also drawn randomly from all possible  $N$  nodes each timestep. Each neighbor was chosen independently from the others, so self-connections and multiple connections to other nodes could occur, although this is not very likely. Hence the topology was also modeled annealed. Simulations were run for  $s = 500$  timesteps. As can be seen in figure 3.11, the simulation converges to stable values in  $m$  and  $d$  already within a small fraction of the complete simulation time. Initial conditions where chosen independently on each node to be  $x_i = +1$  with probability  $m_{start} = 0.5$  and  $x_i = -1$  otherwise (except for the simulations at  $p = 0.93$  and  $p = 0.95$  where two simulation runs were made with  $m_{start} =$ 0.33 and  $m_{start} = 0.66$ , so the distribution of initial conditions is binomial with mean 0.5. On each parameter point  $(p, h)$  the simulation is run in five parallel replicas of the original BN, although with changed initial conditions. Before starting the simulations, the state of  $Nd_{start}$  nodes is flipped in the four replicas, with  $d_{start} = 0.01$ . Neighbor structures (topology) and the coefficients  $c_{ij}$  are identical in those replicas. However, each system is iterated independently on the states of its nodes. Data is collected in the last 100 steps of the simulation. Magnetization  $m$  is averaged over all five replicas, the Hamming distance  $d$  is calculated from the four replicas different from the first.



Figure 3.11: A single simulation run at  $(p, h) = (0.09, 0.8)$ . The two runs with magnetizations  $m_1$  (blue) and  $m_2$  (green) are started with an initial distance  $d_{start} = 0.01$ from each other. The Hamming distance  $d$  (red) between those two BNs is also shown. Magnetization is fluctuating around the stable fixed point, as indicated by the negative value of  $\frac{\partial m'}{\partial m}\Big|_{m^*}$ , seen in figure 3.5(b).



Figure 3.12: Phase diagram of the BN with  $\rho_c^{(cont)}$  and  $K=3$ , as already shown in figure 3.8(d). Green lines indicate the parameters (Simulation lines (1) - (6))where the calculations are verified by simulations.

Several simulations along discrete points on lines in the phase space are conducted. Those lines are shown in green in figure 3.12 and the numerical values are listed in table 3.4. The interval between simulations of those lines are  $\Delta h = 0.02$  and  $\Delta h = 0.002$  for low and high values of  $p$ , respectively.

Simulation-	start			end	
line	h	р	$\Delta h$	h.	$\boldsymbol{p}$
(1)	$-0.10$	0.90	0.002	0.10	0.90
(2)	$-0.10$	0.93	0.002	0.10	0.93
(3)	$-0.10$	0.95	0.002	0.10	0.95
(4)	$-1.00$	0.09	0.02	1.00	0.09
(5)	$-1.00$	0.07	0.02	1.00	0.07
(6)	$-1.00$	0.05	0.02	1.00	0.05

Table 3.4: Parameter lines of the phase space examined with simulations.

In figures 3.13 and 3.14 it is clearly visible, that the (semi-)analytical results presented earlier are in good agreement with the numerical computer simulations. The parameters  $(p, h)$  in the simulation are chosen to show that even in the more complicated areas of the phase space (period-2 and two stable fixed points), the analytical calculation results can be used to predict the simulations.

Figure 3.13 shows several outliers in the simulation around  $h = 0$ . In those simulation the average of the Hamming distance  $d$  is far above the expected value in one or several of the 4 replica simulations. Those could be explained by the simple observation, that the period-2 solution, which is switching from an low magnetization to a high magnetization every timestep, is shifted by a single step between the replicas. Therefore the distance cannot converge to the expected low value.

The simulations for high  $p$  values in figure 3.14 are particularly accurate, except for the highest value ( $p = 0.95$ ). Here the two peaks in the Hamming distance from the calculation



Figure 3.13: Comparing Hamming distance  $d^*$  in simulations (red) and analytical calculations (black line) at low p with varying h ( $h \in [-1, 1]$ ). An explanation for the outliers is given in the text.



Figure 3.14: Comparing Hamming distance  $d^*$  in simulations (red) and analytical calculations (black line) at high p with varying  $h(h \in [-1,1])$ . An explanation for the outliers is given in the text.

belong to the different stable fixed points in the magnetization. In the simulation always the stable fixed point with ordered dynamics  $d^* = 0$  is ultimately reached, but not the fixed point associated with a Hamming distance  $d^* \neq 0$ . To find this  $m^*$  in the disordered region, the simulation must be started very close to this fixed point, not at a more generic value of  $m_{start} = 0.66$  (or  $m_{start} = 0.33$ ), as was used in the simulations performed here. Only at or close to the border between ordered and disordered dynamics the "disordered" fixed point  $m^*$  is reached in some of the replicas of a single simulation, yielding those outliers in the Hamming distance (see especially figure 3.14(c) and to some extend also figure 3.14(b)).

Overall the simulations are in good agreement with the calculation. Almost all errorbars of the simulations contain the "correct" analytical value of the Hamming distance. However, not everything that could be derived analytically, can also be seen in the simulations, as explained with the fixed point  $m^*$  in the disordered dynamics region of the phase space.

# 4 Discussion

In this work the construction of the iteration equations for all orders of the dynamics of Boolean Networks is shown, where the order is the number of parallel evolving networks or also the number of variables on each node. As everything is treated only statistically, the single macroscopic parameter of the first order is the magnetization  $m$ , for which the iteration equation is described in theorem 2.6. For the second order the Hamming distance  $d$  (see proposition 2.13) is one of the macroscopic parameters (or the single one with the both magnetizations  $m^{(X)} = m^{(Y)}$  are set equal, as has been done in the transformations in equation (2.32)). The extension of these first two orders is explained in proposition 2.20. An example for such a higher order parameter would be the frozen core s, which could be seen as belonging to the infinite order. In all these equations the actual state of the BN is important for the derivation. Here lemma 2.5 and 2.12 give expressions for the probabilities of having a certain state in the BN, at least for the first and second order of the dynamics. These probabilities and most expressions from chapter 2 in general have already been proposed and used in [Kesseli et al., 2006], where several of the concepts in chapter 2 are already explained as the so-called "4-state-model".

Furthermore, it has been shown here, and also already in [Kesseli et al., 2006], that a perturbation ansatz for the Hamming distance, which is given by

$$
d'_{S} = \sum_{n=1}^{K} S^{(n)} \binom{K}{n} d^{n} (1-d)^{K-n}, \tag{4.1}
$$

does not allow the second BN to relax to its fixed point  $m^{(\mathbf{Y})*}$ , and is kept at an artificial distance to it, at least below the critical point. The calculation of this property is given in theorem 2.30. This form of the iteration equation of the Hamming distance has been given first in [Derrida, 1987], but for a special BN, where each Boolean function is related to a Linear Threshold function with a symmetric distribution of weights,  $\rho_c(c_i) = \rho_c(-c_i)$ . In theorem 3.4 it has been proved, that for these BNs the coefficients  $\lambda_n$  in the Hamming distance are actually the sensitivities  $S^{(n)}.$  This might be due to the fact, that the iteration equation for the magnetization does not depend on the magnetization itself, and is just a constant. So the "fixed point" is reached after a single time step. This has also been shown in theorem 3.4. However, it is still an open question, whether there are other classes of functions, where the two order parameters  $d^*$  and  $d_S^*$  coincide, i.e. all coefficients are sensitivities,  $\lambda_n = S^{(n)}$ .

The phase transition is defined as the change in the stability of the fixed point  $d^* = 0$ , for which only the first coefficient in the expansion of  $d$  is responsible. That the first coefficient in the Hamming distance is actually the sensitivity  $S^{(1)}$ , has been shown in

lemma 2.28 and theorem 2.29. With the aid of the Boolean derivative, which is in fact similar to the sensitivities, this critical condition can be rewritten to an equation which looks like a continuity equation:

$$
(-1) + \langle \text{div } f \rangle = 0. \tag{4.2}
$$

However, for the quantity, which changes over time and has to be equal to −1, no corresponding expression has been found so far. If this equation would hold, this would be an interesting characterization of the critical condition, as in a critical BN an infinitesimal perturbation neither settles down completely nor percolates through the whole network until a finite fraction is reached, it just flows for an infinite time, giving it the notion of "critical preserved information flow".

This continuity equation could also be interpreted differently with the use of the concept of "effective" variables, as in section 2.4.2. Recall that the sensitivities  $S_i$  for a single variable  $x_j$  are also the probabilities of this variable to occur in a position of an input tuple, where it actually has an effect on the output of the function when changed. Therefore the sum of those sensitivities  $\sum_j S_j = KS^{(1)}$  is also the number of "effective" variables. As the critical condition is  $KS^{(1)} = 1$ , this can be seen as that only a single variable determines the output of the function, constituting this critical flow from a single input to this (single) node on which the function is defined.

These concepts of the Boolean derivative are not yet fully established, as for example the Boolean derivative does not follow a Leibniz rule. This problem has been somehow solved in [Bazsó and Lábos, 2006], where the derivative is expanded to Boolean Lie-algebras, where the Leibniz rule is finally fulfilled. The introduction of this paper outlines this quite nicely, so its first lines are reproduced here:

"The success in understanding the behavior of continuous dynamical systems originates, to a great extent, from the power of infinitesimal calculus. Therefore, it seems reasonable to expect that properly developed calculus can deepen our understanding of iterative dynamics of Boolean functions, discrete dynamical systems and dynamics of computation. [...]"

In the last part of this work Linear Threshold functions were treated with the formalism presented until then. Linear Threshold functions provide an interesting small subclass of all possible Boolean functions. The semi-analytical results in sections 3.2.1 make it plausible, that some results could be extended from a simple binary mixture of the Minority and Majority rule, for which analytical results are derived in section 3.3, to other, more complicated distributions of weights. This is especially true, if a single parameter could express the fraction of weights being either activating or inhibiting  $(c_{ij} > 0$  or  $c_{ij} < 0$ , respectively), as  $p$  in the two distributions  $\rho_c^{(\delta)}$  and  $\rho_c^{(cont)}.$  It has been shown in theorem 3.8, that the parameter region of the ordered phase in this BN actually grows when the connectivity is increased, resulting in a single value of the parameter space in the limit  $K \to \infty$ , see also [Kürten, 2010b]. This result is quite interesting, as in the Kauffman model, where all Boolean functions are allowed in the mixture, the opposite behavior is observed, where the parameter region of the disordered phase grows with increasing connectivity,

spanning the complete parameter space in the limit  $K \to \infty$ . This is important, because biological networks usually have a connectivity larger than the critical value  $K_c = 2$  in the (unbiased) Kauffman model, so that a more realistic topology could be imposed on the BN, where also nodes with a higher in-degree occur, without being restricted to extreme values of the external parameters.

# A List of most used symbols



# B List of iteration equations

In the following pages, the iteration equations for  $z'_{(++)},\,z'_{(+-)},\,z'_{(-+)}$  and  $z'_{(--)}$  of all single Boolean functions f with connectivity  $K = 3$  are listed. The variables are already transformed to magnetization  $m$  and Hamming distance  $d$ , i.e.  $\big(z_{(\pm\pm)}\big) \mapsto (m, d).$  Note that here  $M = \{-1, +1\}$ . The iteration equations for magnetization m' and Hamming distance d' itself can be easily obtained by

$$
m' = z'_{(++)} - z'_{(--)},
$$
  
\n
$$
d' = z'_{(+-)} + z'_{(-+)} = 2z'_{(+-)}.
$$

The tables should be read in the follwing way. The columns separated by double lines are the iteration equations for the four different probabilities  $z'_{(\pm\pm)}$ . The single lines separate the coefficients in a expansion in powers of d, where the powers are  $1(=d^0)$ , d,  $d^2$  and  $d^3$ . For example, rule  $(232)_3$ , i.e. the majority rule, should read as follows:

$$
z'_{(++)} = \left[ -\frac{m^3}{4} + \frac{3m}{4} + \frac{1}{2} \right] + \left[ \frac{3m^2}{4} - \frac{3}{4} \right] d + \left[ \frac{3}{4} \right] d^2 + \left[ -\frac{1}{2} \right] d^3,
$$
  
\n
$$
z'_{(+-)} = \left[ -\frac{3m^2}{4} + \frac{3}{4} \right] d + \left[ -\frac{3}{4} \right] d^2 + \left[ \frac{1}{2} \right] d^3,
$$
  
\n
$$
z'_{(-+)} = \left[ -\frac{3m^2}{4} + \frac{3}{4} \right] d + \left[ -\frac{3}{4} \right] d^2 + \left[ \frac{1}{2} \right] d^3,
$$
  
\n
$$
z'_{(--)} = \left[ \frac{m^3}{4} - \frac{3m}{4} + \frac{1}{2} \right] + \left[ \frac{3m^2}{4} - \frac{3}{4} \right] d + \left[ \frac{3}{4} \right] d^2 + \left[ -\frac{1}{2} \right] d^3.
$$

All iteration equations are obtained by using proposition 2.13. Recall that in the case of single Boolean functions f, given by a truthtable, the coefficients  $Pr[f(x) = \pm 1] Pr[f(y) = \pm 1]$ in the sum over all possible tuples x and y are just either zero or one. Therefore they can be easily obtained by a simple automated program.
















### C Simulation program code

Compile the simulation program with

> gcc -o sim sim.c -lm -lgsl -lgslcblas -fopenmp

The parameter -fopenmp is optional, as it enables using multicore architectures, which are present on almost all modern computers. However, only the different replicas are run on different processors, so for a low replica count  $( $5$ ), this might actually slow the$ simulation down, and the option should be omitted.

A default simulation run is started with

> ./sim -N 10000 -R 3 -s 500 -m 0.5 -d 0.01 -K 3 -p 0.3 -h 1.2 -r \$RANDOM

where **\$RANDOM** is a random variable obtained from the command line environment used as randomseed.

```
\frac{1}{1} #include <stdio.h>
\frac{1}{2} #include <stdlib.h>
\frac{1}{3} #include <unistd.h>
4 #include \langlestring.h>
5 #include \langle \text{math.h} \rangle\frac{1}{6} #include <gsl/gsl_rng.h>
\frac{1}{7} #include <gsl/gsl_randist.h>
8
9 int iterations = 100;
10 int N = 10000;
11 int K = 3;
12 \text{ double } p = 0.5;13 double h = 0.0;
14
15 double start active = 0.50 ;
16 double start_dist = 0.01;
17 int replicas = 3;
18 int perturbation = 0;
19
20 int **nodes,**old_nodes;
21 int *neigh;
22 double ∗weight;
23
24 const gsl_rng_type∗ T;
25 const gsl_rng∗ rg;
```

```
26 unsigned long randseed = 1234567890;
27
28 int *active_nodes;
29 int *dist;
30 int *frozenness;
31
32 void parsecommandline (int argn, char* argv []) {
33 char c;
34 while ((c = getopt(argn, argv, "r:R:N:s:K:m: d:p:h:P:")) := -1){ }35 switch (c) {
36 case 'R': replicas = atoi( optarg );
37 break ;
\case \t'r': \t\t rank \case \t'r': \t\t rank \case \t} = \t \atop \case \t} \case \t'r': \t\t rank \case \t}39 break ;
40 case 'N': N = \text{atoi}(\text{optarg});
<sup>41</sup> break;
2 \cos \theta': iterations = atoi(optarg);
43 break ;
case 'K': K = atoi(optarg);45 break ;
46 case 'm': start_active = atof ( optarg );
<sup>47</sup> break;
48 case 'd': start_dist = atof(optarg);
<sup>49</sup> break;
50 case 'p': p = \text{atof}(\text{optarg});
51 break;
52 case 'h': h = atof(optarg);
53 break ;
54 case 'P': perturbation = atoi(optarg);
55 break ;
66 default: exit(1);57 break:
58 }
59 }
60 }
61
62 int main (int argn, char* argv []) {
\omega int i, j, r, k;
64 double input;
65
66 parsecommandline ( argn,argv ) ;
67
68 gsl_rng_env_setup();
69 T = gsl_rng_default;
rq = qsl\_rnq\_alloc(T);71 gsl_rnq_set (rq, randseed);
72
```

```
73 nodes = (int **)malloc(replicas*sizeof(int*));
74 old nodes = (int * )malloc( replicas* size of (int * ) ) ;
75
76 neigh = (int*)malloc(K*sizeof(int));77 weight = (double*)malloc(K*size of (double));
78
79 dist = (int*)malloc(replicas*sizeof(int));
80 active_nodes = (int*)malloc(replicas*sizeof(int));
81 frozenness = (int*)malloc(replicas*sizeof(int));
82
83 for (r=0; r\leqslant replicas; r++) {
84 active_nodes [r] = 0;
85 frozenness [r] = 0;86 \text{nodes}[r] = (\text{int}*)\text{malloc}(\text{N}*\text{sizeof}(\text{int}));87 old_nodes [r] = (int*)malloc(N*sizeof(int));88 }
89 for (j=0; j\le N; j++) {
90 i f (gsl_rng_uniform ( rg ) < start_active ) {
91 nodes [0][j] = 1;\{ else\}93 nodes [0][\dagger] = -1;94 }
95 \alpha active_nodes[0] \pm nodes[0][j];
96 }
\text{for}(r=1; r\leq r\text{eplicas}; r++) {
98 memcpy(\&nodes[r][0],\&nodes[0][0],N*sizeof(int));
99 active_nodes[r] = active_nodes[0];
100 }
101 printf ("# step m d frozen ... \n' ;
102 for (i=0; i <iterations; i++ }
103 for (r=0; r\leq r\leq r\leq r+1) {
104 memcpy(\&old_nodes [r][0], \&nodes[r][0], N* size of (int) ;
105 active_nodes[r] = 0;
106 dist[r] = 0;
107 frozenness [r] = 0;\inf ((r>0) \&\& (i ==perturbation)) {
109 for (j=0; j\le N*start\_dist; j++) {
k = g s l_{r} n g_{r} (r g_{r});
111 \text{old\_nodes} [r] [k] \neq -1;\{112 \}\{113\}\left\{\n \begin{array}{ccc}\n 114 & & \\
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 119 & & \\
 119 & &amp115 #pragma omp parallel for private (k, r, j)116 for j = 0; j < N; j + +1 \{117 for (k=0; k\lt K; k++) {
\text{neigh}[k] = \text{gsl\_rng\_uniform\_int}(\text{rq},N);if (gs1_rng\_uniform(rg) < p) {
```

```
120 weight [k] = gsl\_rng\_uniform(rg);
121 } else {
122 weight[k] = -1.*gsl_rng_uniform(rg);
\left\{\n \begin{array}{ccc}\n 1 & 2 & 3 \\
 3 &amp; 4 &amp; 5\n \end{array}\n \right\}</math>\left\{\n\begin{array}{ccc}\n1 & 2 & 4 \\
1 & 2 & 3\n\end{array}\n\right\}125 for (r=0; r\leq replicas; r++) {
126 input = 0.;
127 for (k=0; k\lt K; k++) {
128 input += weight[ k] ∗old_nodes [ r ] [ neigh [k ] ] ;
\{129\}130 input - h;
\text{if (input > 0)}132 nodes \lceil r \rceil |j \rceil = 1;
133 } e l s e {
134 nodes [r][j] = -1;\left\{\n\begin{array}{ccc}\n135 & & \\
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169136 active_nodes[r] t= nodes[r][j];
137 frozenness [r] += (n \cdot | j!):<br>
f = (n \cdot | j!);
138 if (r>0) {
139 if (nodes [0][ j] ! = nodes [r][j] dist [r]+;
\left\{\n\begin{array}{ccc}\n140 & & \n\end{array}\n\right\}141 }
\left\{\n \begin{array}{ccc}\n 142 & & \\
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 & & & \\
 & & &143 #pragma omp barrier
144 printf("%5d ",i);
145 for (r=0; r\leqslantreplicas;r++) {
146 printf ( " %8.51f ", ( 1. ∗active_nodes [ r] + 1. ∗N) / ( 2. ∗N ) );
147 printf("% 8.51f",(1.*dist[r]/(1.*N));
148 printf(" \frac{8}{3}.51f ", (1.*frozenness[r]) / (1.0*N));
149 }
150 printf(\sqrt[m]{n});
151 }
152
153 for(r=0; r\leqslantreplicas;r++) {
154 free(nodes[r]);
155 free(old_nodes[r]);
156 }
157 free(nodes);
158 free(old_nodes);
159 free(active_nodes);
160 free(dist);
161 free(neigh);
162 free(weight);
163
164 return 0;
165 }
```
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# List of Figures



# List of Tables



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## Curriculum Vitae

### **Lukas Geyrhofer**

*lukas.geyrhofer@gmx.at* born December 29, 1983

#### Education



#### Research experience



#### **Publications**

O. Zagordi, L. Geyrhofer, V. Roth, N. Beerenwinkel. Deep sequencing of a genetically heterogeneous sample: local haplotype reconstruction and read error correction. RECOMB 2009, LNCS5541:345-358, 2009.

R. Tscheliessnig, L. Geyrhofer, M. Wendland, J. Fischer. Adsorption from oversaturated aqueous solution: Mean force molecular simulations. AIChE Journal, 54(9):2479-2486, 2008.