Gaussian Wave Packet on a Graph

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Abstract. The wave kernel provides a richer and potentially more expressive means of characterising graphs than the more widely studied wave 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 those of the node-based Laplacian. This paper presents the solution of a wave equation on a graph. Wave equation provides an interesting alternative to the heat equation defined using the Edge-based Laplacian. This provides the prerequisites for deeper analysis of graphs and their characterisation. For instance it potentially allows the study of non-dispersive solutions or solitons. In this paper we give a complete solution of the wave equation for a Gaussian wave packet. To simulate the equation on a graph, we assume the initial distribution be a Gaussian wave packet on a single edge of the graph. We show the evolution of this Gaussian wave packet with time on some synthetic graphs.

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

1 Introduction

Traditional graph theory defines a discrete Laplacian, Δ, as an operator which is defined only on the vertices of a graph. This Laplacian has found application in many areas like computer vision, machine learning and pattern recognition. For example Fiedler [1] has used the eigenvector corresponding to second smallest eigenvalue of the Laplacian for graph partitioning. Xiao et al [2] have used heat kernel, which is derived from graph Laplacian, to embed the nodes of a graph in Euclidean space. Zhang et al[3] have used the heat kernel for anisotropic image smoothing. The graph Laplacian was used by Coifman and Lafon[4] for dimensionality reduction of data.

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

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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 ElGhawalby and Hancock [9] has revealed some if 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.

In this paper we present a solution of the edge-based wave equation on a graph. We assume a Gaussian wave packet on one of the edge of the graph, and see its evolution over time. 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 in section 5 we give the solution for the Gaussian wave packet as initial condition. Finally we show simulation of our work on some synthetic graphs.

2 Graphs

A *graph* $G = (V, E)$ consists of a finite nonempty set V of *vertices* and a finite set E of unordered pairs of vertices, called *edges*. A *directed graph* or *digraph* $D = (V_D, E_D)$ consists of a finite nonempty set V_D of vertices and a finite set 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* $L(G) = (V_L, E_L)$ 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

$$V_L = \{(u, v) \in D(G)\}$$

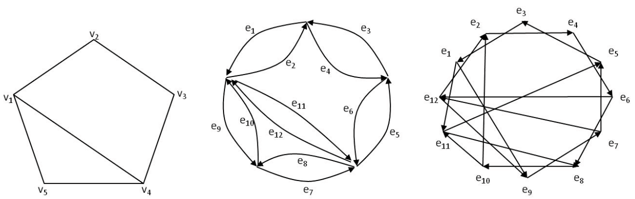
$$E_L = \{((u, v), (v, w)) : (u, v) \in D(G), (v, w) \in D(G)\}$$

The *oriented line graph* $OL(G) = (V_O; E_O)$ 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

$$V_L = \{(u, v) \in D(G)\}$$

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

Figure 1(a) shows a simple graph, 1(b) its digraph, and 1(c) the corresponding oriented line graph.



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

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

3 Edge-Based Eigensystem

In this section we review the eigenvalues and eigenfunctions 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 $\tilde{A}(i,j) = A(i,j)/\sum_{(k,j)\in E} A(k,j)$. 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.

3.2 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 $|E| - |V| + 1$ 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 supported on the vertices.

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. 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 General 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

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

The edge-based wave equation is

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

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

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

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

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

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

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

5 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

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

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

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

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

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

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

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

5.1 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

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

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

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

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.

6 Experiments

In this section, we show the evolution of Gaussian wave packet on some simple graphs. Figure 2 shows the result for a graph with five nodes and seven edges

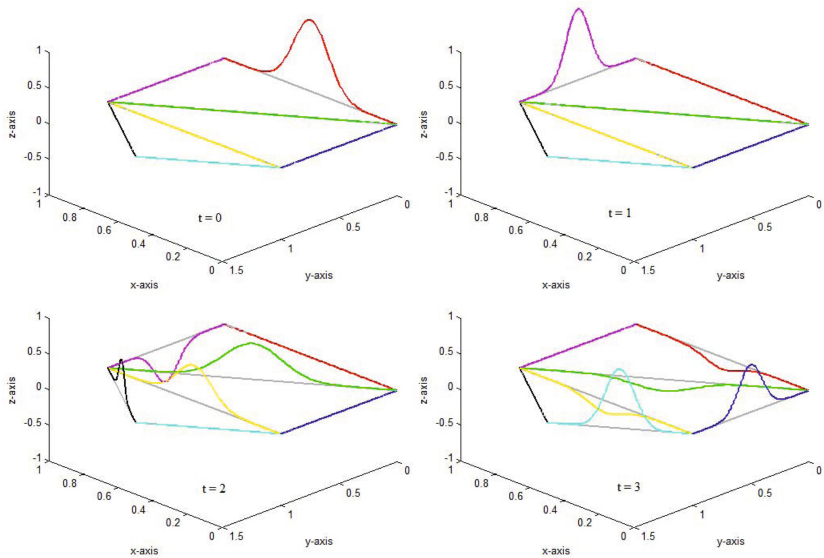


Fig. 2. Graph with 5 vertices and 7 edges

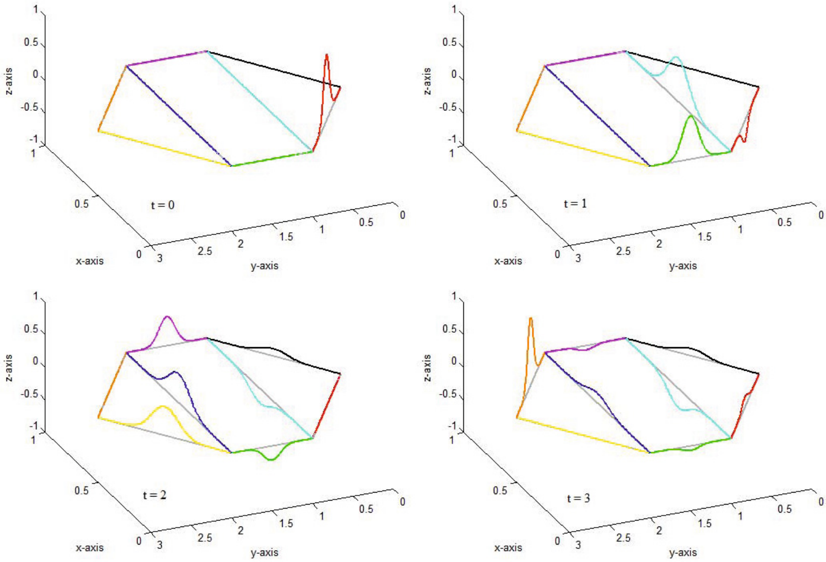


Fig. 3. Graph with 6 vertices and 8 edges

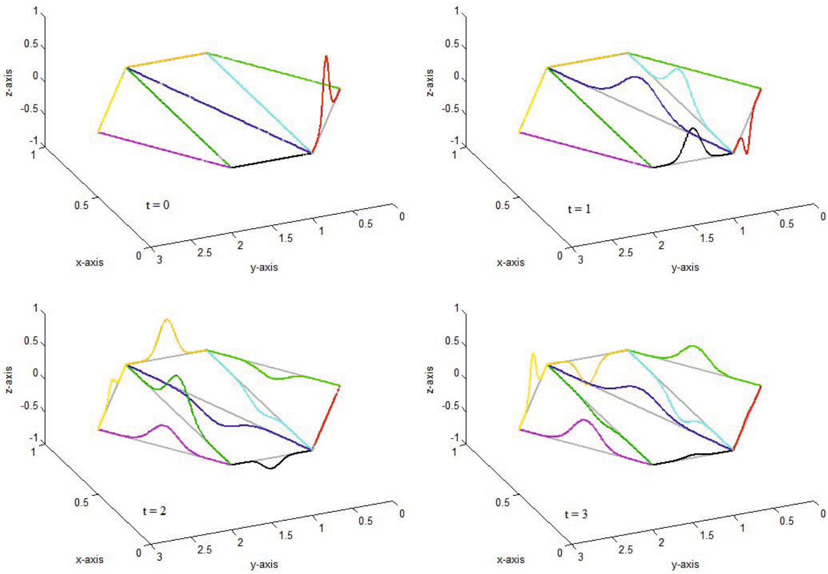


Fig. 4. Graph with 6 vertices and 9 edges

for time $t = 0$, $t = 1$, $t = 2$ and $t = 3$. 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. A similar result is shown for graph with six nodes and eight edges in Figure 3, and for a graph with six nodes and nine edges in Figure 4.

7 Conclusion and Future Work

In this paper we have developed a complete solution of the wave equation on a graph which is based on 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. 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 the wave equation and other equations defined using the edge-based Laplacian for characterizing graphs with higher accuracy.

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