Technical Report

Department of Computer Science
and Engineering
University of Minnesota
4-192 EECS Building
200 Union Street SE
Minneapolis, MN 55455-0159 USA

TR 09-009

Generalized Laplacians and First Transit Times for Directed Graphs

Daniel Boley

March 23, 2009

Generalized Laplacians and First Transit Times for Directed Graphs

Daniel Boley
University of Minnesota
Minneapolis, MN 55455, USA
boley@cs.umn.edu

Abstract

In this paper, we extend previous results on average commute-times for undirected graphs to fully-connected directed graphs, corresponding to irreducible Markov chains. We introduce an unsymmetrized generalized Laplacian matrix and show how its pseudo-inverse directly yields the one-way first-transit times and round-trip commute times with formulas almost matching those for the undirected graph case. We show that the results are equivalent to similar formulas in terms of the Fundamental Matrix for recurrent irreducible Markov chains. We show that the unsymmetrized generalized Laplacian and its pseudo-inverse are positive semi-definite, leading to a natural embedding of the graph in Euclidean space which preserves the round-trip commute times.

1 Introduction

The analysis of graphs using methods from linear algebra and the theory of Markov chains has an extensive literature. For undirected graphs, a graph Laplacian has been used to compute almost optimal cuts of the graph and to bound the size of the minimal cuts in terms of the eigenvalues of the Laplacian, leading to the general method of spectal graph partitioning [4, 6, 21]. The Laplacian has been also been used to compute the average round-trip commute times between any pair of vertices [2, 9, 15, 7], when the graph is modeled by a Markov chain consisting of a random walk over the graph. Undirected graphs lead to reversible Markov chains, for which the final recurring probabilities for each state correspond to the degree of each node [13]. The average commute time has been shown to be equivalent to the effective resistance between two nodes of an electrical network matching the graph, with each edge having a conductance equal to the graph weight on that edge [5, 2, 15]. It has been observed (see e.g. [7] and references therein) that the nodes of an undirected graph can be embedded in Euclidean space in such a way that the distance squared between any two vertices matches the average commute time between those nodes in the original graph. In this embedding, the method of spectral graph partitioning is equivalent to a method of splitting along the main principal component (direction of maximal variance), the key step in the top-down spectral clustering methods of [1, 8].

Relatively less work has been done for directed graphs. We assume throughout this paper that the undirected graphs under consideration are finite and fully connected, i.e. there is a path from any node to any other node. A Markov chain modelling a random walk over this graph will be irreducible, with no transient states. Analyses of the global connectivity properties for directed graphs have been used in defining the concept of Pagerank [18] used by Google, and in the concept of Hubs and Authorities and the HITS algorithm [16]. For example, in the case of Pagerank, the underlying graph consists of web pages and their hyperlinks, and it is made fully connected by adding low probability links between all pairs of web pages.

For fully connected directed graphs, bounds on the minimal cuts and the related Cheeger inequalities, in terms of the eigenvalues of a so-called Laplacian, were proved in [3, 22]. These papers defined the Laplacian to be the symmetric part of the matrix $\mathbf{I} - \mathbf{P}$, or a diagonally scaled version of this matrix, where $\mathbf{P}$ is the Markov chain transition matrix.

In the present paper, we show that the formulas for the average commute times for undirected graphs in [2, 9, 15, 7] can be derived also for directed graphs, using the pseudo-inverse of a diagonally scaled version of $\mathbf{I} - \mathbf{P}$. For undirected graphs, this matrix would be the same as the pseudo-inverse of the Laplacian used in [3, 22], but for directed graphs they differ. They symmetrize first, then take the pseudo-inverse. We take the pseudo-inverse first, then symmetrize. The result is the same only when the matrixes are already symmetric or diagonally symmetrizable, corresponding to undirected graphs and reversible Markov chains.

We further show the close relationship between these formulas for the average commute times and those previously derived using the so-called Fundamental Matrix (see e.g. [11]), both for fully connected directed graphs. Both the Fundamental Matrix and the Laplacian formulations lead to similar formulas and both lead to an embedding in an n-dimensional Euclidean space preserving the round-trip commute times, even for fully connected directed graphs, but only the Laplacian leads to an embedding that is centered around the origin.

2 Assumptions and Preliminaries

Consider a fully connected directed graph with adjacency matrix A. The entries of A are non-negative and equal the weights on the edges – higher weights mean higher affinity. An unweighted graph is a special case in which one assigns a common weight 1 to existing edges and 0 to missing edges. Let $D = \text{Diag}(A \cdot \mathbf{e})$ be the diagonal matrix of row sums of A, where $\mathbf{e}$ is the vector of all ones. Then $\mathbf{P} = D^{-1}A$ is the transition matrix for a Markov chain modelling a random walk across this graph, where the probability of a transition is proportional to the weight on the corresponding edge. For an unweighted graph, the probability of an edge is simply the reciprocal of the number of outgoing edges from a vertex. The assumption that the graph is fully connected yields the properties that (a) the Markov chain is irreducible with no transient states, (b) $\mathbf{P}$ has a simple eigenvalue equal to 1 with right eigenvector $\mathbf{e}$ and left eigenvector $\boldsymbol{\pi}'$ of steady-state recurring probabilities [11, 12, 13], and (c) every element of the vector of final recurring probabilities $\boldsymbol{\pi}'$ is strictly positive [11, 12, 13]. (In this paper, lower case bold letters like $\mathbf{x}$ denote column vectors, $'$ denotes transpose, and $\mathbf{x}'$ is used to denote a row vector. Also, the notation diag($\mathbf{M}$) (with a lower case 'd') denotes the vector of diagonal entries in the matrix $\mathbf{M}$, while Diag($\mathbf{v}$) (with an upper case 'D') denotes the diagonal matrix with diagonal entries taken from the vector $\mathbf{v}$.) All other eigenvalues of $\mathbf{P}$ are at most 1 in absolute value (lying within the closed unit disk on the complex plane) [12]. If, in addition to being irreducible, the chain were aperiodic, then all the other eigenvalues would be strictly less than one in absolute value, but in this paper we do not make any assumptions on the periodicity of the chain. In this paper, we assume that the cost of traversing any edge is equal to 1. We will address the case of directed graphs with edge costs in a future paper.

We partition the $n \times n$ Markov chain transition matrix as $\mathbf{P} = \begin{pmatrix} \mathbf{P}_{11} & \mathbf{p}_{12} \\ \mathbf{p}'_{21} & p_{nn} \end{pmatrix}$. Here $\mathbf{P}_{11}$ is $(n-1) \times (n-1)$, $\mathbf{p}'_{21}$ is a row vector, $\mathbf{p}_{12}$ is a column vector, and p_{nn} is a scalar. Let $\boldsymbol{\pi}' = (\boldsymbol{\pi}'_1, \pi_n) = (\pi_1, \pi_2, \ldots, \pi_{n-1}, \pi_n)$ be the limiting probabilities (a left vector), partitioned into an $(n-1)$-vector and a scalar. Assume $\boldsymbol{\pi}'$ has no non-zero entries. Let $\mathbf{e} = (1, 1, \ldots, 1)'$ of appropriate dimension (usually $n-1$ but sometimes n). Then $\mathbf{Pe} = \mathbf{e}$. This implies

$$\mathbf{p}_{12} = \mathbf{e} - \mathbf{P}_{11}\mathbf{e} = (\mathbf{I} - \mathbf{P}_{11})\mathbf{e} \qquad \text{and} \qquad p_{nn} = 1 - \mathbf{p}'_{21}\mathbf{e}.$$

We will use this Markov model to calculate the expected path length between any two states, which can also be considered the expected first transit times between two states.

3 The Pseudo-Inverse under Small Rank Changes

In order to carry out our development, we need two lemmas regarding the pseudo-inverse under small rank modifications. First we need a lemma regarding the inverse of a submatrix in terms of the pseudo-inverse of a whole matrix. Let $\mathbf{M} = \begin{pmatrix} \mathbf{M}_{11} & \mathbf{m}_{12} \\ \mathbf{m}'_{21} & m_{nn} \end{pmatrix} = \mathbf{L}^{+}$ be the unique Moore-Penrose pseudo-inverse of $\mathbf{L}$, i.e., such that $\mathbf{LM}$ & $\mathbf{ML}$ are symmetric, $\mathbf{LML} = \mathbf{L}$, and $\mathbf{MLM} = \mathbf{M}$ [10]. One property we use is that the left nullspace of $\mathbf{M}$ equals the right nullspace of $\mathbf{L}$ and vice-versa. We will prove the following lemma for general square irreducible matrices $\mathbf{L}$, $\mathbf{M}$ having nullity 1. [The nullity is the dimension of the nullspace.]

Lemma 1. Suppose the $n \times n$ irreducible matrix $\mathbf{L} = \begin{pmatrix} \mathbf{L}_{11} & \mathbf{l}_{12} \\ \mathbf{l}'_{21} & l_{nn} \end{pmatrix}$ has nullity 1, $\mathbf{M} = \mathbf{L}^{+}$ is its pseudo inverse, partitioned similarly, and suppose $(\mathbf{u}', 1)\mathbf{L} = 0$, $\mathbf{L}(\mathbf{v}; 1) = 0$. Here the ';' denotes vertical concatenation *à la* Matlab. Then $\mathbf{L}_{11}^{-1}$ exists and equals

$$\mathbf{L}_{11}^{-1} = \mathbf{X} = (\mathbf{I}\,,\,-\mathbf{v}) \begin{pmatrix} \mathbf{M}_{11} & \mathbf{m}_{12} \\ \mathbf{m}_{21}' & m_{nn} \end{pmatrix} \begin{pmatrix} \mathbf{I} \\ -\mathbf{u}' \end{pmatrix} = (\mathbf{I} + \mathbf{v}\mathbf{v}')\mathbf{M}_{11}(\mathbf{I} + \mathbf{u}\mathbf{u}').$$

Proof. First note that $\mathbf{L}_{11}\mathbf{v} + \mathbf{l}_{12} = \mathbf{0}$ and $\mathbf{u}'\mathbf{L}_{11} + \mathbf{l}_{21}' = \mathbf{0}$, and similarly $\mathbf{M}_{11}\mathbf{u} + \mathbf{m}_{12} = \mathbf{0}$ and $\mathbf{v}'\mathbf{M}_{11} + \mathbf{m}_{21}' = \mathbf{0}$. Hence $(\mathbf{I} + \mathbf{v}\mathbf{v}')\mathbf{M}_{11}(\mathbf{I} + \mathbf{u}\mathbf{u}') = (\mathbf{I}\,,\,-\mathbf{v})\mathbf{M}\begin{pmatrix} \mathbf{I} \\ -\mathbf{u}' \end{pmatrix}$.

Let $\mathbf{X}$ be the expression above, and form:

$$\begin{aligned} \mathbf{L}_{11}\mathbf{X}\mathbf{L}_{11} &= \mathbf{L}_{11}(\mathbf{I}\,,\,-\mathbf{v})\mathbf{M}\begin{pmatrix} \mathbf{I} \\ -\mathbf{u}' \end{pmatrix}\mathbf{L}_{11} &= (\mathbf{L}_{11}\,,\,\mathbf{l}_{12})\mathbf{M}\begin{pmatrix} \mathbf{L}_{11} \\ \mathbf{l}_{21}' \end{pmatrix} \\ &= (\mathbf{I}\,,\,\mathbf{0})\,\mathbf{L}\mathbf{M}\mathbf{L}\begin{pmatrix} \mathbf{I} \\ \mathbf{0}' \end{pmatrix} &= (\mathbf{I}\,,\,\mathbf{0})\,\mathbf{L}\begin{pmatrix} \mathbf{I} \\ \mathbf{0}' \end{pmatrix} = \mathbf{L}_{11}. \end{aligned}$$

Since $\mathbf{L}_{11}$ must have an inverse (because o.w. $\mathbf{L}_{11}\mathbf{x} = 0 \Longrightarrow \mathbf{l}_{21}'\mathbf{x} = 0 \Longrightarrow \mathbf{L}(\mathbf{x}; 0) = 0 \Longrightarrow$ nullity$(\mathbf{L}) \geq 2$), we can multiply both sides of the above by $\mathbf{L}_{11}^{-1}$ to get $\mathbf{L}_{11}\mathbf{X} = \mathbf{I}$.
□

We also need a second lemma regarding a rank-one change to a non-singular matrix which makes it singular. When the matrix obtained after the rank-one change is non-singular, its inverse is given by the well-known Sherman-Morrison formula [12, 10]. When the resulting matrix is singular, the best we can ask for is its pseudo-inverse. The following lemma gives a formulation for this pseudo-inverse.

Lemma 2. Let $\mathbf{A}$ be an $n \times n$ non-singular matrix and suppose $\widetilde{\mathbf{A}} = \mathbf{A} - \mathbf{u}\mathbf{v}'$ is singular. Then the Moore-Penrose pseudo-inverse of $\widetilde{\mathbf{A}}$ is

$$(\widetilde{\mathbf{A}})^{+} = \widetilde{\mathbf{B}} \stackrel{\text{def}}{=} \left(\mathbf{I} - \frac{\mathbf{x}\mathbf{x}'}{\mathbf{x}'\mathbf{x}}\right)\mathbf{A}^{-1}\left(\mathbf{I} - \frac{\mathbf{y}\mathbf{y}'}{\mathbf{y}'\mathbf{y}}\right),$$

where $\mathbf{x} = \mathbf{A}^{-1}\mathbf{u}$, $\mathbf{y}' = \mathbf{v}'\mathbf{A}^{-1}$.

We remark that the quantities $\left(\mathbf{I} - \frac{\mathbf{x}\mathbf{x}'}{\mathbf{x}'\mathbf{x}}\right), \left(\mathbf{I} - \frac{\mathbf{y}\mathbf{y}'}{\mathbf{y}'\mathbf{y}}\right)$ are the symmetric orthogonal projectors onto the subspaces orthogonal to $\mathbf{x}$, $\mathbf{y}$, respectively.

Proof. We establish some facts in sequence:

1. Let $\mathbf{z} \neq 0$ be such that $\widetilde{\mathbf{A}}\mathbf{z} = 0$. Then $\mathbf{A}\mathbf{z} = \mathbf{u}\mathbf{v}'\mathbf{z}$. That means $\mathbf{A}\mathbf{z}$ must be a non-zero multiple of $\mathbf{u}$. Choose the scaling such that $\mathbf{A}\mathbf{z} = \mathbf{u}$. Then it must be the case that $\mathbf{z} = \mathbf{x}$, $\widetilde{\mathbf{A}}\mathbf{x} = 0$, and $\mathbf{v}'\mathbf{x} = 1$. Likewise, we have $\mathbf{y}'\widetilde{\mathbf{A}} = 0$ and $\mathbf{y}'\mathbf{u} = 1$.

2. The right and left nullspaces of $\widetilde{\mathbf{A}}$ each have dimension 1.

3. By direct calculation, $\widetilde{\mathbf{A}}\left(\mathbf{I}-\frac{\mathbf{x}\mathbf{x}'}{\mathbf{x}'\mathbf{x}}\right)=\widetilde{\mathbf{A}}$ and $\left(\mathbf{I}-\frac{\mathbf{y}\mathbf{y}'}{\mathbf{y}'\mathbf{y}}\right)\widetilde{\mathbf{A}}=\widetilde{\mathbf{A}}$.

4. We have

$$\widetilde{\mathbf{A}}\widetilde{\mathbf{B}}=\widetilde{\mathbf{A}}\left(\mathbf{I}-\frac{\mathbf{x}\mathbf{x}'}{\mathbf{x}'\mathbf{x}}\right)\mathbf{A}^{-1}\left(\mathbf{I}-\frac{\mathbf{y}\mathbf{y}'}{\mathbf{y}'\mathbf{y}}\right)=(\mathbf{I}-\mathbf{u}\mathbf{y}')\left(\mathbf{I}-\frac{\mathbf{y}\mathbf{y}'}{\mathbf{y}'\mathbf{y}}\right)=\left(\mathbf{I}-\frac{\mathbf{y}\mathbf{y}'}{\mathbf{y}'\mathbf{y}}\right).$$

   This last quantity is symmetric. Likewise $\widetilde{\mathbf{B}}\widetilde{\mathbf{A}}=\cdots=\left(\mathbf{I}-\frac{\mathbf{x}\mathbf{x}'}{\mathbf{x}'\mathbf{x}}\right)$ is also symmetric.

5. It follows from the above calculations that

$$\widetilde{\mathbf{A}}\widetilde{\mathbf{B}}\widetilde{\mathbf{A}}=\left(\mathbf{I}-\frac{\mathbf{y}\mathbf{y}'}{\mathbf{y}'\mathbf{y}}\right)\widetilde{\mathbf{A}}=\widetilde{\mathbf{A}}$$

6. Finally, we have

$$\begin{aligned}\widetilde{\mathbf{B}}\widetilde{\mathbf{A}}\widetilde{\mathbf{B}} &= \widetilde{\mathbf{B}}\left(\mathbf{I}-\frac{\mathbf{y}\mathbf{y}'}{\mathbf{y}'\mathbf{y}}\right)\\ &= \left(\mathbf{I}-\frac{\mathbf{x}\mathbf{x}'}{\mathbf{x}'\mathbf{x}}\right)\mathbf{A}^{-1}\left(\mathbf{I}-\frac{\mathbf{y}\mathbf{y}'}{\mathbf{y}'\mathbf{y}}\right)\left(\mathbf{I}-\frac{\mathbf{y}\mathbf{y}'}{\mathbf{y}'\mathbf{y}}\right)\\ &= \widetilde{\mathbf{B}}.\end{aligned}$$

We have just verified the four conditions for $\widetilde{\mathbf{B}}$ to be the Moore-Penrose pseudo-inverse of $\widetilde{\mathbf{A}}$ [12, 10]: (i) $\widetilde{\mathbf{A}}\widetilde{\mathbf{B}}$ is symmetric, (ii) $\widetilde{\mathbf{B}}\widetilde{\mathbf{A}}$ is symmetric, (iii) $\widetilde{\mathbf{A}}\widetilde{\mathbf{B}}\widetilde{\mathbf{A}}=\widetilde{\mathbf{A}}$, (iv) $\widetilde{\mathbf{B}}\widetilde{\mathbf{A}}\widetilde{\mathbf{B}}=\widetilde{\mathbf{B}}$.
□

4 Expected First Transit and Commute Times

In this section, we derive a formula for the Expected First Transit Time from any state to any state in terms of the elements of pseudo-inverse of the generalized non-symmetric Laplacian. Specifically we compute the Expected First Transit Time from each of the states $i=1,2,\ldots,n-1$ to state n. This is also the average path length from each state i to state n, where the probability of a given path is proportional to the product of the weights of its edges. In the simplest case of the unweighted graph, the probability of traversing any edge is equal to the reciprocal of the out-degree of each node. Any weights on the edges are reflected in the probabilities of traversing an edge; we assume all edges have the same cost. We will address the case of varying edge costs in a future paper. The expected first transit time from state n to n is 0. Since the states can be numbered arbitrarily, the choice of which state is numbered n is arbitrary. We then arrive at the general formula.

Following [14, 17, 20, 11] we can write the recursive formula for $\mathtt{N}(i,n)$, the expected number of steps to reach node n from node i for the first time as

$$\mathtt{N}(i,n)=1+\sum_{j=1}^{n-1}p_{ij}\mathtt{N}(j,n),\qquad\text{for}\qquad i=1,\ldots,n-1,\tag{1}$$

where by convention, $\mathtt{N}(n,n)=0$. This formula says that the expected time of going from node i to node n is equal to the expected time to go from any immediate neighbor j to n plus the single time step to go from i to j. Putting these times into an $(n-1)$-vector, we obtain a matrix formulation:

$$\mathtt{N}(1\cdots n-1, n) = (\mathbf{I}-\mathbf{P}_{11})^{-1}\mathbf{e} = [\mathbf{D}_1(\mathbf{I}-\mathbf{P}_{11})]^{-1}\boldsymbol{\pi}_1,$$

where $\mathbf{D}_1 = \mathrm{Diag}(\boldsymbol{\pi}_1)$ is an $(n-1)\times(n-1)$ diagonal matrix with $\pi_1,\ldots,\pi_{n-1}$ on the diagonal. We note that $(\mathbf{I}-\mathbf{P}_{11})^{-1}$ must exist by Lemma 1 because of the irreducibility of the Markov chain.

We can actually guarantee that all the eigenvalues of $\mathbf{P}_{11}$ are strictly less than 1 in absolute value as follows. Let $\rho(\mathbf{P}_{11})$ denote the spectral radius of $\mathbf{P}_{11}$. Then $\rho(\mathbf{P}_{11}) \le \|\mathbf{P}_{11}\|_\infty \le \|\mathbf{P}\|_\infty = 1$. But $\mathbf{P}_{11}$ is a non-negative matrix, so it must have an eigenvalue equal to its spectral radius, by Perron-Frobenius theory [12]. Since $(\mathbf{I}-\mathbf{P}_{11})$ is non-singular, 1 is not an eigenvalue of $\mathbf{P}_{11}$, hence the spectral radius of $\mathbf{P}_{11}$ must be strictly less than 1. So we have proved:

Lemma 3. If $\mathbf{P}$ is the transition matrix for an irreducible Markov chain, partitioned as $\mathbf{P} = \begin{pmatrix}\mathbf{P}_{11} & \mathbf{p}_{12}\\ \mathbf{p}'_{21} & p_{nn}\end{pmatrix}$, then the vector of expected first transit times from any state i to state n is

$$\mathtt{N}(\cdot, n) = \begin{pmatrix}[\mathbf{D}_1(\mathbf{I}-\mathbf{P}_{11})]^{-1}\boldsymbol{\pi}_1\\ 0\end{pmatrix}.$$

□

Since the choice of target state n is arbitrary, we would like to obtain an expression for this which has the same form regardless of which is the target state. In order to do this, we need to express the inverse $[\mathbf{D}_1(\mathbf{I}-\mathbf{P}_{11})]^{-1}$ in terms of the pseudo-inverse of the whole matrix $\mathbf{L}=\mathbf{D}(\mathbf{I}-\mathbf{P})$, where $\mathbf{D}=\mathrm{Diag}(\boldsymbol{\pi})$ (an $n\times n$ matrix). We remark that for directed graphs $\mathbf{D}$ is not directly related to the diagonal matrix of out-degrees D, unlike the case for undirected graphs. We have $\mathbf{Le}=\boldsymbol{\pi}-\mathbf{De}=\mathbf{0}$, $\mathbf{e}'\mathbf{L}=\boldsymbol{\pi}'-\boldsymbol{\pi}'\mathbf{P}=\mathbf{0}'$, and $\mathbf{L}$ has non-negative entries, all of which are all less than or equal to 1.

In order to find this inverse, we use Lemma 1, with $\mathbf{v}=\mathbf{e}$, $\mathbf{u}=\mathbf{e}$, $\mathbf{L}=\mathbf{D}(\mathbf{I}-\mathbf{P})$, $\mathbf{M}=[\mathbf{D}(\mathbf{I}-\mathbf{P})]^{+}$, where $\mathbf{D}=\mathrm{Diag}(\boldsymbol{\pi})$ is $n\times n$ diagonal. Then

$$\mathtt{N}(1\cdots n-1, n) = \mathbf{L}_{11}^{-1}\boldsymbol{\pi}_1 = (\mathbf{I}\,,\,-\mathbf{e})\mathbf{M}\begin{pmatrix}\boldsymbol{\pi}_1\\ -\mathbf{e}'\boldsymbol{\pi}_1\end{pmatrix} = (\mathbf{M}_{11}-\mathbf{e}\mathbf{m}'_{21}\,,\,\mathbf{m}_{12}-\mathbf{e}m_{nn})\begin{pmatrix}\boldsymbol{\pi}_1\\ -\mathbf{e}'\boldsymbol{\pi}_1\end{pmatrix}$$

Hence individual transit times are

$$\begin{aligned}\mathtt{N}(i,n) &= \textstyle\sum_{1\le k\le n-1}(m_{ik}-m_{nk})\pi_k + (m_{nn}-m_{in})(1-\pi_n)\\ &= \textstyle\sum_{1\le k\le n}(m_{ik}-m_{nk})\pi_k + (m_{nn}-m_{in})\\ &= \textstyle\sum_{1\le k\le n}(m_{ik}-m_{nk}+m_{nn}-m_{in})\pi_k,\end{aligned} \qquad (2)$$

using the fact that $\sum_{1\le k\le n}\pi_k = 1$, i.e. $\mathbf{e}'\boldsymbol{\pi}_1 = (\pi_1 + \cdots + \pi_{n-1}) = 1 - \pi_n$. This formula, derived for $i = 1, \ldots, n-1$ also holds trivially for $i = n$. Since the choice of n was arbitrary, we can write the corresponding formula for any target state j, encapsulated in the following Theorem.

Theorem 4. Let $\mathbf{P}$ be the Markov transition matrix for an irreducible Markov chain, corresponding to a fully connected directed graph. Let $\mathbf{D} = \mathrm{Diag}(\boldsymbol{\pi})$ be the $n \times n$ diagonal matrix with the steady-state recurring state probabilities on the diagonal, all of which are assumed to be nonzero. Define the Generalized Laplacian $\mathbf{L} = \mathbf{D}(\mathbf{I}-\mathbf{P})$ and let $\mathbf{M} = \mathbf{L}^+$ be its Moore-Penrose pseudo-inverse. Then the one-way expected first transit time from state i to state j (equal to the expected path length from state i to the first pass at state j) is

$$\begin{aligned}\mathtt{N}(i,j) &= \textstyle\sum_{1\le k\le n}(m_{ik}-m_{jk})\pi_k + (m_{jj}-m_{ij}) \\ &= \left[m_{jj} - \textstyle\sum_{1\le k\le n}(m_{jk}\pi_k)\right] - \left[m_{ij} - \textstyle\sum_{1\le k\le n}(m_{ik}\pi_k)\right] \\ &= \textstyle\sum_{1\le k\le n}(m_{ik}-m_{jk}+m_{jj}-m_{ij})\pi_k\end{aligned} \tag{3}$$

The entire matrix of transit times from any state i to any state j is then

$$\begin{aligned}\mathtt{N} &= \mathbf{e}\cdot[\mathrm{diag}(\mathbf{M}-\mathbf{M}\boldsymbol{\pi}\mathbf{e}')]' - (\mathbf{M}-\mathbf{M}\boldsymbol{\pi}\mathbf{e}') \\ &= \mathbf{e}\cdot[\mathrm{diag}(\mathbf{M})]' - \mathbf{e}\boldsymbol{\pi}'\mathbf{M}' - \mathbf{M} + \mathbf{M}\boldsymbol{\pi}\mathbf{e}',\end{aligned} \tag{4}$$

where we have used the identity $\mathrm{diag}(\mathbf{M}-\mathbf{M}\boldsymbol{\pi}\mathbf{e}') = \mathrm{diag}(\mathbf{M}) - \mathbf{M}\boldsymbol{\pi}$.
$\square$

Next we derive the expected round-trip commute time $\mathtt{C}(i,j)$ from state i to the first transition in state j and back to the first transition in state i. This is the expected path length for any path from state i reaching state j for the first time, and then returning to state i for the first time:

$$\mathtt{C}(i,j) = \mathtt{N}(i,j) + \mathtt{N}(j,i) = (m_{jj}-m_{ij}) + (m_{ii}-m_{ji}) \tag{5}$$

We can express this in matrix form as follows. Let $\widehat{\mathbf{L}} = (\mathbf{L}+\mathbf{L}')/2$ be the symmetric part of $\mathbf{L}$. $\widehat{\mathbf{L}}$ also satisfies $\widehat{\mathbf{L}}\mathbf{e} = \mathbf{0}$, $0 \le \widehat{\mathbf{L}} \le 1$ (elementwise) and is, of course, symmetric. We also observe that, since $\mathbf{P}$ is irreducible, so are $\mathbf{L}$ and $\widehat{\mathbf{L}}$.

In terms of the symmetric part of $\mathbf{M}$, the expected commute times are:

$$\mathtt{C}(i,j) = \hat{m}_{jj} - 2\hat{m}_{ij} + \hat{m}_{ii} \tag{6}$$

$$\mathtt{C} = \mathtt{N} + \mathtt{N}' = \mathbf{e}\cdot[\mathrm{diag}(\widehat{\mathbf{M}})]' + [\mathrm{diag}(\widehat{\mathbf{M}})]\cdot\mathbf{e}' - 2\widehat{\mathbf{M}},$$

where $\widehat{\mathbf{M}} = (\mathbf{M}+\mathbf{M}')/2$. We remark that, unless $\mathbf{L}$ were symmetric to begin with, $[(\mathbf{L}+\mathbf{L}')/2]^+ \ne \widehat{\mathbf{M}} = (\mathbf{L}^+ + (\mathbf{L}^+)')/2$ in general. The spectral inequalities in [3, 22] were based on matrices similar to $[(\mathbf{L}+\mathbf{L}')/2]^+$, whereas the analysis here is based on $\widehat{\mathbf{M}}$.

5 Relation to the Modified Fundamental Matrix

Another matrix derived from the Markov chain transition matrix is the so-called Fundamental Matrix. The Fundamental Matrix for irreducible Markov chains (as opposed to a slightly different matrix for absorbing chains) is defined as $\mathbf{Z} = (\mathbf{I} - \mathbf{P} + \mathbf{e}\boldsymbol{\pi}')^{-1}$ [11]. We remark that in [11], the term "ergodic Markov chain" is used to refer to what we call here an irreducible chain, in which every state is reachable from every other state.

In this paper we use the Modified Fundamental Matrix defined as $\widetilde{\mathbf{Z}} = \mathbf{Z}\mathbf{D}^{-1}$, where $\mathbf{D} = \mathrm{Diag}(\boldsymbol{\pi})$. In the following we also define

$$\mathbf{Y} = \widetilde{\mathbf{Z}}^{-1} = \mathbf{D}(\mathbf{I} - \mathbf{P} + \mathbf{e}\boldsymbol{\pi}') = \mathbf{D} - \mathbf{D}\mathbf{P} + \boldsymbol{\pi}\boldsymbol{\pi}' = \mathbf{L} + \boldsymbol{\pi}\boldsymbol{\pi}'.$$

Observe the relations

$$\mathbf{Y}\mathbf{e} = \boldsymbol{\pi}, \quad \mathbf{e}'\mathbf{Y} = \boldsymbol{\pi}' \quad \text{and hence} \quad \widetilde{\mathbf{Z}}\boldsymbol{\pi} = \mathbf{e}, \quad \boldsymbol{\pi}'\widetilde{\mathbf{Z}} = \mathbf{e}'.$$

In order for this discussion to make sense, we must verify that $\widetilde{\mathbf{Z}}$ exists, i.e. that $\mathbf{Y}$ indeed has an inverse.

Lemma 5. [11]. $\mathbf{Y} = \mathbf{D} - \mathbf{D}\mathbf{P} + \boldsymbol{\pi}\boldsymbol{\pi}'$ is non-singular.

Proof. Suppose $\mathbf{Y}\mathbf{x} = 0$ with $\mathbf{x} \neq 0$. Then $0 = \mathbf{e}'\mathbf{Y}\mathbf{x} = (\mathbf{e}'\boldsymbol{\pi})(\boldsymbol{\pi}'\mathbf{x}) = (\boldsymbol{\pi}'\mathbf{x})$. Hence $\mathbf{L}\mathbf{x} = (\mathbf{D} - \mathbf{D}\mathbf{P})\mathbf{x} = \mathbf{Y}\mathbf{x} - \boldsymbol{\pi}\boldsymbol{\pi}'\mathbf{x} = 0$. But $\mathbf{L}$ has a one-dimensional nullspace generated by $\mathbf{e}$, and therefore $\mathbf{x}$ must be a multiple of $\mathbf{e}$. We note that $\mathbf{Y}\mathbf{e} = \boldsymbol{\pi} \neq 0$ arriving at a contradiction.
□

Theorem 6. Let $\mathbf{Z} = (\mathbf{I} - \mathbf{P} + \mathbf{e}\boldsymbol{\pi}')^{-1}$ be the Fundamental Matrix for an irreducible Markov Chain, and $\widetilde{\mathbf{Z}} = \mathbf{Z}\mathbf{D}^{-1}$, where $\mathbf{D} = \mathrm{Diag}(\boldsymbol{\pi})$. Then the one-way expected transit times are

$$\mathtt{N}(i,j) = \frac{z_{ij} - z_{jj}}{\pi_j} = \tilde{z}_{ij} - \tilde{z}_{jj} \tag{7}$$

In matrix form,

$$\mathtt{N} = \mathbf{e} \cdot [\mathrm{diag}(\widetilde{\mathbf{Z}})]' - \widetilde{\mathbf{Z}} \tag{8}$$

The round-trip expected commute times are then

$$\mathtt{C}(i,j) = \frac{z_{ij} - z_{jj}}{\pi_j} + \frac{z_{ji} - z_{ii}}{\pi_i} = \tilde{z}_{ij} + \tilde{z}_{ji} - \tilde{z}_{ii} - \tilde{z}_{jj} \tag{9}$$

In matrix form,

$$\begin{aligned} \mathtt{N} &= \mathbf{e} \cdot [\mathrm{diag}(\widetilde{\mathbf{Z}})]' - \widetilde{\mathbf{Z}} \\ \mathtt{C} &= \mathtt{N} + \mathtt{N}' = \mathbf{e} \cdot [\mathrm{diag}(\widetilde{\mathbf{Z}})]' + [\mathrm{diag}(\widetilde{\mathbf{Z}})] \cdot \mathbf{e}' - \widetilde{\mathbf{Z}} - \widetilde{\mathbf{Z}}' \end{aligned} \tag{10}$$

Proof. The first part of formula (7) is proved in [11] starting with (1). The rest follows by direct calculation or by simply assembling the scalar formulas into a matrix formulation.
□

The remarkable similarity between this theorem and Theorem 4 hints that the Fundamental Matrix is closely related to the pseudo-inverse $\mathbf{M}$ of the Generalized Laplacian. In fact, this is the case, on which we now elaborate.

Theorem 7. The Modified Fundamental Matrix $\widetilde{\mathbf{Z}} = (\mathbf{D} - \mathbf{DP} + \boldsymbol{\pi}\boldsymbol{\pi}')^{-1}$ for an irreducible Markov chain can be written in terms of the pseudo-inverse of the Laplacian, $\mathbf{M} = \mathbf{L}^+ = (\mathbf{D} - \mathbf{DP})^+$ for that same chain as follows:

$$\widetilde{\mathbf{Z}} = \mathbf{M} - \mathbf{M}\boldsymbol{\pi}\mathbf{e}' - \mathbf{e}\boldsymbol{\pi}'\mathbf{M} + (1 + \boldsymbol{\pi}'\mathbf{M}\boldsymbol{\pi})\mathbf{e}\mathbf{e}'$$

Proof. Let $\mathbf{X}$ be the above expression and compute $\mathbf{XY}$, using the facts that $\mathbf{Le} = \mathbf{L}'\mathbf{e} = 0$, and $\mathbf{e}'\boldsymbol{\pi} = 1$:

$$\begin{aligned}\mathbf{XY} &= \mathbf{X}(\mathbf{L} + \boldsymbol{\pi}\boldsymbol{\pi}') = \mathbf{ML} - \mathbf{M}\boldsymbol{\pi}\mathbf{e}'\mathbf{L} - \mathbf{e}\boldsymbol{\pi}'\mathbf{ML} + (1 + \boldsymbol{\pi}'\mathbf{M}\boldsymbol{\pi})\mathbf{e}\mathbf{e}'\mathbf{L} \\ &\quad + \mathbf{M}\boldsymbol{\pi}\boldsymbol{\pi}' - \mathbf{M}\boldsymbol{\pi}\mathbf{e}'\boldsymbol{\pi}\boldsymbol{\pi}' - \mathbf{e}\boldsymbol{\pi}'\mathbf{M}\boldsymbol{\pi}\boldsymbol{\pi}' + (1 + \boldsymbol{\pi}'\mathbf{M}\boldsymbol{\pi})\mathbf{e}\mathbf{e}'\boldsymbol{\pi}\boldsymbol{\pi}' \\ &= \mathbf{ML} - 0 - \mathbf{e}\boldsymbol{\pi}'\mathbf{ML} + 0 + \mathbf{M}\boldsymbol{\pi}\boldsymbol{\pi}' - \mathbf{M}\boldsymbol{\pi}\boldsymbol{\pi}' - (\boldsymbol{\pi}'\mathbf{M}\boldsymbol{\pi})\mathbf{e}\boldsymbol{\pi}' + (1 + \boldsymbol{\pi}'\mathbf{M}\boldsymbol{\pi})(\mathbf{e}'\boldsymbol{\pi})\mathbf{e}\boldsymbol{\pi}'.\end{aligned}$$

Using the fact that $\mathbf{ML} = \mathbf{LM} = \mathbf{I} - \frac{1}{n}\mathbf{e}\mathbf{e}'$ is the orthogonal projector on to the space orthogonal to $\mathbf{e}$, we have

$$\begin{aligned}\mathbf{XY} &= \mathbf{I} - \tfrac{1}{n}\mathbf{e}\mathbf{e}' - \mathbf{e}\boldsymbol{\pi}' + \tfrac{1}{n}\mathbf{e}(\boldsymbol{\pi}'\mathbf{e})\mathbf{e}' + \mathbf{M}\boldsymbol{\pi}\boldsymbol{\pi}' - \mathbf{M}\boldsymbol{\pi}\boldsymbol{\pi}' - (\boldsymbol{\pi}'\mathbf{M}\boldsymbol{\pi})\mathbf{e}\boldsymbol{\pi}' + (1 + \boldsymbol{\pi}'\mathbf{M}\boldsymbol{\pi})\mathbf{e}\boldsymbol{\pi}' \\ &= \mathbf{I}.\end{aligned}$$

Since $\mathbf{Y}$ is non-singular, we must have $\mathbf{X} = \mathbf{Y}^{-1}$.
□

Theorem 8. Defining the Laplacian and Modified Fundamental Matrix for an irreducible Markov chain as in Theorem 7, the pseudo-inverse of the Laplacian can be written in terms of the Modified Fundamental Matrix as follows:

$$\mathbf{M} = \mathbf{L}^+ = \left(\mathbf{I} - \frac{\mathbf{e}\mathbf{e}'}{n}\right)\widetilde{\mathbf{Z}}\left(\mathbf{I} - \frac{\mathbf{e}\mathbf{e}'}{n}\right).$$

Proof. Observing that $\widetilde{\mathbf{Z}} = \mathbf{Y}^{-1}$, $\mathbf{L} = \mathbf{Y} - \boldsymbol{\pi}\boldsymbol{\pi}'$, $\mathbf{e} = \mathbf{Y}^{-1}\boldsymbol{\pi}$, and $\mathbf{e}' = \boldsymbol{\pi}'\mathbf{Y}^{-1}$, the result follows immediately from Lemma 2.
□

We conclude this section with a comparison between formulas (4) and (10). The quantity $\mathtt{N}$ in (10) remains invariant if one replaces $\widetilde{\mathbf{Z}}$ with $\widetilde{\mathbf{Z}} + \mathbf{e}\mathbf{v}'$ for any choice of vector $\mathbf{v}$:

$$\begin{aligned}\mathbf{e}\cdot[\mathrm{diag}(\widetilde{\mathbf{Z}} + \mathbf{e}\mathbf{v}')]' - \widetilde{\mathbf{Z}} - \mathbf{e}\mathbf{v}' &= \mathbf{e}\cdot[\mathrm{diag}(\widetilde{\mathbf{Z}})]' + \mathbf{e}\mathbf{v}' - \widetilde{\mathbf{Z}} - \mathbf{e}\mathbf{v}' \\ &= \mathbf{e}\cdot[\mathrm{diag}(\widetilde{\mathbf{Z}})]' - \widetilde{\mathbf{Z}}. \\ &= \mathtt{N}\end{aligned} \tag{11}$$

By Theorem 7,

$$\mathbf{M} - \mathbf{M}\boldsymbol{\pi}\mathbf{e}' = \widetilde{\mathbf{Z}} + \mathbf{e}\cdot[\boldsymbol{\pi}'\mathbf{M} - (1+\boldsymbol{\pi}'\mathbf{M}\boldsymbol{\pi})\mathbf{e}'] = \widetilde{\mathbf{Z}} + \mathbf{e}\mathbf{v}', \tag{12}$$

with the particular choice $\mathbf{v} = \mathbf{M}'\boldsymbol{\pi} - (1+\boldsymbol{\pi}'\mathbf{M}\boldsymbol{\pi})\mathbf{e}$. Hence formulas (4) and (10) are essentially equivalent.

6 Positive Definite Kernel

If $\widehat{\mathbf{M}}$ were positive semi-definite with rank r, we could factor it as $\widehat{\mathbf{M}} = \mathbf{R}'\mathbf{R}$, where $\mathbf{R}$ would be an $r \times n$ matrix with full row rank. We could then identify the i-th column of $\mathbf{R}$ with the i-th state of the Markov chain (i-th vertex of the original directed graph). This amounts to embedding the vertices of the original graph in r-dimensional Euclidean space, $\mathbb{R}^r$. Letting $\mathbf{R} = (\mathbf{r}_1, \ldots, \mathbf{r}_n)$, In this embedding, the round-trip commute times

$$\mathtt{C}(i,j) = \mathbf{r}_j^{\mathbf{T}}\mathbf{r}_j - 2(\mathbf{r}_i^{\mathbf{T}}\mathbf{r}_j) + \mathbf{r}_i^{\mathbf{T}}\mathbf{r}_i = \|\mathbf{r}_i - \mathbf{r}_j\|_2^2, \tag{13}$$

match the squared distances between the columns of $\mathbf{R}$ representing vertices i and j. The matrix $\widehat{\mathbf{M}}$ would be a positive semi-definite kernel. So we address the issue of positive definiteness in the following.

Theorem 9. Consider the Modified Fundamental Matrix $\widetilde{\mathbf{Z}} = (\mathbf{D} - \mathbf{DP} + \boldsymbol{\pi}\boldsymbol{\pi}')^{-1}$ and define its symmetric part: $\widehat{\mathbf{Z}} = (\widetilde{\mathbf{Z}} + \widetilde{\mathbf{Z}}')/2$. Let $\mathbf{P}$ be as in Lemma 3. Let $\mathbf{D} = \mathrm{Diag}(\boldsymbol{\pi})$ be the $n \times n$ diagonal matrix of final recurring state probabilities, all of which are nonzero. Define $\mathbf{L} = \mathbf{D}(\mathbf{I} - \mathbf{P})$ and $\mathbf{M} = \mathbf{L}^+$. Define the symmetric part $\widehat{\mathbf{M}} = (\mathbf{M} + \mathbf{M}')/2$. Then $\widehat{\mathbf{Z}} = (\widetilde{\mathbf{Z}} + \widetilde{\mathbf{Z}}')/2$ is symmetric positive definite and $\widehat{\mathbf{M}}$ is symmetric positive semi-definite.

To prove this theorem, the following lemma is useful.

Lemma 10. For any given real matrix $\mathbf{A}$, $\mathbf{A} + \mathbf{A}'$ is symmetric positive semidefinite if and only if $\mathbf{x}'\mathbf{A}\mathbf{x} \geq 0$ for any real vector $\mathbf{x}$. We say the 'real field of values' for $\mathbf{A}$ is non-negative. So in words, if the quadratic form for a real matrix is non-negative for all real vectors, the real part of the quadratic form is non-negative also for all complex vectors and hence the symmetric part of the matrix is positive semi-definite.

Proof of Lemma 10. The symmetry of $\mathbf{A} + \mathbf{A}'$ is trivial. Within this proof, let $i = \sqrt{-1}$ and let $\square^H$ denote the conjugate transpose of $\square$. ("if") Suppose $\mathbf{z} = \mathbf{x} + i\mathbf{y}$ for any real vectors $\mathbf{x}, \mathbf{y}$. Then $\mathbf{z}^H\mathbf{A}\mathbf{z} = (\mathbf{x}' - i\mathbf{y}')\mathbf{A}(\mathbf{x} + i\mathbf{y}) = \mathbf{x}'\mathbf{A}\mathbf{x} + \mathbf{y}'\mathbf{A}\mathbf{y} + i(\mathbf{x}'\mathbf{A}\mathbf{y} - \mathbf{y}'\mathbf{A}\mathbf{x}) = \alpha + i\beta$, where $\alpha \geq 0$. Hence $\mathbf{z}^H(\mathbf{A} + \mathbf{A}')\mathbf{z} = 2\alpha \geq 0$. ("only if") For any real vector $\mathbf{x}$: $\mathbf{x}'\mathbf{A}\mathbf{x} = \mathbf{x}^H(\mathbf{A} + \mathbf{A}')\mathbf{x}/2 \geq 0$.
□

Proof of Theorem 9. Let $\mathbf{A} = \mathbf{I} - (\mathbf{L} + \mathbf{L}')/2 = \mathbf{I} - \widehat{\mathbf{L}}$. Observe $\mathbf{A}\mathbf{e} = \mathbf{e}$. $\mathbf{A}$ is symmetric, doubly stochastic, with non-negative entries. Actually, all the entries are in the interval

$[0,1)$. It is also irreducible, since the original $\mathbf{P}$ was. Therefore 1 is a simple eigenvalue of $\mathbf{A}$, and all other eigenvalues are in the interval $[-1,+1)$. Therefore $\widehat{\mathbf{L}} = (\mathbf{L}+\mathbf{L}')/2$ has one simple zero eigenvalue and all its other eigenvalues are in the interval $(0,2]$. Therefore $\widehat{\mathbf{L}}$ is positive semi-definite, with nullity 1. This implies that the 'real field of values' for $\mathbf{L}$ is non-negative: $\mathbf{x}'\mathbf{L}\mathbf{x} \geq 0$ for any real $\mathbf{x}$.

We further observe that $\mathbf{x}'\mathbf{L}\mathbf{x} = 0$ only when $\mathbf{x} = \alpha\mathbf{e}$ for some scalar α. Let $\mathbf{Y} = \widetilde{\mathbf{Z}}^{-1} = \mathbf{L} + \boldsymbol{\pi}\boldsymbol{\pi}'$. Observe that $\mathbf{x}'\mathbf{Y}\mathbf{x} = \mathbf{x}'\mathbf{L}\mathbf{x} + (\mathbf{x}'\boldsymbol{\pi})(\boldsymbol{\pi}'\mathbf{x}) \geq 0$, with $\mathbf{x}'\mathbf{L}\mathbf{x} \geq 0$ and $(\mathbf{x}'\boldsymbol{\pi})(\boldsymbol{\pi}'\mathbf{x}) \geq 0$. The only vector $\mathbf{x}$ for which both $\mathbf{x}'\mathbf{L}\mathbf{x} = 0$ and $(\mathbf{x}'\boldsymbol{\pi})(\boldsymbol{\pi}'\mathbf{x}) = 0$ is $\mathbf{x} = 0$.

Hence $\mathbf{x}'\widetilde{\mathbf{Z}}\mathbf{x} > 0$ for any $\mathbf{x} \neq 0$ and thus $\widehat{\mathbf{Z}} = (\widetilde{\mathbf{Z}} + \widetilde{\mathbf{Z}}')/2$ is symmetric positive definite. Applying Theorem 8, we have $\widehat{\mathbf{M}} = (\mathbf{M}+\mathbf{M}')/2 = \left(\mathbf{I} - \frac{\mathbf{e}\mathbf{e}'}{n}\right)\widehat{\mathbf{Z}}\left(\mathbf{I} - \frac{\mathbf{e}\mathbf{e}'}{n}\right)$ is symmetric positive semidefinite.
□

We remark in passing that since all the entries of the matrix $\mathbf{A}$ in the above proof are in the interval $[0,1)$, all the off-diagonal entries of $\widehat{\mathbf{L}}$ are in the interval $(-1,0]$, and the diagonal entries are in the interval $(0,1]$. We conjecture that this may prove useful in proving further properties about $\widehat{\mathbf{M}}$.

Having established that $\widehat{\mathbf{Z}}$ is symmetric positive definite, we can form its Cholesky factorization: $\widehat{\mathbf{Z}} = \mathbf{S}'\mathbf{S}$ where $\mathbf{S}$ is upper triangular [10]. Then we can write the round-trip commute times as

$$\mathtt{C}(i,j) = \mathbf{s}_j^{\mathbf{T}}\mathbf{s}_j - 2(\mathbf{s}_i^{\mathbf{T}}\mathbf{s}_j) + \mathbf{s}_i^{\mathbf{T}}\mathbf{s}_i = \|\mathbf{s}_i - \mathbf{s}_j\|_2^2, \tag{14}$$

where $\mathbf{s}_i$ is the i-th column of $\mathbf{S}$, representing the embedding of graph vertex i in $\mathbb{R}^n$. If we were to compute the covariance matrix for the vectors $\mathbf{s}_i$, as part of principal component analysis, we would begin by centering the data. Let $\bar{\mathbf{s}} = \frac{1}{n}\sum_i \mathbf{s}_i = \frac{\mathbf{S}\mathbf{e}}{n}$ be the centroid vector for the columns of $\mathbf{S}$ and define $\mathbf{R} = \mathbf{S} - \bar{\mathbf{s}}\mathbf{e}' = \mathbf{S}\left(\mathbf{I} - \frac{\mathbf{e}\mathbf{e}'}{n}\right)$ to be the matrix of centered columns. Then $\mathbf{R}'\mathbf{R}$ would be the covariance matrix, whose eigenvectors are the principal components for the columns of $\mathbf{S}$. On the other hand, from Theorem 8, $\mathbf{R}'\mathbf{R} = \left(\mathbf{I} - \frac{\mathbf{e}\mathbf{e}'}{n}\right)\mathbf{S}'\mathbf{S}\left(\mathbf{I} - \frac{\mathbf{e}\mathbf{e}'}{n}\right) = \widehat{\mathbf{M}}$ is exactly the symmetric part of the pseudo-inverse of the generalized graph Laplacian. We thus conclude that the embedding induced by the Modified Fundamental Matrix is just a rigid translation of the embedding induced by the Generalized Laplacian, the latter being centered around the origin.

7 Some Applications and Consequences

As one possible application, we can get a measure of the importance of a given vertex by adding the average lengths of all paths between any pair of vertices when those paths are restricted to passing through the given vertex, following similar analysis for undirected graphs [19]. If we compare this sum to the sum over all possible paths, we get an estimate on how much the restriction of passing through a given vertex q represents a detour in going from an arbitrary vertex i to another arbitrary vertex j. Since $\sum_i m_{ij} = \sum_j m_{ij} = 0$, equation (3) yields (for all paths)

$$\sum_{ij} \mathtt{N}(i,j) = n \sum_j m_{jj} = n \cdot \mathrm{Trace}(\mathbf{M}) \tag{15}$$

and for paths passing through node q:

$$\begin{aligned} \sum_i \mathtt{N}(i,q) + \sum_j \mathtt{N}(q,j) &= \sum_{ik} (m_{ik} - m_{qk})\pi_k + (m_{qq} - m_{iq}) \\ &\quad + \sum_{kj} (m_{qk} - m_{jk})\pi_k + (m_{jj} - m_{qj}) \\ &= n^2 m_{qq} + n \sum_j m_{jj} \\ &= n^2 m_{qq} + n \cdot \mathrm{Trace}(\mathbf{M}) \end{aligned} \tag{16}$$

Hence the difference between (16) and (15), namely $n^2 m_{qq}$, represents the extra distance traveled between two vertices when forced to pass through vertex q, summed over all n^2 pairs of source/destination vertices.

Under certain conditions, we can derive a weighted undirected graph with expected commute times matching those of the original graph represented by the transition matrix $\mathbf{P}$. We form $\widehat{\mathbf{M}}$ as in Theorem 9, and partially reverse the construction to obtain an adjacency matrix $\widehat{A}$ for the undirected graph. The pseudo-inverse of $\widehat{\mathbf{M}}$ is the new Laplacian $\widehat{L}$ for the new undirected graph. This is not the same as the $\widehat{\mathbf{L}}$ encountered above. The Laplacian of an undirected graph is formed by taking the adjacency matrix $\widehat{A}$, forming the diagonal matrix $\widehat{D}$ of row sums, and setting $\widehat{L} = \widehat{D} - \widehat{A}$. Since we assume the diagonal entries of $\widehat{A}$ are zero, we have $\widehat{D} = \mathrm{Diag}(\widehat{L})$ and $\widehat{A} = \widehat{D} - \widehat{L}$. This construction is valid if all the resulting entries of $\widehat{A}$ are non-negative, i.e., all the off-diagonal entries of $\widehat{L}$ are non-positive. Hence, the steps just outlined here can be carried out only if this property holds.

In this paper, we have illustrated how several properties of undirected graphs carry over to fully connected directed graphs. Such graphs have a generalized Laplacian, which indirectly shares many of the properties of the Laplacian for undirected graphs. In the literature, some properties for undirected graphs were shown for the Laplacian, some for its pseudo-inverse. For directed graphs, many of these properties apply to a symmetrized Laplacian, some to the symmetrized pseudo-inverse, but not necessarily both. This paper presents just one example of a property for undirected graphs that carries over to directed graphs. Using the matrix methods developed herein, we hope to extend this to other properties in the future.

Acknowledgments

This work was partially supported by NSF grant 0534286. The author would like to thank Gyan Ranjan and Zhi-Li Zhang for very helpful discussions and bringing this to the author's attention.

References

[1] D. L. Boley. Principal Direction Divisive Partitioning. *Data Mining and Knowledge Discovery*, 2(4):325–344, 1998.

[2] A. Chandra, P. Raghavan, W. Ruzzo, R. Smolensky, and P. Tiwari. The electrical resistance of a graph captures its commute and cover times. In *Proc. of Annual ACM Symposium on Theory of Computing*, pages 574–586, 1989.

[3] F. Chung. Laplacians and the Cheeger inequality for directed graphs. *Annals of Combinatorics*, 9(1):1–19, 2005.

[4] W. E. Donath and A. J. Hoffman. Lower bounds for the partitioning of graphs. *IBM J. of Res. and Dev.*, 17:410–425, 1973.

[5] P. Doyle and J. Snell. *Random Walks and Electric Networks*. The Math. Assoc. of Am., 1984. `http://front.math.ucdavis.edu/math.PR/0001057`.

[6] M. Fiedler. A property of eigenvectors of nonnegative symmetric matrices and its applications to graph theory. *Czechoslovak Math. J.*, 25(100):619–633, 1975.

[7] F. Fouss, A. Pirotte, R. J.M., and M. Saerens. Random-walk computation of similarities between nodes of a graph with application to collaborative recommendation. *IEEE Transactions on Knowledge and Data Engineering*, 19:355–369, 2007.

[8] J. H. Friedman, J. W. Tukey, and P. A. Tukey. Approaches to analysis of data that concentrate near intermediate-dimensional manifolds. In E. Diday, L. Lebart, J. Pagès, and R. Tomassone, editors, *Data Analysis and Informatics, Proceedings of the Second International Symposium on Data Analysis and Informatics*, pages 3–13. North Holland, 1980.

[9] F. Gobel and A. Jagers. Random walks on graphs. *Stochastic Processes and Their Applications*, 2:311–336, 1974.

[10] G. H. Golub and C. F. Van Loan. *Matrix Computations*. Johns Hopkins Univ. Press, 3rd edition, 1996.

[11] C. M. Grinstead and J. L. Snell. *Introduction to Probability*. American Mathematical Society, 2nd edition, 2006. http://www.dartmouth.edu/~chance/teaching_aids/books_articles/probability_book/book.html.

[12] R. A. Horn and C. R. Johnson. *Matrix Analysis*. Cambridge University Press, Cambridge, 1985.

[13] S. Karlin and H. M. Taylor. *A First Course in Stochastic Processes*. Academic Press, New York, second edition, 1975.

[14] J. Kemeny and J. Snell. *Finite Markov Chains*. Springer-Verlag, 1976.

[15] D. Klein and M. Randic. Resistance distance. *J. Math. Chemistry*, 12:81–95, 1993.

[16] J. Kleinberg. Authoritative sources in a hyper-linked environment. *Journal of ACM*, 46(5):604–632, 1999.

[17] J. Norris. *Markov Chains*. Cambridge Univ. Press, 1997.

[18] L. Page, S. Brin, R. Motwani, and T. Winograd. The pagerank citation ranking: Bringing order to the web. TR SIDL-WP-1999-0120, Computer Systems Laboratory, Stanford Univ., 1998. http://ilpubs.stanford.edu:8090/422/.

[19] G. Ranjan. Personal communication, 2009.

[20] M. Saerens and F. Fouss. A novel way of computing similarities between nodes of a graph, with application to collaborative filtering and subspace projection of the graph nodes, 2006.

[21] J. Shi and J. Malik. Normalised cuts and image segmentation. *IEEE Trans. Pattern Analysis and Machine Intelligence*, 22(8):888–905, 2000.

[22] D. Zhou, J. Huang, and B. Schölkopf. Learning from labeled and unlabeled data on a directed graph. In *Proc. 22nd Int'l Conf. Machine Learning*, pages 1041–1048, 2005.

Appendix - A Simple Example

Consider the Markov chain representing a completely connected directed graph illustrated in Figure 1. The Markov chain has period 2 and has the following state transition matrix and final recurring probabilities

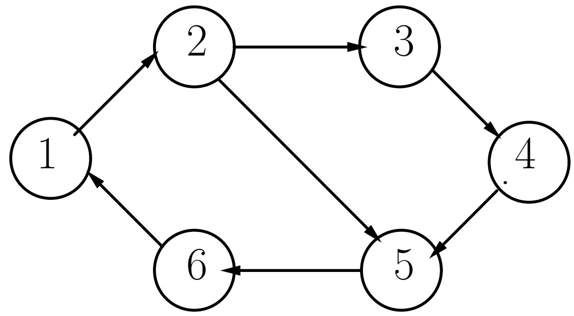

Figure 1: Simple example of a directed graph.

$$\mathbf{P} = \begin{pmatrix} 0 & 1.0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.5 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 1.0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.0 \\ 1.0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{\pi} = \frac{1}{10} \cdot \begin{pmatrix} 2 \\ 2 \\ 1 \\ 1 \\ 2 \\ 2 \end{pmatrix}.$$

Note, since the period is 2, this chain can be in an even state only at even time steps and in an odd state at odd time steps, assuming one starts in an even state at time 0.

The Generalized Laplacian and its Moore-Penrose pseudo-inverse are

$$\mathbf{L} = \frac{1}{10} \cdot \begin{pmatrix} 2 & -2 & 0 & 0 & 0 & 0 \\ 0 & 2 & -1 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 2 & -2 \\ -2 & 0 & 0 & 0 & 0 & 2 \end{pmatrix}, \quad \mathbf{M} = \frac{5}{6} \cdot \begin{pmatrix} 3 & 2 & 0 & -2 & -1 & -2 \\ -2 & 3 & 1 & -1 & 0 & -1 \\ -3 & -4 & 6 & 4 & -1 & -2 \\ -1 & -2 & -4 & 6 & 1 & 0 \\ 1 & 0 & -2 & -4 & 3 & 2 \\ 2 & 1 & -1 & -3 & -2 & 3 \end{pmatrix}$$

The symmetric part of the the pseudo-inverse $\mathbf{M}$, and the Modified Fundamental Matrix are

$$\widehat{\mathbf{M}} = \frac{5}{4} \cdot \begin{pmatrix} 2 & 0 & -1 & -1 & 0 & 0 \\ 0 & 2 & -1 & -1 & 0 & 0 \\ -1 & -1 & 4 & 0 & -1 & -1 \\ -1 & -1 & 0 & 4 & -1 & -1 \\ 0 & 0 & -1 & -1 & 2 & 0 \\ 0 & 0 & -1 & -1 & 0 & 2 \end{pmatrix}, \quad \widetilde{\mathbf{Z}} = \frac{1}{10} \cdot \begin{pmatrix} 31 & 21 & 11 & 1 & 1 & -9 \\ -9 & 31 & 21 & 11 & 11 & 1 \\ -9 & -19 & 71 & 61 & 11 & 1 \\ 1 & -9 & -19 & 71 & 21 & 11 \\ 11 & 1 & -9 & -19 & 31 & 21 \\ 21 & 11 & 1 & -9 & -9 & 31 \end{pmatrix}$$

We observe that the diagonal entries for nodes 3,4 are higher than for the other nodes. This indicates that nodes 3,4 are more on the periphery of the graph, compared to the remaining nodes.

The computed average first transit times from any state to any state, and the average round-trip commute times are

$$\mathtt{N} = \begin{pmatrix} 0 & 1 & 6 & 7 & 3 & 4 \\ 4 & 0 & 5 & 6 & 2 & 3 \\ 4 & 5 & 0 & 1 & 2 & 3 \\ 3 & 4 & 9 & 0 & 1 & 2 \\ 2 & 3 & 8 & 9 & 0 & 1 \\ 1 & 2 & 7 & 8 & 4 & 0 \end{pmatrix}, \quad \mathtt{C} = 5 \cdot \begin{pmatrix} 0 & 1 & 2 & 2 & 1 & 1 \\ 1 & 0 & 2 & 2 & 1 & 1 \\ 2 & 2 & 0 & 2 & 2 & 2 \\ 2 & 2 & 2 & 0 & 2 & 2 \\ 1 & 1 & 2 & 2 & 0 & 1 \\ 1 & 1 & 2 & 2 & 1 & 0 \end{pmatrix}$$

Symmetrizing $\widetilde{\mathbf{Z}}$ and computing its Cholesky factor yields the embedding $\mathbf{S}$ in $\mathbb{R}^6$.

$$\mathbf{S} = \begin{pmatrix} 1.76068 & .340777 & .056796 & .056796 & .340777 & .340777 \\ 0 & 1.72738 & .046686 & .046686 & .280117 & .280117 \\ 0 & 0 & 2.66356 & .786386 & .025367 & .025367 \\ 0 & 0 & 0 & 2.54483 & .018712 & .018712 \\ 0 & 0 & 0 & 0 & 1.70423 & .237298 \\ 0 & 0 & 0 & 0 & 0 & 1.68763 \end{pmatrix}$$

We also subtract the mean vector to get the centered embedding $\mathbf{R}$.

$$\mathbf{R} = \begin{pmatrix} 1.27791 & -.14199 & -.42597 & -.42597 & -.14199 & -.14199 \\ -.39683 & 1.33055 & -.35014 & -.35014 & -.11671 & -.11671 \\ -.58344 & -.58344 & 2.08011 & .202938 & -.55808 & -.55808 \\ -.43037 & -.43037 & -.43037 & 2.11445 & -.41166 & -.41166 \\ -.32358 & -.32358 & -.32358 & -.32358 & 1.38064 & -.08629 \\ -.28127 & -.28127 & -.28127 & -.28127 & -.28127 & 1.40636 \end{pmatrix}$$

To expose the fact that the columns of $\mathbf{R}$ are actually in a 5 dimensional subspace, we can compute the "QR" decomposition [10] $\mathbf{R} = \mathbf{QU}$ where $\mathbf{Q}$ is orthogonal and $\mathbf{U}$ is upper triangular. Since $\mathbf{U}'\mathbf{U} = \mathbf{R}'\mathbf{R} = \widehat{\mathbf{M}}$ and $\mathbf{Ue} = \mathbf{Q}'\mathbf{Re} = 0$, we can use $\mathbf{U}$ as an alternate centered embedding,

$$\mathbf{U} = \begin{pmatrix} -1.5811 & 0 & .790569 & .790569 & 0 & 0 \\ 0 & -1.5811 & .790569 & .790569 & 0 & 0 \\ 0 & 0 & -1.9364 & .645497 & .645497 & .645497 \\ 0 & 0 & 0 & -1.8257 & .912871 & .912871 \\ 0 & 0 & 0 & 0 & -1.1180 & 1.11803 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Finally, we try to construct an undirected graph with round-trip commute times matching those of the original graph.

$$L = (\widehat{\mathbf{M}})^+ = \frac{1}{90} \cdot \begin{pmatrix} 28 & -8 & -2 & -2 & -8 & -8 \\ -8 & 28 & -2 & -2 & -8 & -8 \\ -2 & -2 & 13 & -5 & -2 & -2 \\ -2 & -2 & -5 & 13 & -2 & -2 \\ -8 & -8 & -2 & -2 & 28 & -8 \\ -8 & -8 & -2 & -2 & -8 & 28 \end{pmatrix}, \text{ with diagonal } D = \frac{1}{90} \cdot \begin{pmatrix} 28 \\ 28 \\ 13 \\ 13 \\ 28 \\ 28 \end{pmatrix}.$$

The resulting adjacency matrix and Markov chain transition matrices are

$$A = \frac{1}{90} \cdot \begin{pmatrix} 0 & 8 & 2 & 2 & 8 & 8 \\ 8 & 0 & 2 & 2 & 8 & 8 \\ 2 & 2 & 0 & 5 & 2 & 2 \\ 2 & 2 & 5 & 0 & 2 & 2 \\ 8 & 8 & 2 & 2 & 0 & 8 \\ 8 & 8 & 2 & 2 & 8 & 0 \end{pmatrix}, \quad P_{\text{new}} = \frac{1}{182} \cdot \begin{pmatrix} 0 & 52 & 13 & 13 & 52 & 52 \\ 52 & 0 & 13 & 13 & 52 & 52 \\ 28 & 28 & 0 & 70 & 28 & 28 \\ 28 & 28 & 70 & 0 & 28 & 28 \\ 52 & 52 & 13 & 13 & 0 & 52 \\ 52 & 52 & 13 & 13 & 52 & 0 \end{pmatrix}$$

This adjacency matrix corresponds to a weighted undirected graph.