Analysis of Wave Packet Signature of a Graph

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Abstract. In this paper we investigate a new approach for characterizing both the weighted and un-weighted graphs using the solution of the edge-based wave equation. The reason for using wave equation is that it provides a richer and potentially more expressive means of characterizing graphs than the more widely studied heat equation. The wave equation on a graph is defined using the Edge-based Laplacian. We commence by defining the eigensystem of the edge-based Laplacian. We give a solution of the wave equation and define signature for both weighted graphs and un-weighted graphs. In the experiment section we perform the proposed method on real world data and compare its performance with other state-of-the-art methods.

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

1 Introduction

Graph clustering is one of the most commonly used problems in areas where data are represented using graphs. Since graphs are non-vectorial, we require a method for characterizing graph that can be used to embed the graph in a high-dimensional feature space for the purpose of clustering. Most of the commonly used method for graph clustering are spectral methods which are based on the eigensystem of the Laplacian matrix associated with the graph. For example Xiao et al [1] have used heat kernel for graph characterization. Wilson et al. [2] have made use of graph spectra to construct a set of permutation-invariant features for the purpose of clustering graphs.

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 [3,4], 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

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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 [5]. 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. 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[6].

Wave equation provides potentially richer characterisation of graphs than heat equation. Initial work by Howaida and Hancock [7] 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 [8] have presented a solution of the edge-based wave equation on a graph. In [9] we have used this solution to define a signature, called the wave packet signature (WPS) of a graph. In this paper we extend the idea of WPS to weighted graphs and experimentally demonstrate the properties of WPS. We perform numerous experiments and demonstrate the performance of the proposed methods on both weighted and un-weighted graphs.

2 Edge-Based Eigensystem

In this section we review the eigenvalues and eigenfunction of the edge-based Laplacian[3][5]. 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 $l_e = 1$.

2.1 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 $\tilde{A}(i, j) = A(i, j)/\sum_{(k,j)\in E} A(k, j)$. Let $(\phi(v), \lambda)$ be an eigenvector-eigenvalue pair for this matrix. Note that $\phi(.)$ 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. 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 $\phi(e, x_e) = C(e)\cos(B(e) + \omega x_e)$.

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.

2.2 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[5]. 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 $|E| - |V| + 1$ linearly independent solutions. Similary 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 $|E| - |V|$ linearly independent solutions. This comprises all the principal eigenpairs which are only supported on the edges.

3 Wave Packet Signatures

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

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

Let $\mathcal{W}(z)$ be z wrapped to the range $[-\frac{1}{2}, \frac{1}{2})$, i.e., $\mathcal{W}(z) = z - \left\lfloor z + \frac{1}{2} \right\rfloor$. For the un-weighted graph, we solve the wave equation assuming that the initial condition is a Gaussian wave packet on a single edge of a graph [9]. The solution for this case becomes

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

$$+ \sum_{\omega \in \Omega_c} \frac{C(\omega, e)C(\omega, f)}{4} \left(e^{-a\mathcal{W}(x-t-\mu)^2} - e^{-a\mathcal{W}(x+t+\mu)^2} \right)$$
$$+ \sum_{\omega \in \Omega_c} \frac{C(\omega, e)C(\omega, f)}{4} \left((-1)^{\lfloor x-t-\mu+\frac{1}{2} \rfloor} e^{-a\mathcal{W}(x-t-\mu)^2} \right.$$
$$\left. -(-1)^{\lfloor x+t+\mu+\frac{1}{2} \rfloor} e^{-a\mathcal{W}(x+t+\mu)^2} \right)$$

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.

For a weighted graph, we assume a Gaussian wave packet on every edge of the graph, whose amplitude is multiplied by the weight of that particular edge, and solve the wave equation for this case. Let w_{ij} be the weight of the edge (i, j). The solution in this case becomes

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

To define signature for both weighted and un-weighted graphs, we use the amplitudes of the waves on the edges of the graph over time. For un-weighted graphs, 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. For weighted graph, we assume a wave packet on every edge whose amplitude is multiplied by the weight of the edge. We define the local signature of an edge as

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

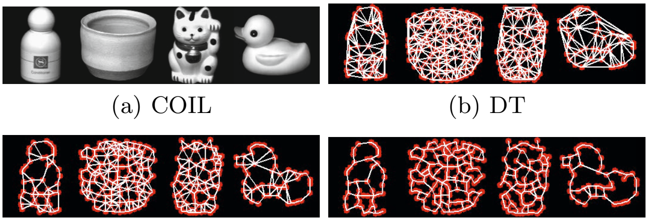
Given a graph G, we define its global wave packet signature as

$$GWPS(G) = hist \left(WPS(\mathcal{X}_1), WPS(\mathcal{X}_2), , ..., WPS(\mathcal{X}_{|E|}) \right) \tag{1}$$

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

4 Experiments

In this section we perform an experimental evaluation of the proposed methods on different graphs. These graphs are extracted from the images in the Columbia object image library (COIL) dataset [10]. 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 [11]. We then construct a Delaunay triangulation (DT) using the selected feature points as vertices of the graph. Figure 1(a) shows some of the object views (images) used for our experiments and Figure 1(b) shows the corresponding Delaunay triangulations.



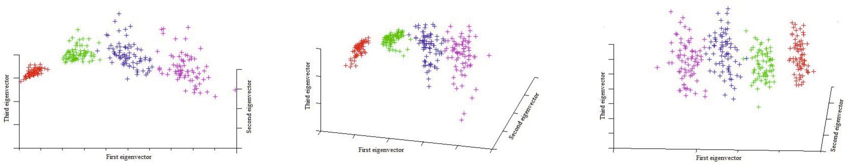
(a) COIL (b) DT

(c) GG (d) RNG

Fig. 1. COIL objects and their extracted graphs

We compute the wave signature for an edge by taking $t_{max} = 100$ and $x_e = 0.5$. We take $t = 20$ to allow the wave packet to be distributed over the whole graph. 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 [12] 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 2(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 [13] and Ihara coefficients [14]. Figure 2 shows



(a) WPS (b) Random Walk (c) Ihara Coefficients

Fig. 2. Graph, its digraph, and its oriented line graph

the embedding results for different methods. To compare the performance, we cluster the feature vectors using *k-means clustering* [15]. 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* [16] 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.

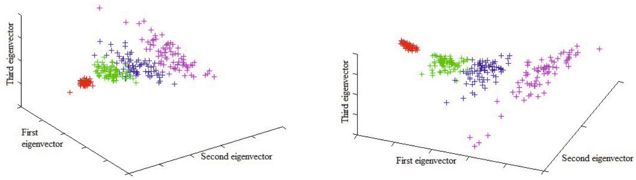
Table 1. Experimental results on Mutag dataset

Method	DT	GG	RNG
Wave Kernel Signature	0.9965	0.9511	0.8235
Random Walk Kernel	0.9526	0.9115	0.8197
Ihara Coefficients	0.9864	0.8574	0.7541

We now compare the performance of the proposed method on Gabriel graphs (GG) and relative neighbourhood graphs (RNG) extracted from the same COIL dataset. The Gabriel graph for a set of n points is a subset of Delaunay triangulation, which connects two data points v_i and v_j for which there is no other point v_k inside the open ball whose diameter is the edge(v_i, v_j). The relative neighbourhood graph is also a subset of Delaunay Triangulation. In this case a lune is constructed on each Delaunay edge. The circles enclosing the lune have their centres at the end-points of the Delaunay edge; each circle has a radius equal to the length of the edge. If the lune contains another node then its defining edge is pruned from the relative neighbourhood graph. Figure 1(c) and 1(d) show the GG and RNG of the corresponding COIL object of Figure 1(a) respectively.

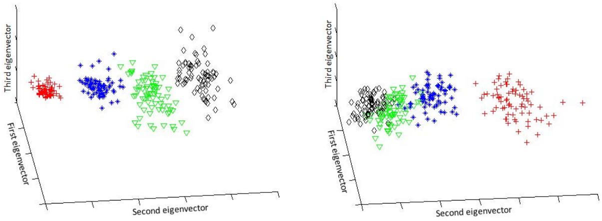
The purpose of comparing the performance on GG and RNG is twofold. First, since both the GG and RNG are subset of DT, it allows us to analyze the performance of the proposed method under controlled structure modification. Second, since both GG and RNG reduce the frequency of cycles of smaller length and introduce branches in the graph, it allows us to analyze the performance of the proposed method on non-cyclic graphs. We compute the performance on GG and RNG in the same way as we did for DT. The visual results of the proposed method on GG and RNG are shown in Figure 3(a) and Figure 3(b) respectively. Table 1 compares the performance of the three methods, which shows that the proposed method performs well under controlled structural modification. Note that a drop in the performance of Ihara coefficient is due to the fact that the Ihara coefficients cannot provide a good measure of similarity for the graphs when branches are present.

We now compare the performance of the proposed WPS on weighted graphs. For this purpose, we have selected the same objects from the COIL dataset. We have extracted the Gabriel graphs for each of these view.The edges are weighted with the exponential of the negative distance between two connected vertices, i.e. $w_{ij} = exp[k||x_i x_j||]$ where x_i and x_j are coordinates of corner points i and j in an image and k is a scalar scaling factor. Figure 4(a) shows the clustering result of WPS, while Figure 4(b) shows the clustering result of truncated Laplacian. To



(a) clustering GG (b) clustering RNG

Fig. 3. Clustering results



(a) WPS (b) Truncated Laplacian

Fig. 4. Clustering results on Weighted graphs

compare the performance we have computed the rand indices for both methods. The rand index for WPS is 0.9931, while for truncated Laplacian is 0.8855.

Finally we look at the characteristic of the proposed WPS. The histogram distribution of the WPS closely follows Gaussian distribution. Figure 5 shows distribution of WPS of a single view of 3 different objects in COIL dataset and a Gaussian fit for each signature. Figure 6(a) and 6(b) show the values of standard deviation of all the DT and GG respectively of all 72 views of 4 different objects of COIL dataset. Table 2 shows the mean value of the standard deviation and a standard error for each of the 4 objects.

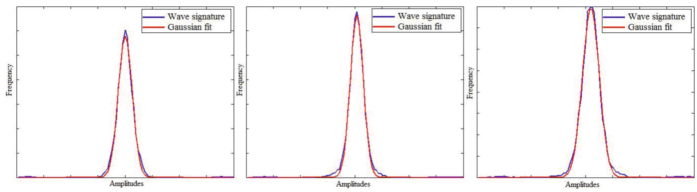
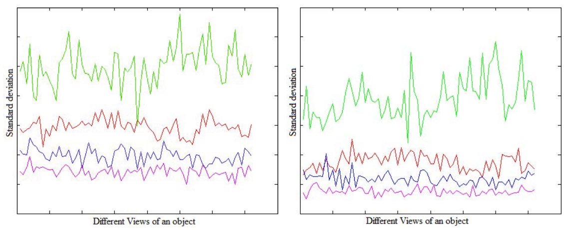


Fig. 5. Gaussian Fit



(a) DT (b) GG

Fig. 6. Standard Deviation

Table 2. Average value of standard deviation

	Standard Deviation	Standard Error
Object 1	0.1400	1.54×10^{-3}
Object 2	0.0989	6.57×10^{-4}
Object 3	0.0793	5.64×10^{-4}
Object 4	0.0685	4.07×10^{-4}

5 Conclusion and Future Work

In this paper we have used the solution of the wave equation on a graph to characterize both weighted and un-weighted graphs. The wave equation is solved using the edge-based Laplacian of a graph. 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. 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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