Graph Characterization Using Gaussian Wave Packet Signature

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Abstract. In this paper we present a new approach for characterizing graphs using the solution of the wave equation. The wave equation provides a richer and potentially more expressive means of characterizing graphs than the more widely studied heat equation. Unfortunately the wave equation whose solution gives the kernel is less easily solved than the corresponding heat equation. There are two reasons for this. First, the wave equation can not be expressed in terms of the familiar node-based Laplacian, and must instead be expressed in terms of the *edge-based Laplacian*. Second, the eigenfunctions of the edge-based Laplacian are more complex than that of the node-based Laplacian. In this paper we present a solution to the wave equation, where the initial condition is Gaussian wave packets on the edges of the graph. We propose a global signature of the graph which is based on the amplitudes of the waves at different edges of the graph over time. We apply the proposed method to both synthetic and real world datasets and show that it can be used to characterize graphs with higher accuracy.

Keywords: Edge-based Laplacian, Wave Equation, Gaussian wave packet, Graph Characterization.

1 Introduction

Graphs-based methods are frequently used to solve problems in many areas including computer vision machine learning and pattern recognition. This is due to the fact that most real world data can be conveniently represented by graphs or meshes. For example a color or a gray-scale image can be represented using a planar graph, where vertices are corners of the objects and edges represent some geometric relationship between the vertices. Similarly a chemical data structure can be represented using a graphs, where vertices represent atoms and edges represent bonds between the edges. A three-dimensional shapes can be conveniently represented using a mesh that approximates the bounding surface of the body. Once the graph of the object is extracted, we can use these graphs to find both the local and global properties of the object itself.

One of the most popular way of characterizing graph structure is to use spectral methods, which make use of the eigenvalues and eigenvectors of the Laplacian matrix. The Laplacian matrix is defined using the adjacency matrix of the

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graph and can be used to link equations from analysis to graph. Over the recent years many researchers have successfully used the solutions of partial differential equations defined using the Laplacian matrix to characterize graphs. For example, Xiao et al [1] have used heat kernel, which is derived from graph Laplacian, to embed the nodes of a graph in Euclidean space. Zhang et al[2] have used the heat kernel for anisotropic image smoothing. Sun et al[3] have used the heat kernel on mesh for defining signatures for 3D shapes and this is referred to as Heat Kernel Signature. Aubry et al[4] have used the solution of Schrödinger equation to define Wave Kernel Signature, which represents the average probability of measuring a quantum mechanical particle at a specific location. There are many other applications of graph Laplacian in the literature.

The discrete Laplacian defined over the vertices of a graph, however, cannot link most results in analysis to a graph theoretic analogue. For example the wave equation $u_{tt} = \Delta u$, defined with discrete Laplacian, does not have finite speed of propagation. In [5,6], Friedman and Tillich develop a calculus on graph which provides strong connection between graph theory and analysis. Their work is based on the fact that graph theory involves two different volume measures. i.e., a "vertex-based" measure and an "edge-based" measure. This approach has many advantages. It allows the application of many results from analysis directly to the graph domain.

While the method of Friedman and Tillich leads to the definition of both a divergence operator and a Laplacian (through the definition of both vertex and edge Laplacian), it is not exhaustive in the sense that the edge-based eigenfunctions are not fully specified. In a recent study we have fully explored the eigenfunctions of the edge-based Laplacian and developed a method for explicitly calculating the edge-interior eigenfunctions of the edge-based Laplacian [7]. This reveals a connection between the eigenfunctions of the edge-based Laplacian and both the classical random walk and the backtrackless random walk on a graph. The eigensystem of the edge-based Laplacian contains eigenfunctions which are related to both the adjacency matrix of the line graph and the adjacency matrix of the oriented line graph.

As an application of the edge-based Laplacian, we have recently presented a new approach to characterizing points on a non-rigid three-dimensional shape[8]. This is based on the eigenvalues and eigenfunctions of the edge-based Laplacian, constructed over a mesh that approximates the shape. This leads to a new shape descriptor signature, called the Edge-based Heat Kernel Signature (EHKS). The EHKS was defined using the heat equation, which is based on the edge-based Laplacian. This has applications in shape segmentation, correspondence matching and shape classification.

Wave equation provides potentially richer characterisation of graphs than heat equation. Initial work by Howaida and Hancock [9] has revealed some of its potential uses. They have proposed a new approach for embedding graphs on pseudo-Riemannian manifolds based on the wave kernel. However, there are two problems with the rigourous solution of the wave equation; a) we need to compute the edge-based Laplacian, and b) the solution is more complex than the heat equation. Recently we [10] have presented a solution of the edge-based wave equation on a graph. We assume that initial condition is a Gaussian wave packet on the edge of the graph, and show the evolution of this wave packet over time.

In this paper we propose a new signature for characterizing graphs, which is based on the solution of edge-based wave equation. The signature is constructed by assuming a Gaussian wave packet on a single edge of the graph and use the amplitude of the wave on different edges over different times to construct a unique signature for the graph.The remainder of this paper is organized as follows. We commence by introducing graphs and some definitions. In section 3, we introduce the eigensystem of the edge-based Laplacian. In section 4, we give a general solution of the wave equation, and the solution for the Gaussian wave packet as initial condition. In section 5, we define the proposed wave packet signature for the graph. Finally, in the experiment section, we apply the proposed method to both synthetic and real-world dataset.

2 Graphs

A *graph* $G = (\mathcal{V}, \mathcal{E})$ consists of a finite nonempty set $\mathcal{V}$ of *vertices* and a finite set $\mathcal{E}$ of unordered pairs of vertices, called *edges*. A *directed graph* or *digraph* $D = (\mathcal{V}_D, \mathcal{E}_D)$ consists of a finite nonempty set $\mathcal{V}_D$ of vertices and a finite set $\mathcal{E}_D$ of ordered pairs of vertices, called *arcs*. So a digraph is a graph with an orientation on each edge. A digraph D is called *symmetric* if whenever (u, v) is an arc of D, (v, u) is also an arc of D. There is a one-to-one correspondence between the set of symmetric digraphs and the set of graphs, given by identifying an edge of the graph with an arc and its inverse arc on the digraph on the same vertices. We denote by $D(G)$ the symmetric digraph associated with the graph G.

The *line graph* $L(G) = (\mathcal{V}_L, \mathcal{E}_L)$ is constructed by replacing each arc of $D(G)$ by a vertex. These vertices are connected if the head of one arc meets the tail of another. Therefore

$$\mathcal{V}_L = \{(u, v) \in D(G)\}$$

$$\mathcal{E}_L = \{((u, v), (v, w)) : (u, v) \in D(G), (v, w) \in D(G)\}$$

The *oriented line graph* $OL(G) = (\mathcal{V}_O; \mathcal{E}_O)$ is constructed in the same way as the $L(G)$ except that reverse pairs of arcs are not connected, i.e. $((u, v), (v, u))$ is not an edge. The vertex and edge sets of $OL(G)$ are therefore

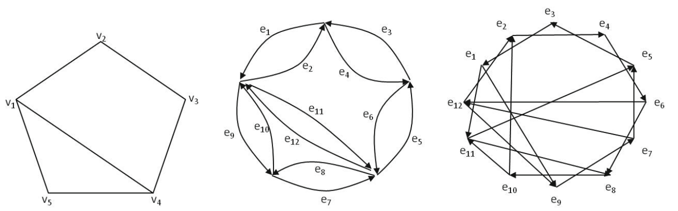
$$\mathcal{V}_O = \{(u, v) \in D(G)\}$$

$$\mathcal{E}_O = \{((u, v), (v, w)) : (v, w)), (u, v) \in D(G), (v, w) \in D(G), u \neq w\}$$

The *complement* or *inverse* of a graph G is a graph with the same vertex set but whose edge set consists of the edges not present in G. The complement is denoted by $\overline{G} = (\overline{\mathcal{V}}, \overline{\mathcal{E}})$, where

$$\overline{\mathcal{V}} = \mathcal{V}$$

$$\overline{\mathcal{E}} = \{(u, v) : (u, v) \notin \mathcal{E}\}$$



(a) Graph (b) Diagraph (c) Oriented line graph

Fig. 1. Graph, its digraph, and its oriented line graph

Figure 1(a) shows a simple graph, 1(b) its digraph, and 1(c) the corresponding oriented line graph. A random walk on the vertices of $L(G)$ represents the sequence of edges traversed in a random walk on the original graph G. Similarly, a random walk on the $OL(G)$ represents the sequence of edges traversed in a random walk on G where backtracking steps are not allowed (a backtrackless walk).

3 Edge-Based Eigensystem

In this section we review the eigenvalues and eigenfunction of the edge-based Laplacian[5][7]. Let $G = (\mathcal{V}, \mathcal{E})$ be a graph with a boundary ∂G. Let $\mathcal{G}$ be the geometric realization of G. The geometric realization is the metric space consisting of vertices $\mathcal{V}$ with a closed interval of length l_e associated with each edge $e \in \mathcal{E}$. We associate an edge variable x_e with each edge that represents the standard coordinate on the edge with $x_e(u) = 0$ and $x_e(v) = 1$. For our work, it will suffice to assume that the graph is finite with empty boundary (i.e., $\partial G = 0$) and $l_e = 1$.

3.1 Vertex Supported Edge-Based Eigenfunctions

The vertex-supported eigenpairs of the edge-based Laplacian can be expressed in terms of the eigenpairs of the normalized adjacency matrix of the graph. Let A be the adjacency matrix of the graph G, and $\tilde{A}$ be the row normalized adjacency matrix. i.e., the $(i,j)th$ entry of $\tilde{A}$ is given as $\tilde{A}(i,j) = A(i,j)/\sum_{(k,j)\in\mathcal{E}} A(k,j)$. Let $(\phi(v), \lambda)$ be an eigenvector-eigenvalue pair for this matrix. Note $\phi(.)$ is defined on vertices and may be extended along each edge to an edge-based eigenfunction. Let ω^2 and $\phi(e, x_e)$ denote the edge-based eigenvalue and eigenfunction. Here $e = (u, v)$ represents an edge and x_e is the standard coordinate on the edge (i.e., $x_e = 0$ at v and $x_e = 1$ at u). Then the vertex-supported eigenpairs of the edge-based Laplacian are given as follows:

1. For each $(\phi(v), \lambda)$ with $\lambda \neq \pm 1$, we have a pair of eigenvalues ω^2 with $\omega = \cos^{-1}\lambda$ and $\omega = 2\pi - \cos^{-1}\lambda$. Since there are multiple solutions to

$\omega = \cos^{-1}\lambda$, we obtain an infinite sequence of eigenfunctions; if $\omega_0 \in [0, \pi]$ is the principal solution, the eigenvalues are $\omega = \omega_0 + 2\pi n$ and $\omega = 2\pi - \omega_0 + 2\pi n, n \geq 0$. The eigenfunctions are $\phi(e, x_e) = C(e)\cos(B(e) + \omega x_e)$ where

$$C(e)^2 = \frac{\phi(v)^2 + \phi(u)^2 - 2\phi(v)\phi(u)\cos(\omega)}{\sin^2(\omega)}$$

$$\tan(B(e)) = \frac{\phi(v)\cos(\omega) - \phi(u)}{\phi(v)\sin(\omega)}$$

There are two solutions here, $\{C, B_0\}$ or $\{-C, B_0 + \pi\}$ but both give the same eigenfunction. The sign of $C(e)$ must be chosen correctly to match the phase.

2. $\lambda = 1$ is always an eigenvalue of $\tilde{A}$. We obtain a principle frequency $\omega = 0$, and therefore since $\phi(e, x_e) = C\cos(B)$ and so $\phi(v) = \phi(u) = C\cos(B)$, which is constant on the vertices.
3. If the graph is bipartite then $\lambda = -1$ is an eigenvalue of $\tilde{A}$. We obtain a principle frequency $\omega = \pi$, and therefore since $\phi(e, x_e) = C\cos(B + \pi x_e)$ and so $\phi(v) = -\phi(u)$, implying an alternating sign eigenfunction.

3.2 Edge-Interior Eigenfunctions

The edge-interior eigenfunctions are those eigenfunctions which are zero on vertices and therefore must have a principle frequency of $\omega \in \{\pi, 2\pi\}$. Recently we have shown that these eigenfunctions can be determined from the eigenvectors of the adjacency matrix of the oriented line graph[7]. We have shown that the eigenvector corresponding to eigenvalue $\lambda = 1$ of the oriented line graph provides a solution in the case $\omega = 2\pi$. In this case we obtain $|\mathcal{E}| - |\mathcal{V}| + 1$ linearly independent solutions. Similarly the eigenvector corresponding to eigenvalue $\lambda = -1$ of the oriented line graph provides a solution in the case $\omega = \pi$. In this case we obtain $|\mathcal{E}| - |\mathcal{V}|$ linearly independent solutions. This comprises all the principal eigenpairs which are only supported on the edges.

3.3 Normalization of Eigenfunctions

Note that although these eigenfunctions are orthogonal, they are not normalized. To normalize these eigenfunctions we need to find the normalization factor corresponding to each eigenvalue and divide each eigenfunction with the corresponding normalization factor. Let $\rho(\omega)$ denotes the normalization factor corresponding to eigenvalue ω. Then

$$\rho^2(\omega) = \sum_{e \in \mathcal{E}} \int_0^1 \phi^2(e, x_e)\, dx_e$$

Evaluating the integral, we get

$$\rho(\omega) = \sqrt{\sum_{e \in \mathcal{E}} C(e)^2 \left[\frac{1}{2} + \frac{\sin(2\omega + 2B(e))}{4\omega} - \frac{sin(2B(e))}{4\omega}\right]}$$

Once we have the normalization factor to hand, we can compute a complete set of orthonormal bases by dividing each eigenfunction with the corresponding normalization factor. Once normalized, these eigenfunctions form a complete set of orthonormal bases for $L^2(\mathcal{G}, \mathcal{E})$.

4 Solution of the Wave Equation

Let a graph coordinate $\mathcal{X}$ defines an edge e and a value of the standard coordinate on that edge x. The eigenfunctions of the edge-based Laplacian are

$$\phi_{\omega,n}(\mathcal{X}) = C(e,\omega)\cos\left(B(e,\omega) + \omega x + 2\pi n x\right)$$

The edge-based wave equation is

$$\frac{\partial^2 u}{\partial t^2}(\mathcal{X}, t) = \Delta_E u(\mathcal{X}, t) \tag{1}$$

We look for separable solutions of the form $u(\mathcal{X}, t) = \phi_{\omega,n}(\mathrm{X})g(t)$. This gives

$$\phi_{\omega,n}(\mathcal{X})g''(t) = g(t)\left(\omega + 2\pi n\right)^2 \phi(\omega, n)$$

which gives a solution for the time-based part as

$$g(t) = \alpha_{\omega,n}\cos\left[(\omega + 2\pi n)t\right] + \beta_{\omega,n} sin\left[(\omega + 2\pi n)t\right]$$

By superposition, we obtain the general solution

$$\begin{aligned} u\left(\mathcal{X}, t\right) = \sum_{\omega}\sum_{n} & C(e,\omega)\cos\left[B(e,\omega) + \omega x + 2\pi n x\right] \\ & \left\{\alpha_{\omega,n}\cos\left[(\omega + 2\pi n)t\right] + \beta_{\omega,n} sin\left[(\omega + 2\pi n)t\right]\right\} \end{aligned} \tag{2}$$

4.1 Initial Conditions

Since the wave equation is second order partial differential equation, we can impose initial conditions on both position and speed

$$u(\mathcal{X}, 0) = p(\mathcal{X})$$

$$\frac{\partial u}{\partial t}(\mathcal{X}, 0) = q(\mathcal{X})$$

and we obtain

$$p(\mathcal{X}) = \sum_{\omega}\sum_{n} \alpha_{\omega,n} C(e,\omega)\cos\left[B(e,\omega) + \omega x + 2\pi n x\right]$$

$$q(\mathcal{X}) = \sum_{\omega}\sum_{n} \beta_{\omega,n}(\omega + 2\pi n) C(e,\omega)\cos\left[B(e,\omega) + \omega x + 2\pi n x\right]$$

We can obtain these coefficients using the orthogonality of the eigenfunctions. So we get

$$\alpha_{\omega,n} = \sum_e C(e,\omega)\frac{1}{2}\left[F_{\omega,n} + F^*_{\omega,n}\right]$$

where

$$F_{\omega,n} = e^{iB}\int_0^1 dxp(e,x)e^{i\omega x}e^{i2\pi n}$$

similarly

$$\beta_{\omega,n}(\omega + 2\pi n) = \sum_e C(e,\omega)\frac{1}{2}\left[G_{\omega,n} + G^*_{\omega,n}\right]$$

where

$$G_{\omega,n} = e^{iB}\int_0^1 dxq(x,e)e^{i(\omega+2\pi n)x} = e^{iB}\int_0^1 dxp'(x,e)e^{i(\omega+2\pi n)x}$$

4.2 Gaussian Wave Packet

Let the initial position be a Gaussian wave packet $p(e,x) = e^{-a(x-\mu)^2}$ on one particular edge and zero everywhere else. Then we have

$$\begin{aligned} F_{\omega,n} &= e^{iB}\int_0^1 dxe^{-a(x-\mu)^2}e^{i\omega x}e^{i2\pi nx} \\ &= e^{iB}e^{i\mu\omega}e^{-\frac{\omega^2}{4a}}\int_0^1 dxe^{-a\left(x-\mu-\frac{i\omega}{2a}\right)^2}e^{i2\pi nx} \end{aligned}$$

Let the Gaussian is fully contained on one edge. i.e., $p(x,e)$ is only supported on this edge, then

$$F_{\omega,n} = e^{iB}e^{i\mu\omega}e^{-\frac{\omega^2}{4a}}\int_{-\infty}^{\infty} dxe^{-a\left(x-\mu-\frac{i\omega}{2a}\right)^2}e^{i2\pi nx}$$

Solving, we get

$$F_{\omega,n} = \sqrt{\frac{\pi}{a}}e^{i[B+\mu(\omega+2\pi n)]}e^{-\frac{1}{4a}(\omega+2n\pi)^2}$$

Similarly we obtain

$$F^*_{\omega,n} = \sqrt{\frac{\pi}{a}}e^{-i[B+\mu(\omega+2\pi n)]}e^{-\frac{1}{4a}(\omega+2n\pi)^2}$$

and so

$$\alpha_{\omega,n} = \sqrt{\frac{\pi}{a}}e^{-\frac{1}{4a}(\omega+2n\pi)^2}C(e,\omega)\cos[B + \mu\,(\omega + 2\pi n)] \tag{3}$$

Since $p(x,e)$ is zero at both ends the coefficients β can be found straightforwardly.

$$\beta_{\omega,n} = \sqrt{\frac{\pi}{a}}e^{-\frac{1}{4a}(\omega+2n\pi)^2}C(e,\omega)\sin[B + \mu\,(\omega + 2\pi n)] \tag{4}$$

4.3 Complete Reconstruction

Let f be the edge on which the initial function is non-zero. Let the Gaussian is fully contained on one edge. Then

$$u(\mathcal{X},t) = \sum_{\omega} \sqrt{\frac{\pi}{a}} C(\omega,e)C(\omega,f) \sum_{n} e^{-\frac{1}{4a}(\omega+2\pi n)^2}$$
$$\cos\left[B(\omega,e)+\omega x+2\pi n x\right]\cos\left[B(\omega,f)+(\omega+2\pi n)(t+\mu)\right]$$

For a particular sequence with principal eigenvalue ω, we need to calculate

$$u_\omega = \sum_n \sqrt{\frac{\pi}{a}} e^{-\frac{1}{4a}(\omega+2\pi n)^2} \cos\left[B(\omega,e)+\omega x+2\pi n x\right]\cos\left[B(\omega,f)+(\omega+2\pi n)(t+\mu)\right]$$

Writing the cosine in exponential form, we obtain

$$\begin{aligned} u_w = & \sum_n \sqrt{\frac{\pi}{a}} e^{-\frac{1}{4a}(\omega+2\pi n)^2} \\ & \times \frac{1}{4}\left[e^{i[B(e,\omega)+B(f,\omega)]} e^{i(\omega+2\pi n)(x+t+\mu)} + e^{-i[B(e,\omega)+B(e,\omega)]} e^{-i(\omega+2\pi n)(x+t+\mu)}\right. \\ & \left. + e^{i[B(e,\omega)-B(f,\omega)]} e^{i(\omega+2\pi n)(x-t-\mu)} + e^{-i[B(e,\omega)-B(e,\omega)]} e^{-i(\omega+2\pi n)(x-t-\mu)}\right] \end{aligned}$$

We need to evaluate terms like terms like $\sum_n \frac{\pi}{a} e^{-\frac{1}{4a}} e^{i[B(e,\omega)+B(f,\omega)]} e^{i(\omega+2\pi n)(x+t+\mu)}$, where the values of ω and n depend on the particular eigenfunction sequence under evaluation.

Let $\mathcal{W}(z)$ be z wrapped to the range $[-\frac{1}{2},\frac{1}{2})$, i.e.,

$$\mathcal{W}(z) = z - \left\lfloor z + \frac{1}{2} \right\rfloor$$

Solving for all cases, the complete solution becomes

$$\begin{aligned} u(\mathcal{X},t) = & \sum_{\omega\in\Omega_a} \frac{C(\omega,e)C(\omega,f)}{2} \left(e^{-a\mathcal{W}(x+t+\mu)^2} \cos\left[B(e,\omega)+B(f,\omega)+\omega\left\lfloor x+t+\mu+\frac{1}{2}\right\rfloor\right]\right. \\ & \left. + e^{-a\mathcal{W}(x-t-\mu)^2} \cos\left[B(e,\omega)-B(f,\omega)+\omega\left\lfloor x-t-\mu+\frac{1}{2}\right\rfloor\right]\right) \\ & + \frac{1}{2|E|}\left(\frac{1}{4}e^{-a\mathcal{W}(x+t+\mu)^2} + \frac{1}{4}e^{-a\mathcal{W}(x-t-\mu)^2}\right) \\ & + \sum_{\omega\in\Omega_c} \frac{C(\omega,e)C(\omega,f)}{4}\left(e^{-a\mathcal{W}(x-t-\mu)^2} - e^{-a\mathcal{W}(x+t+\mu)^2}\right) \\ & + \sum_{\omega\in\Omega_c} \frac{C(\omega,e)C(\omega,f)}{4}\left((-1)^{\left\lfloor x-t-\mu+\frac{1}{2}\right\rfloor} e^{-a\mathcal{W}(x-t-\mu)^2}\right. \\ & \left. -(-1)^{\left\lfloor x+t+\mu+\frac{1}{2}\right\rfloor} e^{-a\mathcal{W}(x+t+\mu)^2}\right) \end{aligned} \quad (5)$$

where Ω_a represents the set of vertex-supported eigenvalues and Ω_b and Ω_c represent the set of edge-interior eigenvalues respectively. i.e., π and 2π.

5 Wave Packet Signatures

Once a complete solution of the edge-based wave equation is known, we can use it to define both local and global signatures for graphs and meshes. In this paper we define a global signature for characterizing graphs which is based on amplitudes of waves on the edges of the graph over time. To define the signature we assume that the initial condition is a Gaussian wave packet on a single edge of the graph. For this purpose we select the edge $(u, v) \in E$, such that u is the highest degree vertex in the graph and v is the highest degree vertex in the neighbours of u. We define the local signature of an edge as

$$WPS(\mathcal{X}) = [u(\mathcal{X}, t_0), u(\mathcal{X}, t_1), u(\mathcal{X}, t_2), ...u(\mathcal{X}, t_n)] \tag{6}$$

Given a graph G, we define its global wave packet signature as

$$GWPS(G) = hist\left(WPS(\mathcal{X}_1), WPS(\mathcal{X}_2), , ..., WPS(\mathcal{X}_{|E|})\right) \tag{7}$$

where hist(.) is the histogram operator which bins the list of arguments $WPS(\mathcal{X}_1)$, $WPS(\mathcal{X}_2), , ..., WPS(\mathcal{X}_{|E|})$.

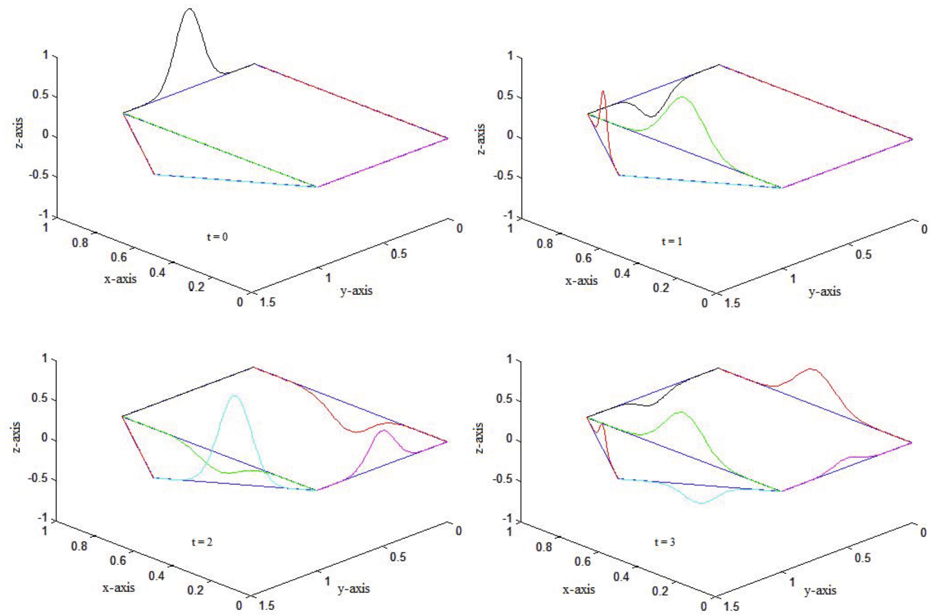
6 Experiments

In this section we apply our proposed method on both synthetic and real world datasets.

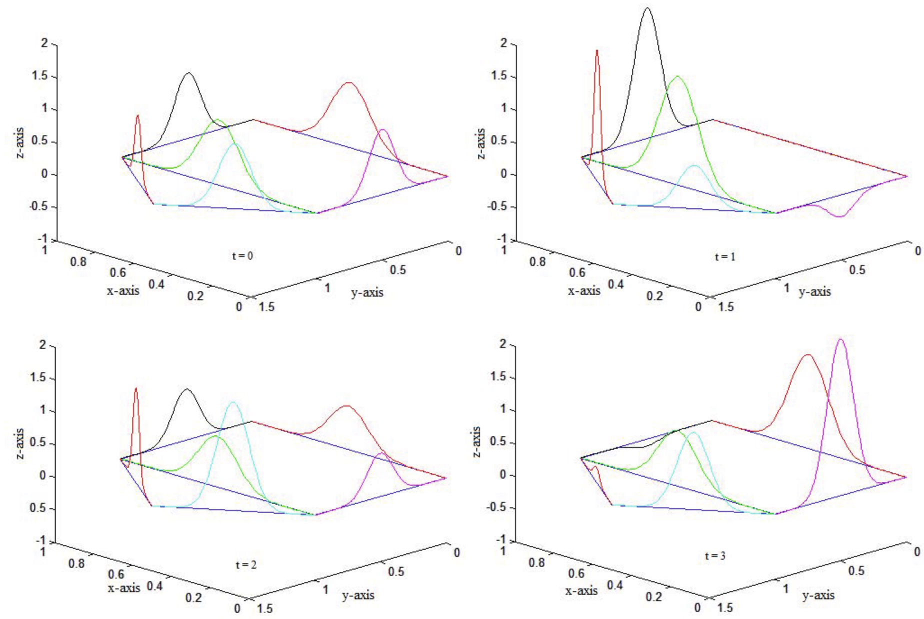
6.1 Synthetic Dataset

To show the evolution of Gaussian wave packet on a graph, we take a simple graph with 5 nodes and 6 edges. We assume the initial condition as a Gaussian wave packet on a single edge and zero everywhere else. Figure 2(a) shows the results for the times $t = 0$, $t = 1$, $t = 2$ and $t = 3$ in a three dimensional space. Note that when the wave packet hits a node with degree greater than 2, some part of the packet is reflected back while the other part is equally distributed to the connecting edges. Figure 2(b) shows a similar analysis but with a different initial condition. Here we assume that initially a Gaussian wave packet exist on every edge of the graph and show its evolution for the times $t = 0$, $t = 1$, $t = 2$ and $t = 3$.

One of the advantage of using the solution of equations defined using edge-based Laplacian is that it is less prone to the problem of failing to distinguish graphs due to cospectrality of the Laplacian or adjacency matrices. This is due to the fact that the structure of edge-interior eigenfunctions of the edge-based Laplacian are determined by the eigenvectors of the oriented line graph which is closely related to discrete time quantum walk on a graph [11]. Figure 3(a) and Figure 3(b) show two pairs of graphs with 9 and 10 vertices respectively, which are cospectral with respect to both their adjacency matrices and the adjacency matrices of their complements. Figure 4(a) and Figure 4(b) show the global wave

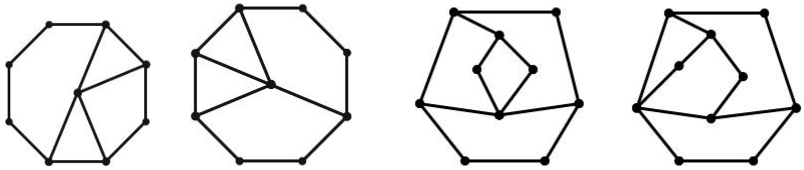


(a) Evolution of a single wave packet



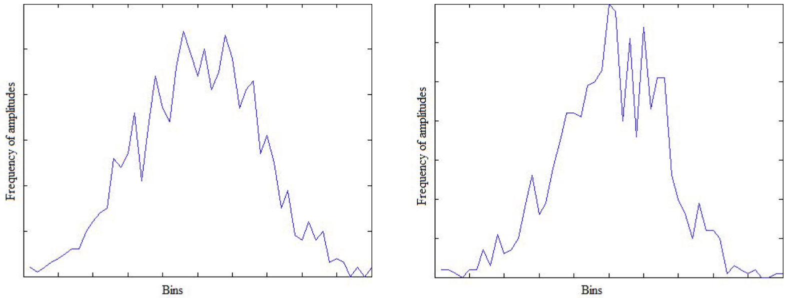
(b) Evolution of multiple wave packets

Fig. 2. Solution of wave equation on a graph with 6 vertices and 8 edges

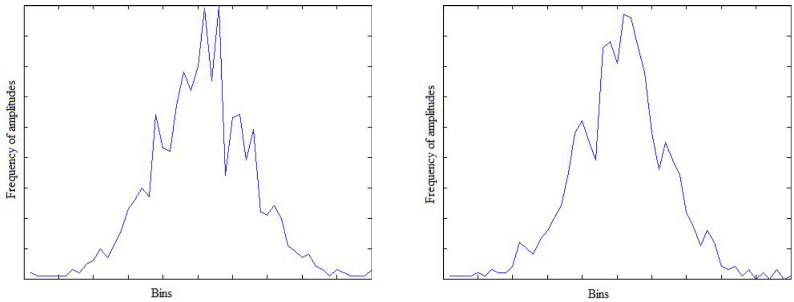


(a) cospectral graphs with 9 nodes (b) cospectral graphs with 10 nodes

Fig. 3. Examples of cospectral graphs



(a) Histogram for the graphs of Figure 3(a)



(b) Histogram for the graphs of Figure 3(b)

Fig. 4. Histograms for cospectral graphs

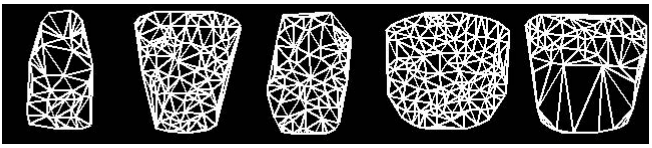
packet signature for the graphs of Figure 3(a) and Figure 3(b). Results show the ability of the wave equation to distinguish cospectral graphs. This is due to the fact that although these graphs cannot be distinguished by random walks on the graph, backtrackless walks on the other hand can distinguish such graphs[12].

6.2 Real-World Dataset

Finally, we apply the proposed method on real world dataset. Our dataset consists of graphs extracted from the images in the Columbia object image library

(COIL) dataset [13]. This dataset contains views of 3D objects under controlled viewer and lighting condition. For each object in the database there are 72 equally spaced views. The objective here is to cluster different views of the same object onto the same class. To establish a graph on the images of objects, we first extract feature points from the image. For this purpose, we use the Harris corner detector [14]. We then construct a Delaunay graph using the selected feature points as vertices. Figure 5(a) shows some of the object views (images) used for our experiments and Figure 5(b) shows the corresponding Delaunay triangulations.

(a) COIL

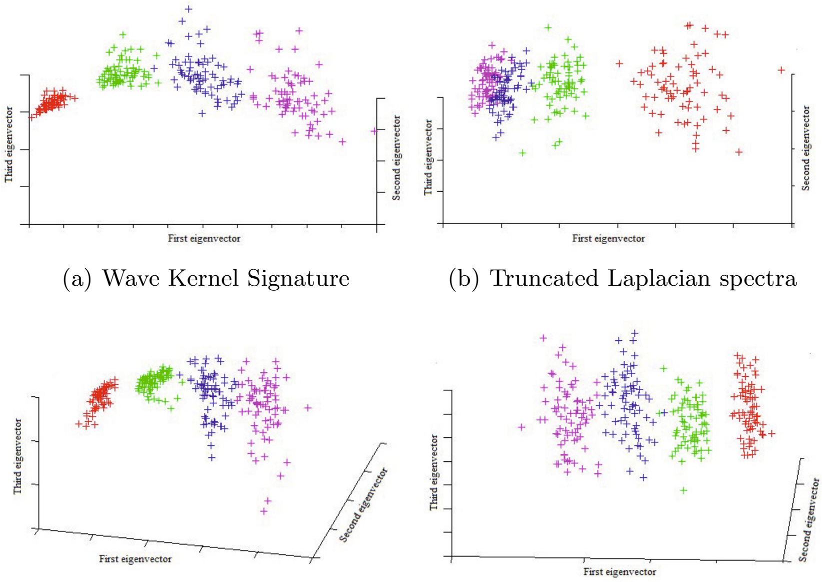


(b) Delaunay triangulation

Fig. 5. COIL objects and their Delaunay triangulations

We compute the wave signature for an edge by taking $t_{min} = 10$, $t_{max} = 100$ and $x_e = 0.5$. We then compute the GWPS for the graph by fixing 100 bins for histogram. To visualize the results, we have performed principal component analysis (PCA) on GWPS. PCA is mathematically defined [15] as an orthogonal linear transformation that transforms the data to a new coordinate system such that the greatest variance by any projection of the data comes to lie on the first coordinate (called the first principal component), the second greatest variance on the second coordinate, and so on. Figure 6(a) shows the results of the embedding of the feature vectors on the first three principal components.

To measure the performance of the proposed method we compare it with truncated Laplacian, random walk [16] and Ihara coefficients [17]. Figure 6 shows the embedding results for different methods. To compare the performance, we cluster the feature vectors using *k-means clustering* [18]. k-means clustering is a method which aims to partition n observations into k clusters in which each observation belongs to the cluster with the nearest mean. We compute *Rand index* [19] of these clusters which is a measure of the similarity between two data clusters. The rand indices for these methods are shown in Table 1. It is clear from the table that the proposed method can classify the graphs with higher accuracy.



(a) Wave Kernel Signature (b) Truncated Laplacian spectra

(c) Random Walk Kernel (d) Ihara Coefficients

Fig. 6. Graph, its digraph, and its oriented line graph

Table 1. Experimental results on Mutag dataset

Method	Accuracy
Wave Kernel Signature	0.9965
Random Walk Kernel	0.9526
Truncated Laplacian Spectra	0.8987
Ihara Coefficients	0.9864

7 Conclusion and Future Work

In this paper we have used the solution of the wave equation on a graph to characterize graphs. The wave equation is solved using the edge-based Laplacian of a graph. We assume the initial distribution be a Gaussian wave packet and shown its evolution with time on different graphs. We use the amplitudes of the wave over different edges to define a signature for graph characterization. The advantage of using the edge-based Laplacian over vertex-based Laplacian is that it allows the direct application of many results from analysis to graph theoretic domain. For example it allows the study of non-dispersive solutions or solitons. In future our goal is to use the solution of other equations defined using the edge-based Laplacian for defining local and global signatures for graphs.

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