Fast Algorithm for Relaxation Processes in Big-data Systems

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Relaxation processes driven by the Laplacian matrix in complex networks can be found in many real-world big-data systems, for example, search engines on web pages and dynamic load balancing protocols in mesh networks. To numerically implement such processes, a fast-running algorithm for the calculation of the inverse of the Laplacian matrix is needed. Yet, such algorithms have not been developed in complex networks, in which the fast-Fourier acceleration method cannot be used. Here, we introduce a fast-running algorithm that computes the pseudo inverse of a given Laplacian matrix using the renormalization method of the Gaussian integral. Through this method, the inverse of the Laplacian matrices of real-world networks containing millions of nodes can be obtained within reasonable computing times. Thus, this proposed algorithm could be used very widely in analyzing the relaxation processes occurring on large-scale networked systems.

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Fast analyses of big datasets \cite{1} are increasingly requested in diverse interdisciplinary areas in this information era. Given the limitations of available computing resources in space and time, designing and implementing scalable and efficient algorithms are essential for practical applications. One of the problems most often encountered in such problems is the analysis of huge sparse matrices, for example, the Laplacian matrix $L$ of a large-scale complex network. The matrix $L$ plays important roles in a wide range of problems such as diffusion processes, random walks \cite{2,3}, synchronization phenomena \cite{4}, epidemics \cite{5}, and load balancing in parallel computing \cite{6}. For instance, the spectrum of a Laplacian matrix determines the number of minimum spanning tree, minimal cuts \cite{7,8} and Kirchhoff index \cite{9}. We remark that there are many other large sparse matrices that appear and are analyzed in various disciplines \cite{10,11}. For example, the adjacency matrix $A$ represents the connection topology of a given network. In this Letter, we investigate how to compute the generalized inverse, so-called Moore-Penrose pseudo inverse of those matrices, which is useful for computing the first passage property of the Markov chains and the correlation function, etc. \cite{10,12}.

As a concrete example, in the study of disordered media, the entries of the pseudo-inverse is encoded as the current distribution of the random resistor networks where the scaling behavior of the distribution described as $d_f$ and $d_w$ are the fractal dimension and the random walk dimension of the substrates. Due to the slow convergence of the Jacobci relaxation method, where the time complexity grows as $t^{d_f+d_w}$ with the lateral size $l$ of the system, it had been a challenging task to obtain the entries of pseudo-inverse numerically. To resolve such difficulty, Batrouni et al. \cite{13,14} developed an algorithm based on Fourier acceleration which greatly improves the relaxation time of the Jacobi method. To general complex networks, however, the natural extension of the algorithm has not been clarified yet, because the Fourier transformation is not well defined in complex networks.

We begin by introducing a couple of formulae used for the algorithm. For an $N \times N$ positive definite real symmetric matrix $H$ and an arbitrary column vector $|J\rangle$ of size $N$, we consider the Gaussian integral given by

$$Z \equiv \int_{-\infty}^{\infty} \prod_{j=1}^{N} d\phi_j \exp \left[ \frac{1}{2} \langle \phi | H | \phi \rangle + i \langle J | \phi \rangle \right]$$

$$= \sqrt{\frac{(2\pi)^N}{\det H}} e^{-\frac{1}{2} \langle J | H^{-1} | J \rangle}, \quad (1)$$

where we introduced the state $|\phi\rangle = (\phi_1, \phi_2, \ldots, \phi_N)\dagger$ and $i$ is the imaginary unit $\sqrt{-1}$. If we introduce a $2N$-dimensional vector $|\psi\rangle$ by gluing $|J\rangle$ and $|\phi\rangle$ as

$$\psi_j = \begin{cases} J_j & \text{for } 1 \leq j \leq N, \\ \phi_{j-N} & \text{for } N+1 \leq j \leq 2N, \end{cases} \quad (2)$$

and a $2N \times 2N$ real symmetric matrix $\tilde{H}$

$$\tilde{H}_{j\ell} = \begin{cases} \delta_{j\ell} & \text{for } 1 \leq j, \ell \leq N, \\ H_{j-N,\ell-N} & \text{for } N+1 \leq j, \ell \leq 2N, \\ 0 & \text{otherwise,} \end{cases} \quad (3)$$

then Eq. $(1)$ could be rewritten as

$$Z = \int_{-\infty}^{\infty} \prod_{\ell=N+1}^{2N} d\psi_{\ell} \exp \left[ \frac{1}{2} \langle \psi | \tilde{H} | \psi \rangle \right]. \quad (4)$$

The evaluation of the Gaussian integral in Eq. $(4)$ can be performed by integrating out $\psi$ variables one by one and decimating the elements of $\tilde{H}$ accordingly. The dimension of the matrix $\tilde{H}$ is reduced by one at each stage. We consider a graph $G$ with the adjacency matrix $A$ with its elements given by

$$A_{j\ell} = \begin{cases} 1 & \text{if } \tilde{H}_{j\ell} \neq 0, \\ 0 & \text{otherwise.} \end{cases} \quad (5)$$
ψ is transformed to \(G\) in the graph representation, the corresponding graph \(G\) where \(\tilde{G}\) is positive definite, \(\tilde{G}\) is detailed later. Once that ordering is determined, one can rearrange the indices of \(\tilde{H}\) such that \(\ell\) decreases from \(j = 2N\) to \(j = N + 1\). Now, we integrate out \(\psi_{2N}\) in Eq. (4) to transform \(\tilde{H}\) into \(\tilde{H}^{(1)}\) of size \((2N - 1) \times (2N - 1)\). Since \(\tilde{H}\) is positive definite, \(\tilde{H}_{2N2N}\) is positive. Collecting the terms involving \(\psi_{2N}\), we find that

\[
\int_{-\infty}^{\infty} d\psi_{2N} \exp \left( \frac{1}{2} \tilde{H}_{2N2N} \psi_{2N}^2 + i B_{2N} \psi_{2N} \right) = \frac{2\pi i}{\sqrt{\tilde{H}_{2N2N}}} \exp \left( -\frac{i}{2} B_{2N}^2 \right),
\]

where \(B_{2N} = \sum_j A_{2N} \tilde{H}_{2N} \psi_j\). Noting that \(B_{2N}^2 = \sum_{j,\ell} A_{2N} A_{2N} \tilde{H}_{2N} \tilde{H}_{2N} \psi_j \psi_\ell\), one can identify the renormalized Hamiltonian \(\tilde{H}^{(1)}\) in the Gaussian integral as

\[
Z = \sqrt{\frac{2\pi i}{\tilde{H}_{11}}} Z^{(1)},
\]

\[
Z^{(1)} = \int_{-\infty}^{\infty} \prod_{j=2N+1}^{2N-1} d\psi_j \exp \left[ \frac{1}{2} \langle \psi | \tilde{H}^{(1)} | \psi \rangle \right],
\]

where \(\tilde{H}_{j\ell}^{(1)} = \tilde{H}_{j\ell}\) for all \(1 \leq j, \ell \leq (2N - 1)\) unless both \(j\) and \(\ell\) are the neighbor nodes of the decimated node \(2N\) in \(G\). If \(A_{j2N} A_{2N} > 0\), the corresponding matrix element \(\tilde{H}_{j\ell}\) is changed to \(\tilde{H}_{j\ell}^{(1)} = \tilde{H}_{j\ell} - \tilde{H}_{2N} \tilde{H}_{2N} / \tilde{H}_{2N2N}\). In the graph representation, the corresponding graph \(G\) is transformed to \(G^{(1)}\) by eliminating the node \(2N\) and adding links to every pair of the nodes that were adjacent to the node \(2N\) but disconnected in \(G\) (see Fig. 1). Accordingly, the adjacency matrix evolves from \(A\) to \(A^{(1)}\).

We repeat this procedure \(N\) times to integrate out all \(\psi_j = \phi_j - N\) variables for \(N + 1 \leq j \leq 2N\). Consequently the extended matrix \(H\) evolves as \(\tilde{H}^{(0)} = \tilde{H} \rightarrow \tilde{H}^{(1)} \rightarrow \cdots \rightarrow \tilde{H}^{(N)}\). The \(N \times N\) matrix \(\tilde{H}^{(N)}\) obtained at the last stage represents the coupling between \(j\)'s and is equal to \(\tilde{H}^{-1}\) in Eq. (1). The adjacency matrix \(A\) also evolves as \(A = A^{(0)} \rightarrow A^{(1)} \rightarrow \cdots \rightarrow A^{(N)}\).

If we introduce \(v_n\), the index of the node that is eliminated in \(G^{(n)}\) to obtain \(G^{(n+1)}\), then it is given by \(v_n = 2N - n\) for \(n = 0, 1, \ldots, N - 1\). Then, the above procedure can be written as

\[
\tilde{H}^{(n+1)}_{j\ell} = \tilde{H}^{(n)}_{j\ell} - A^{(n)} \tilde{H}^{(n)}_{jv_n} \tilde{H}^{(n)}_{v_n \ell},
\]

and

\[
A^{(n+1)}_{j\ell} = A^{(n)}_{j\ell} + A^{(n)}_{jv_n} A^{(n)}_{v_n \ell} (1 - A^{(n)}_{j\ell}),
\]

for \(1 \leq j, \ell \leq v_n+1 = v_n - 1\). We remark that \(\tilde{H}^{(n)}_{v_n v_n} \neq 0\) for all \(n = 0, 1, 2, \ldots, N - 1\) and therefore one can apply Eq. (6) for all \(n\).

\(H^{(N)}\) is unique and independent of the order of decimating nodes. However, the ordering \(v_n\) is important to reduce the computational cost. For instance, as shown in Eq. (9), if a node with degree \(k\) is removed, its \(k\) links are removed but its neighbors get interconnected, resulting in the maximum possible increase of links by \(k(k - 1)/2 - k\) which incurs large memory requirement if hub nodes are eliminated.

The appearance of new links as in Fig. 1 and Eq. (9) are called fill-in in the context of graph theory and there have been much efforts to find the ideal ordering that suppresses those fill-ins. Eliminating nodes in a graph, so called graph elimination game, is encountered in the Cholesky factorization, which is generally used to solve linear problem \(M|x| = |b|\) for positive definite matrix \(M\). While the ideal ordering which minimizes the fill-ins is hard to find, NP-complete, heuristic methods have been proposed, such as the minimum-degree ordering, the reverse Cuthill-McKee ordering, and the nested-dissection ordering \[16\].

In decimating \(\phi_j = \psi_{j-N}\) variables in Eq. (1), every pair of nodes that are adjacent to the decimated node should update their corresponding matrix element. These pairs of nodes \((j, \ell)\) are classified into three groups according to the types of their associated variables, \((\phi, \phi), (J, J_N), (\phi, J_N)\). For the problems that we plan to apply our algorithm to, only \(O(N)\) entries of \(H\), e.g., the diagonal elements or a few off-diagonal elements of \(H^{-1} = H^{(N)}\) are wanted, so the updating cost of the pairs involving \(J\) is not dominant compared to that of the \((\phi, \phi)\) pairs. Therefore, we choose the ordering scheme that minimizes the fill-ins for \((\phi, \phi)\). To fix the order of decimating nodes and rearrange the node indices so that nodes are eliminated from the one with \(j = 2N\) to \(N + 1\) in \(H\), we perform the node elimination in \(G\) representing \(H\) as follows:
i) Construct graph $G^{(0)} = G$ representing $H$.

ii) $n \leftarrow 0$.

iii) Choose the node having the minimum degree in $G^{(n)}$ and record its index in $w(n)$.

iv) Assign a link to every disconnected pair of neighbor nodes of $w(n)$ and eliminate the node $w(n)$ and its links, which yields $G^{(n+1)}$.

v) If $n < N$, $n \leftarrow n + 1$ and go to the step 3. Otherwise, for each node of index $i = 1, 2, \ldots, N$ of $H$, assign a new index $w(N-i)$.

Next, we consider the relaxation dynamics in complex network described by the Laplacian matrix with elements $L_{ij} = \delta_{ij} - A_{ij}/k_j$, where $k_j = \sum_k A_{jk}$ is the degree of node $j$. Its symmetrized version defined as $\bar{L}$ with elements $\bar{L}_{ij} = \delta_{ij} - A_{ij}/\sqrt{k_i k_j}$ is more useful to study physical problems such as the mean first passage time of random walks [10] [12] [17]. This symmetrized Laplacian matrix has positive eigenvalues and one non-degenerate zero eigenvalue. Moreover, the eigenvector of the zero eigenvalue does not have any zero entries, i.e., $e_i^{(1)} \neq 0$ for all $1 \leq i \leq N$. Such a matrix is called a semi-positive definite symmetric (SPDS) matrix for simplicity. We define the pseudo-inverse matrix $\bar{L}^+$ by dropping the zero-eigenvalue mode in its representation as

$$\bar{L}^+ = \sum_{n=2}^{N} \frac{e_i^{(n)} e_i^{(n)^T}}{\lambda_n},$$

(10)

where $\lambda_n$’s are the eigenvalues of $\bar{L}$ with $\lambda_1 = 0$ and $|e_i^{(n)}|$’s are the corresponding eigenvectors.

The pseudo-inverse $\bar{L}^+$ contains important information of random walk dynamics. For instance, the mean-first passage time (MFPT) $T_{is}$ from a node $s$ to $i$ is represented as

$$T_{is} = \begin{cases} \frac{2\ell}{\ell_i} \left( \frac{\bar{L}^+}{\ell_i} - \frac{1}{\sqrt{\ell_i}} \delta_{is} \right) & \text{for } i \neq s, \\ \frac{2\ell}{\ell_i} \delta_{is} & \text{for } i = s \end{cases}$$

(11)

The generalized MFPT $T_i$ of node $i$ denotes the MFPT to the target node $i$ averaged over all possible starting nodes in the stationary state [19] and is represented by the diagonal element of the pseudo inverse of the Laplacian as

$$T_i = \sum_s k_s \frac{2L}{2L} T_{is} = \frac{2L}{\ell_i} \bar{L}^+_{ii} + 1.$$  

(12)

The MFPT of random walks is represented in terms of $O(N)$ entries of the pseudo-inverse matrices of dimension $N - 1$. Our algorithm presented is suitable for computing these quantities. In general, the inverse of a sparse matrix is not guaranteed to be sparse. Therefore given the limitation of space and time of computation, it is not always available to obtain all the entries of the inverse matrix of a large sparse matrix.

Here we present the algorithm for computing the entries of the pseudo-inverse of a general SPDS matrix $V$. Since $V$ is not invertible, we introduce $H(\mu)$ defined as $H(\mu) = \mu I + V$ where $\mu$ is a positive real value and $I$ is the identity matrix of the same dimension as $V$. Then $H(\mu)$ is positive definite and therefore we can apply Eq. (1) to obtain

$$H^{-1}_j(\mu) = \frac{e_j^{(1)}}{\mu} + \sum_{n=2}^{N} \frac{e_j^{(n)} e_j^{(n)^T}}{\lambda_n} + O(\mu^1),$$

(13)

where $\lambda_n(n = 1, 2, \ldots, N)$ are the eigenvalues of $V$ and $e^{(n)}$’s are the corresponding eigenvectors $e^{(n)} = (e_1^{(n)}, e_2^{(n)}, \ldots, e_N^{(n)})^T$. Therefore, the pseudo-inverse $V^+$ of $V$ can be obtained by using $H^{-1}$ as

$$V_j^+ = \frac{\partial}{\partial \mu} H^{-1}_j(\mu) \bigg|_{\mu=0}.$$  

(14)

Whereas Eq. (14) implies that one can obtain $V^+$ once $H^{-1}(\mu)$ is known, it is actually impossible to compute $H^{-1}$ as a function of $\mu$. On the other hand, Eq. (14) suggests that only a few first terms, up to $O(\mu^2)$, in the expansion of $H^{-1}$ are sufficient to obtain $V^+$ as

$$\tilde{H}_j(\mu) = \left( 1 + \frac{\mu}{2} \frac{d}{d\mu} + \frac{\mu^2}{2!} \frac{d^2}{d\mu^2} \right) \tilde{H}_j \bigg|_{\mu=0} + O(\mu^3) = \tilde{H}_{0,j} + \tilde{H}_{1,j} \mu + \tilde{H}_{2,j} \mu^2 + O(\mu^3).$$

(15)

Our idea is to apply Eq. (8) to trace the evolution of the three leading matrices $\tilde{H}_0$, $\tilde{H}_1$, and $\tilde{H}_2$. One striking difference for the SPDS matrix is that the zeroth order of diagonal matrix element of the last node becomes zero due to the zero eigenvalue of SPDS matrix. Therefore, one should derive another version of the component-wise updating rules of Eq. (8) for the last integration. The details will be published elsewhere [20].

Let us mention the space and time complexity of the algorithm. The computing time $\mathcal{T}$ of the algorithm depends on the network topology and the ordering scheme. If the number of neighbors of the decimated nodes is $O(1)$, each step in the algorithm takes $O(1)$ time and the whole algorithm will take $O(N)$ time as the integrations are repeated $N$ times. In this case, the number of non-zero elements of $H$ remains at $O(N)$. On the other hand, if the number of neighbors of the decimated node is of order $N$ and thereby $O(N^2)$ elements should be updated at each integration, the computation time scales as $N^3$. Also, $H$ becomes dense and $O(N^2)$ memory is needed.

To address the performance of the proposed algorithm specifically, we investigate the computing time $\mathcal{T}$ taken to obtain all the diagonal elements of the symmetric Laplacian matrix $\bar{L}$ of diverse networks including artificial and
FIG. 2. (Color Online) Scaling of the computing time $T$ for the generalized MFPT in model networks of $N$ nodes. The model networks are (a) the 2D Sierpinski gasket and 2D percolation cluster at the critical point and (b) the random SF networks (BA model) with the mean degree $\langle k \rangle = 2, 4$ and $\langle k \rangle = 4$ (which is marked as *) with the same mean degree $\langle k \rangle = 4$ using the conventional eigendecomposition.

real ones. As shown in Eq. (12), the diagonal component $L^*_j$ is the generalized MFPT to node $j$, $T_j$, in a network having the symmetric Laplacian matrix $\bar{L}$.

The performance of our algorithm varies with the network topology. In Fig. 2, we present the computing time $T$ as a function of the number of nodes $N$ of the Sierpinski gasket ($d_f = \ln 3/\ln 2$ and $d_s = 2\ln 3/\ln 5$), two-dimensional (2D) percolation clusters ($d_f = 91/48$ and $d_s = 1.32$) [21], the Barabási-Albert (BA) model as a candidate of random scale-free (SF) networks ($d_f \to \infty$, $d_s \to \infty$), and the $(1,2)$-flower networks ($d_f = 91/48$, $d_s = 2\ln 3/\ln 2$) [22]. The scaling exponent $z$, where $T \sim N^z$, of the computing time of our algorithm turns out to be different across these networks. We check how the performance of the algorithm depends on the fractal dimension or the spectral dimension of the embedded structure. It seems that the algorithm performance is better for the networks having smaller spectral dimension. The details will be published elsewhere [20].

For comparison to other method, we also show the result of BA model with $\langle k \rangle = 4$ (which is marked as *) in Fig. 2 using the conventional eigendecomposition method, the time complexity of which is $O(N^3)$. Even though the two data plots for BA model with $\langle k \rangle = 4$ have the same slope, it turns out that our result is relatively faster than the conventional method. Since the conventional method does not depend on the network structure, we can claim that our algorithm outperforms the method using the eigendecomposition for all tested networks.

The scaling behaviors of the computing time in model networks suggest that our algorithm can be useful in analyzing the Laplacian matrices of large real-world systems. We constructed the Laplacian matrices $\bar{L}$ of the email-communication network, the World-Wide-Web, road networks in the United States, and the collaboration networks, all archived in the Stanford Large Network Dataset Collection [1]. These selected networks commonly have a large number of nodes, $N$ ranging between $2 \times 10^5$ and $2 \times 10^6$ while the mean degree $\langle k \rangle = 2L/N$ is not so large, ranging between 2 and 20. The properties of those real-world networks and the computing time of the algorithm are summarized in Table I. It is worthy to note that the computing time is especially short for road networks compared with the WWW although the size of road networks is larger. The trace of the pseudo inverse, $\text{Tr} \bar{L}^*/N$ is related to the generalized MFPT by Eq. (12) and we present the values in Table I. The road networks show larger values of $\text{Tr} \bar{L}^*/N$ than the WWW which implies the road networks possesses smaller spectral dimension. It should be noted that the computing time is shorter in the model networks of lower dimensionality. Although we only dealt with random walks in our paper, this method can be applied to any general Markov chain satisfying detailed balance, such as the Edwards-Wilkinson dynamics on complex networks [6].

In summary, we have presented a fast algorithm that computes the entries of the pseudo-inverse of a symmetricized version of the Laplacian matrix for relaxation processes in complex networks. The algorithm turns out to be much efficient than the direct simulation of the Markov chain particularly when underlying network is sparse in connections. In this algorithm, we follow an heuristic method in which the decimation process follows the order of nodes with minimum degree. Even though this method is not always optimal to reduce the computing time, we could obtain the elements of pseudo inverses of the Laplacian matrices of real-world networks within an affordable range of computing times. Therefore, we think that our algorithm could be useful for studying the relaxation processes in big-data systems.

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TABLE I. Basic properties of real-world networks and the computing time on them. The number of nodes ($N$), the number of links ($L$), the mean degree ($\langle k \rangle = 2L/N$), the clustering coefficient (C.C.), the trace of the symmetric Laplacian matrix $\text{Tr} \bar{L}^*/N$, and the computing time ($T$) for the generalized MFPT are given for each network.

| Network          | $N$    | $L$    | $\langle k \rangle$ | C.C | $\text{Tr} \bar{L}^*/N$ | $T$ (sec) |
|------------------|--------|--------|----------------------|-----|-------------------------|----------|
| Email-EuAll      | 224832 | 339925 | 3.02                | 0.07| 21.3529                | 87.5     |
| web-Stanford     | 255265 | 1941926| 15.2                | 0.60| 18.7769                | 2833     |
| web-NotreDame    | 325729 | 1090108| 6.69                | 0.23| 39.5499                | 6608     |
| roadNet-CA       | 1957027| 2760388| 2.82                | 0.05| 916.898                | 351      |
| roadNet-TX       | 1351137| 1879201| 2.78                | 0.05| 862.147                | 165      |
| com-DBLP         | 334863 | 925872 | 5.53                | 0.40| NA                      | NA       |

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For the networks with large values of $\langle k \rangle$, the computation time and the required memory of the algorithm may be very large. It can happen that a large amount of memory is needed for networks with moderate values of $\langle k \rangle$, like the collaboration network that we tried to analyze but failed with the 24GB memory of our computers.