On Fast Computation of Directed Graph Laplacian Pseudo-Inverse

Daniel Boley  
*University of Minnesota*  
boley@umn.edu  

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**Abstract**

The Laplacian matrix and its pseudo-inverse for a strongly connected directed graph is fundamental in computing many properties of a directed graph. Examples include random-walk centrality and betweenness measures, average hitting and commute times, and other connectivity measures. These measures arise in the analysis of many social and computer networks. In this short paper, we show how a linear system involving the Laplacian may be solved in time linear in the number of edges, times a factor depending on the separability of the graph. This leads directly to the column-by-column computation of the entire Laplacian pseudo-inverse in time quadratic in the number of nodes, i.e., constant time per matrix entry. The approach is based on “off-the-shelf” iterative methods for which global linear convergence is guaranteed, without recourse to any matrix elimination algorithm.

**Keywords:** Graph Laplacian; Directed Graphs; Pseudo-Inverse.

1. Introduction.

Many computations on networks depend on efficient solvers for matrix systems of linear equations, matrix pseudo-inverses, and/or eigenvalue problems. Examples include the well-known pagerank, centrality measures, betweenness measures, graph cuts, distances or affinities between nodes, trust/influence propagation, etc. Many of these can be found via the solution of special linear systems based on the graph Laplacian. This has spawned many papers on efficient, almost linear time solvers for these special linear systems such as [28] for symmetric systems for undirected graphs to more recent papers reporting almost linear time for non-symmetric Eulerian Laplacians for directed graphs [8, 9]. For the purpose of this paper, a matrix is Eulerian if the individual row sums match the individual columns sums. These fast methods use a careful ordering of the nodes, an approximate factorization using Gaussian elimination used as a preconditioner to an iterative method based on, e.g., Richardson iteration. The theoretical running time for the methods of [8, 9] can be bounded by $O(m \log^c (n \kappa \varepsilon))$ with high probability $(1 - \delta)$, where $m$ is the number of edges, $n$ the number of nodes, $\kappa$ is the matrix condition number, and $\varepsilon$ is the desired accuracy, with $O(n \log^c / (\delta \varepsilon^6))$ fillin from the factorization. In this short paper we use a different approach to obtain an algorithm for the pseudo-inverse of a non-symmetric Eulerian Laplacian. Our approach is to use only iterative methods in widespread use in practice, and which also enjoy provable linear convergence guarantees and per-iteration costs linear in the number of edges in the graph. We also propose a computational process to obtain an Eulerian scaling.

Consider a directed graph with adjacency matrix $A \in \mathbb{R}^{n \times n}$ where $a_{ij}$ is the weight on the edge $i \rightarrow j$ if such an edge exists, otherwise $a_{ij} = 0$. If $I$ is the vector of all ones of appropriate dimension, then $d = A I$ is the vector of out-degrees, and $P = \text{DIAG}(d)^{-1} A$ is the matrix of transition probabilities for a random walk over this directed graph. Throughout this paper we assume the graph is strongly connected implying
that $P$ is irreducible. Let $\pi$ be the vector of stationary probabilities over this graph, i.e., the vector satisfying $\pi^T P = \pi^T$ and $\pi^T I = I$, and let $\Pi = \text{Diag}(\pi)$ be the diagonal matrix with the stationary probabilities $\{\pi_i\}$ on the diagonal. A directed graph has several scalings for the Laplacian \[4\]
\[
L^r = \Pi - \Pi P \\
L^a = D - A = D - DP \\
L^p = I - P \\
L^d = I - \Pi^{1/2} P \Pi^{-1/2}
\]
random walk Laplacian
unnormalized Laplacian
normalized Laplacian
diagonally scaled Laplacian
and corresponding pseudo-inverses
\[
M^r = (L^r)^+, \quad M^d = (L^d)^+, \quad M^p = (L^p)^+, \quad \text{etc.}
\]
It is well known that one can obtain many graph properties from the Laplacian or its pseudo-inverse, e.g., the average length $h(i, j)$ of a random walk starting from node $i$ before reaching node $j$ and the average round-trip commute time $c(i, j)$ \[18\], \[23\], \[12\], \[15\], \[19\], \[20\], \[4\] (even for strongly connected directed graphs):
\[
h(i, j) = \frac{m_{ij}^d}{\pi_j} - \frac{m_{ji}^d}{\sqrt{\pi_i \pi_j}}
\]
\[
c(i, j) = \frac{m_{ij}^d}{\pi_j} + \frac{m_{ji}^d}{\pi_i} - \frac{m_{ij}^d + m_{ji}^d}{\sqrt{\pi_i \pi_j}}
\]
The pseudo-inverse also yields the average number of visits to an individual node $j$ for random walks starting in node $i$ before reaching $k$: \[14\], \[3\]:
\[
v(i, j, k) = (m_{ij}^r - m_{kj}^r - m_{ik}^r + m_{kk}^r)\pi_j,
\]
and the probability of such a random walk to pass node $j$ at all:
\[
\text{Prob}(\text{pass } j \text{ on walks } i \rightarrow k) = v(i, j, k)/v(j, j, k).
\]
By summing $v(i, j, k)$ across various dimensions, one can obtain various centrality and betweenness measures for individual nodes \[14\].

Given an arbitrary directed graph with $n$ nodes, one can augment the graph with an extra node $n+1$ such that, upon every transition in a random walk over the graph, there is a small probability $\alpha$ that the walker "evaporates" to node $n+1$, and thence the walker transitions to an arbitrary node with equal probability (or biased probabilities in a personalized setting). This is a process very similar to teleportation in the pagerank setting. The result is a strongly connected directed graph to which we can apply the methods of this paper. In this case the average number of visits $v(i, j, n+1)$ or average path lengths $h(i, j)$ would yield a continuum of affinity estimates from $i$ to $j$, approximating random walk affinity for $\alpha$ near $0$ and shortest path affinity for $\alpha$ near $1$. This has been used to model, e.g., trust propagation in social networks \[22\], \[5\].

The main contributions of this paper are: (A) we show how an off-the-shelf iterative method in widespread use yields a method to find the the pseudo-inverse of an Eulerian Laplacian with a provable complexity guarantee that is linear in the number of edges times a factor related to the connectness of the graph; (B) we show how another off-the-shelf method yields a method to find a Eulerian scaling for a non-Eulerian Laplacian with similar complexity guarantees; and (C) we illustrate the methods with some examples showing the linear complexity can be observed in practice with the off-the-shelf numerical procedures. The constructions proposed in this paper are kept as simple as possible to highlight a minimal set of assumptions
needed to form the basis for a fast Laplacian solver. Most of the theoretical properties used in this paper are well-known, but we include a few brief proofs to make this paper more self-contained.

The rest of this paper begins with a Lemma which reduces the pseudo-inverse computation to a simple matrix inversion. Then we present the overall algorithm to find an Eulerian scaling and compute the necessary inverses, followed by an outline of the complexity analysis, which includes the convergence theory and the cost per iteration. We end with a short table of experiments showing the methods translate directly to an implementable numerical algorithm with the costs that grow approximately as the theory predicts.

2. Preliminary Construction.

In this paper we study mainly the Laplacian matrices $L^r$ and $L^d$. The matrix $L^r$ can be thought of as the unnormalized Laplacian for a weighted digraph with adjacency matrix $\Pi \Pi^T$. This last matrix has all row sums and column sums equal to each other: $\Pi \Pi^T = (\Pi \Pi^T)^T \pi = \pi$, and hence is called Eulerian [8, 9].

The matrix $\Pi^{1/2} \Pi^{-1/2}$ has a similar property: $\Pi^{1/2} \Pi^{-1/2} \sqrt{\pi} = (\Pi^{1/2} \Pi^{-1/2})^T \sqrt{\pi} = \sqrt{\pi}$. Here $\sqrt{\pi} = [\sqrt{\pi_1}, \ldots, \sqrt{\pi_n}]^T$. For the purposes of this paper, we call a matrix whose weighted row sums equal its weighted column sums (with the same weights) a [generalized] Eulerian matrix.

The main point of this section is to present the mapping between the pseudo-inverse computation for an Eulerian Laplacian and the computation of related ordinary inverses. In the following lemma we present two such mappings. Part (a) connects the pseudo-inverse of the Eulerian Laplacian matrix with the ordinary inverse of a symmetric rank-1 modification to that matrix. The rank-1 modification is exactly in the direction corresponding to the nullspace of the original Laplacian. This construction is well known (see, e.g., [12, 4]). Part (b) shows how the ordinary inverse of the $(n - 1) \times (n - 1)$ principal submatrix of a Eulerian Laplacian can be obtained directly from the pseudo-inverse of the entire matrix via small rank changes, and part (c) gives reverse mapping, from the ordinary inverse of the submatrix to the pseudo-inverse of the entire matrix. These connections will allow the use of off-the-shelf iterative methods for the ordinary inverse in order to obtain the desired pseudo-inverse.

Lemma 1. Let $C$ be an $n \times n$ non-singular matrix and suppose $A = C - \alpha uu^T$ is singular with $Au = A^T u = 0$. Partition $A$ and $u$ as follows:

$$A = \begin{bmatrix} A_{11} & a_{12} \\ a_{21}^T & a_{22} \end{bmatrix}, \quad u = \begin{bmatrix} u_1 \\ u_n \end{bmatrix}. \quad (3)$$

Assume $u^T u = 1$ and $u_n > 0$. Then

(a) the left and right nullspaces of $A$ are $\nullsp(A) = \nullsp(A^T) = \text{span}(u)$, and the Moore-Penrose pseudo-inverse of $A$ is given as:

$$A^\dagger \overset{\text{def}}{=} B = -uu^T/\alpha.$$

(b) $A_{11}^{-1}$ exists and can be written in terms of $A^\dagger = B$:

$$A_{11}^{-1} = [I_{n-1}, -u_1/u_n] B \begin{bmatrix} I_{n-1} \\ -u_1^T/u_n \end{bmatrix}$$

$$= B_{11} - u_1 u_{1n} b_{21}^T - b_{12} u_1^T u_{1n} + u_1 u_{1n}^T,$$

where we have partitioned $B$ as in (3).
(c) We can write $A$ and $B = A^\dagger$ in terms of $A_{11}$ and $u$ as follows

$$
A = \begin{bmatrix}
A_{11} & -A_{11}u_1 \frac{1}{u_n} \\
-u_1^T \frac{1}{u_n} A_{11} & u_1^T A_{11} u_1 \frac{1}{u_n^2}
\end{bmatrix} = \begin{bmatrix}
I_{n-1} & -u_1 \frac{1}{u_n} \\
-u_1^T \frac{1}{u_n} & A_{11}
\end{bmatrix} \begin{bmatrix}
I_{n-1}, & -u_1 \frac{1}{u_n}
\end{bmatrix};
$$

\[(5)\]

$$
B = \begin{bmatrix}
B_{11} & b_{12} \\
b_{21}^T & b_{nn}
\end{bmatrix} = \begin{bmatrix}
I_{n-1} - u_1 u_1^T \\
-u_n \cdot u_1^T
\end{bmatrix} A_{11}^{-1} \begin{bmatrix}
I_{n-1} - u_1 u_1^T, & -u_n \cdot u_1
\end{bmatrix}
$$

where the individual blocks are

$$
B_{11} = A_{11}^{-1} - u_1 t^T - w u_1^T + (u_1^T w) \cdot u_1 u_1^T
$$
$$
b_{12} = u_n^2 (u_1^T w) \cdot u_1 - u_n w
$$
$$
b_{21} = u_n^2 (u_1^T w) \cdot u_1^T - u_n t^T
$$
$$
b_{nn} = u_n^2 (u_1^T w)
$$

where $w = A_{11}^{-1} u_1$, $t = u_1^T A_{11}^{-1}$.

Proof.

(a) A simple calculation yields $AB = BA = I_n - uu^T$, and a further simple calculation yields $ABA = A$ and $BAB = B$. Hence $B$ satisfies the conditions to be the Moore-Penrose pseudo inverse.

(b) $Au = 0$ and $u^T A = 0^T$ imply

$$
A_{11} u_1 = -a_{12} u_n, \quad u_1^T A_{11} = -u_1^T a_{21} u_n
$$
$$
a_{21} u_1 = -a_{nn} u_n, \quad u_1 a_{12} = -a_{nn} u_n
$$

Likewise, $Bu = 0$ and $u^T B = 0^T$ imply

$$
B_{11} u_1 = -b_{12} u_n, \quad u_1^T B_{11} = -b_{21}^T u_n
$$
$$
b_{21} u_1 = -b_{nn} u_n, \quad u_1^T b_{12} = -b_{nn} u_n
$$

These yield the equivalence for the two formulas for $A_{11}^{-1}$ in (4) and the formulas for $A$ in (5). To verify (4) is indeed the inverse of $A_{11}$, we multiply (4) by $A_{11}$ to obtain the identity:

$$
[I_{n-1}, \ -u_1 / u_n] B \begin{bmatrix}
I_{n-1}^{-1} & -u_1 / u_n
\end{bmatrix} A_{11}
$$

$$
= [I_{n-1}, \ -u_1 / u_n] B \begin{bmatrix}
A_{11}^{-1} & -a_{21}
\end{bmatrix}
$$

$$
= [I_{n-1}, \ -u_1 / u_n] \begin{bmatrix}
I_{n-1} - u_1 u_1^T \\
-u_n u_1^T
\end{bmatrix} = I_{n-1}
$$

(c) Using the second formulas for $A$, $B$ in (5), calculations similar to the proof of (b) yield $AB = BA = I_n - uu^T$ and then $ABA = A$, $BAB = B$.

3. Algorithm for Eulerian Laplacians.

We study the computation of the pseudo-inverses of $L^d$ and $L^f$. Using Lemma of, we can write these as follows:

$$
[a] \quad M^d = (L^d)^\dagger = (L^d + \sqrt{\pi} \sqrt{\pi}^T)^{-1} - \sqrt{\pi} \sqrt{\pi}^T
$$
$$
[b] \quad M^f = (L^f)^\dagger = (L^f + I f^T/(n \eta))^\dagger - I f^T \eta,
$$

\[(6)\]
for some arbitrary $\eta \neq 0$ (we use $\eta = 1$ below). Lemma \[\] applies here because both $L'$ and $L^d$ have nullity 1 and are generalized Eulerian.

The overall algorithm begins with a computation of the stationary probabilities. These probabilities are used to scale the Laplacian to an Eulerian scaling. The final step is to solve for the pseudo-inverse of the Eulerian Laplacian by applying an iterative method to (6). The detailed steps are given in Algorithm \[\].

**Algorithm 1.**

**Input:** $P$ - probability transition matrix for a random walk over the graph.

**Output:** Stationary probabilities $\pi$ and either [a] pseudo-inverse $M^d = (L^d)^+ = (I - I^{1/2} \Pi \Pi^{-1/2})^+$, and/or [b] pseudo-inverse $M' = (L')^+ = (\Pi - \Pi \Pi)$. Note: items marked [a] are needed only for $M^d$ while items marked [b] are needed only for $M'$.

1. Compute $\pi$, the vector of stationary probabilities:
   Use the modified subspace iteration method with $\ell$ starting vectors [29] on $P^T$ to compute eigenvector corresponding to the eigenvalue $\lambda = 1$. Here $\ell$ is larger than the period of the graph.
2. Set [a] $L^d = I - \Pi^{1/2} \Pi \Pi^{-1/2}$, where $\Pi^{1/2} = \text{diag}(\sqrt{\pi})$, and/or [b] $L' = \Pi - \Pi \Pi$, where $\Pi = \text{diag}(\pi)$.
3. Compute pseudo-inverses of Eulerian Laplacians:
   - [a] $M^d = (L^d)^+$ and/or
   - [b] $M' = (L')^+$ column-by-column:
     - For $j = 1, \ldots, n$
       - (a) Solve linear systems
         - [a] $(L^d + \sqrt{\pi} \pi^T)x^d = e_j$, or
         - [b] $(L' + I^T/n)x = e_j$, with restarted GMRES.
       - (b) Fill in the $j$-th column of pseudo-inverse:
         - [a] $M^d_{i,j} = x^d - \sqrt{\pi}j \cdot \sqrt{\pi}$, and/or
         - [b] $M'_{i,j} = x - 1/n$.

4. **Complexity of Algorithm 1: Convergence.**

The two most expensive steps in Algorithm 1 are steps [1] and [3a] both involving an iterative method. Their cost is a product of the cost per iteration times the number of iterations. The remaining steps all have cost at most $O(n^2)$ for the entire matrix, i.e., constant time per matrix entry.

In step [1] the modified subspace iteration (Alg [3] [29]) computes the Schur decomposition on a small $\ell \times \ell$ matrix which is the orthogonal projection of the original matrix $P^T$ onto a $\ell$ dimensional subspace. If $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of $P$ with $1 \geq |\lambda_2| \geq \cdots \geq |\lambda_n|$, where $1 \geq |\lambda_\ell| > |\lambda_{\ell+1}|$, and $\lambda_1 = 1$ is a simple eigenvalue, then Stewart [29] showed that the leading eigenvector (corresponding to $\lambda_1 = 1$) converges as:

$$\frac{\|P^T x^{[k]} - x^{[0]}\|}{\|P^T x^{[0]} - x^{[0]}\|} \leq O(|\lambda_{\ell+1}|^k)$$

where $\lambda_1^{[k]}$ denotes the approximation to the eigenvalue $\lambda_1 = 1$ at the $k$-iteration. In the following we use $c_1, c_2, \ldots$ to represent small positive constants in the costs bounds, all of which are less than 10. If the random walk is aperiodic, then we are guaranteed that $1 > |\lambda_2| \geq \cdots \geq |\lambda_\ell| \geq \cdots$. If the random walk is periodic with period $\per$, it suffices to have $\ell > \per$ in order to guarantee that $\lambda_{\ell+1} < \lambda_1 = 1$. To obtain an error at most $tol$ requires at least $k^*$ iterations with

$$k^* \geq \frac{\log(tol) + \log(\|P^T x^{[0]} - x^{[0]}\|)}{\log(|\lambda_{\ell+1}|)}$$
As written in Algorithm 3 in the Appendix, the cost per iteration is \( \text{cost}_{Mv} \cdot (\ell + 1) + c_5(n\ell^2) + c_6(\ell^3) \) where the first term accounts for the matrix vector products, the second term accounts for the orthogonalization (Alg 3, step 2) and the third term accounts for the \( \ell \times \ell \) Schur decomposition (step 3). Here \( Mv \) is the number of matrix vector products. Each matrix-vector product requires \( \text{cost}_{Mv} = 2 \cdot \text{nnz}(\text{matrix}) \) flops (one multiply and one add per matrix entry). Here each matrix entry corresponds exactly to an edge in the graph. So the total cost per iteration is

\[
\text{cost}^{\text{subspace}}_1 = c_2 \#\text{edges} \cdot (\ell + 1) + c_3 n \ell^2 + c_4 \ell^3,
\]

for some small constants \( c_2, c_3, c_4 \) at most 10. We remark that for undirected graphs, this eigenvector is a multiple of the vector of degrees, so this step would be essentially free.

We remark that there are many choices of algorithms to compute this eigenvector, similar to the many choices to compute the pagerank vector, many of which can be faster \[13\]. For the purposes of providing a simple convergence formula leading to a simple complexity bound, this subspace iteration is quite sufficient.

The other costly step is step 3a to compute the inverse \( M^d \). This line is called \( n \) times, each time solving a linear system to obtain one column of the inverse, using restarted GMRES. In order to apply an analysis similar to the one for step 1, we must show that GMRES (without any preconditioning) is guaranteed to converge. In order to do that, we show that the symmetric part of the modified Laplacian matrices in question are positive definite, in the following lemma.

**Lemma 2.** If \( P \) is the probability transition matrix for a strongly connected directed graph, and \( \pi > 0 \) is the vector of stationary probabilities, then

\[
S(L^d) + \sqrt{\pi} \sqrt{\pi}^T = (L^d + (L^d)^T) / 2 + \sqrt{\pi} \sqrt{\pi}^T
\]

\[
S(L^r) + 11^T = (L^r + (L^r)^T) / 2 + 11^T
\]

are symmetric positive definite.

**Proof (sketch).** We show the symmetric part of the non-symmetric Laplacian is the Laplacian for a weighted undirected graph and hence is an M-matrix \[2\] which is positive semidefinite. Consider the weighted undirected graph with adjacency matrix \( \tilde{A} = (\Pi P + P^T \Pi) / 2 \). This is a weighted undirected graph with the same nodes as the original graph and an edge wherever the original graph has an edge in either direction. The vector of stationary probabilities for this graph is \( \pi \), proportional to the weighted degrees of the nodes in the new graph. The associated unnormalized Laplacian is \( 1/2(L^r + (L^r)^T) \), which is therefore symmetric positive semi-definite with nullspace equal to \( \text{span}(I) \) \[7\]. The associated diagonally scaled Laplacian is \( 1/2(L^d + (L^d)^T) = 1/2 \Pi^{-1/2}(L^r + (L^r)^T) \Pi^{-1/2} \), which is therefore also symmetric positive semi-definite with nullspace equal to \( \text{span}(\sqrt{\pi}) \). The probability transition matrix for the new graph is \( \tilde{P} = \Pi^{-1} \tilde{A} = (P + \Pi^{-1} P^T \Pi) / 2 \). Adding a symmetric rank-1 matrix \( (11^T \text{ or } \sqrt{\pi} \sqrt{\pi}^T) \) makes the respective Laplacian matrices non-singular, moving the 0 eigenvalue to a positive number without moving the remaining eigenvalues.

We can now notice that the Laplacian matrices \( S(L^r) + \sqrt{\pi} \sqrt{\pi}^T, S(L^d) + 11^T \) have just the right scaling to belong to a class of matrices for which GMRES (or any similar Krylov space minimum residual method) converges. We have the following theorem that is an immediate consequence of Theorem 5 in the Appendix.

**Corollary 3.** Let \( A \) be a real matrix such that \( S(A) = (A + A^T) / 2 \) is symmetric positive definite and let \( \lambda_{\min}[S(A)] > 0 \) denote the smallest eigenvalue for \( S(A) \). The residual \( r_k \) obtained by restarted GMRES \[26\] (restarting after \( \ell \) inner steps) after \( k \) outer steps satisfies

\[
\frac{\|r_k\|_2}{\|r_0\|_2} \leq \left( 1 - \frac{(\lambda_{\min}[S(A)])^2}{\|A\|_2^2} \right)^{k\ell/2}
\]
The cost of one outer step of restarted GMRES is $\text{cost}^\text{GMRES}_1 \ell \cdot \text{cost}_M + c_7(n\ell^2 + \ell^3)$ (see appendix).

In summary, the total cost to find the vector of stationary probabilities is

$$\text{cost}^\text{subspace} = k^* (\ell + 1) \cdot \text{cost}_M + c_8(2n\ell^2 + \ell^3),$$

where $\rho = \lambda_{\ell+1}(P)$. The total cost to find each column of the pseudo-inverse with a residual error of $\text{tol}$ is

$$\text{cost}^\text{GMRES} = k^* (\ell \cdot \text{cost}_M + c_7(n\ell^2 + \ell^3)),\text{cost}^\text{total} = n k^* (\ell \cdot \text{cost}_M + c_9(n + n\ell^2 + \ell^3))$$

where $\sigma = \left(1 - \frac{\lambda_{\min}[S(A)]^2}{\|A\|^2} \right)^{\ell/2}$, yielding a total cost to obtain the entire pseudo-inverse of the Eulerian Laplacian:

$$\text{cost}^\text{total} = n k^* (\ell \cdot \text{cost}_M + c_9(n + n\ell^2 + \ell^3))$$

5. General Pseudo-Inverses.

Here we show how to extend the previous to obtain the inverses or pseudo-inverses of general Laplacian matrices derived from strongly connected directed graphs. The approach is to apply a row/column diagonal scaling to the non-Eulerian Laplacian to obtain a related Eulerian matrix (similar to [8]), compute the pseudo-inverse using the previous methods, and undo the diagonal scaling. This can be applied to any Laplacian $\tilde{L}$ that has all the following properties:

(Pa) $\tilde{L}$ is irreducible,

(Pb) all the off-diagonal entries are non-positive,

(Pc) there is a strictly positive vector $x$ so that $\tilde{L}x = 0$.

Matrices satisfying property (Pb) are called Z-matrices. Alternatively, we can start with an $(n-1) \times (n-1)$ matrix $\tilde{L}_{11}$ which shares properties (Pa) and (Pb), but has the property

(Pc’) there is a strictly positive vector $w$ so that $\tilde{L}_{11}w$ is strictly positive.

Then we use Lemma 4 below to embed $\tilde{L}_{11}$ inside an $n \times n$ matrix $\tilde{L}$ enjoying properties (Pa), (Pb), (Pc) and hence apply the same procedures. Matrices satisfying (Pa), (Pb), (Pc’) are non-singular M-matrices and include matrices that are strictly row-diagonally dominant [2]. There are many other ways to characterize M-matrices (see [2]).

The pseudo-inverse of a diagonally scaled matrix is not the diagonally scaled pseudo-inverse of the original, but the ordinary inverse of a diagonally scaled matrix is the diagonally scaled ordinary inverse of the original. Hence one can apply the diagonal scaling to the leading principal submatrix of a Laplacian to map the problem to the Eulerian scaling. The following lemma provides a way to map from a matrix pseudo-inverse to the ordinary inverse of its principal submatrix and vice versa, using only fast rank-one updates. Alternatively, one can use $\Pi$ as a preconditioner on the unscaled Laplacian.

**Lemma 4.** Let $C$ be an $n \times n$ non-singular matrix and suppose $A = C - \alpha uv^T$ is singular with $Au = A^Tv = 0$, $v^Tu = 1$ and $u_n > 0$, $v_n > 0$. Then
(a) the left and right nullspaces of $A$ are $\text{nullsp}(A) = \text{span}(u)$, and $\text{nullsp}(A^T) = \text{span}(v)$. The Moore-Penrose pseudo-inverse of $A$ is given as:

$$A^\dagger = B \overset{\text{def}}{=} (I_n - uu^T u^u) C^{-1} (I_n - vv^T v^v)$$

$$= C^{-1} - uy^T u^u - \frac{1}{v^v} xv^T + \frac{u^T x}{(u^u)(v^v)} uv^T,$$

where $y^T = u^T C^{-1}, \ x = C^{-1} v$.

(b) $A^{-1}_{11}$ exists and can be written in terms of $A^\dagger = B, u, v$:

$$A^{-1}_{11} = \left( I_{n-1} + u_1 u_1^T \frac{1}{u_1^T u_1} \right) B_{11} \left( I_{n-1} + v_1 v_1^T \frac{1}{v_1^T v_1} \right)$$

$$= \left[ I_{n-1}, - u_1 / u_1 \right] B \left[ I_{n-1}^T / v_1, -v_1^T / v_1 \right],$$

$$= B_{11} - u_1 \frac{1}{u_1} b_{21}^T - b_{12} v_1^T \frac{1}{v_1} + u_1 v_1^T \frac{b_{21}}{v_1 v_1},$$

where we have partitioned $B$ as above.

(c) We can write $A$ and $B = A^\dagger$ in terms of $A_{11}, u, v$ as follows

$$A = \begin{bmatrix} A_{11} & -A_{11} u_1 \frac{1}{u_1} \\ -v_1^T \frac{1}{v_1} A_{11} & \text{Diag} \left( \frac{1}{u_1} \right) \end{bmatrix} = \begin{bmatrix} I_{n-1}^T / v_1 \end{bmatrix} A_{11} \left[ I_{n-1}, - u_1 \frac{1}{u_1} \right]$$

$$B = \begin{bmatrix} B_{11} & b_{12} \\ b_{21}^T & b_{nn} \end{bmatrix} = \begin{bmatrix} I_{n-1}^T / v_1 - \frac{u_1 u_1^T}{u_1^T u_1} u_1^T v_1 \\ -u_1 \frac{1}{u_1^T u_1} u_1^T \end{bmatrix} A_{11} \left[ I_{n-1} - \frac{v_1 v_1^T}{v_1^T v_1}, -v_1 v_1 \right]$$

where the individual blocks of $B$ are

$$B_{11} = A_{11}^{-1} - u_1 t^T - wu_1^T + \frac{u_1 w}{v^v} \cdot u_1 v_1^T$$

$$b_{12} = \frac{u_1 w}{v^v} \cdot v_1 - w$$

$$b_{21}^T = \frac{v_1^T v_1}{v_1^T v_1} \cdot u_1 - t^T$$

$$b_{nn} = \frac{u_1 w}{u_1^T u_1} (u_1^T w)$$

where $w = \frac{u_1}{u_1^T u_1} A_{11}^{-1} v_1, \ t^T = \frac{u_1 w}{v^v} u_1^T A_{11}^{-1}$

**Proof.** The proof follows the same lines as that of Lemma [1], after noting that $AB = I - \frac{uv^T}{v^v}$, and $BA = I - \frac{uv^T}{v^v}$.

Using this lemma, we briefly outline a feasible procedure to obtain the pseudo-inverse for an admissible Laplacian matrix consisting of a sequence of diagonal scalings and the Eulerian Laplacian Algorithm [1].

Suppose we have a matrix $\hat{L}$ satisfying properties (Pa), (Pb), (Pc), together with a strictly positive vector $x$ such that $0 = \hat{L} x$. For a strongly connected digraph with adjacency matrix $\hat{A}$, and vector of out-degrees $\hat{d}$, the unnormalized Laplacian, $\hat{L} = \text{Diag}(\hat{d}) - \hat{A}$ is such a matrix, with $x = 1$. Define $\hat{\hat{L}} \overset{\text{def}}{=} (\hat{\hat{D}} - \hat{\hat{A}}) = \hat{L} \cdot \text{Diag}(x)$, where $\hat{D}$ is the diagonal part of $\hat{L}$ and $\hat{\hat{A}}$ has the rest. This matrix has the property that $\hat{\hat{L}} \hat{1} = 0$. In this case, $\hat{P} = \hat{D}^{-1} \hat{\hat{A}}$ is the probability transition matrix for a random walk.
over this graph, with stationary probabilities $\pi$. We can then follow the following steps to compute the pseudo-inverse of $\tilde{L}$.

**Algorithm 2.**

**Input:** $\tilde{L}$ satisfying (Pa)--(Pc) and a strictly positive vector $x$ such that $\tilde{L}x = 0$.

**Output:** Pseudo-inverse of $\tilde{L}$.

1. Form $\hat{\tilde{L}} \overset{\text{def}}{=} (\hat{D} - \hat{A}) = \tilde{L} \cdot \text{Diag}(x)$, where $\hat{D}$ is the diagonal part of $\tilde{L}$.
2. Compute $\pi$, the vector of stationary probabilities by computing the leading eigenvector for $\hat{P}^T = (\hat{D}^{-1} \hat{A})^T$ as in Algorithm 1 step 1.
3. Form $\hat{L}_d = \Pi^{1/2} (I - \hat{D}^{-1} \hat{A}) \Pi^{-1/2} = \Pi^{1/2} (\hat{D}^{-1} \hat{L}) \Pi^{-1/2}$.
4. Compute pseudo-inverse $(\hat{L}_d)^\dagger$ as in Algorithm 1 step 3.
5. Use Lemma 1b to obtain the $(n-1) \times (n-1)$ matrix $(\hat{L}_{11})^{-1}$ from $(\hat{L}_d)^\dagger$. Here $u = \sqrt{\pi}$.
6. Form the $(n-1) \times (n-1)$ matrix $(\tilde{L}_{11})^{-1} = (\text{Diag}(x_1, \ldots, x_{n-1})) \Pi_1^{1/2} (\hat{L}_{11})^{-1} \Pi_1^{1/2} \hat{D}_1^{-1}$.
7. Use Lemma 4c to obtain $\tilde{L}^\dagger$ from $(\tilde{L}_{11})^{-1}$. Here $u = I$ and $v = \pi$.

**6. Performance.**

To illustrate how the theoretical complexity corresponds to practice we generate a sequence of synthetic graphs using preferential attachment [1] with $2n$ edges plus an extra set of $n$ randomly placed one-way edges to make the graph a digraph. Table 1 shows the time to compute the stationary probabilities $\pi$ and the time to solve a single linear system involving $\hat{L}_d$ using GMRES. We also show the number of matrix-vector products, which is solely a function of the number of overall iterations, which in turn is entirely dependent on the eigenvalue distribution of Laplacian. This, of course, depends on the nature of the underlying graph and would have to be analysed on a case-by-case basis. In the sequence of synthetic graphs constructed for this illustration, it is seen that the number of iterations is a slowly growing function of the dimension. Except for the modest increase in the number of matrix-vector products, the cost of the methods approximately double when the dimension $n$ is doubled. Using Matlab R2018a on a 2.5GHz linux desktop, each experiment was repeated 4 times with averages shown in Table 1.

Table 1 also shows performance on an Epinions data set [25], augmented with an evaporating node with an evaporating probability of 0.05 followed by a uniformly random restart (akin to the pagerank teleportation probability [24]). In other words, at every transition the walker has a 5% chance of “evaporating” to the extra node, and from the extra node the walker transitions to one of the original nodes with equal probability. Including the extra node and associated links and 9 old nodes not otherwise connected to any other node, the resulting graph has 75,889 nodes and 660,613 links.

**7. Discussion and Conclusions.**

We have used several off-the-shelf matrix iterative methods to compute the pseudo-inverse of a digraph Laplacian matrix in time that is amortized to almost constant time per matrix entry. Each column of the pseudo-inverse can be computed in time linear in the number of edges times a factor depending on how difficult it is to cut the graph into separate connected components. The methods proposed here depend exclusively on iterative methods and do not make any use of an elimination scheme that results in fill-ins, unlike methods using a variant of Gaussian elimination. They are relatively efficient and enjoy a plethora of available implementations.

For simplicity, we have described the methods to compute the entire pseudo-inverse, but of course this is impractical for larger graphs. However, it is straightforward to rearrange Algorithm 1 to compute the final
Table 1: Performance on synthetic graphs & one social network

| $n$   | $\text{dim}$ | $\#Mv$ | time (ms) | $\text{dim}$ | $\#Mv$ | time (ms) |
|-------|--------------|--------|-----------|--------------|--------|-----------|
| 1024  | 237          | 3.919  | 59        | 7.097        |
| 2048  | 286          | 5.297  | 65        | 9.331        |
| 4096  | 303          | 11.685 | 68        | 23.451       |
| 8192  | 369          | 28.223 | 74        | 51.270       |
| 16384 | 429          | 56.804 | 82        | 82.047       |
| 32768 | 347          | 88.941 | 77        | 135.895      |
| 65536 | 391          | 192.741| 83        | 265.114      |
| 131072| 429          | 427.461| 86        | 483.605      |
| 262144| 528          | 1130.698| 95        | 1136.207     |

Epinions data set

| $n$   | $\text{dim}$ | $\#Mv$ | time (ms) |
|-------|--------------|--------|-----------|
| 75889 | 682          | 477.362| 68        |
|       |              |        | 304.657   |

pseudo-inverse one column at a time or in parallel, each with one GMRES linear system solution taking $O(m)$ operations per iteration. The overall complexity is entirely dependent on the convergence rate for the iterative GMRES and eigensolver, which in turn depends on the smallest eigenvalues of $I - P$ and $L + L^T$, respectively. The former is related to the mixing rate of the random walk, while the latter is closely related to the Cheeger constant \[6\]. In both cases a tiny eigenvalue corresponds to a graph that can be split with a small cut. Any iterative method would depend on similar quantities in some fashion.

Appendix

8. Compute Stationary Probabilities. The vector of stationary probabilities $\pi$ is the eigenvector of $P^T$ corresponding to the eigenvalue $\lambda = 1$. Since the underlying graph is strongly connected, the Perron Frobenius theory guarantees eigenvalue $\lambda = 1$ is simple. The number of other eigenvalues of modulus 1 is equal to the periodicity of the graph or random walk. For instance, a bipartite graph will have an eigenvalue $-1$. If $\text{per}$ is the period of the graph and we use $\ell > \text{per}$ vectors in the following algorithm then the algorithm is guaranteed to converge at a rate bounded by $|\lambda_{\ell+1}(P)| < 1$ \[29\] since $\lambda = 1$ is known and is a simple eigenvalue of largest modulus.

Algorithm 3. Modified Subspace Iteration. \[29\]

Input: matrix $A$, hyperparameters: $\text{tol}$, initial guess $X[0] \in \mathbb{R}^{n \times \ell}$.

Output: $z = $ eigenvalue corresponding to eigenvalue 1.

1. Set $Z = \text{orthogonalize}(X[0])$, where $Z_{:,1}$ is all non-negative.
2. Repeat until convergence:
   (a) Set $Q = \text{orthogonalize}(AZ)$.
   (b) Compute $\ell \times \ell$ Schur Decomposition $[UTU^T] = Q^T AQ$ with the diagonal entries of $T$ ordered to put the entry closest to 1 in the 1,1 position.
   (c) Set $Z = QU$. Ensure the first column $Z_{:,1}$ is all non-negative (flipping signs of rows of $Z$ to make the first column all non-negative, if necessary).
3. Return $z = Z_{:,1}$.
9. **Restarted GMRES.** The heart of the computation of the pseudo-inverse is the use of Lemma 1 to convert a pseudo-inverse computation to an ordinary inverse computation. The restarted GMRES algorithm has received much attention in the literature (see [26] and references therein) with many enhancements for numerical stability that do not impact the cost by more than a constant factor. For the purposes of showing the overall cost of the algorithm, we show a simplified sketch of the basic algorithm. By using restarted GMRES we bound the cost of each iteration.

**Algorithm 4. Arnoldi-based Restarted GMRES.**

**Input:** Matrix $A$, right hand side $b$, hyperparameters: restart count $\ell$, outer iteration limit $\text{maxit}$, tolerance $\text{tol}$, initial vector $x^{[0]}$.

**Output:** solution $x$ such that $\|r\| = \|Ax - b\| < \text{tol}$.

1. Compute $r^{[0]} = b - Ax^{[0]}$
2. For $k = 0, 1, 2, \ldots \text{maxit}$:
   a. Set $\beta = \|r^{[k]}\|_2$ and set $v_1 = r^{[k]} / \beta$.
   b. If $\beta < \text{tol}$, return solution $x = x^{[k]}$.
   c. Generate orthonormal Arnoldi basis $V_{\ell+1} = [v_1, \ldots, v_{\ell+1}]$ for the Krylov space $\text{span}\{r_0, AV_0, \ldots, A^{\ell}r_0\}$, and upper Hessenberg matrix $H_{\ell} \in \mathbb{R}^{(\ell+1)\times \ell}$ such that $AV_{\ell} = V_{\ell+1}H_{\ell}$.
   d. Compute $y^{[k]} = \text{arg min}_{y} \|\beta e_1 - H_{\ell}y\|_2$.
   e. Set $x^{[k+1]} = x^{[k]} + V_{\ell}y^{[k]}$

The cost of one outer step of restarted GMRES is $\ell \cdot \text{cost}_{Mv} + O(n\ell^2 + \ell^3)$ [26]. Here $\text{cost}_{Mv}$ is the cost of one matrix vector product involving sparse matrix $A$. This takes one floating multiply and one floating add for each non-zero matrix element. So the cost is $\text{cost}_{Mv} = O(\text{nnz}(A))$. The number of outer iterations required is controlled by the eigen-structure of the symmetric part $S(A) = (A + A^T)/2$, which is related to the separability of the underlying graph [6]. Note step (d) is an $(\ell + 1) \times \ell$ least squares problem costing $O(\ell^2)$ to solve, due to the special Hessenberg structure of $H$.

Regarding the number of GMRES iterations, we have the following bound which yields Theorem 5 as an immediate consequence.

**Theorem 5.** [11, 10, 21, 17]. Let $A$ be a matrix such that $S(A) \overset{\text{def}}{=} (A + A^H)/2$ is Hermitian positive definite and let $\lambda_{\text{min}}[S(A)] > 0$ denote the smallest eigenvalue for $S(A)$. The residual $r_k$ obtained by GMRES [27] after $k$ steps applied to the linear system $Ax = b$ satisfies

$$\frac{\|r_k\|_2}{\|r_0\|_2} \leq \left(1 - \frac{\lambda_{\text{min}}[S(A)]^2}{\|A\|_2^2}\right)^{k/2}$$

We give a sketch of a proof, referring to [11, 10, 21, 17] for detailed proofs, including several tighter bounds. First we need the following Lemma

**Lemma 6.** Let $A \in \mathbb{R}^{n \times n}$ and $v \in \mathbb{C}^n$ with $\|v\|_2 = 1$ be given. Let $\alpha_v = [(Av)^H v] / [(Av)^H (Av)]$. Then

$$\|v - \alpha_v Av\|^2 \leq 1 - \lambda_{\text{min}}[S(A)] \cdot \lambda_{\text{min}}[S(A^{-1})] \leq 1 - \frac{\lambda_{\text{min}}[S(A)]^2}{\|A\|^2}$$

(8)

**Proof.** $\alpha_v$ is the value achieving the minimum in the scalar least squares problem $\min_{\alpha} \|v - \alpha Av\|_2^2$ and hence satisfies the Galerkin condition $(Av)^H (v - \alpha_v Av) = 0$. So we have

$$\|v - \alpha Av\|^2 = v^H (v - \alpha_v Av) = 1 - \alpha_v \cdot v^H Av = 1 - \frac{w^H A^{-1}w \cdot v^H Av}{w^H w},$$
\[ w = Av. \] A well known result on field of values for any matrix \( M \) whose Hermitian part \( S(M) = (M + M^H)/2 \) is positive definite is the inequality \[ \left| \frac{x^H M x}{x^H x} \right| \geq \text{Re} \left( \frac{x^H M x}{x^H x} \right) \geq \lambda_{\min}[S(M)] > 0. \]

Hence the first inequality follows. The remaining inequality follows from the identity \[ S(A^{-1}) = A^{-1} \cdot S(A) \cdot A^{-H}. \]

Inverting both sides and taking norms yields \[ (\lambda_{\min}[S(A^{-1})])^{-1} \leq \frac{\|A\|^2}{\lambda_{\min}[S(A)]}. \]

**Sketch of Proof of Theorem 5.** GMRES on a matrix \( A \) with initial residual \( r_0 \) will find in \( k \) steps a solution with a residual \( r_k \) satisfying \( \|r_k\| = \min_{p \in \mathbb{P}_k} \|p(A)r_0\| \), where \( \mathbb{P}_k \) is the set of all polynomials \( p \) of degree up to \( k \) satisfying \( p(0) = 1 \). In particular, after a single step \( \|r_1\| = \min_{p \in \mathbb{P}} \|p(A)r_0\| \leq \|(I - \alpha(r_0))Ar_0\| \), where \( \alpha(r_0) = [(Ar_0)^H r_0]/[(Ar_0)^H (Ar_0)] \). Hence we have the bound from Lemma 6 \( \|r_1\| \leq \|r_0\| \cdot \sqrt{1 - \lambda_{\min}S(A)\lambda_{\min}S(A^{-1})} \). This amounts to a single step of a variant of the classical Richardson iteration. Repeating this Richardson iteration yields \( r_k^{[\text{rich}]} = \left( I - \alpha(r_{k-1}^{[\text{rich}]} \right)A \cdots \left( I - \alpha(r_1^{[\text{rich}]} \right)A \left( I - \alpha(r_0)A \right)r_0. \)

The norm of the residual after \( k \) Richardson steps would be bounded above by the convergence rate and bounded below by the norm of the GMRES residual:

\[ \|r_k^{[\text{GMRES}]}\| = \min_{p \in \mathbb{P}_k} \|p(A)r_0\| \leq \|r_k^{[\text{rich}]}\| \leq (1 - \lambda_{\min}[S(A)]\lambda_{\min}[S(A^{-1})])^{k/2} \]

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