Preface

Invariants associated with mathematical objects or data sets should be informative and interpretable, easy to compute, and stable in the presence of small perturbations. In particular, they should allow us to quickly distinguish qualitatively different structures. Certain invariants that satisfy these requirements can be obtained from the spectra, that is, the collection of eigenvalues, of linear operators for functions defined on that structure. And arguably the most useful ones are Laplace-type operators. Such a Laplace-type operator can be defined when a structure consists of elements that may stand in relations permitting the definition of a neighborhood relation. Then, one compares the value of a function at an element to the average of the function values at its neighbors. Such Laplace operators were first investigated for smooth structures, such as domains in Euclidean space or Riemannian manifolds. There were some analytical issues to be overcome, which among other things, stimulated the development of functional analysis and the theory of elliptic partial differential equations.

In this monograph, we look at structures that are discrete and finite, and therefore, there are no such analytical difficulties. Nevertheless, both historically and in our own research, the smooth theory could inspire much of the discrete theory. The neighborhood structures that we are considering could be those of a graph, a hypergraph, or a simplicial complex. In the case of a graph, we only have relations between pairs of elements. When relations can involve larger sets of elements, we obtain a hypergraph. And when any nontrivial subset of related elements also supports a relation, we get a simplicial complex. Although a simplicial complex can be considered as a special case of a hypergraph, the theories that we develop and explore for the two types of structures are quite different. An important insight underlying our theory is that a hypergraph should not be viewed as a deficient simplical complex, but rather as a structure in its own right that can be enhanced with an orientation.

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In graph theory, one usually considers the algebraic Laplacian which has many useful properties. While our theory is general, when the analysis becomes more specific, we shall mostly consider the normalized Laplacian instead for several reasons. The normalized Laplacian satisfies a conservation law and is therefore naturally related to diffusion processes and random walks. Also, the analogy with the smooth case seems stronger than that with the algebraic Laplacian. And finally, it seems better suited for the more abstract aspects of the theory that cover not only graphs but also hypergraphs and simplicial complexes.

So, what can the spectrum of a Laplace operator tell us about the geometry of the underlying structure? Perhaps most importantly, the smallest nonvanishing eigenvalue estimates how difficult it is to divide the structure, by severing as few relations as possible, into two large components, known as Cheeger cut (Cheeger had established such a relation in the Riemannian case). This has long been known for graphs, but we will derive new results in this direction for simplicial complexes and hypergraphs. Also, we will systematically investigate the nodal sets of the corresponding eigenfunction, although the nodal decomposition need not necessarily provide an optimal Cheeger cut. In order to understand this and other phenomena more deeply, we will also systematically study nonlinear versions of the Laplace operator, for a parameter $1 \leq p \leq \infty$. Here, $p = 2$ corresponds to the standard Laplacian, while the extreme cases $p = 1$ and $p = \infty$ are the most difficult, but also most insightful. An important tool that we shall systematically utilize will be the Lovász extension that turns a discrete optimization problem into a continuous one.

The Laplacian spectrum does not determine the underlying structure completely. For instance, there are isospectral graphs, that is, non-isomorphic graphs with the same Laplacian spectrum. Nevertheless, many classes of (hyper)graphs can be characterized by their spectral properties, and we can also look at the spectral asymptotics for families of (hyper)graphs. Moreover, small changes, such as additions or deletions of vertices or edges, have only a small influence on the spectrum, and this can be made precise by interlacing inequalities. Our corresponding analysis will depend on the systematic use of so-called Rayleigh quotients. These are functions defined on a sphere in some Euclidean space whose critical values yield the eigenvalues and whose critical points provide the corresponding eigenfunctions. This naturally leads to Morse theoretical conceptualizations, and it provides us with the opportunity to illustrate the geometry of Floer theory.

For the hypergraph Laplacian, there are various possibilities. On the one hand, we can study a previously introduced linear operator that uses orientations, which led us to the concept of a chemical hypergraph where a hyperedge

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is conceived as representing a chemical reaction that connects two sets of vertices: the educts and the products. On the other hand, we can also define a tensorial Laplace operator whose eigenvalue equations are polynomial and no longer linear as in the graph case. Both approaches yield mathematical interesting results that is useful for the quantitative and qualitative analysis of hypergraphs.

Our original interest in the spectral theory of discrete structures was partly motivated by questions arising from the analysis of empirical data in fields such as biology, neuroscience, chemistry, or the social sciences. Many such data arise as networks and can therefore be modeled as graphs, simplicial complexes, or hypergraphs. We have gene regulation, protein interaction, and neural or friendship networks, for example, which can be modeled as graphs. In topological data analysis, simplicial complexes are constructed from discrete metric data. Chemical reaction systems or coauthorship networks between scientists are naturally considered as hypergraphs. Spectra of linear operators naturally led to useful invariants for investigating, characterizing, or classifying such structures. Spectral methods have therefore found, and continue to find, many applications in network analysis across a wide range of empirical domains. The systematic study of network properties was first undertaken by social scientists. Since we did not want to start a mathematical monograph with a discussion of social science literature, these applications will be discussed only in Chapter 13. Of course, we need to be selective there and will highlight only a few key examples.

This motivation also had consequences for our research design. Empirical data are neither fully regular nor completely random. Therefore, on the one hand, we have not explored in depth the theory of graphs with specific regular structures. For instance, the important theory of expander graphs uses the strong regularity assumption that all vertices in a graph have the same number of neighbors. This is also the case for the Cayley graphs, which represent the structure of a discrete group geometrically. More generally, algebraic graph theory is a well-researched field, but this is not the thrust of our research. On the other hand, we have also not delved into random graph theory. This theory started with the work of Erdös and Rényi, who connected a given set of vertices in a purely random manner and then investigated how the resulting structure almost surely depended on the density of the random connections. This has found many applications in mathematics and statistical physics, for instance, in the direction of Wigner's semicircle law for spectra of random matrices. More generally, methods from random graph theory are powerful for deriving existence results for graphs with particular structural properties. Even though, according to some such arguments, almost all graphs may exhibit a particular

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property, the proofs are not explicit, and it may still be a challenge to exhibit a concrete graph with the property in question. Also, in network analysis and statistical physics, several other schemes for the construction of random graphs with specific features, in particular those exhibiting power law behavior, have been proposed, and again, this is an active field of research that is not covered in our book.

Thus, we investigate the spectral properties of general graphs, simplicial complexes, and hypergraphs, with a theory that is as systematic and comprehensive as possible. However, we have found that complete generality is not feasible, in the sense that hypergraphs should better not be considered as generalized or somehow deficient simplicial complexes. To recall, in a hypergraph, sets of vertices are related or connected by hyperedges. For a simplicial complex, it is required that whenever such a vertex set is related, then all its subsets stand in relation as well. Simplicial complexes are therefore well suited for the schemes of algebraic topology, more precisely (co)homology theory with its boundary relations. Thus, the (co)homology theory of simplicial complexes is clear and canonical. While people have also proposed such theories for hypergraphs, none can be considered clear or canonical. In that situation, one of the key insights underlying this book, as indicated previously, is that Laplace operators of hypergraphs should be constructed in a fundamentally different way with no analog for simplicial complexes. In fact, we impose and utilize an additional structure on hypergraphs, that of an orientation of hyperedges, and this eventually drives the theory.

As already mentioned, we have to relate the properties of spectra to the geometry of the underlying objects. For this book, the most important of these relations are the Cheeger-type inequalities. In such inequalities, a bound on an eigenvalue indicates how easy or difficult it is to separate a structure into disjoint substructures by cutting as few relations as possible. Other such inequalities estimate how close a structure is to or how different it is from a bipartite structure, that is, one where we have two classes of elements, with relations only between elements of opposite classes.

In fact, a general theory of Cheeger-type inequalities constitutes the core of this book. A Cheeger-type inequality relates an eigenvalue of a Laplace operator with a global quantity of the underlying structure, expressing how difficult it is to cut that structure into two large pieces. The larger the part of the structure, for instance, an edge set for a graph, needed for the cut, the larger that constant, and according to the inequality, that is bounded from above and below by an eigenvalue of the Laplacian. There are two conceptual issues. First, the Cheeger-type constant is a discrete quantity, whereas the Laplacian and its eigenvalues are continuous objects, in the sense that they succumb to

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the tools of analysis. This issue will be systematically resolved via Lovász-type extensions that turn a discrete optimization problem into a continuous one. The second issue is that the Cheeger-type constant is an L^1-quantity, whereas the Laplacian naturally operates on L^2-spaces. That issue will be resolved by looking at L^p-Laplacians. The case $p \to 1$ is the most difficult, but also the most useful, as it turns the inequality into an equality. Equipped with such techniques, we can also derive novel Cheeger-type inequalities for simplicial complexes and hypergraphs.

We shall supply many examples, particularly those that exhibit certain extremal properties of the spectra that we investigate.

Our interest is with *finite* structures. Recently, two monographs [171, 174] appeared that address the spectral theory of infinite graphs. They are complementary to ours. Another book [178] also addresses relations between the spectrum and the geometry of the underlying graph, but with a focus on the trace formula and inverse problems, that is, topics not covered in our book. In fact, Kurasov considers graphs as metric spaces, which leads to infinite spectra. This is very different from our approach that works with finite structures.

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