Edge-based Laplacians, the Wave Equation and Wave Packet Signatures

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Background

Discrete Laplacians, heat+wave kernels and all that.
Outline

• Well known vertex Laplacian can be used to solve simple differential equations on graphs.

• Does not account for differential effects due to edges of graph – to get realistic solutions of wave equation require edge-based Laplacian.

• Full spectrum of edge-based Laplacian only recently reported.

• Aim is to investigate effect of using EBL to model packet propagation on graphs and to use this a more detailed signature.
Background

Differential equations on graphs and their use as characterisations or signatures
Laplacian and Heat Kernel

• Recently there has been considerable recent interest in the discrete Laplacian in graph characterisation
  – Discrete Laplacian is analogue of Laplace-Beltrami operator on manifold
    \[ L = D - A \]
    \[ \hat{L} = I - D^{-\frac{1}{2}}AD^{-\frac{1}{2}} \]

• The heat kernel has been extensively used

• Is a solution of the heat equation
  \[ \frac{\partial H}{\partial t} = \Delta H \]
  Laplace-Beltrami (manifold)
  \[ \frac{\partial H}{\partial t} = -LH \]
  Discrete Laplacian (graph)
Heat Kernel Characterisations

• Heat equation

\[ \frac{\partial f}{\partial t} = -\Delta f \]

• Fundamental solution of heat equation gives heat kernel \( H \)

• Heat kernels have been used for structural characterisations of graphs
  – Bai Xiao et al [2010]

• Idea:
  – Graph Laplacian from graph representing some object or shape
  – Structure of corresponding heat kernel gives a shape signature
Heat Kernel Trace

\[ Tr[h_t] = \sum_i \exp[-\lambda_i t] \]

Shape of heat-kernel distinguishes graphs...can we characterise its shape using moments
Heat Kernel Signature

• The heat kernel signature has been used to characterise 3D shapes
  • Sun et al (2009)
• Sample self-heat of vertices over time
  • Closely related to heat kernel trace

• Characterised individual vertices
• Overall signature from histogram of all HKS

\[ \text{HKS} = [H_{t_0}(x, x), H_{t_1}(x, x), H_{t_2}(x, x), \ldots] \]
Wave Kernels

- There are other differential equations which might be interesting

\[ \frac{\partial^2 f}{\partial t^2} = \Delta f \]

Wave equation

- Wave kernel signature (WKS) Aubry (2011)

- The wave equation on a graph using the discrete Laplacian has a notable ‘problem’
  - Infinite speed of propagation
  - Some signal received everywhere instantaneously

- Results from calculus seem un-natural using the discrete Laplacian.

- Need improved calculus on graphs
Wave Equation

• A better model of transmission in networks?
Calculus on graphs

Bringing edges into the picture
Graph Calculus

- Work by Friedman & Tillich [2004]

- Try to develop a calculus which is linked more closely to traditional analysis

- Key Idea: Geometric graph

- Now the graph lives in two spaces
  - Node-space $\mathcal{V}$: Point-like measure
  - Edge-space $\mathcal{E}$: interval (Lebesque measure)

- Graph functions exist on vertices and on edges
Graph Laplacian

• This leads to a two-part Laplacian

\[ \Delta \equiv \Delta_V dV + \Delta_E dE \]

\[ \Delta_V f = \frac{1}{\mathcal{V}(u)} \sum_{e,u \in e} n_{e,u} \cdot \nabla_{e} f(u) \]

\[ \Delta_E f = -\nabla_{calc} \cdot \nabla f \]

• The V-part is essentially a type of discrete Laplacian
  – vertex-based Laplacian

• The E-part is like a normal 1D Laplacian \( \nabla^2 \) along the edges
  – edge-based Laplacian
Vertex- and Edge-functions

- Function $f$ on the graph
  - $f$ exists both at vertices and along the edge intervals

- If $\Delta_E f = 0$ then the function is said to be vertex-based and if $\Delta_V f = 0$ it is edge-based.

- $\Delta_E f = 0$ implies the function is linear on edges in which case
  - $f$ exists on vertices
  - $f$ is linear between vertices
  - continuity means $f$ is fully defined by the vertex values
  - Laplacian is a discrete Laplacian

- The new and old frameworks co-incide when edge functions are linear
Edge-based Eigensystem

• The eigenfunctions of the edge-based Laplacian are of two types
  – Vertex-supported eigenfunctions
  – Edge-interior eigenfunctions

• Vertex-supported eigenfunctions can be expressed in terms of the eigenpairs of the normalized adjacency matrix of the graph.

• Edge-interior eigenfunctions can be computed from the eigenpairs of the oriented line graph of the original graph.
Edge-based Eigenfunctions

• (Oriented) Line graph:

Oriented Line graph: Random walk, no backtracking

Line graph: Random walk
Eigensystem of the Edge-based Laplacian

Overview of Wilson, Aziz and Hancock, Linear Algebra and Applications, 2013.
Calculus on graphs

Let $G = (V,E)$ be a graph with a boundary $\partial G$. Let $\mathcal{G}$ be the geometric realization of $G$.

The geometric realization is the metric space consisting of vertices $V$ with a closed interval of length $l_e$ associated with each edge.

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 $l_e = 1$. 
Vertex-supported Eigenfunctions

• Let $A$ be the adjacency matrix of the graph $G$, and $\tilde{A}$ be the normalized adjacency matrix (row normalization). 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 $(\varphi, \lambda)$ be an eigenvector-eigenvalue pair for this matrix. Note $\varphi(.)$ is defined only on vertices and may be extended along each edge to an edge-based eigenfunction.

• Let $\omega^2$ and $\varphi(e, x_e)$ 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 $u$).
Vertex-supported Eigenfunctions

• For each \((\phi(v), \lambda)\) with \(\lambda \neq \pm 1\), we have a pair of eigenvalues \(\omega^2\) with
  \[
  \omega = \cos^{-1} \lambda \quad \text{and} \quad \omega = 2\pi - \cos^{-1} \lambda.
  \]
• Since there are multiple solutions to \(\omega = \cos^{-1} \lambda\), we obtain an infinite number of eigenvalues and infinite sequence of eigenfunctions with increasing frequencies.
• If \(\omega_0 \in [0, \pi]\) is the principal solution, the eigenvalues are \(\omega^2\) where
  \[
  \omega = \omega_0 + 2\pi n \quad \text{and} \quad \omega = 2\pi - \omega_0 + 2\pi n, \ n \geq 0.
  \]
• The eigenfunctions are
  \[
  \phi(e, x_e) = C(e) \cos(B(e) + \omega x_e)
  \]
  where
  \[
  C(e)^2 = (\phi(v)^2 + \phi(u)^2 - 2\phi(v)\phi(u) \cos(\omega)) / \sin^2(\omega) \quad \text{and}
  \]
  \[
  \tan(B(e)) = (\phi(v) \cos(\omega) - \phi(u)) / \phi(v) \sin(\omega)
  \]
• 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.
Constant Eigenfunctions

• \( \lambda = 1 \) is always an eigenvalue of \( \tilde{A} \). We obtain a principle frequency \( \omega = 0 \), and therefore since \( \varphi(e, x_e) = C \cos(B) \) and so \( \varphi(v) = \varphi(u) = C \cos(B) \), which is constant on the vertices.

• If the graph is bipartite, then \( \lambda = -1 \) is an eigenvalue of \( \tilde{A} \). We obtain a principle frequency \( \omega = \pi \), and then since \( \varphi(e, x_e) = C \cos(B + \pi x_e) \), so \( \varphi(v) = C \cos(B) = -\varphi(u) \) implying an alternating sign eigenfunction.
Edge-interior Eigenfunctions

• The edge-interior eigenfunctions are those eigenfunctions which are zero on vertices and therefore must have a principle frequency of $\omega \in \{\pi, 2\pi\}$.

• These eigenfunctions can be determined from the eigenvectors of the adjacency matrix of the oriented line graph.

• Eigenvector corresponding to the 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.

• Similarly the eigenvector corresponding to the 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.
Normalization of Eigenfunctions

• Note that although these eigenfunctions are orthogonal, they are not necessarily 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 \( \omega \). Then

\[
\rho^2(\omega) = \int_G \varphi^2(e, x_e) \, dx_e
= \sum_{e \in E} \int_0^1 C(e)^2 \cos^2(B(e) + \omega x_e) \, dx_e
\]

• 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. Therefore the orthonormalized eigenfunctions corresponding to eigenvalues \( \omega^2 \) are

\[
\varphi(e, x_e) = C(e) / \rho(\omega) \cos(B(e) + \omega x_e).
\] Once normalized, these eigenfunctions form a complete set of orthonormal bases for \( L^2(G, E) \).
Gaussian Wavepacket

Using edge-based Laplacian to solve wave equation for a Gaussian wave packet propagating with finite speed.
General Solution of the Wave Equation

- With edge coordinate \( \chi \) and time \( t \), edge-based wave equation is

\[
\frac{\partial^2 u(\chi, t)}{\partial t^2} = \Delta_E u(\chi, t)
\]

- Seek separable solutions of the form

\[
u(\chi, t) = \phi_{\omega, n}(\chi) g(t)
\]

with edge-based eigenfunctions

\[
\phi_{\omega, n}(\chi) = C(e, \omega) \cos(B(e, \omega) + \omega x + 2n\pi x)
\]

- Gives a temporal solution

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

- By superposition, we obtain the general solution

\[
u(\chi, t) = \sum_{\omega} \sum_{n} C(e, \omega) \cos(B(e, \omega) + \omega x + 2n\pi x)
\]

\[
\{\alpha_{\omega, n} \cos((\omega + 2n\pi) t) + \beta_{\omega, n} \sin((\omega + 2n\pi) t)\}
\]
Initial Conditions

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

\[ u(\chi,0) = p(\chi) \]

\[ \frac{\partial u}{\partial t}(\chi,0) = q(\chi) \]

and we obtain

\[ p(\chi) = \sum_{\omega} \sum_{n} \alpha_{\omega,n} C(e, \omega) \cos[B(e, \omega) + \omega x + 2n\pi x] \]

\[ q(\chi) = \sum_{\omega} \sum_{n} \beta_{\omega,n} (\omega x + 2n\pi) C(e, \omega) \cos[B(e, \omega) + \omega x + 2n\pi x] \]

We can find these coefficients using the orthonormality of eigenfunctions. So we get

\[ \alpha_{\omega,n} = \sum_{e} C(e, \omega) \frac{1}{2} [F_{\omega,n} + F_{\omega,n}^*] \]

where

\[ F_{\omega,n} = e^{iB} \int_{0}^{1} dx p(e, x) e^{i\omega x} e^{i2\pi n} \]

similarly

\[ \beta_{\omega,n} (\omega x + 2n\pi) = \sum_{e} C(e, \omega) \frac{1}{2} [G_{\omega,n} + G_{\omega,n}^*] \]

where

\[ G_{\omega,n} = e^{iB} \int_{0}^{1} dx q(e, x) e^{i\omega x} e^{i2\pi n} \]
Gaussian Wave Packet

- We assume the initial position be a Gaussian wave packet

\[ p(e, x) = \exp\{-a(x-\mu)^2\} \]

- on one particular edge and zero everywhere else. Then we have

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

- Solving, we get

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

- And so

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

- Similarly

\[
\beta_{\omega, n} = \sqrt{\frac{\pi}{a}} e^{-\frac{1}{4a}(\omega+2\pi n)^2} C(e, \omega) \sin[B + \mu(\omega + 2\pi n)]
\]
General Solution of the Wave Equation

Solution of wave equation with Gaussian wave packet as initial condition

\[
    u(\mathcal{X}, t) = \sum_{\omega \in \Omega_a} \frac{C(\omega, e)C(\omega, f)}{2} \left( e^{-aW(x+t+\mu)^2} \cos \left[ B(e, \omega) + B(f, \omega) + \omega \left[ x + t + \mu + \frac{1}{2} \right] \right] \right)
    \]

\[
    + e^{-aW(x-t-\mu)^2} \cos \left[ B(e, \omega) - B(f, \omega) + \omega \left[ x - t - \mu + \frac{1}{2} \right] \right] \right)
    \]

\[
    + \frac{1}{2|E|} \left( \frac{1}{4} e^{-aW(x+t+\mu)^2} + \frac{1}{4} e^{-aW(x-t-\mu)^2} \right)
    \]

\[
    + \sum_{\omega \in \Omega_b} \frac{C(\omega, e)C(\omega, f)}{4} \left( e^{-aW(x-t-\mu)^2} - e^{-aW(x+t+\mu)^2} \right)
    \]

\[
    + \sum_{\omega \in \Omega_c} \frac{C(\omega, e)C(\omega, f)}{4} \left( (-1)^{\left\lfloor x-t+\frac{1}{2} \right\rfloor} e^{-aW(x-t-\mu)^2} - (-1)^{\left\lfloor x+t+\frac{1}{2} \right\rfloor} e^{-aW(x+t+\mu)^2} \right)
    \]

where \(\Omega_a\) represents the set of vertex-supported eigenvalues and \(\Omega_b\) and \(\Omega_c\) represent the set of edge-interior eigenvalues. i.e., \(\pi\) and \(2\pi\). Also

\[
    W(\tilde{z}) = \tilde{z} - \left\lfloor \tilde{z} + \frac{1}{2} \right\rfloor
    \]
Evolution of Gaussian wave packet on a graph
Evolution of Gaussian wave packet on a graph with 5 vertices and 7 edges
Wave packet signature

Local signature for edge sampled at different times

\[ WPS(\chi) = [u(\chi, t_0), u(\chi, t_1), u(\chi, t_2), \ldots, u(\chi, t_n)] \]

Global signature histograms over edges

\[ GWPS(G) = \text{hist}[WPS(\chi_1), WPS(\chi_2), WPS(\chi_3), \ldots, WPS(\chi_{|E|})] \]
Cospectral Graphs

(a) Cospectral graphs, each with 9 vertices and 12 edges

(b) Cospectral graphs, each with 10 vertices and 13 edges
Wavepacket Signature

(a) Histogram for the graphs of Figure 8.2(a)

(b) Histogram for the graphs of Figure 8.2(b)
Figure 6.4: Cospectral graphs with respect to their Laplacian matrices

Figure 6.5: Histogram for the graphs of Figure 6.4, which are cospectral with respect to their Laplacian matrices
Unweighted Graphs

Wave Kernel Signature

Truncated Laplacian

Random Walk Kernel

Ihara Coefficients

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<th>Delaunay Triangulation</th>
<th>Gabriel Graphs</th>
<th>RN Graphs</th>
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Gaussian Fits to GWPS
Width of GWPS

(a) Delaunay triangulations

(b) Gabriel graphs
Weighted graphs

- The edges are weighted with the exponential of the negative distance between two connected vertices, i.e., $\omega_{i,j} = \exp(k \|x_i - x_j\|)$, where $x_i$ and $x_j$ are coordinates of points $i$ and $j$ in the image and $k$ is a scalar scaling factor.

Truncated Laplacain
Rand Index: 0.8855

WPS
Rand Index: 0.9931
Three-dimensional Shape Analysis

Develop new heat kernel signature based on Gaussian heat packet
Three-dimensional Shape Analysis

• Motivation
  – to define informative and discriminative feature descriptors that characterize each point on the surface of the shape. This has applications in
    • Correspondence Matching
    • Shape Segmentation
    • Shape Classification
  – usually represented by a mesh that approximates the bounding surface of the three-dimensional shape (convenient for visualization but not suitable for many other applications)
Edge-based Heat Equation

• The proposed signature is based on the heat diffusion process governed by the equation

\[ \frac{\partial H_t}{\partial t} = -\Delta_E H_t \]

where \( \Delta_E \) is the edge-based Laplacian and \( H_t \), called heat kernel, is the solution to the above equation. The heat kernel has the following eigen-decomposition:

\[ H_t(x, y) = \sum_{i=0}^{\infty} e^{-\omega_i^2 t} \phi(x)\phi(y) \]
Edge-based heat kernel for Gaussian Heat Packet

\[
h(x, t) = \sum_{\omega} \sqrt{\frac{\pi}{a}} C(\omega, e) C(\omega, f) \sum_{n} e^{-\frac{1}{4a}(\omega+2\pi n)^2} e^{-(\omega+2n\pi)^2t} \\
cos \left[ B(\omega, e) + \omega x + 2\pi nx \right] cos \left[ B(\omega, f) + (\omega + 2\pi n)\mu \right].
\]
Shape Descriptors

• Local descriptors are found by sampling the retained heat at a number of time points:
  $$EHKS(x) = [H_{t_0}(x,x), H_{t_1}(x,x), \ldots, H_{t_k}(x,x)]$$

• Global descriptors is a histogram of local signatures at different time intervals.
  $$GEHKS(S) = \text{hist}(EHKS(x_1), EHKS(x_2), \ldots, EHKS(x_n))$$
Discrete Settings

• The simplest way of defining the adjacency matrix of the mesh using the un-weighted (0-1) or the weighted (distance or proximity) matrix is sensitive to the regularity of the particular triangulation and give little information about the shape itself.

• We use the angle information between the edges and the area around each vertex to define the adjacency matrix.

• Existing techniques use the eigensystem of the Laplace-Beltrami operator that captures the geometric and topological properties of the underlying surface by using the area and angle information.
Discrete Settings

• Let $M$ is a matrix whose $(i, j)$th entry is defined as

$$M(i, j) = \begin{cases} \frac{\cot \alpha_{ij} + \cot \beta_{ij}}{2} & \text{if } (i, j) \in E \\ 0 & \text{otherwise} \end{cases}$$

• Let $S$ be a diagonal matrix whose $i$th diagonal entry is the area associated with the triangles abetting the vertex $i$. We define the symmetric adjacency matrix as $A = S^{1/2}MS^{1/2}$. The $(i, j)$th entry of the adjacency matrix, in terms of the elements of the matrices $M$ and $S$, is given as follows

$$A(i, j) = \begin{cases} \sqrt{S(i, i)S(j, j)}M(i, j) & \text{if } (i, j) \in E \\ 0 & \text{otherwise} \end{cases}$$

• Once the adjacency matrix is known, we can compute the proposed signature by finding the eigensystem of the normalized adjacency matrix.
Experimental setting

• SHREC dataset: three-dimensional objects each with different deformations

• We compute the EHKS by uniformly sampling 100 points for different values of $t$ over the time interval $[t_{\text{min}}; t_{\text{max}}]$. We select the minimum values of time as $t_{\text{min}} = 4 \ln 10/\lambda_300$ and $t_{\text{max}} = 4 \ln 10/\lambda_2$. 
Eigenfunctions of Edge-based Laplacian

\[ EGPS(p) = \left( \frac{1}{\omega} \varphi_1(p), \frac{1}{\omega} \varphi_2(p), \frac{1}{\omega} \varphi_3(p) \ldots \right) \]
Feature Points Segmentation

EHKS on six deformed shapes of a human body

Clustering of feature points. 15 different poses. with 5 points on each hand, foot and head.
Segmentation using EHKS
EHKS vs WKS
Correspondence matching

Edge-based Heat Kernel Signature

Wave Kernel Signature
Example of Dense Matching
Robustness under Gaussian noise

• We add Gaussian noise with standard deviation $\sigma=0.3$ to the point positions of the shape.

• Figure shows 50 best matches for each point
GEHKS

- Shape Classification

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Future Directions

• The edge-based Laplacian is a new tool linking manifolds and graphs
  — Richer structure

• Geometric aspects make it suitable for analysing problems when time, distance and speed of transmission are important

• Analyse a wider range of differential equations
  — Fokker-Planck, Quantum evolution

• Apply to finite-speed network transmission problems
  — Spread of information
  — Disease transmission and epidemiology

• New network descriptors