1
Functional Complexity Based on Topology

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1.1
Introduction

Complexity measures have been proposed as measures for computational, statistical, or structural complex features in various contexts; for review, see [1]. A complexity measure for patterns, for example, arising in chaotic systems, has been proposed in [2]. It is a measure theoretic concept that applies to ensembles of patterns. It is natural in the sense that it reflects the intuitive notion of a complex pattern being neither completely random nor completely regular, but having some structure instead. Complexity of hierarchical systems has been studied in [3]. The complexity measure has the property of isolating the most diverse trees as the ones with maximal complexity. Intuitively one would expect that the complexity of a hierarchy is related to its diversification, that is, to the number of nonisomorphic subtrees found at that level. The proposals given by Ceccatto and Huberman [3] reproduce this expectation. Recently, information storage and transfer was analyzed in [4,5]. A number of complexity measures that are based on various notions of graph entropy have been proposed. Graph entropies are supposed to characterize the structural information content of graphs; what is meant by "information" depends on the context. For review, see [6]. In particular, such measures are used in applications to chemical structures of molecule graphs whose vertices represent atoms and edges represent chemical bonds [7]. Moreover, in connection with molecule graphs, various "distance-related topological indices" are defined [8], for which the connotation of "topology" and spirit of derivation is very different from ours, although the wording may suggest an apparent overlap.

Our complexity measure is based on a proposal presented in [9]. We do not restrict our considerations to graphs that are trees and do not study branching properties of trees. Our graphs can represent a generic network as a dynamical system with n input and m output channels with directed or undirected edges. We restrict the graphs to one type of nodes, one type of edges, and one type of connectivities of nodes via these edges. There may be an arbitrary number of loops. The structural complexity of a graph needs to be considered with an associated dynamics. Hence, the result of our complexity measure will sensitively depend on the dynamics, of

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which the graph is just a rough abstraction that is supposed to indicate the mutual interactions. In our applications, a whole dynamical system may be assigned to a single node, and a path of regulation or transportation to an edge, where the edge can be equipped with its own dynamics.

Given a graph and the associated dynamics, we determine the complexity measure in two steps. The first one, called the vertex resolution, leads to a proliferation of patterns assigned to this graph, and the second one leads to a selection of only those patterns that are topologically inequivalent. This way we "get rid" off the entropy, generated by symmetries of the initial graph and generated patterns. Therefore, our approach is complementary to measures based on entropies of graphs.

Both steps, the vertex resolution and the restriction to topologically inequivalent contributions, are motivated by dynamical systems. Vertex resolutions "break up" the vertices into parts in all allowed ways leading to rewiring of edges, or a fusion or fission of interaction paths between the vertices; vertices represent nodes which in a broad sense transform an input in k_{in} channels to an output in k_{out} channels, regulating the flux of cargo, traffic, energy, fluid, or information. Their splitting may create or destroy loops, an important basic motif in networks. Not all patterns, resulting from this process of partitioning the edges assigned to a vertex, are dynamically allowed, as we will see later.

The selection of topologically inequivalent graphs is motivated by the fact that whole classes of dynamical systems are known to exist, whose space of attractors and their associated functions are to a large extent determined by their topology, that is, by fixing the mutual interaction. (Attractors are understood as stationary states that can be fixed points, limit cycles, or chaotic attractors of the dynamics. Their relation and interpretation in terms of a "function" is not always obvious, but sometimes possible.) The conjecture then is that changing the topology changes the function or functionality of these systems, so that the complexity measure gives a hint on the functional flexibility of the dynamical systems, natural and artificial ones, represented by the considered graph.

In particular, the concept of functionality applies to networks in life science and in information science. Network motifs have been studied as characteristic building blocks for complex networks [10]. They are local subgraphs or wiring patterns that occur throughout the network significantly more often than in randomized networks. As a result, motifs shared by ecological food webs are specifically different from those in genetic networks. More generally, it has been found in [10] that motifs in networks of information processing are typically distinct from networks of energy transporting. Information processing may refer to nets as diverse as those of gene regulation, neurons, and electric circuits. The overall conclusion is that frequently repeated motifs should represent certain functions.

At a first place, to make these concepts well defined, in particular the topological equivalence of two graphs, we use the framework of LCE-graphs, in which LCE stands for "linked cluster expansions" used in statistical physics. The appropriated definitions are introduced in Section 1.2.1, followed by a definition of the vertex resolution patterns of a graph in Section 1.2.2. Section 1.2.3 contains a short

excursion to link invariants and Kauffman states, which are usually used for calculating Jones polynomials as link invariants. The reason for this excursion is a close correspondence between the decomposition of a link into Kauffman states and our scheme of vertex resolutions. We are then ready to define a measure for functional complexity in Section 1.2.4. In Section 1.3, we illustrate with examples from dynamical systems a number of cases, in which the topology determines the function. We start with a very simple system of phase oscillators in Section 1.3.1. Next we indicate applications to transport networks of information (Section 1.3.2) or of cargo (Section 1.3.3), to Boolean networks in Section 1.3.4, and to topological quantum systems in Section 1.3.5. In Section 1.3.6, we sketch a dynamical system, of which the steering dynamics on the highest level of its hierarchical organization is stored in the topology of a knot. In Section 1.4, we draw the conclusions. Throughout this contribution, we will use "lines" and "edges", and "vertices" and "nodes", in a synonymous way, respectively.

1.2
A Measure for the Functional Complexity of Networks

1.2.1
Topological Equivalence of LCE-Graphs

As usual in the context of networks, our graphs consist of nodes and edges (or vertices and lines), the edges may be directed or undirected; in principle, we can formulate our notions of topological equivalence for graphs with two type of connectivity: nodes are connected via edges, and edges are connected via a different kind of nodes. Such a type of connectivity was naturally introduced in the context of the graphical representation of a generalized high-temperature expansion in spin glasses, if not only the spins interact via their couplings, but the couplings self-interact with their own dynamics, see [11,12]. For simplicity, we focus here on undirected graphs with only one type of connectivity, represented by graphs with internal and external lines – internal lines to describe internal interactions and external lines for input and output channels in the general context.

Let us now define in detail the notion of an LCE-graph and the topological equivalence of two such graphs. The notions are obtained as special case of those introduced in [11]. An LCE-graph is a structure

$$\Gamma = (\mathcal{L}_\Gamma, \mathcal{B}_\Gamma, E_\Gamma, \mathcal{R}^{\mathcal{L}}_\Gamma) \tag{1.1}$$

Here $\mathcal{L}_\Gamma$ and $\mathcal{B}_\Gamma$ are two mutually disjoint sets of internal lines of Γ and vertices of Γ, respectively. E_Γ are maps that assign the number of external lines to every vertex $v \in \mathcal{B}_\Gamma$. $\mathcal{R}^{\mathcal{L}}_\Gamma$ are incidence relations that map internal lines to their endpoint vertices. Lines are treated as undirected; the generalization to directed ones is easily done. We consider $\overline{\mathcal{B}_\Gamma \times \mathcal{B}_\Gamma}$ as the set of unordered pairs of vertices (v, w) with $v, w \in \mathcal{B}_\Gamma$. Then we have $\mathcal{R}^{\mathcal{L}}_\Gamma : \mathcal{L}_\Gamma \to \overline{\mathcal{B}_\Gamma \times \mathcal{B}_\Gamma}$. We say v and w are the endpoint vertices of $l \in \mathcal{L}_\Gamma$ if $\mathcal{R}^{\mathcal{L}}_\Gamma(l) = (v, w)$. A line with only one vertex attached is an external line. In a

concrete realization, the incidence relations $\mathcal{R}_\Gamma^{\mathcal{L}}$ may be realized as a matrix $(\mathcal{I}_\Gamma^{\mathcal{L}}(i,j))$, $i,j \in \{1,\ldots,n\}$ with

$$\mathcal{I}_\Gamma^{\mathcal{L}} : \overline{\mathcal{B}_\Gamma \times \mathcal{B}_\Gamma} :\to \mathbf{N}_0 \tag{1.2}$$

defined in the following way. Given a graph Γ with n vertices, m internal lines, L external lines, and a labeling of vertices and internal lines. $\mathcal{I}_\Gamma^{\mathcal{L}}(i,j)$ is a symmetric $n \times n$ matrix with $\mathcal{I}_\Gamma^{\mathcal{L}}(i,j)$ equal to the number of internal lines (i.e., a natural number $\in \mathbf{N}_0$ including 0) connecting i and j for $i \neq j$, $i,j \in \{1,\ldots,n\}$. As long as we do not allow self-lines (i.e., lines starting and ending at the same vertex), the diagonal elements $\mathcal{I}_\Gamma^{\mathcal{L}}(i,i)$ may be reserved for storing the number of external lines attached to vertex i. The matrix $\mathcal{I}_\Gamma^{\mathcal{L}}$, representing the incidence relations, would be suited for computer implementations of LCE-graphs as it allows computer-aided algorithmic generation of graphs.

Now we can formulate in a purely algebraic way when are two LCE-graphs topologically equivalent. Two LCE-graphs

$$\Gamma_i = (\mathcal{L}_i, \mathcal{B}_i, E_i, \mathcal{R}_i^{\mathcal{L}}) \quad i = 1,2 \tag{1.3}$$

are called topologically equivalent if there are two invertible maps

$$\begin{aligned} f_{\mathcal{B}} &: \mathcal{B}_1 \to \mathcal{B}_2 \\ f_{\mathcal{L}} &: \mathcal{L}_1 \to \mathcal{L}_2 \end{aligned} \tag{1.4}$$

between the sets of vertices, and the set of internal lines of these graphs Γ_1 and Γ_2 such that

$$\mathcal{R}_2^{\mathcal{L}} \circ f_{\mathcal{L}} = \overline{f}_{\mathcal{B}} \circ \mathcal{R}_1^{\mathcal{L}} \tag{1.5}$$

and

$$E_2 \circ f_{\mathcal{B}} = E_1 \tag{1.6}$$

Here $\circ$ is understood as the composition of maps, and

$$\begin{aligned} \overline{f}_{\mathcal{B}} &: \overline{\mathcal{B}_1 \times \mathcal{B}_1} \to \overline{\mathcal{B}_2 \times \mathcal{B}_2} \\ \overline{f}_{\mathcal{B}}(v,w) &\mapsto (f_{\mathcal{B}}(v), f_{\mathcal{B}}(w)) \end{aligned} \tag{1.7}$$

For example, (1.5) means that the following compositions of maps are equivalent: first assign via $\mathcal{R}_1^{\mathcal{L}}$ the endpoint vertices to a given internal line l_1 of the first graph Γ_1 and map them to the corresponding vertices in Γ_2 via $\overline{f}_{\mathcal{B}'}$, or, alternatively, first map the given internal line of the first graph Γ_1 to the corresponding internal line l_2 of the second graph via $f_{\mathcal{L}}$, and then associate the endpoint vertices with this line there via $\mathcal{R}_2^{\mathcal{L}}$. Both orders are equivalent if graphs are topologically equivalent. Equation (1.6) states the equivalence of assigning the external lines either to the vertex of the first graph or to the corresponding vertex of the second graph. Figure 1.1 shows four graphs, of which three (a), (b), and (c) are topologically inequivalent, but two (c) and (d) are equivalent. Below we will define admissible vertex resolutions. The graphs (c) and (d), "fragmentized" into two pieces, would not be admissible as contribution to a connected two-point correlation function.

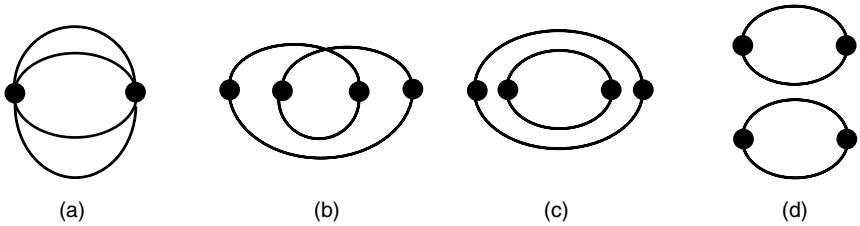

Figure 1.1 Topologically (in) equivalent graphs: (c) and (d) are equivalent, whereas (a), (b), and (c) are not.

1.2.2 Vertex Resolution Patterns

Apart from operations like adding or removing vertices, or lines, with or without the attached structures, one operation is of interest in this context that is the resolution of vertices. Let Γ be an LCE-graph, $v \in \mathcal{B}_\Gamma$ a vertex with n lines ending upon it, and let $\Pi \in \mathcal{P}(\mathcal{L}_v)$ be any partition of the set of lines $\mathcal{L}_v$ ending on v. $\mathcal{P}(\mathcal{L}_v)$ is the set of all partitions of lines ending on v. (A partition is a disjoint union of subsets P of lines ending on v such that it gives $\mathcal{L}_v$.). We remove the vertex v and draw for every subset $P \in \Pi$ of lines a new vertex $v(P)$, so that all lines $l \in P$ enter the vertex $v(P)$ rather than v before its removal. This procedure is called a vertex resolution of v. For example, see Figure 1.2 showing three partitions of the original set of four lines, where we left out partitions into vertices with single lines attached. Also we left out permutations from two other possible pairings of lines, which should be taken into account when the lines are labeled. Note that this resolution procedure amounts to a rewiring of lines. It then depends on the dynamical constraints whether the resulting (resolution pattern of a) graph Γ is allowed or not. For example, the graph may become disconnected and fragmentize into several pieces as a result of the resolution procedure. Such a resolution is forbidden if the considered graphs must be connected. More generally, a vertex resolution is called admissible if it satisfies all constraints from the dynamics or from the choice of observables.

A remark may be in order on what has led us to introduce the concept of vertex resolutions. In the original formal context of so-called dynamical linked cluster expansions [11], the graphs (c) and (d) of Figure 1.1, which now fragmentize into independent parts, could remain connected if one allows self-interactions of spin

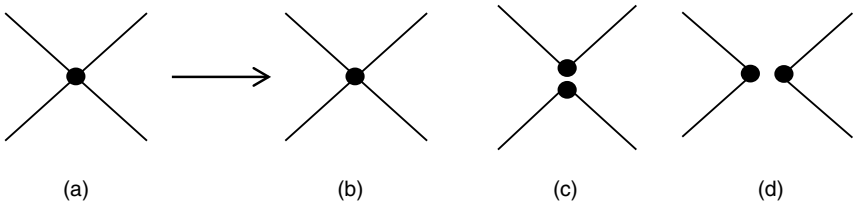

Figure 1.2 Three possible resolution patterns (b), (c), and (d) of the graph in (a).

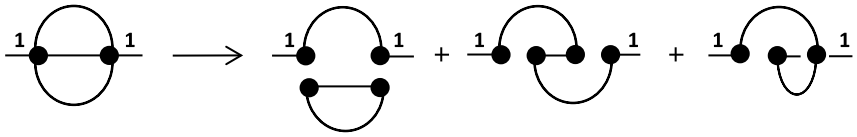

Figure 1.3 Propagation of a "color" labeled as 1 along different paths in three resolution patterns.

couplings, represented by lines. These graphs would then contribute to a connected two-point function, for example. But also in connection with linked cluster expansions, one is naturally led to consider resolutions as shown in Figure 1.3 when calculating symmetry factors of an internal symmetry like color or flavor symmetry. For example, assuming an underlying $O(N)$-symmetry of the system, one of N "colors" ("flavors", "features", or "bits") may propagate along each line. In calculating the internal symmetry factor, one looks for all possible paths along which feature 1, say, out of N, can propagate from the input channel through the graph to yield feature 1 in the output channel, while a closed loop may carry any one of the N features, and only one feature can propagate along a line at the same time. As shown in Figure 1.3, feature 1 can propagate along the upper line, say l_1, along with N possible features for the loop of the remaining lines, l_2 and l_3, or it can propagate along l_1, l_2, l_3, or l_1, l_3, l_2, or it could choose the intermediate line l_2, or the lower line l_3 first, yielding $3 \times (N + 2)$ possibilities altogether.

Consider the special case of vertices of degree 4 in a closed graph without external lines, and interpret the vertices as crossings of two lines, resulting from a two-dimensional projection of under- or overcrossings in links (for the definition of "link," see Section 1.2.3) in three dimensions. In this case, our vertex resolutions contain a decomposition of two-dimensional link diagrams into a sum over Kauffman states as we show in the following section.

1.2.3
Kauffman States for Link Invariants

Let us briefly recall some basic facts about knots and links. A "knot" as defined by mathematicians is a submanifold of $\mathbb{R}^3$ that is diffeomorphic to S^1, the circle. An example for a two-dimensional projection of a trefoil is shown in Figure 1.4. The over- or undercrossings of the "rope" in three dimensions are indicated with continuous or broken lines, respectively. A "link" is a submanifold of $\mathbb{R}^3$ that is diffeomorphic to a disjoint union of circles. The circles are components of the link. A link with two components is the Hopf link, as shown in Figure 1.5. For classifying knots or links, a number of link invariants have been proposed such as the Jones polynomial. Kauffman's approach to Jones polynomials made it a simple construction [13]. The first step is to define the Kauffman bracket of a link L, $\langle L \rangle$, which is then used to construct the Jones polynomial. The Kauffman bracket is a function of three variables, A, B, and d. Choosing $B = A^{-1}$, $d = -(A^2 + A^{-2})$, the Kauffman bracket will be invariant under Reidemeister moves. Now, rather than summing over the crossings of the link L, the Kauffman

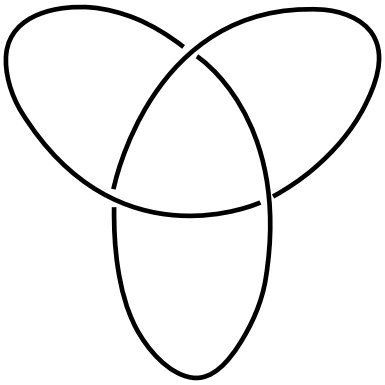

Figure 1.4 Trefoil knot.

bracket sums over states σ, which we here will call Kauffman states. Such a state of L assigns to each crossing c of L a number σ_c that is either A or B, so that a link of N vertices has 2^N possible states. Given a state σ of a link L, we orient each crossing c such that the overcrossing line points upward to the right and the broken line upward to the left as on the left-hand sides of Figures 1.6 and 1.7. Assigning the variable A to this crossing means to avoid it according to Figure 1.6, and assigning the variable B implies an avoiding according to Figure 1.7. This way all crossings are avoided and the resulting diagram consists of a finite set of circles, embedded in the plane, as indicated in Figure 1.8 for

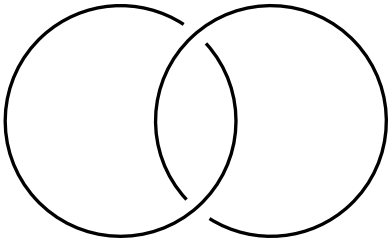

Figure 1.5 Hopf link.

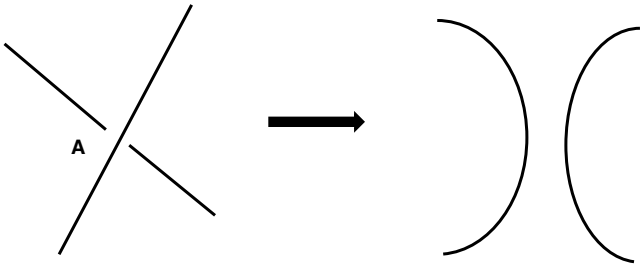

Figure 1.6 First possibility of avoiding the crossing. In this case, the variable A is assigned to the crossing.

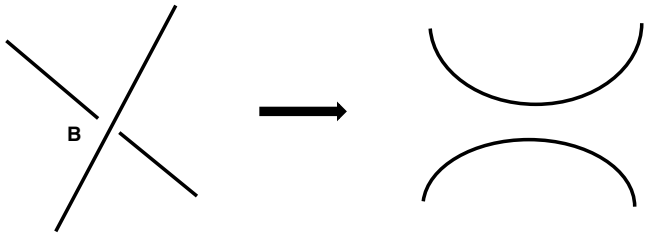

Figure 1.7 Second possibility of avoiding the crossing, here labeled as *B*.

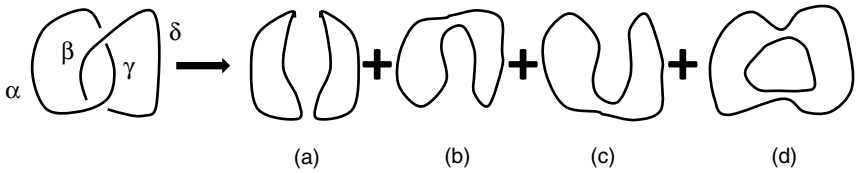

Figure 1.8 Kauffman states of the Hopf link.

the Hopf link. The Kauffman bracket is then defined by a sum over all Kauffman states according to

$$\langle L \rangle = \sum_{\sigma} d^{||\sigma||} \prod_{\text{crossings c}} \sigma_{\text{c}} \tag{1.8}$$

where $||\sigma||$ denotes the number of circles of the state σ. (For the Hopf link, the Kauffman bracket is then given by $\langle L \rangle = d^2A^2 + dAB + dAB + d^2B^2$). Now it should be obvious why we have made this excursion to link invariants in connection with our resolution patterns. For the special case that our graphs have no external lines, and the vertices of the links have all degree 4 corresponding to two crossing lines, our decomposition into patterns contains the decomposition into Kauffman states as a subset of all partitions. The kind of summation reminds to a sum over states of a partition function, and the relation can be made precise in both cases, see [10,14]. In Section 1.3.6, we will indicate a possible application of these link diagrams as generating functions of dynamical processes that arise from different Kauffman states of these links.

1.2.4
Definition of the Complexity Measure

We are now prepared to define a measure for the functional complexity of networks. It is defined as

$$\text{FCM} := \frac{\sum'_{i\in(1,\ldots,N)} PA_i(\Gamma)}{\sum_{\text{all admissible patterns } j} PA_j(\Gamma),} \tag{1.9}$$

that is, it counts the total number of topologically inequivalent admissible resolution patterns PA_i of the graph Γ of that network (here defined for an LCE-graph),

normalized over all admissible patterns. The prime stands for the restriction to topologically inequivalent and admissible patterns. A resolution pattern is obtained by allowing any $r_v (0 \leq r_v \leq n_v)$ resolutions of vertices, n_v denoting the total number of vertices of Γ. It is admissible if it is compatible with the constraints imposed by the dynamics. Two resolution patterns are topologically equivalent if there exist two invertible maps (1.4) between their associated graphs Γ_1 and Γ_2 that satisfy (1.5)–(1.7).

Examples for dynamical constraints are as follows:

- After the resolution of vertices, the resulting graph should stay connected.
- Vertices should have an even number of lines attached. This constraint may reflect an underlying symmetry of the dynamics, which forbids an odd number of attached lines.
- There are no lines that start and end at the same vertex (i.e., no self-lines or tadpoles).
- Conservation laws should be respected at each vertex.
- Rewiring of edges should avoid geometric frustration. It may happen that the vertex resolution leads to the creation of loops such as in the first resolution pattern of Figure 1.3. If the edges are not directed but represent repressing interactions, a loop with an odd number of such edges will lead to geometric frustration [15]. In case of directed edges, representing repressing interactions, an even number of such edges in a loop leads to geometric frustration. If the network shall be designed in a way to avoid geometric frustration, such resolution patterns would be excluded.

In our definition of the complexity measure, we count all admissible resolution patterns of graphs with equal weight. In general, it may happen that certain topologically inequivalent patterns are admitted, but dynamically strongly suppressed in some small parameters like a coupling constant. For such cases, the measure should be generalized accordingly.

The scaling of this measure with the number N of (unresolved) vertices is bounded by $k_{\max}^N$ if $k_{\max}$ denotes the maximal degree of vertices in the network. The actual scaling, however, can be quite different from this exponential proliferation of patterns due to the dynamical constraints.

Our conjecture is that the restriction to topologically inequivalent resolution patterns projects on inequivalent functionalities. We shall give examples in the following sections.

1.3 Applications

The definitions in the previous sections with graphs induced by linked cluster expansions mainly served to illustrate that the notions of topologically inequivalent resolution patterns of graphs (which are themselves graphs) can be well defined and tested in a computer-aided way by analyzing their matrix representations. From now on, we consider any interpretation of such graphs for which the concept of vertex resolution is meaningful.

1.3.1
Creation of a Loop

Let us start with a very simple example in which it is only the topology that determines the attractor of the dynamics, here a synchronized state of a system of interacting phase oscillators. Consider an open chain of coupled phase oscillators, assigned to the nodes of the chain, which are coupled to their nearest neighbors apart from those at the boundaries which have only a neighbor on one side. Depending on the choice of parameters, the oscillators can then oscillate either completely independently of each other or in full synchrony with a fixed phase difference between them. Now let us choose the parameters such that the oscillators are in an incoherent state for open boundary conditions along the chain. As we have shown in [16], the mere closure of the open chain to a closed loop is then sufficient to induce synchronization of the whole set without any other change of parameters. The switch to a synchronized state induced by a change in the topology holds for a whole range of parameters, for which the chain of oscillators is dephased.

More generally, loops, whether undirected, or directed as feedback loops or feedforward loops, play an important role as a basic motif in network dynamics.

1.3.2
Networks of Information

Recently, a discrete-time Gaussian model was analyzed with respect to its capability of storing information on individual nodes, given the network structure and the weights of the edges [4,5]. The authors show that directed feedback or directed cycles and feedforward loop motifs dominantly contribute to the capability of information storage. For example, in this model, feedforward loops let information pass to another node along paths of different lengths, so that the information arrives at different instants of time. This effectively amounts to an intermediate storage of this information at another place within the network. (The active information storage is calculated in terms of certain entropies.) Moreover, the longer such loops, the longer the memory which in principle can be incorporated in such networks.

If our decomposition of nodes in the context of neural networks leads to resolution patterns of graphs that yield a number of loops with a variety of loop lengths, such a network architecture is flexible in its memory capacity and depth. In contrast to loops, a full decomposition of the network graph into trees of different roots would reflect the possibility of a fully parallel transport of information over time.

1.3.3
Transport Networks of Cargo

For transport networks of cargo, the edges correspond to roads or tracks, and the logistics of transport is much determined by the traffic regulations at the crossings.

A large value for the complexity measure here would reflect many ways of partitioning the road network for optimizing the speed of transport, the avoidance of traffic jams, the amount of transported cargo, but also a time-ordered supply to have the cargo at the right time at the right place. Different partitions, corresponding to different vertex resolutions, would stand for different strategies to satisfy the logistic requirements. Here we do not only think of macroscopic traffic networks and traffic regulations in cities; one may think of smart energy grids with an efficient design for the transport of power based on renewable energy. On the one hand, one would like to make the network robust against a global electric power outage, so that some redundancy in the number of cables seems to be required. On the other hand, one should avoid Braess' paradox [17] that is well known to occur in traffic systems. It is also known for power networks that the addition of a single route may induce an outage rather than improving the robustness. Such considerations would lead to constraints on the admissible partitions of the road network. In more formal terms, the design should avoid geometric frustration ("frustration" in a similar sense as it is used in spin systems (see [15]), since frustration amounts to conflicting regulations at crossing points of loops. Calculating then our complexity measure for such a traffic network of a given fixed size would not be conclusive on its own, but its scaling with the system size together with a dynamical process of traffic (energy transport) would be conclusive for the network's transport capacity.

Much more fancy transport networks than the artificial ones on the macroscopic scale can be found in natural networks on the mesoscale, realized in the cytoskeleton of eukaryotic cells. The cytoskeleton provides structure and organization of cells, but also drives their change of shape and movement and transforms applied stress, transmitting or resisting it [18]. Within the cytoskeleton, there are three networks: actin filaments together with crosslinkers on the smallest scale, intermediate filaments, and microtubules on the largest scale. Microtubules play a key role in particular for intracellular transport. It is a focus of current research what exactly regulates this traffic, and how traffic jams or malfunctions are avoided in a healthy organism. In contrast to the static networks on the macroscopic scale (often also equipped with static traffic regulations), the networks on the nano- and microscales have a highly dynamic structure. "Roads" and crosslinkers are regularly created and destroyed as in our purely formal vertex "fission" and "fusion" events, in which connections to other edges can be lost or are newly created. Yet we are far off from establishing a direct connection between the functional complexity of this complex viscoelastic material in the cell and our complexity measure that would only indicate the number of inequivalent arrangements of traffic lines. In any case, here the topological aspect is certainly not sufficient to capture the very rich, sophisticated functional behavior of the cytoskeleton, since the very material properties of the involved networks matter as well as metric features related to the range of forces, the very size of the cargo, tracks and crosslinkers, and the very timing of the processes.

Therefore, in regard to an optimal design of a flexible topology of transport networks, one should take into account the nature of the material that is transported, whether it is cargo, energy flux, fluid, single information bits, or signals for

regulation. This leads us to the next class of networks for which the topology decides about certain functions which the network can perform.

1.3.4 Boolean Networks of Gene Regulation

Boolean networks provide a prominent example for systems in which it is the topology that determines to a large extent the dynamical attractors, and the attractors can be identified with certain functions. Boolean modeling of gene regulatory networks was very successful for the segment polarity gene network [19], dealing with genes involved in the embryonic pattern formation in the fruit fly *Drosophila melanogaster*. As it was shown in [19], it is the topology of the regulatory network that essentially determines the dynamics and the overall function, and it is much less the kinetic details of this system which matter. To expose more clearly the connection between function and topology (connectivity), the original graph of the segment polarity network is expanded toward the inclusion of so-called complementary and composite "pseudonodes," in particular to represent more clearly the logical functions and to account for the two possible signs of interaction ((+) for activating and (−) for repressing interaction). This extension toward further vertices is different from our resolution patterns, but in a similar spirit to reflect further details of the dynamics in the graphical representation.

Another prominent example for a successful description of a genetic system in terms of Boolean functions is provided by the yeast cell cycle [20]. Again it is the topology in which the regulatory functions are arranged that determine the dynamic attractors and their basins of attraction, whose size reflects the robustness against perturbations. In case of the modeling of the yeast cell cycle, one is in the lucky situation, as the intimate relation is obvious not only between Boolean functions and topology but also between biological function and topology, since the attractors can be interpreted in biological terms, such as an attractor corresponding to the G1 state, that is the biological stationary state of the cell cycle, here of yeast. In this system, it is possible to observe how the biologically realized cell-cycle sequence of protein states is an attractive trajectory in the Boolean dynamics with a global range of attraction [20].

It is particularly this kind of systems behind our idea that inequivalent topologies go along with different functionalities.

1.3.5 Topological Quantum Systems

Next we come to an extreme case of a class of systems, in which the functions exclusively depend on the topology. These are quantum systems in which the quantum mechanical amplitude of a particular process depends only on the topology of this process. This means, if the paths, which particles trace out in space-time, are topologically equivalent, they will be equally likely. Theories that describe such topological quantum systems are called topological quantum field theories [21]. In

these systems, the amplitude for a particular process is a knot invariant of the space-time paths followed by the particles during this process. Out of a two-particle, two-hole system, one can construct a two-state quantum system or a single quantum bit. This suggests the possibility to use topological quantum systems as quantum computers. Different types of braids (structures formed by intertwining three or more paths) correspond to different quantum computation, so that there is a direct relation between the topology and the function (of performing a calculation). Different realizations of such quantum systems are currently explored. Computations performed in this way would be much more robust against noise of various origin, since they only depend on the topology, but not on other details of the space-time paths.

1.3.6
Steering Dynamics Stored in Knots and Links

Let us finally sketch a toy model for a dynamical system with a hierarchical organization. On the highest level, the steering level, we store the instructions and initializations for dynamical processes taking place on a lower level. These instructions are stored along closed strings which are knotted. To be definite, let us consider the Hopf link of Figure 1.5. Next we let a nanomachine walk along the knotted link, that is along the different pieces of the path, labeled as α, β, γ, and δ in Figure 1.8. During its walk, the machine translates the instructions into operations A, B, Γ, and Δ, acting upon the dynamics on the underlying level. These operations need not commute. The function of the resulting dynamics on the underlying level will likely reflect the order A, B, Γ, and Δ of the non-commuting operations, corresponding to the order in which the instructions were read off. Now we offer the nanomachine two options at each crossing to avoid the over- or undercrossing of another string, the two options just corresponding to Figures 1.6 and 1.7. In this case, the instructions along the Hopf link would be read off either in pairings of two pieces to one cycle each, α with β for the first cycle and γ with δ for the second cycle (Figure 1.8a), or, alternatively, α with δ for the first and β with γ for the second cycle (Figure 1.8d), or to a single cycle in the order α, δ, γ, and β (Figure 1.8b), or to another single cycle in the order of α, β, γ, and δ (Figure 1.8c), up to cyclic permutations. For noncommuting operations, the versatility of the dynamical performance of the whole system would then be determined by (the Kauffman states of) the Hopf link, associated with the steering level.

A desirable feature of such an organization in general would be that the dynamics on the steering level depends mainly on the topology, since this guarantees a highly robust performance, while less robustness is required for the lower levels in view of the maintenance of the system as a whole. Of course, one may wonder what steers the superimposed dynamics that determines the decisions of the nanomachines at the crossings while they are reading out the instructions along the path. This may be some feedback from the overall performance after the instructions are carried out.

1.4 Conclusions

As we have seen, along with the versatile interpretation of graphs that represent dynamical processes on and of networks, our manipulation of graphs in terms of fusion and fission of nodes and edges has different applications, ranging from transport networks of cargo, energy, or flux to those of transport of information and to regulatory gene networks, described by Boolean functions. After all one may wonder why we distinguish at all between graphs of these networks and their possible resolution patterns if it is mainly the latter which may be directly related to certain functions. The answer is best provided by the answer to an analogous question: Why do we consider links like the Hopf link rather than the associated Kauffman states? The graphs classify the dynamical system, and the resolution patterns correspond to concrete and particular realizations. In the toy model of the last section, it would be the link invariant that would characterize a whole class of dynamical systems by their steering dynamics. In general, we expect a close relation between function (performance) and topology in regulatory systems, which are not sensitive to kinetic details or metric measures such as the size and distance of the involved objects.

Characterizing a complex performance of a dynamical system by a single number such as our complexity measure is certainly not conclusive if we know this number just for a single system size. However, the scaling of this measure with the system size can be revealing. As we have indicated in Section 1.2.4, the scaling need not be exponential in the number of vertices, but can be rather nontrivial due to the presence of dynamical constraints that should be satisfied by the admissible vertex resolutions. Since the measure sensitively depends on the very choice of the dynamics, there are no universal scaling laws; results in concrete applications, however, will be useful for deciding the storage capacity of a network, the robustness of large regulatory systems, or the feasibility of a calculation. In our original application of counting the (topologically inequivalent) resolution patterns of vertices, occurring in a generalized linked cluster expansion for spin glass systems [10,11], this number was a measure for the computational complexity of the problem, so that a computer-aided algorithmic generation of graphs was needed to go to higher orders in the expansion. For a neural network, this number may give a hint on the storage capacity in terms of the abundance of special loop motifs. In nonrandom Boolean networks, it would be interesting to see whether the number reflects a non-exponential scaling with the system size if all dynamic constraints are taken into account that apply to genetic systems, and if the sequential, nonrandom order of regulations is respected in the Boolean modeling. Here it is most interesting to understand why not all in principle allowed combinations ("resolution patterns") are realized in nature, since the observed number of stable attractors (supposed to represent the stable cell states) is relatively low as compared to the huge number that would be possible without additional constraints.

In summary, it is not all kind of dynamical systems to which we would apply this measure, but those in which the topology of the network has the main influence on the stationary states of the system.

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