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Lx = b

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Lx=bLaplacian Solvers and Their Algorithmic Applications

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Abstract

The ability to solve a system of linear equations lies at the heart of areas such as optimization, scientific computing, and computer science, and has traditionally been a central topic of research in the area of numerical linear algebra. An important class of instances that arise in practice has the form $L\mathbf{x} = \mathbf{b}$, where L is the Laplacian of an undirected graph. After decades of sustained research and combining tools from disparate areas, we now have Laplacian solvers that run in time nearlylinear in the sparsity (that is, the number of edges in the associated graph) of the system, which is a distant goal for general systems. Surprisingly, and perhaps not the original motivation behind this line of research, Laplacian solvers are impacting the theory of fast algorithms for fundamental graph problems. In this monograph, the emerging paradigm of employing Laplacian solvers to design novel fast algorithms for graph problems is illustrated through a small but carefully chosen set of examples. A part of this monograph is also dedicated to developing the ideas that go into the construction of near-linear-time Laplacian solvers. An understanding of these methods, which marry techniques from linear algebra and graph theory, will not only enrich the tool-set of an algorithm designer but will also provide the ability to adapt these methods to design fast algorithms for other fundamental problems.

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The ability to solve a system of linear equations lies at the heart of areas such as optimization, scientific computing, and computer science and, traditionally, has been a central topic of research in numerical linear algebra. Consider a system $A\mathbf{x} = \mathbf{b}$ with n equations in n variables. Broadly, solvers for such a system of equations fall into two categories. The first is Gaussian elimination-based methods which, essentially, can be made to run in the time it takes to multiply two $n \times n$ matrices, (currently $O(n^{2.3...})$ time). The second consists of iterative methods, such as the conjugate gradient method. These reduce the problem to computing n matrix-vector products, and thus make the running time proportional to mn where m is the number of nonzero entries, or sparsity, of A.¹ While this bound of n in the number of iterations is tight in the worst case, it can often be improved if A has additional structure, thus, making iterative methods popular in practice.

An important class of such instances has the form $L\mathbf{x} = \mathbf{b}$, where L is the Laplacian of an undirected graph G with n vertices and m edges

¹ Strictly speaking, this bound on the running time assumes that the numbers have bounded precision.

with m (typically) much smaller than n^2 . Perhaps the simplest setting in which such *Laplacian systems* arise is when one tries to compute currents and voltages in a resistive electrical network. Laplacian systems are also important in practice, e.g., in areas such as scientific computing and computer vision. The fact that the system of equations comes from an underlying undirected graph made the problem of designing solvers especially attractive to theoretical computer scientists who entered the fray with tools developed in the context of graph algorithms and with the goal of bringing the running time down to O(m). This effort gained serious momentum in the last 15 years, perhaps in light of an explosive growth in instance sizes which means an algorithm that does not scale near-linearly is likely to be impractical.

After decades of sustained research, we now have a solver for Laplacian systems that runs in $O(m \log n)$ time. While many researchers have contributed to this line of work, Spielman and Teng spearheaded this endeavor and were the first to bring the running time down to $\tilde{O}(m)$ by combining tools from graph partitioning, random walks, and lowstretch spanning trees with numerical methods based on Gaussian elimination and the conjugate gradient. Surprisingly, and not the original motivation behind this line of research, Laplacian solvers are impacting the theory of fast algorithms for fundamental graph problems; giving back to an area that empowered this work in the first place.

That is the story this monograph aims to tell in a comprehensive manner to researchers and aspiring students who work in algorithms or numerical linear algebra. The emerging paradigm of employing Laplacian solvers to design novel fast algorithms for graph problems is illustrated through a small but carefully chosen set of problems such as graph partitioning, computing the matrix exponential, simulating random walks, graph sparsification, and single-commodity flows. A significant part of this monograph is also dedicated to developing the algorithms and ideas that go into the proof of the Spielman–Teng Laplacian solver. It is a belief of the author that an understanding of these methods, which marry techniques from linear algebra and graph theory, will not only enrich the tool-set of an algorithm designer, but will also provide the ability to adapt these methods to design fast algorithms for other fundamental problems.

How to use this monograph. This monograph can be used as the text for a graduate-level course or act as a supplement to a course on spectral graph theory or algorithms. The writing style, which deliberately emphasizes the presentation of key ideas over rigor, should even be accessible to advanced undergraduates. If one desires to teach a course based on this monograph, then the best order is to go through the sections linearly. Essential are Sections 1 and 2 that contain the basic linear algebra material necessary to follow this monograph and Section 3 which contains the statement and a discussion of the main theorem regarding Laplacian solvers. Parts of this monograph can also be read independently. For instance, Sections 5–7 contain the Cheeger inequality based spectral algorithm for graph partitioning. Sections 15 and 16 can be read in isolation to understand the conjugate gradient method. Section 19 looks ahead into computing more general functions than the inverse and presents the Lanczos method. A dependency diagram between sections appears in Figure 1. For someone solely interested in a near-linear-time algorithm for solving Laplacian systems, the quick path to Section 14, where the approach of a short and new proof is presented, should suffice. However, the author recommends going all



Fig. 1 The dependency diagram among the sections in this monograph. A dotted line from i to j means that the results of Section j use some results of Section i in a black-box manner and a full understanding is not required.

the way to Section 18 where multiple techniques developed earlier in the monograph come together to give an $\tilde{O}(m)$ Laplacian solver.

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Bangalore 15 January 2013 Nisheeth K. Vishnoi Microsoft Research India

Notation

- The set of real numbers is denoted by \mathbb{R} , and $\mathbb{R}_{\geq 0}$ denotes the set of nonnegative reals. We only consider real numbers in this monograph.
- The set of integers is denoted by Z, and Z_{≥0} denotes the set of nonnegative integers.
- Vectors are denoted by boldface, e.g., \mathbf{u}, \mathbf{v} . A vector $\mathbf{v} \in \mathbb{R}^n$ is a column vector but often written as $\mathbf{v} = (v_1, \dots, v_n)$. The transpose of a vector \mathbf{v} is denoted by \mathbf{v}^{\top} .
- For vectors \mathbf{u}, \mathbf{v} , their inner product is denoted by $\langle \mathbf{u}, \mathbf{v} \rangle$ or $\mathbf{u}^\top \mathbf{v}$.
- For a vector \mathbf{v} , $\|\mathbf{v}\|$ denotes its ℓ_2 or Euclidean norm where $\|\mathbf{v}\| \stackrel{\text{def}}{=} \sqrt{\langle \mathbf{v}, \mathbf{v} \rangle}$. We sometimes also refer to the ℓ_1 or Manhattan distance norm $\|\mathbf{v}\|_1 \stackrel{\text{def}}{=} \sum_{i=1}^n |v_i|$.
- The outer product of a vector \mathbf{v} with itself is denoted by $\mathbf{v}\mathbf{v}^{\top}$.
- Matrices are denoted by capitals, e.g., A, L. The transpose of A is denoted by A^{\top} .
- We use t_A to denote the time it takes to multiply the matrix A with a vector.

6 Notation

- The A-norm of a vector **v** is denoted by $\|\mathbf{v}\|_A \stackrel{\text{def}}{=} \sqrt{\mathbf{v}^\top A \mathbf{v}}$.
- For a real symmetric matrix A, its real eigenvalues are ordered $\lambda_1(A) \leq \lambda_2(A) \leq \cdots \leq \lambda_n(A)$. We let $\Lambda(A) \stackrel{\text{def}}{=} [\lambda_1(A), \lambda_n(A)]$.
- A positive-semidefinite (PSD) matrix is denoted by $A \succeq 0$ and a positive-definite matrix $A \succ 0$.
- The norm of a symmetric matrix A is denoted by $||A|| \stackrel{\text{def}}{=} \max\{|\lambda_1(A)|, |\lambda_n(A)|\}$. For a symmetric PSD matrix A, $||A|| = \lambda_n(A)$.
- Thinking of a matrix A as a linear operator, we denote the image of A by Im(A) and the rank of A by rank(A).
- A graph G has a vertex set V and an edge set E. All graphs are assumed to be undirected unless stated otherwise. If the graph is weighted, there is a weight function $w: E \mapsto \mathbb{R}_{\geq 0}$. Typically, n is reserved for the number of vertices |V|, and m for the number of edges |E|.
- $\mathbb{E}_{\mathcal{F}}[\cdot]$ denotes the expectation and $\mathbb{P}_{\mathcal{F}}[\cdot]$ denotes the probability over a distribution \mathcal{F} . The subscript is dropped when clear from context.
- The following acronyms are used liberally, with respect to (w.r.t.), without loss of generality (w.l.o.g.), with high probability (w.h.p.), if and only if (iff), right-hand side (r.h.s.), left-hand side (l.h.s.), and such that (s.t.).
- Standard big-o notation is used to describe the limiting behavior of a function. \tilde{O} denotes potential logarithmic factors which are ignored, i.e., $f = \tilde{O}(g)$ is equivalent to $f = O(g \log^k(g))$ for some constant k.

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Part I Basics



This section reviews basics from linear algebra, such as eigenvalues and eigenvectors, that are relevant to this monograph. The spectral theorem for symmetric matrices and min–max characterizations of eigenvalues are derived.

1.1 Spectral Decomposition of Symmetric Matrices

One way to think of an $m \times n$ matrix A with real entries is as a linear operator from \mathbb{R}^n to \mathbb{R}^m which maps a vector $\mathbf{v} \in \mathbb{R}^n$ to $A\mathbf{v} \in \mathbb{R}^m$. Let dim(S) be dimension of S, i.e., the maximum number of linearly independent vectors in S. The rank of A is defined to be the dimension of the image of this linear transformation. Formally, the image of Ais defined to be $\operatorname{Im}(A) \stackrel{\text{def}}{=} {\mathbf{u} \in \mathbb{R}^m : \mathbf{u} = A\mathbf{v}}$ for some $\mathbf{v} \in \mathbb{R}^n}$, and the rank is defined to be $\operatorname{rank}(A) \stackrel{\text{def}}{=} \dim(\operatorname{Im}(A))$ and is at most $\min\{m, n\}$.

We are primarily interested in the case when A is square, i.e., m = n, and symmetric, i.e., $A^{\top} = A$. Of interest are vectors \mathbf{v} such that $A\mathbf{v} = \lambda \mathbf{v}$ for some λ . Such a vector is called an eigenvector of A with respect to (w.r.t.) the eigenvalue λ . It is a basic result in linear algebra that every real matrix has n eigenvalues, though some of them could

10 Basic Linear Algebra

be complex. If A is symmetric, then one can show that the eigenvalues are real. For a complex number z = a + ib with $a, b \in \mathbb{R}$, its conjugate is defined as $\bar{z} = a - ib$. For a vector \mathbf{v} , its conjugate transpose \mathbf{v}^* is the transpose of the vector whose entries are conjugates of those in \mathbf{v} . Thus, $\mathbf{v}^*\mathbf{v} = \|\mathbf{v}\|^2$.

Lemma 1.1. If A is a real symmetric $n \times n$ matrix, then all of its eigenvalues are real.

Proof. Let λ be an eigenvalue of A, possibly complex, and \mathbf{v} be the corresponding eigenvector. Then, $A\mathbf{v} = \lambda \mathbf{v}$. Conjugating both sides we obtain that $\mathbf{v}^* A^\top = \overline{\lambda} \mathbf{v}^*$, where \mathbf{v}^* is the conjugate transpose of \mathbf{v} . Hence, $\mathbf{v}^* A \mathbf{v} = \overline{\lambda} \mathbf{v}^* \mathbf{v}$, since A is symmetric. Thus, $\lambda ||\mathbf{v}||^2 = \overline{\lambda} ||\mathbf{v}||^2$ which implies that $\lambda = \overline{\lambda}$. Thus, $\lambda \in \mathbb{R}$.

Let $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ be the *n* real eigenvalues, or the *spectrum*, of *A* with corresponding eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_n$. For a symmetric matrix, its *norm* is

$$||A|| \stackrel{\text{def}}{=} \max\{|\lambda_1(A)|, |\lambda_n(A)|\}.$$

We now study eigenvectors that correspond to distinct eigenvalues.

Lemma 1.2. Let λ_i and λ_j be two eigenvalues of a symmetric matrix A, and \mathbf{u}_i , \mathbf{u}_j be the corresponding eigenvectors. If $\lambda_i \neq \lambda_j$, then $\langle \mathbf{u}_i, \mathbf{u}_j \rangle = 0$.

Proof. Given $A\mathbf{u}_i = \lambda_i \mathbf{u}_i$ and $A\mathbf{u}_j = \lambda_j \mathbf{u}_j$, we have the following sequence of equalities. Since A is symmetric, $\mathbf{u}_i^{\top} A^{\top} = \mathbf{u}_i^{\top} A$. Thus, $\mathbf{u}_i^{\top} A\mathbf{u}_j = \lambda_i \mathbf{u}_i^{\top} \mathbf{u}_j$ on the one hand, and $\mathbf{u}_i^{\top} A\mathbf{u}_j = \lambda_j \mathbf{u}_i^{\top} \mathbf{u}_j$ on the other. Therefore, $\lambda_j \mathbf{u}_i^{\top} \mathbf{u}_j = \lambda_i \mathbf{u}_i^{\top} \mathbf{u}_j$. This implies that $\mathbf{u}_i^{\top} \mathbf{u}_j = 0$ since $\lambda_i \neq \lambda_j$.

Hence, the eigenvectors corresponding to different eigenvalues are orthogonal. Moreover, if \mathbf{u}_i and \mathbf{u}_j correspond to the same eigenvalue λ , and are linearly independent, then any linear combination

1.1 Spectral Decomposition of Symmetric Matrices 11

is also an eigenvector corresponding to the same eigenvalue. The maximal eigenspace of an eigenvalue is the space spanned by all eigenvectors corresponding to that eigenvalue. Hence, the above lemma implies that one can decompose \mathbb{R}^n into maximal eigenspaces U_i , each of which corresponds to an eigenvalue of A, and the eigenspaces corresponding to distinct eigenvalues are orthogonal. Thus, if $\lambda_1 < \lambda_2 < \cdots < \lambda_k$ are the set of distinct eigenvalues of a real symmetric matrix A, and U_i is the eigenspace associated with λ_i , then, from the discussion above,

$$\sum_{i=1}^{k} \dim(U_i) = n.$$

Hence, given that we can pick an orthonormal basis for each U_i , we may assume that the eigenvectors of A form an orthonormal basis for \mathbb{R}^n . Thus, we have the following spectral decomposition theorem.

Theorem 1.3. Let $\lambda_1 \leq \cdots \leq \lambda_n$ be the spectrum of A with corresponding eigenvalues $\mathbf{u}_1, \ldots, \mathbf{u}_n$. Then, $A = \sum_{i=1}^n \lambda_i \mathbf{u}_i \mathbf{u}_i^{\top}$.

Proof. Let $B \stackrel{\text{def}}{=} \sum_{i=1}^{n} \lambda_i \mathbf{u}_i \mathbf{u}_i^{\top}$. Then, $B \mathbf{u}_j = \sum_{i=1}^{n} \lambda_i \mathbf{u}_i \mathbf{u}_i^{\top} \mathbf{u}_j$

$$= \lambda_j \mathbf{u}_j$$
$$= A \mathbf{u}_j.$$

The above is true for all j. Since \mathbf{u}_j s are orthonormal basis of \mathbb{R}^n , we have for all $\mathbf{v} \in \mathbb{R}^n$, $A\mathbf{v} = B\mathbf{v}$. This implies A = B.

Thus, when A is a real and symmetric matrix, Im(A) is spanned by the eigenvectors with nonzero eigenvalues. From a computational perspective, such a decomposition can be computed in time polynomial in the bits needed to represent the entries of A.¹

¹To be very precise, one can only compute eigenvalues and eigenvectors to a high enough precision in polynomial time. We will ignore this distinction for this monograph as we do not need to know the *exact* values.

12 Basic Linear Algebra

1.2 Min–Max Characterizations of Eigenvalues

Now we present a variational characterization of eigenvalues which is very useful.

Lemma 1.4. If A is an $n \times n$ real symmetric matrix, then the largest eigenvalue of A is

$$\lambda_n(A) = \max_{\mathbf{v} \in \mathbb{R}^n \setminus \{\mathbf{0}\}} \frac{\mathbf{v}^\top A \mathbf{v}}{\mathbf{v}^\top \mathbf{v}}.$$

Proof. Let $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ be the eigenvalues of A, and let $\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_n$ be the corresponding orthonormal eigenvectors which span \mathbb{R}^n . Hence, for all $\mathbf{v} \in \mathbb{R}^n$, there exist $c_1, \ldots, c_n \in \mathbb{R}$ such that $\mathbf{v} = \sum_i c_i \mathbf{u}_i$. Thus,

$$\langle \mathbf{v}, \mathbf{v} \rangle = \left\langle \sum_{i} c_{i} \mathbf{u}_{i}, \sum_{i} c_{i} \mathbf{u}_{i} \right\rangle$$

= $\sum_{i} c_{i}^{2}$.

Moreover,

$$\mathbf{v}^{\top} A \mathbf{v} = \left(\sum_{i} c_{i} \mathbf{u}_{i} \right)^{\top} \left(\sum_{j} \lambda_{j} \mathbf{u}_{j} \mathbf{u}_{j}^{\top} \right) \left(\sum_{k} c_{k} \mathbf{u}_{k} \right)$$
$$= \sum_{i,j,k} c_{i} c_{k} \lambda_{j} (\mathbf{u}_{i}^{\top} \mathbf{u}_{j}) \cdot (\mathbf{u}_{j}^{\top} \mathbf{u}_{k})$$
$$= \sum_{i} c_{i}^{2} \lambda_{i}$$
$$\leq \lambda_{n} \sum_{i} c_{i}^{2} = \lambda_{n} \langle \mathbf{v}, \mathbf{v} \rangle.$$

Hence, $\forall \mathbf{v} \neq 0, \ \frac{\mathbf{v}^{\top} A \mathbf{v}}{\mathbf{v}^{\top} \mathbf{v}} \leq \lambda_n$. This implies,

$$\max_{\mathbf{v}\in\mathbb{R}^n\setminus\{\mathbf{0}\}}\frac{\mathbf{v}^{\top}A\mathbf{v}}{\mathbf{v}^{\top}\mathbf{v}}\leq\lambda_n.$$

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Now note that setting $\mathbf{v} = \mathbf{u}_n$ achieves this maximum. Hence, the lemma follows.

If one inspects the proof above, one can deduce the following lemma just as easily.

Lemma 1.5. If A is an $n \times n$ real symmetric matrix, then the smallest eigenvalue of A is

$$\lambda_1(A) = \min_{\mathbf{v} \in \mathbb{R}^n \setminus \{\mathbf{0}\}} \frac{\mathbf{v}^\top A \mathbf{v}}{\mathbf{v}^\top \mathbf{v}}.$$

More generally, one can extend the proof of the lemma above to the following. We leave it as a simple exercise.

Theorem 1.6. If A is an $n \times n$ real symmetric matrix, then for all $1 \le k \le n$, we have

$$\lambda_k(A) = \min_{\mathbf{v} \in \mathbb{R}^n \setminus \{\mathbf{0}\}, \mathbf{v}^\top \mathbf{u}_i = 0, \forall i \in \{1, \dots, k-1\}} \frac{\mathbf{v}^\top A \mathbf{v}}{\mathbf{v}^\top \mathbf{v}},$$

and

$$\lambda_k(A) = \max_{\mathbf{v} \in \mathbb{R}^n \setminus \{\mathbf{0}\}, \mathbf{v}^\top \mathbf{u}_i = 0, \forall i \in \{k+1, \dots, n\}} \frac{\mathbf{v}^\top A \mathbf{v}}{\mathbf{v}^\top \mathbf{v}}.$$

Notes

Some good texts to review basic linear algebra are [35, 82, 85]. Theorem 1.6 is also called the Courant–Fischer–Weyl min–max principle.

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