GRASS: GRAph Spectral Sparsification Leveraging Scalable Spectral Perturbation Analysis

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Abstract—Spectral graph sparsification aims to find ultra-sparse subgraphs whose Laplacian matrix can well approximate the original Laplacian eigenvalues and eigenvectors. In recent years, spectral sparsification techniques have been extensively studied for accelerating various numerical and graph-related applications. Prior nearly-linear-time spectral sparsification methods first extract low-stretch spanning tree from the original graph to form the backbone of the sparsifier, and then recover small portions of spectrally-critical off-tree edges to the spanning tree to significantly improve the approximation quality. However, it is not clear how many off-tree edges should be recovered for achieving a desired spectral similarity level within the sparsifier. Motivated by recent graph signal processing techniques, this paper proposes a similarity-aware spectral graph sparsification framework that leverages efficient spectral off-tree edge embedding and filtering schemes to construct spectral sparsifiers with guaranteed spectral similarity (relative condition number) level. An iterative graph densification scheme is also introduced to facilitate efficient and effective filtering of off-tree edges for highly ill-conditioned problems. The proposed method has been validated using various kinds of graphs obtained from public domain sparse matrix collections relevant to VLSI CAD, finite element analysis, as well as social and data networks frequently studied in many machine learning and data mining applications. For instance, a sparse SDD matrix with 40 million unknowns and 180 million nonzeros can be solved (1E-3 accuracy level) within two minutes using a single CPU core and about 6GB memory.

Index Terms—Spectral graph theory, iterative matrix solver, graph partitioning, circuit analysis, perturbation analysis

I. INTRODUCTION

Spectral methods are playing increasingly important roles in many graph and numerical applications [32], such as scientific computing [30], numerical optimization [5], data mining [24], graph analytics [16], [18], [43], machine learning [9], [10], [34], graph signal processing [26], and VLSI computer-aided design [12], [39], [40]. For example, classical spectral graph partitioning (data clustering) algorithms embed original graphs into low-dimensional space using the first few nontrivial eigenvectors of graph Laplacians and subsequently perform graph partitioning (data clustering) on the low-dimensional graphs to obtain high-quality solution [24], [33]. To further push the limit of spectral methods for large graphs, mathematics and theoretical computer science researchers have extensively studied many theoretically-sound research problems related to spectral graph theory. Recent spectral graph sparsification research [2], [6], [20], [24], [27], [29] allows computing nearly-linear-sized subgraphs (sparsifiers) that can robustly preserve the spectra (i.e., eigenvalues and eigenvectors) of the original graph’s Laplacian, which immediately leads to a series of theoretically nearly-linear-time numerical and graph algorithms for solving sparse matrices, graph-based semi-supervised learning (SSL), spectral graph partitioning (data clustering), and max-flow problems [5], [19], [29], [30]. For example, sparsified circuit networks allow for developing more scalable computer-aided (CAD) design algorithms for designing large VLSI systems [12], [39]; sparsified social (data) networks enable to more efficiently understand and analyze large social (data) networks [32]; sparsified matrices can be immediately leveraged to accelerate the solution computation of large linear system of equations [41]. To this end, a spectral sparsification algorithm leveraging an edge sampling scheme that sets sampling probabilities proportional to edge effective resistances (of the original graph) has been proposed in [27]. However, it becomes a chicken-and-egg problem since calculating effective resistances (leverage scores for edge sampling) requires solving the original graph Laplacian matrix multiple times (even when using JohnsonLindenstrauss (JL) lemma [27]) and thus can be extremely expensive for very large graphs.

This paper aims to address the standing question whether there exists a practically-efficient, nearly-linear time spectral graph sparsification algorithm that can immediately enable the development of nearly-linear time sparse SDD matrix solvers and other graph-based algorithms for large-scale, real-world problems. Our work is built upon the recent spectral perturbation analysis framework that allows for highly-scalable spectral sparsification of large (weighted) undirected graphs [12], [13], which also shows connections with the Courant-Fischer theorem for generalized eigenvalues as well as recent graph signal processing techniques [26].

Our method starts by extracting a spectrally-critical spanning tree subgraph as a backbone of the sparsifier, and subsequently recovers a small portion spectrally-critical off-tree edges to the spanning tree. In many scientific computing and graph-related applications, it is usually desired to construct sparsifiers according to a given spectral similarity level: introducing too few edges may lead to poor approximation of the original graph, whereas too many edges can result in rather high computational complexity. For example, when using a preconditioned conjugate gradient (PCG) method to solve a symmetric diagonally dominant (SDD) matrix for multiple right-hand-side (RHS) vectors, it is hoped the PCG solver would converge to a good solution as fast as possible, which usually requires the sparsifier (preconditioner) to be highly spectrally-similar to the original problem or achieve relatively a small condition number; on the other hand, in many graph
partitioning tasks, only the Fiedler vector (the first nontrivial eigenvector) of graph Laplacian is needed \cite{28}, so even a sparsifier with a much lower spectral similarity should suffice. To this end, this work introduces a similarity-aware spectral graph sparsification framework that leverages efficient spectral off-tree edge embedding and filtering schemes to construct spectral sparsifiers with guaranteed spectral similarity. The contribution of this work has been summarized as follows:

1) We present a nearly-linear time yet practically-efficient framework for constructing ultra-sparsifier subgraph from a spanning tree subgraph via efficient spectral perturbation analysis of generalized eigenvalue problem. The proposed algorithm allows effectively fixing the largest generalized eigenvalues, by recovering the most spectrally-critical off-tree edges to the spanning-tree subgraph.

2) We present a similarity-aware spectral sparsification framework by leveraging scalable spectral off-tree edge embedding and filtering schemes motivated by recent graph signal processing techniques \cite{26}. Such a scheme enables to flexibly trade off the complexity and spectral similarity of the sparsified graph.

3) For highly ill-conditioned problems, we introduce an iterative graph densification scheme to more effectively fix the most problematic eigenvalues by progressively improving the ultra-sparsifier subgraphs. Compared to the single-pass spectral sparsification scheme, the proposed scheme can always achieve greater reduction of relative condition numbers, thereby leading to more effective spectral approximation of the original graph Laplacian.

4) Extensive experiments have been conducted to validate the proposed method in various numerical and graph-related applications, such as solving sparse SDD matrices, spectral graph partitioning, as well as compression of large social and data networks. Very promising results for even extremely ill-conditioned VLSI, thermal and finite element analysis problems have been obtained.

The rest of this paper is organized as follows. Section \ref{sec:background} provides a brief introduction to graph Laplacians and the state of the art in spectral sparsification of graphs. In Sections \ref{sec:method} and \ref{sec:results} a scalable similarity-aware spectral sparsification method based on spectral perturbation analysis is described in detail. Section \ref{sec:applications} describes extensive experimental results for a variety of real-world, large-scale sparse Laplacian matrix and graph problems, which is followed by the conclusion of this work in Section \ref{sec:conclusion}.

II. BACKGROUND

A. Graph Laplacian Matrices and Quadratic Forms

Consider a weighted, undirected and connected graph $G = (V,E,\omega)$, where $V$ denotes a set of vertices, $E$ denotes a set of edges, and $\omega$ denotes a weight function that assigns a positive weight to each edge. As shown in Fig. \ref{fig:resistor_network}, the Laplacian matrix of graph $G$ can be defined as follows:

$$
\mathbf{L}_G(p,q) = \begin{cases} 
-\omega(p,q) & \text{if } (p,q) \in E \\
\sum_{(p,t) \in E} \omega(p,t) & \text{if } (p,q) = (p,t) \\
0 & \text{if otherwise.}
\end{cases}
$$

\hspace{1cm} (1)

Fig. 1. A resistor network (conductance value of each element is shown) and its graph Laplacian matrix.

It can be shown that every graph Laplacian matrix is an SDD matrix, which also can be considered as an admittance matrix of a resistor circuit network. For any real vector $x \in \mathbb{R}^V$, the Laplacian quadratic form of graph $G$ is defined as:

$$
x^T \mathbf{L}_G x = \sum_{(p,q) \in E} \omega_{p,q} (x(p) - x(q))^2,
$$

\hspace{1cm} (2)

which can be considered as the Joule heat dissipated in the resistor network when $x$ is a voltage vector.

B. Graph Sparsification and Its Applications

Classic graph sparsification problem can be described as follows: given a graph $G = (V,E,\omega)$ and its Laplacian matrix $\mathbf{L}_G$, graph sparsification aims to find a subgraph (a.k.a graph sparsifier) $P = (V,E_s,\omega_s)$ and its Laplacian $\mathbf{L}_P$ so that the sparse subgraph will retain all vertices but significantly less number of edges compared to the original graph.

Graph sparsifiers typically fall into the following two categories: the cut sparsifier \cite{4} and spectral sparsifier \cite{29}. The cut sparsifier preserves the values of cuts in a graph as shown in Fig. \ref{fig:cut_sparsifier} whereas spectral sparsifier preserves eigenvalues and eigenvectors of the original graph. It has been shown that a good cut sparsifier may not always be a good spectral sparsifier, while the spectral sparsifier is always a stronger notion than the cut sparsifier \cite{29}.

To illustrate the role of graph sparsification in numerical computation applications, consider the following example of the standard PCG algorithm for solving SDD matrices. PCG can find an $\epsilon$-accurate solution in at most $O(\kappa(\mathbf{L}_G,\mathbf{L}_P)^{1/2} \log \epsilon^{-1})$ iterations, where the relative condition number $\kappa(\mathbf{L}_G,\mathbf{L}_P)$ is defined as follows:

$$
\kappa(\mathbf{L}_G,\mathbf{L}_P) = \frac{\lambda_{\max}}{\lambda_{\min}},
$$

\hspace{1cm} (3)
C. Spectral Graph Sparsification

Graphs $G$ and $P$ are said to be $\sigma$-spectrally similar if for all real vectors $x \in \mathbb{R}^n$ the following holds [3]:

$$\frac{x^\top L_P x}{\sigma} \leq x^\top L_G x \leq \sigma x^\top L_P x. \quad (5)$$

It can be shown that the relative condition number $\kappa(L_G, L_P) \leq \sigma^2$. Note that a graph sparsifier that can result in a smaller relative condition number will also be spectrally similar to the original graph, and thus can lead to faster convergence of iterative methods, such as Krylov-subspace iterative methods. For complete graphs the Ramanujan graphs are among the best spectral graph sparsifiers [2], whereas for arbitrary graphs the linear-sized Twice-Ramanujan graphs can achieve the same spectral similarity with twice as many as the edges in Ramanujan graphs [2], [20]. However, it still remains unclear if there is a practically-efficient algorithm for constructing linear-sized spectral sparsifiers.

In this work, we define spectrally-critical edges to be the ones that can mostly perturb the graph spectral properties, such as the first few Laplacian eigenvalues and eigenvectors. Recent approaches for constructing nearly-linear-sized spectral sparsifiers aim to dramatically reduce relative condition number, which typically include the following two key steps (as shown in Fig. 3) [17], [19], [27], [30]:

1) Extract an initial spanning tree from the original graph as a backbone of the sparsifier;

2) Recover a small number of spectrally-critical off-tree edges to the spanning tree to form an ultra-sparsifier subgraph.

Note that since the smallest generalized eigenvalue $\lambda_{\min}$ of a spanning tree subgraph (without scaling) is no smaller than 1, we always have $\lambda_{\max} \geq \kappa(L_G, L_P) = \frac{\lambda_{\max}}{\lambda_{\min}}$.

For step 1), recent theoretical computer science research results suggest that low-stretch spanning trees should be constructed since they will result in an upper bound of $\lambda_{\max} < O(m \log n (\log \log n)^2)$ that can immediately lead to the development of nearly-linear time algorithms for solving SDD matrices [19], where $m$ denotes the number of nonzeros and $n$ the number of equations in the matrix. Towards this goal, nearly-linear time low-stretch spanning tree algorithms based on star- and petal-decomposition methods have been proposed [1], [11].

For step 2), it requires to recover the most spectrally-critical off-tree edges to the spanning tree for constructing the ultra-sparsifier, thereby drastically improving spectral approximation of the sparsifier. To this end, effective-resistance based edge sampling scheme [27] can be adopted for recovering these off-tree edges. However, calculating effective resistances (leverage scores for edge sampling) requires solving graph Laplacian multiple times (even when using the Johnson-Lindenstrauss Lemma [27]) and thus can be rather expensive for very large graphs. It is also suggested to use stretch to replace effective resistance for edge sampling, which is more computationally efficient but will increase the number of edges sampled [19].

III. SPECTRAL GRAPH SPARSIFICATION VIA EFFICIENT SPECTRAL PERTURBATION ANALYSIS

In this paper, we introduce a practically-efficient, nearly-linear time spectral graph sparsification algorithm that can be efficiently applied to sparsify large-scale real-world graphs (Laplacian matrices). We show that for an initial spectrally-critical spanning-tree subgraph, such as a low-stretch spanning tree, the proposed algorithm can always efficiently identify the most spectrally-critical off-tree edges to be added to the spanning tree, thereby drastically reducing the relative condition number of the preconditioned system. As a result, an ultra-sparse yet spectrally-similar subgraph can be constructed and leveraged for solving sparse SDD matrices as well as other graph related problems in nearly-linear time.

A. Overview of Our Approach

The overview of the proposed method for similarity-aware spectral sparsification of undirected graphs has been summarized as follows. For a given input graph, the following key procedures are involved in the proposed algorithm flow: (a) low-stretch spanning tree [1], [11] extraction based on its original graph Laplacian; (b) spectral (generalized eigenvalue) embedding and filtering of off-tree edges by leveraging the recent spectral perturbation analysis framework [12]; (c) iterative sparsifier improvement (graph densification) by gradually adding small portions of dissimilar off-tree edges to the spanning tree.

In the rest of this paper, we assume that $G = (V, E, w)$ is a weighted, undirected and connected graph, whereas $P =$

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\(\lambda_{\min}\) and $\lambda_{\max}$ denote the smallest and largest nonzero generalized eigenvalue$^1$ that satisfy:

$$L_G u = \lambda L_P u, \quad (4)$$

with $u$ denoting the eigenvector corresponding to the generalized eigenvalue $\lambda$. It is desired that the preconditioner $L_P$ matrix should be very similar to $L_G$ and result in a much smaller relative condition number. It is also desired that $L_P$ should be much sparser than $L_G$ so that the overall cost of the preconditioned iterations can be much lower than directly solving the original matrix. It is obvious that a graph sparsifier with good spectral approximation of the original matrix can be immediately adopted as a preconditioner for solving SDD or SDD-like matrices [14], [15], [19], [30], [36]–[38].
Define \( e_p \in \mathbb{R}^V \) to be a vector with only the \( p \)-th element being 1 and others being 0. Also define \( e_{p,q} = e_p - e_q \). Then the trace of \( L_p^T L_G \) becomes [31]:

\[
\text{Tr} \left( L_p^T L_G \right) = \sum_{i=1}^{n} \lambda_i = \sum_{(p,q) \in E} \omega_{p,q} \text{Tr} \left( L_p^T e_{p,q} e_{p,q}^T \right) = \sum_{(p,q) \in E} \omega_{p,q} \left( e_{p,q}^T L_p^T e_{p,q} \right) = \sum_{(p,q) \in E} \omega_{p,q} e_{p,q}^T L_p^T e_{p,q} = st_p(G) \geq \lambda_1 = \lambda_{\text{max}}.
\]

The above result indicates that the total stretch \( st_p(G) \) is bounded by \( \lambda_1 \). Therefore, it is suggested that a spanning tree with low stretch should be constructed so that the preconditioned system will have a small relative condition number. It has been shown that if each of the largest eigenvalues can be fixed (dramatically decreased) by recovering a small number of off-tree edges to the spanning tree, an ultra-sparsifier with totally \( n + o(n) \) edges can be created to provide a good spectral approximation of \( G \) [17], [19], [30]. For instance, it has been shown that an ultra-sparsifier with a relative condition number \( \alpha k^2 \) can be constructed by adding at most \( n/k \) off-tree edges to the spanning tree subgraph [30].

C. Perturbation Analysis of Generalized Eigenvalue Problems

Consider the following first-order eigenvalue perturbation problem:

\[
L_G \left( u_i + \delta u_i \right) = \left( \lambda_i + \delta \lambda_i \right) \left( L_p + \delta L_p \right) \left( u_i + \delta u_i \right), \tag{9}
\]

where a perturbation \( \delta L_p \) is applied to \( L_p \), leading to the perturbations in generalized eigenvalues and eigenvectors \( \lambda_i + \delta \lambda_i \) and \( u_i + \delta u_i \) for \( i = 1, \ldots, n \), respectively. By keeping only the first-order terms, (9) becomes:

\[
L_G \delta u_i = \lambda_i L_p \delta u_i + \delta \lambda_i L_p u_i + \lambda_i \delta L_p u_i. \tag{10}
\]

Expressing \( \delta u_i \) with the original eigenvectors \( u_j \) leads to:

\[
\delta u_i = \sum_{j=1}^{n} \zeta_{ij} u_j, \tag{11}
\]

where \( u_j \) can always be constructed to satisfy:

\[
u_j^T L_p u_j = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}. \tag{12}
\]

Substituting (11) into (10) leads to:

\[
\sum_{j=1}^{n} \zeta_{ij} \lambda_j L_p u_j = \lambda_i L_p \left( \sum_{j=1}^{n} \zeta_{ij} u_j \right) + \delta \lambda_i L_p u_i + \lambda_i \delta L_p u_i. \tag{13}
\]

Multiplying \( u_i^T \) to both sides of (13) results in:

\[
u_i^T \left( \sum_{j=1}^{n} \zeta_{ij} \lambda_j L_p u_j \right) = \lambda_i u_i^T L_p \left( \sum_{j=1}^{n} \zeta_{ij} u_j \right) + \delta \lambda_i u_i^T L_p u_i + \lambda_i u_i^T \delta L_p u_i, \tag{14}
\]
which immediately leads to:
\[ \delta \lambda_i = -\lambda_i \frac{u_i^\top \delta L_p u_i}{u_i^\top L_p u_i} = -\lambda_i u_i^\top \delta L_p u_i. \]  (15)

Expanding \( \delta L_p \) that includes multiple extra off-tree edges \((p, q)\) leads to:
\[ \delta L_p = \sum_{(p, q) \in E \setminus E_s} \omega_{p, q} e_{p, q} e_{p, q}^\top. \]  (16)

The above leads to the following based on (15):
\[ \delta \lambda_i = -\lambda_i \sum_{(p, q) \in E \setminus E_s} w_{p, q} u_i^\top e_{p, q} e_{p, q}^\top u_i. \]  (17)

It is obvious from (17) that the reduction of \( \lambda_i \) is proportional to the Joule heat produced by the extra off-tree edges when its unperturbed eigenvector \( u_i \) is applied as a node-voltage vector. For instance, the voltage difference between nodes \( p \) and \( q \) is computed by
\[ v_{p, q} = u_i^\top e_{p, q}, \]  (18)
which results in the following Joule heat for the off-tree edge \((p, q)\):
\[ h_{p, q} = \omega_{p, q} v_{p, q}^2. \]  (19)

Therefore, the perturbation of eigenvalue \( \lambda_i \) becomes:
\[ \delta \lambda_i = -\lambda_i \sum_{(p, q) \in E \setminus E_s} h_{p, q}. \]  (20)

Consequently, adding the off-tree edges with the largest Joule heat values computed using the dominant generalized eigenvector \((u_1)\) that corresponds to the largest eigenvalue \( (\lambda_1) \) will dramatically reduce the relative condition number thereby improving the spectral approximation of the subgraph. Repeating the above procedures for all large eigenvalues will lead to very good spectral graph sparsifiers.

D. Why Dominant Generalized Eigenvectors?

As shown in the previous perturbation analysis, dominant generalized eigenvectors can help identify the most spectrally-critical off-tree edges. Alternatively, the following Courant-Fischer theorem can be leveraged for better understanding why generalized eigenvectors should be used for spectral sparsification tasks. Assigning each node in the graph with an integer value either 0 or 1, the corresponding Laplacian quadratic form measures the boundary size (cut) of a node set. For example, if a node set \( Q \) is defined as
\[ Q \overset{\text{def}}{=} \{ q \in V : x(q) = 1 \}, \]  (21)
then the number of edges going out of \( Q \) becomes:
\[ x^\top L_G x = \text{cut}(Q, \overline{Q}) = |\partial_G(Q)|, \]  (22)
where the boundary of \( Q \) in \( G \) is defined as
\[ \partial_G(Q) \overset{\text{def}}{=} \{(p, q) \in E : p \notin Q, q \in Q \}. \]  (23)

Courant-Fischer theorem for generalized eigenvalues
\[ \lambda_{\text{max}} = \max_{\|x\|_2 = 1} \frac{x^\top L_G x}{x^\top L_P x} \rightarrow \max \text{ cuts in } G \Rightarrow \max \text{ mismatch in } P. \]  

The Courant-Fischer theorem for generalized eigenvalue problems allows finding dominant eigenvalues and eigenvectors by solving the following optimization task:
\[ \lambda_{\text{max}} = \max_{\|x\|_2 = 1} \frac{x^\top L_G x}{x^\top L_P x} = \max_{x \in \{0, 1\}} \frac{|\partial_G(Q)|}{|\partial_P(Q)|}, \]  (24)
where \( 1 \in \mathbb{R}^V \) is the all-one vector, and the boundary of \( Q \) in \( P \) is defined as
\[ \partial_P(Q) \overset{\text{def}}{=} \{(p, q) \in E : x(p) \notin Q \} \],  (25)
which leads to the following equations:
\[ x^\top L_G x = |\partial_G(Q)|, x^\top L_P x = |\partial_P(Q)|. \]  (26)

Then (24) indicates that finding the dominant generalized eigenvector would be closely related to finding \( Q \) such that \( |\partial_G(Q)| / |\partial_P(Q)| \) or the ratio of the boundary sizes in the original graph \( G \) and subgraph \( P \) is maximized. As a result, \( \lambda_{\text{max}} = \lambda_1 \) becomes the upper bound of the mismatch in boundary (cut) size between \( G \) and \( P \), as shown in Fig. 6.

E. Problem Formulation

Once \( Q \) or \( \partial_G(Q) \) is found using dominant generalized eigenvectors, we can recover a small number of edges from \( \partial_G(Q) \) to \( P \) in order to dramatically reduce the maximum mismatch \( (\lambda_1) \), and thus improve the spectral approximation of \( P \). To this end, we propose the following problem formulation for spectral graph sparsification:
\[ \min_{L_P} \left\{ \max_{x} \left( \frac{x^\top L_G x}{x^\top L_P x} \right) + \beta \|L_P\|_1 \right\}, \]  (27)
where \( L_P \) denotes Laplacian matrix of the subgraph \( P \), \( x^\top 1 = 0 \) and \( |x| \neq 0. \) (27) aims to minimize the largest generalized eigenvalue by adding the minimum amount of edges into the subgraph \( P \), which can be solved iteratively by repeating the following two steps: 1) compute the generalized eigenvector corresponding to the largest (dominant) eigenvalue, and 2) identify the most spectrally-critical off-tree edges that can mostly decrease the dominant eigenvalue(s) and add them into
the subgraph $P$. Once the dominant eigenvalue is small enough (e.g., $\lambda = 10$), $P$ will be highly spectrally similar to the original graph $G$.

However, computing the dominant eigenvalue and its eigenvector can sometimes be too costly for large-scale graph Laplacian matrices, even when state-of-the-art eigenvalue decomposition methods are adopted [25]. Additionally, there can still be too many eigenvalues to be fixed in order to achieve a desired spectral similarity level (relative condition number).

F. Edge Embedding with Approximate Dominant Eigenvector

To more efficiently identify critical off-tree edges, approximate dominant generalized eigenvectors and eigenvalues of $Q$ can be exploited. To this end, a generalized power iteration procedure that can be computed in nearly-linear time has been proposed in [12]. In the rest of this paper, we assume that a very small positive diagonal element is added to a randomly selected row of the graph Laplacian matrix to convert the very small positive diagonal element is added to a randomly (4) can be exploited. To this end, a generalized power iteration composition methods are adopted [25]. Additionally, there can Laplacian matrices, even when state-of-the-art eigenvalue de-

\[ L \text{ (e.g., } P \text{)} \]

Once the dominant eigenvalue is small enough $\lambda_1$, 10 $\lambda_t \in \mathbb{R}$.

which leads to the edge-based expansion of the quadratic form for $\delta L_{P, \max}$ as follows:

\[
Q_{\delta L_{P, \max}}(h_t) = h_t^\top \delta L_{P, \max} h_t = \sum_{i=1}^{n} (\alpha_i \lambda_i^t)^2 (\lambda_i - 1) = \sum_{(p,q) \in E \setminus E_s} \alpha_i^2 \lambda_i^2 (u_i^\top e_{p,q})^2.
\]

(35)

It is obvious that (31), or (35) will allow ranking each off-tree edge according to its spectral-criticality level. (35) also indicates that adding all off-tree edges with nonzero Joule heat values back to $P$ will immediately bring all generalized eigenvalues to 1. It should be noted that the required number of generalized power iterations can be rather small (e.g. $t = 2$) in practice to observe good result.

G. Spectrally-unique Off-tree Edges

Define a spectrally-unique off-tree edge $(p_i, q_i)$ to be the off-tree edge that can completely and only fix one large (dominant) generalized eigenvalue $\lambda_i$, though each edge will usually influence more than one eigenvalues and eigenvectors according to (35). Then the following truncated expansion of the Laplacian quadratic form can be obtained when considering the top $k$ most dominant yet spectrally-unique off-tree edges for fixing the top $k$ largest eigenvalues:

\[
Q_{\delta L_{P, \max}}(h_t) \approx \sum_{i=1}^{k} \sum_{(p,q) \in E \setminus E_s} \alpha_i^2 \lambda_i^2 (u_i^\top e_{p,q})^2,
\]

where we should be able to find $\gamma_i \neq 0$ such that:

\[
eq \sum_{i=1}^{k} \alpha_i^2 \lambda_i^2 (\lambda_i - 1),
\]

(36)

while the following will also be satisfied:

\[
\gamma_i, i = j, \quad 0, i \neq j.
\]

(38)

Obviously, for random coefficients $\alpha_i$, the following must be satisfied for a spectrally-unique off-tree edge:

\[ w_{p_i, q_i} \gamma_i^2 = \lambda_i - 1. \]

(39)

Consequently, if there is an off-tree edge $(p_i, q_i)$ with weight $w_{p_i, q_i}$, that satisfies:

\[ e_{p_i} - e_{q_i} = \pm \sqrt{\lambda_i - 1} L P u_i, \]

(40)

adding this off-tree edge back to the spanning tree will completely fix the corresponding eigenvalue $\lambda_i$. Then the effective resistance of edge $(p_i, q_i)$ in $P$ becomes:

\[ R_{e_i}^{\text{eff}} = (e_{p_i}^\top L P e_{p_i, q_i} = \gamma_i^2 u_i^\top L P u_i = \gamma_i^2. \]
which immediately leads to:
\[ Q_{\delta L_{P_{\max}}(h_t)}(\mathbf{h}_t) \approx \sum_{i=1}^{k} \alpha_i^2 \lambda_i^2 w_{p_{i},q_{i}}^2 R_{e_{i}} \approx \sum_{i=1}^{k} \alpha_i^2 \lambda_i^{2t+1}. \] (42)

Since the stretch of off-tree edge \((p_i,q_i)\) is computed by \(st_P(p_i,q_i) = w_{p_i,q_i} R_{e_{i}}^{\text{eff}}\) \[42\] also indicates that \(st_P(e_{i}) \approx \lambda_i\) holds for spectrally-unique off-tree edges. Consequently, the key off-tree edges identified by \([35]\) or \([42]\) will have the largest stretch values and therefore most significantly impact the largest eigenvalues of \(L_{G_{P_{\max}}}^{1/2}\). \(42\) also can be considered as a randomized version of \(\text{Trace}(L_{P_{\max}}^1 L_{G})\) that is further scaled up by a factor of \(\lambda_i^2\).

H. Rank-One Update with A Spectrally-Unique Edge

The updated generalized eigenvalue \(\lambda'_i\) after adding one spectrally-unique off-tree edge \((p_i,q_i)\) with weight \(w_{p_i,q_i}\) back to the spanning tree for fixing eigenvalue \(\lambda_i\) can be derived based on the Sherman-Morrison Formula and Matrix Determinant Lemma. Define matrix \(A_P\) to be:
\[ A_P = L_{G_{P_{\max}}}^{1/2} L_{P_{\max}}^{-1} L_{G_{P_{\max}}}^{1/2}, \] (43)
which has the same set of eigenvalues of matrix \(L_{P_{\max}}^{-1} L_{G}\). After adding the off-tree edge \((p_i,q_i)\), the updated \(A_P\) is denoted by \(A'_P\), that is expressed as:
\[ A'_P = L_{G_{P_{\max}}}^{1/2} (L_{P} + w_{p_i,q_i} \mathbf{e}_{p_i,q_i} \mathbf{e}_{p_i,q_i}^\top)^{-1} L_{G_{P_{\max}}}^{1/2} \]
\[ = A_P - \frac{w_{p_i,q_i} L_{G_{P_{\max}}}^{1/2} \mathbf{e}_{p_i,q_i} \mathbf{e}_{p_i,q_i}^\top L_{G_{P_{\max}}}^{1/2}}{1 + w_{p_i,q_i} \mathbf{e}_{p_i,q_i}^\top L_{P_{\max}}^{-1} \mathbf{e}_{p_i,q_i}} = A_P - v_P v_P^\top, \] (44)
where \(v_P\) is defined as:
\[ v_P = \frac{\sqrt{w_{p_i,q_i} L_{G_{P_{\max}}}^{1/2} \mathbf{e}_{p_i,q_i}}}{\sqrt{1 + w_{p_i,q_i} \mathbf{e}_{p_i,q_i}^\top L_{P_{\max}}^{-1} \mathbf{e}_{p_i,q_i}}} \]
\[ = \frac{\gamma_i v_{p_{i},q_{i}} L_{P_{\max}}^{1/2} \mathbf{u}_{i}}{\sqrt{1 + w_{p_{i},q_{i}} \gamma_i}}. \] (45)

The characteristic polynomial of \(A'_P = A_P - v_P v_P^\top\) can be computed as follows:
\[ p_{A'_P}(x) = p_{A_P}(x) - v_P^\top v_P = \det(xI - A_P + v_P v_P^\top) \]
\[ = \det(xI - A_P) \det(1 - (xI - A_P)^{-1} v_P v_P^\top). \] (46)

According to Matrix Determinant Lemma, we have:
\[ p_{A'_P}(x) = p_{A_P}(x) \left(1 + v_P^\top(xI - A_P)^{-1} v_P\right). \] (47)

Denoting \(z_i\) for \(i = 1, \ldots, n\) the unit-length orthonormalized eigenvectors of matrix \(A_P\) that correspond to eigenvalues \(\lambda_i\) respectively, we have:
\[ (xI - A_P)^{-1} = \sum_{i=1}^{n} \frac{z_i z_i^\top}{x - \lambda_i}, \] (48)
which leads to:
\[ p_{A'_P}(x) = p_{A_P}(x) \left(1 + \sum_{i=1}^{n} \frac{(v_P^\top z_i)^2}{x - \lambda_i}\right). \] (49)

It has been shown in \([2]\) that \([49]\) indicates: 1) the latest eigenvalues after rank-one update will always be reduced if \((v_P^\top z_i)^2 > 0\); 2) the greater value of \((v_P^\top z_i)^2\) will result in greater reduction in \(\lambda_i\). Therefore, if an off-tree edge satisfies \((v_P^\top z_i)^2 \gg 0\) for multiple eigenvectors \(z_i\), adding this edge back to the spanning tree subgraph will substantially reduce multiple eigenvalues at the same time; on the other hand, a spectrally-unique off-tree edge will substantially reduce only one eigenvalue. It can be shown that:
\[ L_{G_{P_{\max}}}^{1/2} L_{P_{\max}}^{-1} L_{G_{P_{\max}}}^{1/2} \left( L_{G_{P_{\max}}}^{1/2} \mathbf{u}_i \right) \left( L_{G_{P_{\max}}}^{1/2} \mathbf{u}_i \right) \]
\[ = \lambda_i \left( L_{G_{P_{\max}}}^{1/2} \mathbf{u}_i \right) \left( L_{G_{P_{\max}}}^{1/2} \mathbf{u}_i \right) = \lambda_i z_i. \] (50)

Therefore, the updated eigenvalue \(\lambda'_i\) after adding the off-tree edge can be computed by solving \(p_{A'_P}(x) = 0\), which leads to:
\[ \lambda'_i = \lambda_i - \frac{\lambda_i}{\lambda_i^2 + \gamma_i^2}. \] (52)

For achieving the desired \(\lambda'_i\) after adding the off-tree edge, the edge weight should be set as:
\[ w_{p_{i},q_{i}} = \frac{\lambda_i - \lambda'_i}{\lambda_i^2 + \gamma_i^2}. \] (53)

It can be shown that when the desired \(\lambda'_i = 1\), we have \(w_{p_{i},q_{i}} = \frac{\lambda_i^2}{\gamma_i^2 + \lambda_i^2}\), which is equivalent to \([39]\). As a result, considering the nearly-worst case eigenvalue distribution \(\lambda_i \leq \delta_{L_{P_{\max}}}/(\delta_{L_{G_{P_{\max}}}})\), shown in Fig. \(4\), a \(\sigma\)-similar spectral sparsifier with \(n - 1 + O(n \log n / \log \log n)\) edges can be obtained in \(O(m)\) time using the proposed method when an initial low-stretch spanning tree is given.

I. Algorithm Flow and Complexity

The detailed algorithm flow of the proposed spectral graph sparsification approach has been summarized as follows:

1) Extract a spanning tree subgraph (e.g. a scaled low-stretch spanning tree \([1]\), \([11]\)) from the original graph; 
2) Perform \(t\)-step generalized power iterations to compute \(h_t\) with an initial random vector; 
3) Compute the spectral criticality of each edge based on the Laplacian quadratic form of \(\delta L_{P_{\max}}\) using \([35]\); 
4) Rank each edge using its spectral criticality levels; 
5) Add a small portion of dissimilar off-tree edges back to the spanning tree to form the ultra-sparse spectral graph sparsifier.

It should be noted that the proposed spectral graph sparsification approach allows ranking all off-tree edges according to their spectral criticality levels in a very efficient and effective way. Compared to the state-of-the-art sampling-based approaches that rely on effective resistance calculations, the proposed method can achieve the very similar goal of ranking spectrally critical off-tree edges.

The complexity of the proposed spectral perturbation based approach can be analyzed by considering two key steps: (a) spanning tree construction based on the original graph, and (b) ultra-sparsifier construction based on the spanning tree. Recent research has shown that low-stretch spanning trees in (a) can
be constructed in nearly-linear time \([1], [11]\). For instance, the petal-decomposition algorithm requires \(O(m \log n \log \log n)\) time to generate a low-stretch spanning tree with a total stretch of \(O(m \log n \log \log n) \) \([1]\); the \(t\)-step generalized power iterations in (b) can be achieved in linear time for a fixed \(t\) since factorization of a tree-graph Laplacian matrix can be accomplished within linear \(O(m)\) time. Consequently, the overall complexity of the proposed spectral perturbation based sparsification algorithm is almost linear.

IV. SIMILARITY-AWARE SPECTRAL SPARSIFICATION BY EDGE FILTERING

Although \([55]\) and \([42]\) provide a spectral ranking for each off-tree edge, it is not clear how many off-tree edges should be recovered to the spanning tree for achieving a desired spectral similarity level. To this end, we introduce a simple yet effective spectral off-tree edge filtering scheme motivated by recent graph signal processing techniques \([26]\).

A. Spectral Sparsification: A Low-Pass Filter on Graphs

To more efficiently analyze signals on general undirected graphs, graph signal processing techniques have been extensively studied recently \([26]\). There is a clear analogy between traditional signal processing based on classical Fourier analysis and graph signal processing: 1) the signals at different time points in classical Fourier analysis correspond to the signals at different nodes in an undirected graph; 2) the more slowly oscillating functions in time domain correspond to the graph Laplacian eigenvectors associated with lower eigenvalues and more slowly varying (smoother) components across the graph. For example, the first few nontrivial eigenvectors associated with the smallest non-zero eigenvalues of a path graph Laplacian have been illustrated in Fig. 7, where the increasing eigenvalues correspond to increasing oscillation frequencies in the path graph. A comprehensive review of fundamental signal processing operations, such as filtering, translation, modulation, dilation, and down-sampling to the graph setting has been provided in \([26]\).

Spectral sparsification aims to maintain a simplest subgraph sufficient for preserving the slowly-varying or “low-frequency” signals on graphs, which therefore can be regarded as a “low-pass” graph filter. In other words, such spectrally

sparsified graphs will be able to preserve the eigenvectors associated with low eigenvalues more accurately than high eigenvalues, and thus will retain “low-frequency” graph signals sufficiently well, but not so well for highly-oscillating (signal) components due to the missing edges.

In practice, preserving the spectral (structural) properties of the original graph within the spectral sparsifier is key to design of many fast numerical and graph-related algorithms \([5], [19], [27], [30]\). For example, when using spectral sparsifier as a preconditioner in preconditioned conjugate gradient (PCG) iterations, the convergence rate only depends on the spectral similarity (or relative condition number) for achieving a desired accuracy level, while in spectral graph partitioning and data clustering tasks only the first few eigenvectors associated with the smallest nontrivial eigenvalues of graph Laplacian are needed \([24], [28]\).

B. Off-Tree Edge Filtering with Joule Heat

To only recover the off-tree edges that are most critical for achieving the desired spectral similarity level, we propose the following scheme for truncating spectrally-unique off-tree edges based on each edge’s Joule heat. For a spanning-tree preconditioner, since there will be at most \(k\) generalized eigenvalues that are greater than \(st_p(G)/k\), the following simple yet nearly worst-case generalized eigenvalue distribution can be assumed:

\[
\lambda_i = \frac{2\lambda_{\max}}{i + 1} = \frac{st_p(G)}{i + 1}, i \geq 1.
\]  

(54)

To most economically select the top-\(k\) spectrally-unique off-tree edges that will dominantly impact the top-\(k\) largest generalized eigenvalues, the following sum of quadratic forms (Joule heat levels) can be computed based on \([42]\) by performing \(t\)-step generalized power iterations with \(r\) multiple random vectors \(\text{ht}_1, \ldots, \text{ht}_r\):

\[
Q_{\text{sp} \rightarrow \text{max}}(\text{ht}_1, \ldots, \text{ht}_r) \approx \sum_{j=1}^{r} \sum_{i=1}^{k} (\alpha_{i,j})^2 \left(\frac{2\lambda_{\max}}{i + 1}\right)^{2t+1}.
\]

(55)

The goal is to select top \(k\) spectrally-unique off-tree edges for fixing the top \(k\) largest generalized eigenvalues such that the resulting upper bound of the relative condition number will become \(\sigma^2 = \frac{\overline{\lambda}_{\min}}{\overline{\lambda}_{\max}}\), where \(\overline{\lambda}_{\max}\) and \(\overline{\lambda}_{\min}\) denote the largest and smallest eigenvalues of \(L_p^1 L_G\) after adding top-\(k\) spectrally-unique off-tree edges. Then we have:

\[
k = 2\lambda_{\max}/\overline{\lambda}_{\max} - 1.
\]

(56)

When using multiple random vectors for computing \([55]\), it is expected that \(\sum_{j=1}^{r} \alpha_{k,j}^2 \approx \sum_{j=1}^{r} \alpha_{1,j}^2\), which allows us to define the normalized edge Joule heat \(\theta_k\) for the \(k\)-th spectrally-unique off-tree edge through the following simplifications:

\[
\theta_k = \frac{\text{heat}\lambda_k}{\text{heat}\lambda_1} = \left(\frac{\sum_{j=1}^{r} \alpha_{k,j}^2}{\sum_{j=1}^{r} \alpha_{1,j}^2}\right)^{\frac{2t+1}{\lambda_{\max}}/\lambda_{\max}} \approx \left(\frac{\sigma^2 \overline{\lambda}_{\min}}{\lambda_{\max}}\right)^{2t+1}.
\]

(57)
The key idea of the proposed similarity-aware spectral sparsi-
ification is to leverage the normalized Joule heat [57] as a thresh-
old for filtering off-tree edges: only the off-tree edges with
normalized Joule heat values greater than \( \theta_p \) will be selected
for inclusion into the spanning tree for achieving the desired
spectral similarity (\( \sigma \)) level. Although the above scheme is
derived for filtering spectrally-unique off-tree edges, general
off-tree edges also can be filtered using similar strategies.
Since adding the off-tree edges with largest Joule heat to the
subgraph will mainly impact the largest generalized eigenval-
es but not the smallest ones, we will assume \( \lambda_{\text{min}} \approx \lambda_{\text{min}} \)
and use the following edge truncation scheme for filtering
general off-tree edges: the off-tree edge \((p, q)\) will be included
into the sparsifier if its normalized Joule heat value is greater
than the threshold determined by:

\[
\theta_{(p,q)} = \frac{\text{heat}_{(p,q)}}{\text{heat}_{\text{max}}} \geq \theta_{\sigma} \approx \left(\frac{\sigma^2 \lambda_{\text{min}}}{\lambda_{\text{max}}}\right)^{2^{t+1}}, \quad (58)
\]

where \( \theta_{\sigma} \) denotes the threshold for achieving the \( \sigma \)-spectral
similarity in the sparsifier, and \( \text{heat}_{\text{max}} \) denotes the maximum
Joule heat of all off-tree edges computed by [35] with multiple
initial random vectors.

\section{C. Estimation of Extreme Eigenvalues}

To achieve the above spectral off-tree edge filtering scheme, we
need to compute \( \theta_{\sigma} \) in (58) that further requires to
estimate the extreme eigenvalues \( \lambda_{\text{max}} \) and \( \lambda_{\text{min}} \) of \( L_P \) \( L_G \).
In this work, we propose the following efficient methods for
computing these extreme generalized eigenvalues.

1) \textit{Estimating} \( \lambda_{\text{max}} \) \textit{via Power Iterations} : Since general-
ized power iterations converge at a geometric rate determined
by the separation of the two largest generalized eigenvalues
\( \lambda_{\text{max}} = \lambda_1 > \lambda_2 \), the error of the estimated eigenvalue will
decrease quickly when \( |\lambda_2/\lambda_1| \) is small. It has been shown that
the largest eigenvalues of \( L_P \) \( L_G \) are well separated from each other [31],
which thus leads to very fast convergence of generalized power iterations for estimating \( \lambda_1 \). To achieve
scalable performance of power iterations, we can adopt rec-
cent graph-theoretic algebraic multigrid (AMG) methods for
solving the sparsified Laplacian matrix \( L_P \) [21, 41].

2) \textit{Estimating} \( \lambda_{\text{min}} \) \textit{via Node Coloring}: Since the smallest
est eigenvalues of \( L_P \) \( L_G \) are crowded together [31], using
(shifted) inverse power iterations may not be efficient due
to the extremely slow convergence rate. To the extent of
our knowledge, none of existing eigenvalue decomposition
methods can efficiently compute \( \lambda_{\text{min}} \).

This work exploits the following Courant-Fischer theorem
for generalized eigenvalue problems:

\[
\lambda_{\text{min}} = \min_{|x| \neq 0} \frac{x^T L_G x}{x^T L_P x}, \quad (59)
\]

where \( x \) is also required to be orthogonal to the all-one vector.
[59] indicates that if we can find a vector \( x \) that minimizes the
ratio between the quadratic forms of the original and
sparsified Laplacians, \( \lambda_{\text{min}} \) can be subsequently computed.
By restricting the values in \( x \) to be only 1 or 0, which can be
considered as assigning one of the two colors to each node in
graphs \( G \) and \( P \), the following simplifications can be made:

\[
\lambda_{\text{min}} \leq \min_{|x| \neq 0} \frac{x^T L_G x}{x^T L_P x} = \min_{x(i) \in \{0,1\}} \frac{\sum_{p \neq q} w_{pq} x(p) x(q)}{\sum_{p \neq q} w_{pq} x(p) x(q)} \quad (60)
\]

which will always allow estimating an upper bound for \( \lambda_{\text{min}} \).
To this end, we first initialize all nodes with 0 value and
subsequently try to find a node \( p \) such that the ratio between
quadratic forms can be minimized:

\[
\lambda_{\text{min}} \leq \min_{p \in V} L_G(p, p). \quad (61)
\]

The above procedure for estimating \( \lambda_{\text{min}} \) only requires finding
the node with the smallest node degree ratio and thus can be
easily implemented and efficiently performed for even very
large graph problems. Our results for real-world graphs show
that the proposed method is highly efficient and can very well
estimate the smallest generalized eigenvalues when compared
with existing generalized eigenvalue methods [25].

\section{D. Iterative Sparsification for Ill-Conditioned Problems}

To achieve more effective edge filtering for similarity-aware
spectral graph sparsification, we propose to iteratively recover
off-tree edges to the sparsifier through an incremental graph
densification procedure. Each densification iteration adds a
small portion of “filtered” off-tree edges to the latest spe-
clar sparsifier, while the spectral similarity is estimated to
determine if more off-tree edges are needed. The \( i \)-th graph
densification iteration includes the following steps:

1) Update the subgraph \( L_P \) as well as its solver by leveraging recent graph-theoretic algebraic
multigrid methods [21, 41].
2) Estimate the spectral similarity by computing \( \lambda_{\text{max}} \) and
\( \lambda_{\text{min}} \) using the methods described in Section IV-C.
3) If the spectral similarity is not satisfactory, continue with
the following steps; otherwise, terminate the subgraph
densification procedure.
4) Perform \( t \)-step generalized power iterations with
\( O(\log |V|) \) random vectors to compute the sum of
Laplacian quadratic forms [55].
5) Rank and filter each off-tree edge according to its
normalized Joule heat value using the threshold \( \theta_{\sigma} \) in
(58);
6) Check the similarity of each selected off-tree edge and
only add dissimilar edges to the latest sparsifier.

\section{V. EXPERIMENTAL RESULTS}

The proposed spectral perturbation based spectral graph
sparsification method (GRASS) has been implemented in
\texttt{C++} and available for download \footnote{https://sites.google.com/mtu.edu/zhuofeng-graphspar
2}. The proposed spectral graph sparsification algorithm allows developing nearly-linear
time algorithms for tackling SDD or SDD-like sparse matrix
problems, spectral graph partitioning problems, as well as
graph-based regression problems [14, 19, 30, 37, 43].
In this paper, a sparse SDD matrix algorithm has been implemented and compared to the state-of-the-art sparse matrix solver, Cholmod [7]. Test cases demonstrated in this paper cover a great variety of sparse SDD matrix problems obtained from realistic VLSI power grid problems [22], [35], and the sparse matrix collection from the University of Florida that includes integrated circuit simulation problems, three-dimensional thermal analysis problems, finite-element analysis, etc [8]. Additionally, a spectral graph partitioning engine is also implemented, which has been dramatically accelerated by taking advantage of the proposed spectral sparsification approach. All experiments are performed using a single CPU core of a computing platform running 64-bit RHEW 6.0 with a 2.67GHz 12-core CPU.

### A. A Scalable Iterative Solver For Power Grid Analysis

The spectral sparsifier obtained by the proposed algorithm (without weight re-scaling for the spanning tree and off-tree edges) is leveraged as a preconditioner in a PCG solver. The preconditioner is factorized by the same Cholmod solver [7]. The right-hand-side (RHS) input vector \( b \) is generated randomly and the solver is set to converge to an accuracy level \(|Ax - b| < 10^{-3}|b|\) for all test cases. \(|V|\) denotes the number of nodes, \(\text{NNZ}\) denotes the number of nonzero elements in the original matrix, \(T_D\) (\(T_I\)) denotes the total solution time including both the matrix factorization and solving steps of the direct (iterative) solver, \(M_D\) (\(M_I\)) denotes the memory cost for sparse matrix factorizations, \(N_I\) denotes the number of iterations for the PCG solver to converge to the required accuracy level, \(\lambda_{\text{max}}\) calculates the reduction rate of the largest eigenvalue using the proposed spectral sparsification approach when compared to the initial spanning tree preconditioner, and \(N^{\text{ST}}\) is the ratio of required iteration numbers using the initial spanning-tree preconditioners and the new subgraph preconditioners.

### B. Estimation of Extreme Eigenvalues

In Table IV the extreme generalized eigenvalues \(\lambda_{\text{min}}\) and \(\lambda_{\text{max}}\) estimated by the proposed methods (Section IV-C) are compared with the ones \(\lambda_{\text{min}}\) and \(\lambda_{\text{max}}\) computed by the “eigs” function in Matlab for sparse matrices in [35], while the relative errors \(\epsilon_{\lambda_{\text{min}}}\) and \(\epsilon_{\lambda_{\text{max}}}\) are also shown. \(\lambda_{\text{max}}\) is estimated using less than ten generalized power iterations.

### C. Spectral Ranking of Off-tree Edges

We illustrate the results of spectral edge ranking and filtering according to Joule heat levels computed by one-step generalized power iteration using [35] in Fig. 8 for two sparse matrices in [8]. The thresholds of normalized edge Joule heat values required for spectral edge filtering are labeled using red dash lines. It is observed in Fig. 8 that there is a sharp change of the top normalized edge Joule heat values, which indicates that there are not many large eigenvalues of \(L_p^T L_p\) in both

---

**Table I**

| CKTs | \(|V|\) | \(\text{NNZ}\) | \(T_D\) | \(T_I\) | \(N_I\) | \(\lambda_{\text{max}}\) | \(N^{\text{ST}}\) |
|------|-------|-------|--------|--------|-----|----------------|--------|
| thupg1 | 4704 | 768 (0.06G) | 4.2s (0.3G) | 183s (1.0G) | 24 | 41.9 | 66X |
| thupg2 | 4704 | 352 (0.6G) | 8.3s (0.3G) | 368s (1.0G) | 34 | 78.1 | 65X |

**Table II**

| CKTs | \(|V|\) | \(\text{NNZ}\) | \(T_D\) | \(T_I\) | \(N_I\) | \(\lambda_{\text{max}}\) | \(N^{\text{ST}}\) |
|------|-------|-------|--------|--------|-----|----------------|--------|
| ibmpg1 | 1240 | 1240 (0.06G) | 1.2s (0.3G) | 3.2s (0.3G) | 32 | 42.1 | 86X |
| ibmpg2 | 1240 | 600 (0.3G) | 6.1s (0.3G) | 34s (0.3G) | 32 | 79.1 | 86X |

**Table III**

| Test Cases | \(|V|\) | \(T_D\) | \(T_I\) | \(N_I\) | \(\lambda_{\text{max}}\) | \(N^{\text{ST}}\) |
|-----------|-------|--------|--------|-----|----------------|--------|
| ibmpg1 | 1240 | 1240 (0.06G) | 1.2s (0.3G) | 3.2s (0.3G) | 32 | 42.1 | 86X |
| ibmpg2 | 1240 | 600 (0.3G) | 6.1s (0.3G) | 34s (0.3G) | 32 | 79.1 | 86X |

**Table IV**

| Test Cases | \(\lambda_{\text{min}}\) | \(\lambda_{\text{max}}\) | \(\epsilon_{\lambda_{\text{min}}}\) | \(\epsilon_{\lambda_{\text{max}}}\) |
|-----------|----------------|----------------|----------------|----------------|
| ibmpg1 | 0.71 | 0.99 | 0.02 | 0.01 |
| ibmpg2 | 0.71 | 0.99 | 0.02 | 0.01 |

Accurate analysis of on-chip power grids is indispensable for designing modern VLSI chips since it can help reveal critical design issues related to power supply noise, electromigration, etc. However, modern power grid designs can integrate billions of components, which results in super-linear runtime/memory cost when using direct solution methods. The proposed spectral sparsification technique allows developing nearly-linear time iterative solvers for power grid analysis problems. Additionally, even more general transistor-level SPICE-accurate circuit simulations can potentially benefit from the proposed spectral graph sparsification algorithm [14], [36], [37]. Table I and Table II demonstrate the DC analysis results of IBM and THU power grid design benchmarks [22], [35], showing nearly-linear runtime/memory cost. Similar runtime scalability is observed from Table III for solving sparse matrices from [8]. In all test cases, the proposed spectral graph sparsification algorithm can find tree-like ultrasparse with high spectral similarity. For example, we achieve \(\kappa(L_p, L_p) \approx 16\) (\(\kappa \approx 4\)), for all IBM power grid test cases, which allows solving the sparse matrices within just a small number of PCG iterations (e.g. \(N_I < 14\)).
cases and agrees well with the prior theoretical analysis [31]. We also demonstrate the results of Joule heat levels (spectral criticality) of off-tree edges computed by (35) for a random vector using one-step generalized power iteration (t = 1) for a “hair-comb” spanning tree shown in Fig. [9]. It is not difficult to show that such a spanning tree can not well match the top part of the original 2D grid, so the Joule heat levels of off-tree edges at the top should be much greater than the ones at the bottom part. In fact, it has been shown that the “hair-comb” spanning tree for a $\sqrt{n} \times \sqrt{n}$ 2D mesh will have a total stretch of $\Theta(n \sqrt{n})$ that is mainly contributed by the off-tree edges with largest stretch values near the top part of the mesh grid [23]. Using the proposed similarity-aware spectral graph sparsification framework, we are able to efficiently identify and recover the most spectrally-critical off-tree edges, thereby dramatically reducing the largest generalized eigenvalues. For example, the “hair-comb” spanning tree of a $200 \times 200$ mesh grid can be dramatically improved in terms of spectral similarity by recovering top 400 spectrally-critical off-tree edges: $\sigma^2$ is reduced from about 64,000 to about 100 ($640 \times$ reduction), which can also be indicated by the Joule heat distributions before and after adding these off-tree edges as illustrated in Fig. [9].

D. Preservation of Long-Range Effects in the Sparsifier

The similarity-aware spectral sparsifier extracted using the proposed framework will effectively preserve low-frequency graph signals or long-range effects due to the good preservation of graph spectral (structural or global) properties. As an example shown in Fig. [10], the responses of the original on-chip power grid and its spectrally sparsified grid ($\sigma^2 = 50$) are obtained by solving $Ax = b$ and $\tilde{A}x = b$ respectively, where $A$ ($\tilde{A}$) denotes the original (sparsified) conductance matrix and $b$ denotes a unit excitation right-hand-side (RHS) vector with only a single element being 1 and others being 0. Note that we applied a global edge scaling procedure [40] to the sparsified power grid network in order to match the original node-wise effective resistances in $\tilde{A}$. If we consider the RHS vector $b$ as the original input graph signal, and the voltage response vector $x$ as the output after graph signal processing, the power grid system can be naturally regarded as a low-pass filter for graph signals. Consequently, the solutions obtained by solving the original and sparsified power grid problems using a unit excitation source can be understood as the impulse responses of low-pass filters commonly studied in classic Fourier analysis. Fig. [10] obviously indicates the good preservation of long range effects or low-frequency components on the spectral sparsifier obtained using the proposed method.

E. An SDD Matrix Solver with Similarity-Aware Sparsification

Fig. [11] shows the spectral drawings [18] of an airfoil graph [8] as well as its spectrally-similar ($\sigma = 5$) subgraph computed by the proposed similarity-aware spectral sparsification algorithm.

The spectral sparsifiers obtained by the proposed similarity-aware algorithm are also leveraged as preconditioners in a PCG solver. The RHS input vector $b$ is generated randomly and the solver is set to converge to an accuracy level $\|Ax - b\| < 10^{-8}\|b\|$ for all test cases. In Table V “|V|” and “|E|” denote the numbers of nodes and edges in the original graph, whereas “|E_{\sigma^2}|”, “|N_{\sigma^2}|” and “|T_{\sigma^2}|” denote the number of edges in the sparsifier, the number of PCG iterations required for converging to the desired accuracy level, and the total time of graph sparsification for achieving the spectral similarity of $\sigma^2$, respectively. As observed in all test cases, there are very clear trade-offs between the graph density, computation time, and spectral similarity for all spectral sparsifiers extracted using the proposed method: sparsifiers with higher spectral similarities (smaller $\sigma^2$) allow converging to the required solution accuracy level in much fewer PCG iterations, but need to retain more edges in the subgraphs and thus require longer time to compute (sparsify).

Similar runtime scalability is observed from Table V for solving sparse matrices from [8]. In all test cases, the proposed spectral graph sparsification algorithm can find tree-like ultrasparsifiers with high spectral similarity. In Fig. [12] the relative residual plot (versus PCG iteration number) has been shown using three preconditioners. As observed, the PCG iterations with the preconditioner obtained by directly running the Cholesky decomposition algorithm for the spectrally-sparsified matrix computed by GRASS converge much faster than the ones with preconditioners generated by using standard incomplete Cholesky decomposition algorithm (with drop tolerances of 0.01 and 0.001); it is also observed that the number of non-zeros (nnz) in the preconditioner matrix created by GRASS is the lowest.

F. A Scalable Spectral Graph Partitioner

It has been shown that by applying only a few inverse power iterations, the approximate Fiedler vector ($u_f$) that corresponds to the smallest nonzero eigenvalue of the (normalized) graph Laplacian matrix can be obtained for obtaining high-quality graph partitioning solution [30]. Therefore, using the
spectral sparsifiers computed by the proposed spectral sparsification algorithm can immediately accelerate the PCG solver for inverse power iterations, leading to scalable performance for graph partitioning problems \cite{30}. In fact, if the spectral sparsifier is already a good approximation of the original graph, its Fiedler vector can be directly used for partitioning the original graph.

We implement the accelerated spectral graph partitioning algorithm, and test it with sparse matrices in \cite{8} and several 2D mesh graphs synthesized with random edge weights. As shown in Table VI, the graphs associated with sparse matrices have been partitioned into two pieces using sign cut method \cite{28} according to the approximate Fiedler vectors computed by a few steps of inverse power iterations. The direct solver \cite{7} and the preconditioned iterative solver are invoked within each inverse power iteration for updating the approximate Fiedler vectors $u_f$ and $\tilde{u}_f$, respectively. $|V^+|/|V^−|$ denotes the ratio of nodes assigned with positive and negative signs according to the approximate Fiedler vector, and “Rel.Err.” denotes the relative error of the proposed solver compared to the direct solver computed by $|V^+|/|V^−|$, where $|V^\pm|$ denotes the number of nodes with different signs in $u_f$ and $\tilde{u}_f$. “$T_D$” (” $T_I$”) and “$M_D$” (” $M_I$”) denote the total solution time (excluding sparsification time) and memory cost of the direct (iterative) method. We extract sparsifiers with $\sigma^2 \leq 200$ for all test cases.

It can be observed that the proposed preconditioned spectral
graph partitioner only results in a very small portion of nodes (0.07% to 4%) assigned with different signs when comparing with the original spectral graph partitioner, while achieving significant runtime and memory savings (4–10×). The approximate Fiedler vector computed by our fast solver for the test case “mesh_1M” is also illustrated in Fig. 13, showing rather good agreement with the true solution.

G. Sparsification of Other Complex networks

As shown in Table VII, a few finite element, protein, data and social networks have been spectrally sparsified to achieve $\sigma^2 \approx 100$ using the proposed similarity-aware method. “$T_{tot}$” is the total time for extracting the sparsifier, “$T_{eig}$” denotes the ratio of the largest generalized eigenvalues before and after adding off-tree edges into the spanning tree sparsifier, and $T_{eig}^o(T_{eig}^s)$ denotes the time for computing the first ten eigenvectors of the original (sparsified) graph Laplacians using the “eig” function in Matlab. Since spectral sparsifiers can well approximate the spectral (structural) properties of the original graph, the sparsified graphs can be leveraged for accelerating many numerical and graph-related tasks. For example, spectral clustering (partitioning) using the original “RCV-80NN” (80-nearest-neighbor) graph cannot be performed on our server with 50GB memory, while it only takes a few minutes using the sparsified one.

H. Nearly-linear Runtime Scalability

Our results show that the proposed method can extract the similarity-aware spectral sparsifier in nearly-linear time as shown in Fig. 14. It should be noted that each spectral sparsifier needs to be extracted once and can be reused or incrementally updated many times [15], [38].

VI. Conclusions

This paper introduces a nearly-linear time yet practically efficient spectral graph sparsification algorithm that can be immediately leveraged to develop nearly-linear time sparse matrix solvers and spectral graph (data) partitioning (clustering) algorithms. A novel spectral perturbation based approach is proposed for constructing an ultra-sparse spectral graph sparsifier by adding the most spectrally-critical off-tree edges back to the initial spanning tree subgraph, so that key spectral properties of the original graph can be very well approximated. Additionally, we also propose a similarity-aware spectral graph sparsification framework that leverages efficient spectral off-tree edge embedding and filtering schemes to construct spectral sparsifiers with guaranteed spectral similarity (relative condition number) level. An iterative graph densification scheme is introduced to facilitate efficient and effective filtering of off-tree edges for highly ill-conditioned problems. Extensive experimental results show the runtime of the SDD solver and the spectral graph partitioner scales nearly-linearly with the graph size for a variety of large-scale, real-world problems, such as VLSI power grid analysis, circuit simulation, finite element problems, transportation and social networks, etc. For instance, a sparse matrix with 40 million unknowns and 180 million nonzeros can be solved within two minutes using a single CPU core and about 6GB memory.
