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Spectral Methods

1 Individual Project's contribution to the CRP

1.1 Aims and Objectives

The foundations of spectral graph theory were laid in the fifties and sixties of the 20th century. Eigenvalues of the adjacency matrix and (signless) Laplacian matrix of graphs have since then received much attention as a means of characterizing classes of graphs and for obtaining bounds on properties such as the diameter, girth, chromatic number, connectivity and many others [1, 3–6, 8]. The corresponding eigenvectors of such matrices hold a lot of information of the underlying class. Hence they have been used quite successfully for heuristics for hard combinatorial problems including graph partitioning, coloring, clustering, and graph drawing, see, e.g., Bıyıkoğlu et al. [2]. They have been used for page ranking algorithms and there is even an attempt to find optimal moves for the board game Go. An important example is combinatorial optimization. There Grover [9] and others (e.g., [10]) made the astonishing observation that the cost function (shifted by the average cost) is in many cases an eigenfunction of the Laplacian of the graph that represents the configuration space of the optimization problem (called *landscape*). Such optimization problems occur frequently in mathematical biology and finding heuristics for good solutions is often crucial, see PI Stadler.

Near products. It is a well-known fact that eigenvectors of Cartesian products can be easily constructed by the Kronecker product of the eigenvectors of its factors. Thus it is possible to derive the product structure from the set of eigenvectors. For approximate products (where some edges are deleted and/or additional edges are inserted) this simple structure is disturbed. However, for small changes the deviations may be small enough to use eigenvector for a guess of the approximate product structure.

Landscapes. Landscapes in combinatorial optimization are characterized naturally in terms of their projection on the eigenspaces of the Laplace matrix of the underlying graph. The number of nodal domains can be seen a measure for the roughness of a cost function in fitness landscapes (see PI Stadler). This number is generally bounded from above by Courant's nodal domain theorem, see Davies et al. [7]. For example, there exists just one such nodal domain for the principle eigenvector and Fiedler vectors have exactly two such nodal domains. For higher order eigenvalue the bound is not sharp in general and can be improved for particular graph classes, see [2] for examples. We plan to explore the nodal domains for landscapes and their connection to other geometric properties like saddle point and local optima of such eigenvectors.

Aims. The geometry of eigenvectors can give valuable information about the underlying optimization problem. Thus one aim of this IP is to explore the geometric properties of such eigenvectors which are important for molecular biology (see PI Stadler for further details).

A second aim of the project is to investigate possible relations between the structure of eigenvectors and spectral plots of a graph and (approximate) product structures as described by PI Leydold and AP Imrich. This will be conducted in close collaboration with these partners.

For our third objective consider the following problem that arise in geometric graph theory. Given a distance matrix D of points and a radius r we can create a graph $G_r(D)$ in the following way: vertices x and y are adjacent if and only if their distance D_{xy} does not exceed r. Then for a certain monotone graph property P one can ask for the threshold θ such that $G_r(D)$ has property P for all $r \geq \theta$. Another question is for a threshold where we see certain subgraphs (called motifs). We can also ask about the effect of transformations of the distance matrix D. Here we are interested in connections between eigenvalues and eigenvectors of the the distance matrix D

and those of the resulting graph $G_r(D)$. In particular the influence of simple transformations will be investigated.

1.2 Methodologies

Eigenvectors and eigenvalues are simply described: They must satisfy the eigenvalue equation. From this starting point a couple of tools are available like the Courant-Fisher Theorem (minimax theorem), Perron-Frobenius Theorem, and perturbation theory for matrices. There exists literature that investigates the influence of graph rearrangements on graph eigenvalues. The influence on the valuation of the corresponding eigenvector is, however, less investigated, see Bıyıkoğlu et al. [2]. We found that the concepts of Perron vectors and geometric nodal domains quite useful in exploring the structure of eigenvectors.

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