

Executive Summary of Minor Research Project entitled

THE LAPLACIAN SPECTRUM OF GRAPHS AND  
STUDY OF INVERSE EIGEN VALUE PROBLEMS.

Spectral Graph Theory is the study of the spectra of certain matrices defined from a given graph, including the adjacency matrix, the Laplacian matrix and other related matrices. Graph Spectra have been studied extensively for more than fifty years. For the past two decades, the interest has been developed in the study of the generalized Laplacian matrix of a graph, that is, real symmetric matrices with negative off-diagonal entries in the positions described by the edges of the graph and zero in all other off-diagonal positions. Spectral Graph Theory has traditionally used the spectra of specific matrices associated with the graph such as the adjacency matrix, Laplacian matrix or other normalized forms to provide information about the graph. For certain families of graphs it is possible to characterize a graph by the spectrum of certain matrices associated with the graph. More generally, this is not possible, but many useful information about the graph can be obtained from the spectra of these various matrices.

Just as astronomers study stellar spectra to determine the make-up of distant stars one of the main goals in the graph theory is to deduce the principal properties and structure of a graph from its graph spectrum. We will see that eigenvalues are closely related to almost all major invariants of a graph, linking one extremal property to another. Further speaking, eigenvalues play a central role in our fundamental understanding of graphs. The study of eigenvalues realizes increasing rich connections with many other areas of mathematics. A major development is the relation between spectral graph theory and differential geometry. There is an interesting analogy between Spectral Riemannian Geometry and Spectral Graph Theory. Algebraic spectral methods are also very useful especially for extremal examples and constructions. Also there are wide applications in the field of chemistry.

Eigenvalues are associated with the stability of molecules. Graph spectra arise naturally in various problems of theoretical physics, quantum mechanics, for example in minimizing energies of Hamiltonian systems. The progress on expander graphs and eigenvalues was initiated by problems in communication networks. Applications of graph eigenvalues occur in numerous areas in different guises.

Also my work includes the study of numerous graph invariants including connectivity, expanding properties, the limit points of laplacian spectra of graphs, laplacian spectra and invariants of graphs, a relation between the matching number and laplacian spectrum of graph and bounds of laplacian spectrum based on the domination number. Also a comparison between the spectra of graphs and trees are studied. A review of the Inverse Eigen Value Problem also done.

In this project I have discussed many representations of a graph as matrices and a review of study has done regarding which representation is comparatively more reliable. The main difficulty we encounter is the co spectrality between graphs. A deep study has made and I have presented a paper in this area. The Spectrum of a graph has been widely used in graph theory to characterize the properties of a graph and extract information from its structure. It is also used as a tool for graph representation for pattern matching tasks. Its use has not gained wide acceptance as a representation for matching and comparison of graphs. There are two main reasons for this; firstly more than one graph may share the same spectrum and secondly, the spectrum may change dramatically with a small change structure. Graph structures have been used to represent structural and relational arrangements of entities in many vision problems. The key problem in utilizing graph representations lies in measuring their structural similarity. This is a difficult problem because there are no explicit labeling of the parts and correspondences must be established before similarity can be assessed. Spectral Graph theory provides a method to the problem of graph similarity. This approach is based on a branch of mathematics that is concerned with

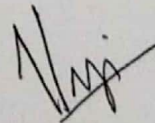


characterizing the structural properties of graphs using the eigen vectors and eigen values of its related matrices.

Two graphs are said to be co spectral if they have the same eigen values with respect to the matrix representation being used. Trees cannot be uniquely defined by the spectrum. This result does not tell us the size that trees need to be before this becomes a problem. The trees need to be very large in size in order to have a significant chance of finding a cospectral pair. However, the matrix representation chosen for the graph has a large impact on the chance of finding cospectral pair.

Survey shows that the adjacency matrix appears to be the worst representation in terms of producing a large number of cospectral pairs. The laplacian is superior in this regard and the signless Laplacian even better. The normalized laplacian initially appears to be inferior, but the fraction of cospectral graphs rapidly falls and becomes far smaller than for other representations for larger graphs. The normalized laplacian produces approximately 0.2% co spectral graphs with 11 vertices. In contrast, the signless laplacian, laplacian, and adjacency matrix produces 3.8%, 9%, 21 % respectively.

The results show that the use of the Laplacian or related matrices can drastically reduce the problem of cospectrality between trees. As a graph similarity measure, Laplacian matrix and spectrum seems to be superior. The adjacency matrix is the weakest representation of the ones investigated. While the performance of the signless laplacian is similar to that of the Laplacian, the normalized Laplacian seems to be less effective



**SIGNATURE OF PRINCIPAL INVESTIGATOR**



Now we shall discuss how the graph properties can be extracted from the spectra of these matrices.

From the spectrum of the adjacency matrix the following details can be extracted. Let the characteristic polynomial of  $A$  be  $p(x) = x^n + a_{n-2}x^{n-2} + \dots + a_1x + a_0$ . Note that  $a_{n-1} = 0$  as  $\text{trace}(A) = 0$ .

1. The number of edges in  $G = -a_{n-2} = \frac{\text{trace}(A^2)}{2} = \frac{\sum \alpha_i^2}{2}$
2. The number of triangles in  $G = \frac{-a_{n-3}}{6} = \frac{\text{trace}(A^3)}{6} = \frac{\sum \alpha_i^3}{6}$

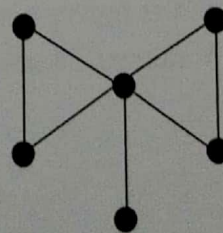
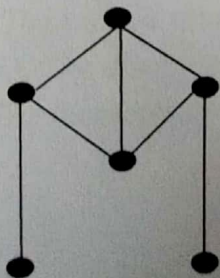
From the Laplacian spectrum the following properties of graph structure can be viewed.

1. If  $G = (V, E)$  be a simple graph with  $n$  vertices, then the multiplicity of  $n$  as an eigen value of  $L(G)$  is at least  $s-1$  if and only if  $G$  contains a complete  $s$ -partite graph on  $V$  as a subgraph.
2. If a connected graph  $G$  has a pendant vertex, then the multiplicity of an eigen value  $n$  of  $L(G)$  is at most 1.
3. If  $G$  is a simple connected graph with an eigen value  $(0 < \lambda < 1)$ , then the diameter of  $G$  is at least 3.
4. If  $G$  is a simple connected graph of order  $n (> 2)$  and  $G$  has a pendant vertex, then the smallest non zero eigen value is less than or equal to 1. More over, the smallest non zero eigen value is strictly less than 1 if the pendant vertex is not adjacent to the highest degree vertex.
5. For a graph  $G$  on  $n$  vertices,  $\sum_i \lambda_i \leq n$ , with equality holding if and only if  $G$  has no isolated vertices.
6. For  $n \geq 2$ ,  $\lambda_1 \leq \frac{n}{n-1}$  with equality holding if and only if  $G$  is the complete graph on  $n$  vertices. Also for a graph  $G$  without isolated vertices, we have  $\lambda_{n-1} \geq \frac{n}{n-1}$

One important use of Spectral graph theory is to determine whether two graphs are isomorphic. If two graphs have different spectra or equivalently different characteristic polynomials then clearly they are not isomorphic. However, non-isomorphic graphs can be cospectral. Two graphs are said to be **cospectral** if they have the same eigen values with respect to the matrix representation used.

Example: Given below are cospectral graphs with characteristic polynomial

$$p(x) = x^6 - 7x^4 - 4x^3 + 7x^2 + 4x - 1$$





**Theorem:**

If  $G$  is not  $K_n$ , then  $\lambda_2 \leq \kappa_0$ . The diameter of a connected graph  $G$  is less than the number of distinct eigen values of the adjacency matrix.

**4. GRAPH DISTANCE**

There are a number of ways to measure the distance between two graphs; the most appropriate is the **edit distance**. The edit distance is defined by a sequence of operations, which includes edge and vertex deletion and insertion that transform one graph into another. Each of these operations has an associated cost, and the total cost of a sequence of edits is the sum of the individual costs. The sequence of minimal cost which transforms one graph into another is the edit distance between graphs.

The spectral distance between the graphs  $G_1$  and  $G_2$  is the Euclidean distance between the spectra.  $d_s(G_1, G_2) = \sqrt{\sum_i (s_i - t_i)^2}$ . When the spectra are of different sizes then the smaller spectra are adjoined with the zero values. This is equivalent to adding disjoint vertices to the smaller graphs to make both graphs the same vertex cardinality.

If the spectrum is to be a good representation, the spectral distance should be related to the edit distance between the graphs.

**5. CLASSIFICATION AND CLUSTERING**

These are the two central tasks in pattern recognition and they are of huge practical importance. Similarity based classification is an important task for graphs particularly on large graph databases. In such situations the spectrum of the graph would be an ideal tool, as it is easy to compute from the corresponding matrix representation. If the spectrum of a matrix is a good representation then we should be able to group similar graphs together.

**6. APPLICATIONS****1. Spectral Embeddings**

Considering the Laplacian as a quadratic form measuring the difference between values of a vector across all edges in a graph, we see that a Laplacian eigen vector of low eigen value must have values that are very similar on adjacent vertices. This property makes Laplacian eigen vectors of low eigen value useful for generating embeddings of arbitrary graphs into Euclidean space. This is the basis for a number of nonlinear dimensionality reduction techniques. The problem is: given a set of data points in a very high dimensional space, we want to embed the points in a lower dimensional space such that the distance between the points are approximately preserved. But sometimes, it may not be possible to preserve the distance between the farther points; hence we wish to preserve distances between the nearby points.

**2. Graph Colouring Heuristics**

The eigen vector corresponding to the highest eigen value in the case of a wheel graph oscillated between  $+1$  and  $-1$  on adjacent vertices. This leads to a heuristic idea for graph colouring



problems: we can look at eigen vectors with high eigen value and colour vertices with different colours according to their value in that eigen vector. .

### **3. Graph isomorphism**

Two graphs are isomorphic if and only if there is a permutation of the labelling of the vertices such that the two graphs have all the same edges. Hence  $H$  and  $G$  are isomorphic if and only if  $P^T L(G)P = L(H)$  for some permutation  $P$ . Since the eigen values are invariant under unitary transformations, and permutations are a subset of unitary transformations, it follows that  $H$  and  $G$  must have the same eigen values if they are isomorphic. The converse is not true. But there are some tricks for some converses. If we can find an eigen value whose eigen vector has all of its entries distinct, then that eigen vector defines a unique permutation of vertices.

### **7. CONCLUSIONS**

All the matrix representations can reduce the problem of cospectrality between graphs and trees. When the trees are large enough, almost all trees are cospectral. For all these representations, there is a close relationship between the edit distance and the spectral distance. As a graph similarity measure, the Laplacian matrix seems to be superior. The adjacency matrix is the weakest of all representations and its spectrum is not used to represent the underlying graph. The signless Laplacian performs similar to the Laplacian, but the normalized laplacian seems to be less effective.