

# LAPLACIAN LINEAR SOLVERS

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# TOPICS

## Prerequisites

- Linear Algebra
- The Graph Laplacian

## Graphs as Electrical Circuits

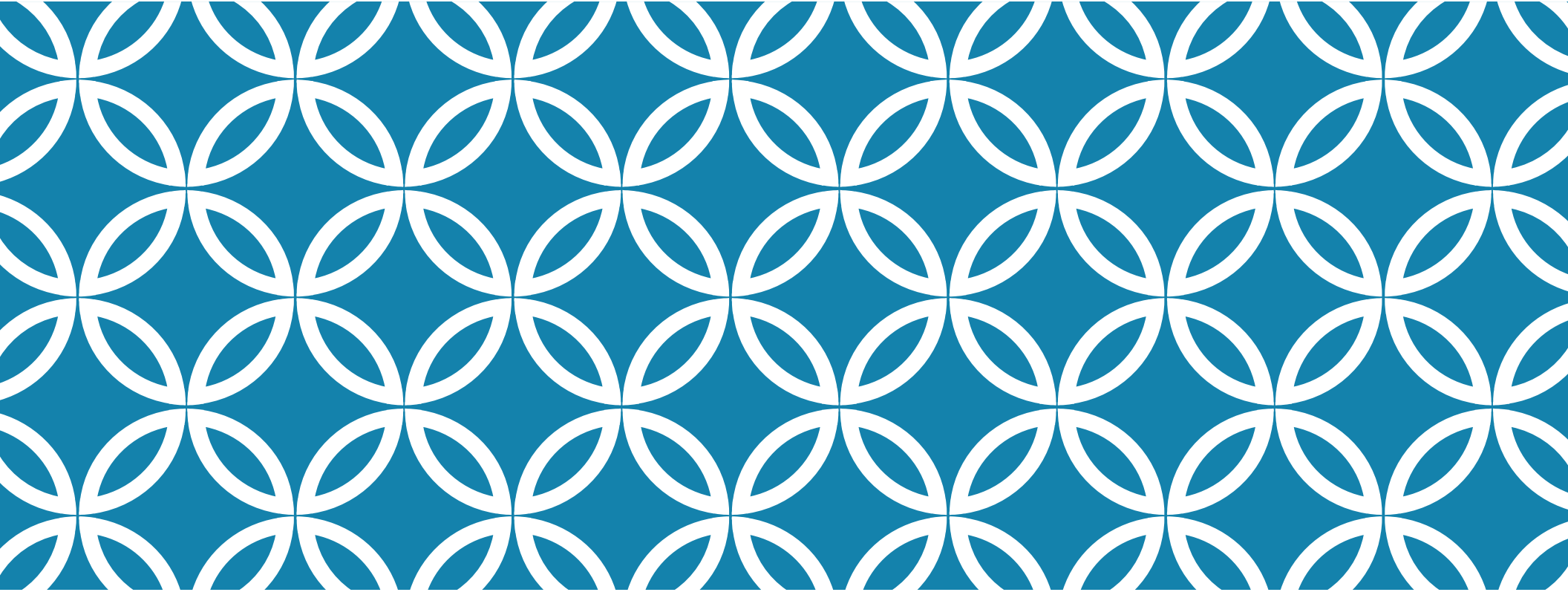
## Graph Sparsification via Effective Resistances

## Cholesky Decomposition

## Iterative Linear Solvers

- The Gradient Method
- The Conjugate Gradient Method

## Laplacian Linear Solvers



# PREREQUISITES



# BASIC LINEAR ALGEBRA

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

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

**Lemma 1.3:** Let  $\lambda_1 \leq \dots \leq \lambda_n$  be the spectrum of  $A$  with the  $\mathbf{u}_1, \dots, \mathbf{u}_n$  being the corresponding eigenvectors. Then  $A = \sum_{i=1}^n \lambda_i \mathbf{u}_i \mathbf{u}_i^T$ . Here  $\mathbf{u}_1, \dots, \mathbf{u}_n$  are orthonormal.

**Theorem 1.4:** If  $A$  is a  $n \times n$  real symmetric matrix, then for all  $1 \leq k \leq n$ ,

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

And

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

# THE GRAPH LAPLACIAN

We define the adjacency matrix  $A$  and the degree matrix  $D$  of a graph  $G = (V, E)$  as follows:

$$A_{i,j} = \begin{cases} 1 & \text{if } ij \in E \\ 0 & \text{otherwise} \end{cases}$$
$$D_{i,j} = \begin{cases} d_i & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

The Graph Laplacian of  $G$  is then defined as  $L = D - A$ .

We define the  $n \times n$  matrices  $L_e$ , where  $e = ij \in E$  as follows:  $L(i, i) = L(j, j) = 1, L(i, j) = L(j, i) = -1$ .

# PROPERTIES OF THE LAPLACIAN

**Lemma 2.1:** If  $L$  is the graph Laplacian of  $G = (V, E)$ ,  $L = \sum_{e \in E} L_e$ .

**Lemma 2.2:** Let  $L$  be a graph Laplacian. Then  $L$  is positive semidefinite.

**Lemma 2.3:** Let  $L$  be a graph Laplacian. Then  $\mathbf{1} = (1, \dots, 1)$  is an eigenvector of  $L$  with eigenvalue 0.

**Theorem 2.4:** Let  $L$  be the graph Laplacian of  $G = (V, E)$ . Then,  $\lambda_2 > 0$  iff  $G$  is connected.

**Theorem 2.5:** Let  $B \in \{-1, 0, 1\}^{m \times n}$  be any arbitrary incidence matrix of  $G$ . Then  $B^T B = L$ .

## PROOF OF THEOREM 2.5

We have  $(B^T B)_{i,j} = \sum_e B_{e,i} B_{e,j}$ .

When  $i = j$ , the only nonzero terms are for those edges which are incident to  $i$ , and the product is 1. Hence, the sum is the degree of the vertex.

For other entries, the term is only nonzero when  $e$  is shared by  $i$  and  $j$ . We can see in that case,  $B_{e,i} B_{e,j} = -1$ . Therefore,  $(B^T B)_{i,j} = -1, \forall i \neq j, ij \in E$ .

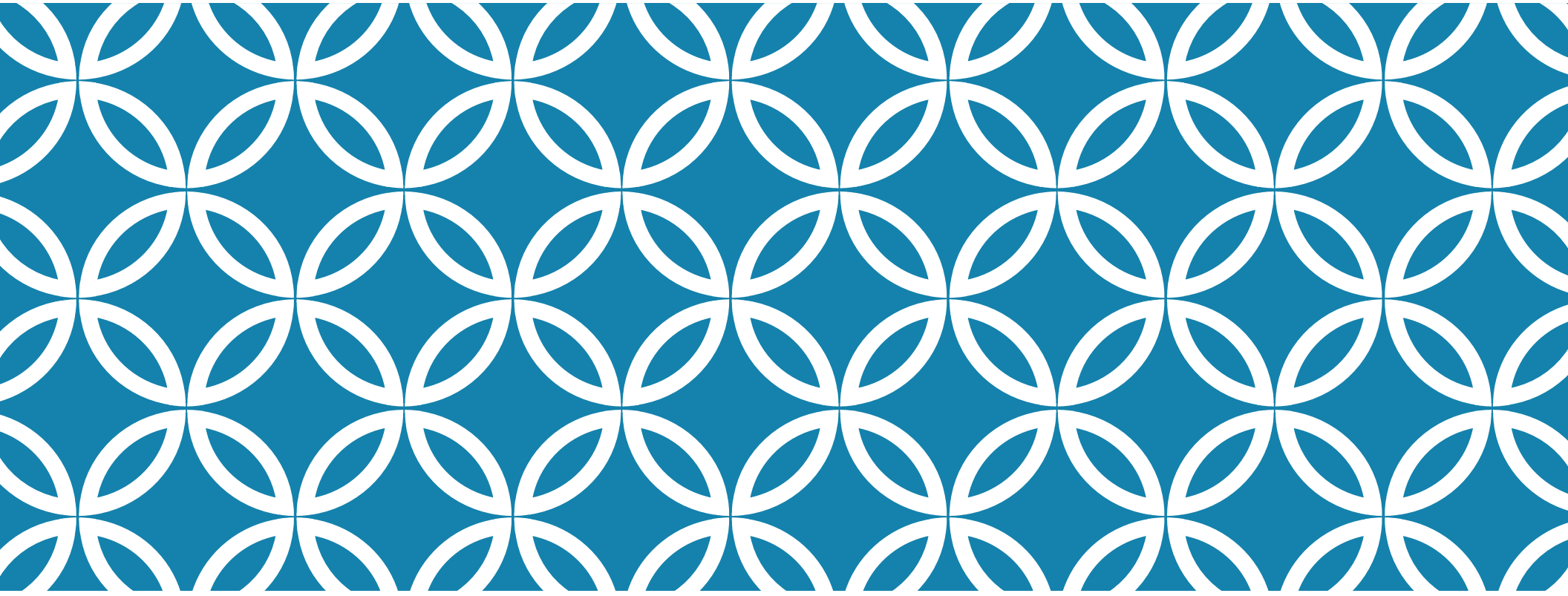
# WHAT ARE WE TRYING TO PROVE?

**Theorem 3:** There exists an algorithm which takes as input a graph Laplacian  $L$ , a vector  $\mathbf{b}$ , and an error value  $\varepsilon > 0$  and returns  $\mathbf{x}$  such that:

$$\|\mathbf{x} - L^+\mathbf{b}\|_L \leq \varepsilon \|L^+\mathbf{b}\|_L$$

Where  $\|\mathbf{b}\|_L = \sqrt{\mathbf{b}^T L \mathbf{b}}$ . This algorithm runs in  $\tilde{O}\left(m \log \frac{1}{\varepsilon}\right)$  time, where  $m$  is the number of non-zero entries in  $L$ . Here  $L^+$  is the Moore-Penrose pseudoinverse.





# GRAPHS AS ELECTRICAL NETWORKS



# DEFINING THE CIRCUIT

We can associate every edge to be a resistor with a resistance of 1.

Consider a voltage vector  $\mathbf{v} \in \mathbb{R}^n$ , which represents the voltage at each vertex, a current vector  $\mathbf{i} \in \mathbb{R}^m$ , which represents the current through each edge, and  $\mathbf{c} \in \mathbb{R}^n$  representing the external current supplied to each vertex. Note that  $\langle \mathbf{c}, \mathbf{1} \rangle = 0$ , as no charge can accumulate in the network.

From Kirchoff's current law, we have:

$$B^T \mathbf{i} = \mathbf{c}$$

From Ohm's Law, we have:

$$\mathbf{i} = B\mathbf{v}$$

This gives us:

$$B^T B\mathbf{v} = L\mathbf{v} = \mathbf{c} \Rightarrow \mathbf{v} = L^+ \mathbf{c}$$

# GRAPHS AS ELECTRICAL NETWORKS

Therefore, the current through an edge  $ij$  is  $(\mathbf{e}_i - \mathbf{e}_j)L^+ \mathbf{c}$ , as the resistance is 1.

We use this to define the effective resistance of  $e = ij$ :

$$R_{eff}(e) = (\mathbf{e}_i - \mathbf{e}_j)^T L^+ (\mathbf{e}_i - \mathbf{e}_j)$$

We can now consider the currents through any edge, when a unit current is passed through another edge. This would be given by (in matrix notation)

$$\Pi = BL^+B^T$$

# PROPERTIES OF $\Pi$

**Lemma 4.1:**  $\Pi$  is symmetric.

- This is because  $L^+$  is symmetric.

**Lemma 4.2:**  $\Pi^2 = \Pi$

- Proof:  $\Pi^2 = BL^+ \overbrace{B^T B}^{=L} L^+ B^T = B \overbrace{L^+ L L^+}^{=L^+} B^T = BL^+ B^T = \Pi$

**Lemma 4.3:** The eigenvalues of  $\Pi$  are either 1 or 0.

- Proof: Let  $v$  be an eigenvector. We have  $\lambda v = \Pi v = \Pi^2 v = \lambda^2 v$ , which implies  $\lambda = 0, 1$ .

**Lemma 4.4:** If  $G$  is connected,  $\text{rank}(\Pi) = n - 1$

- Proof:  $B$  is full column rank and the rank of  $L^+$  is  $n - 1$  if  $G$  is connected. Therefore, the rank of  $\Pi$  is  $n - 1$ .

# A FINAL NOTE ON EFFECTIVE RESISTANCES

**Theorem 4.5**<sup>[1]</sup>: Let  $T$  be a spanning tree chosen uniformly at random from all the spanning trees in  $G$ . Then the probability that an edge  $e$  belongs to the tree is:

$$\mathbb{P}[e \in T] = R_{eff}(e) = \Pi(e, e)$$

[1]: C. D. GODSIL AND G. ROYLE, ALGEBRAIC GRAPH THEORY. SPRINGER, 2001.

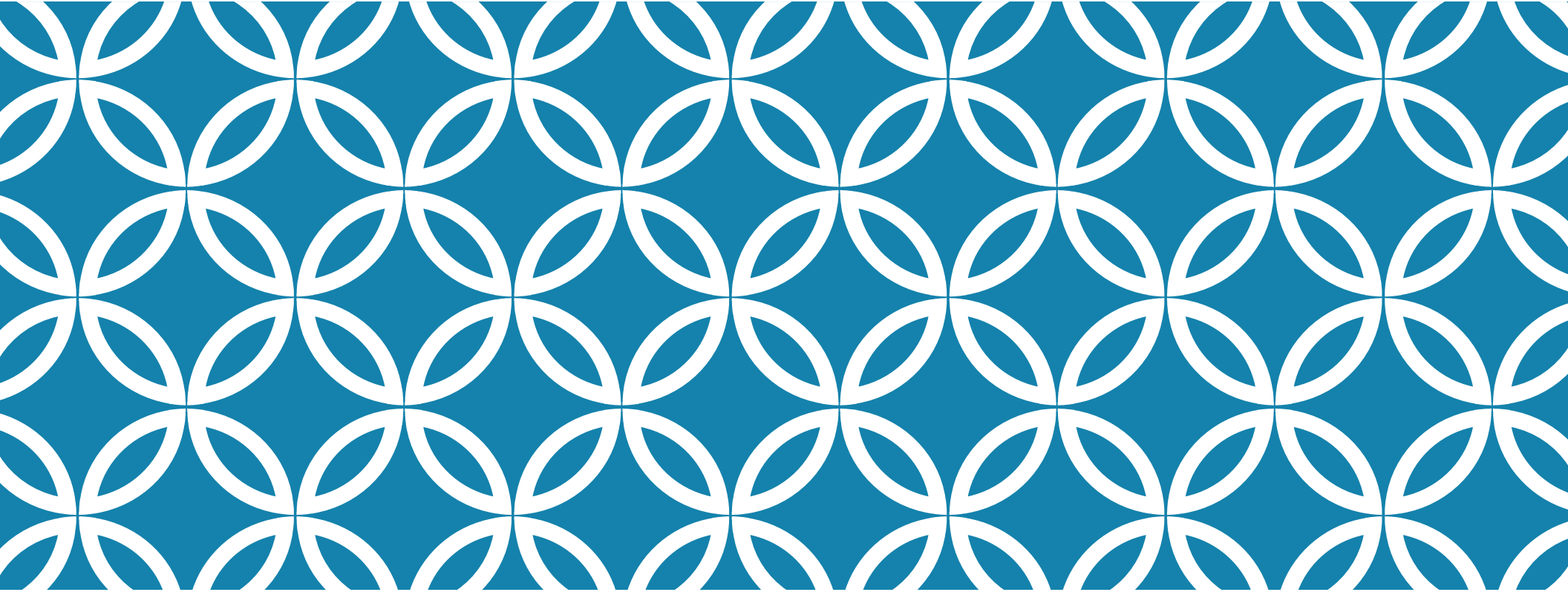
# WEIGHTED GRAPHS

Let  $W \in \mathbb{R}^{m \times m}$  such that  $W(e, e) = w(e)$ , where  $w$  is the weight vector.

We define:

$$L = B^T W B$$
$$\Pi = W^{\frac{1}{2}} B L^+ B^T W^{\frac{1}{2}}$$

If we consider the resistance of an edge to be the inverse of its weight, then all the results proved before apply, with  $\mathbf{i} = W B \mathbf{v}$ , as according to Ohm's law. The definition of  $R_{eff}$  remains the same, but it used the new definition of the Laplacian.



# GRAPH SPARSIFICATION

Sparsification via Effective Resistances

# INTRODUCTION

As already introduced, graphs are connected to electrical networks.

This connection can be used to spectrally sparsify graphs.

The goal of cut sparsification is, for a given graph  $G = (V, E)$  and parameter  $\varepsilon$ , to find a weighted graph  $H = (V, E')$  such that for any cut  $(S, \bar{S})$  of  $V$ , the weight of the edges in  $H$  that cross the cut is within a multiplicative factor  $1 \pm \varepsilon$  of the number of edges in  $G$  that cross this cut, while keeping the number of edges in  $H$  small.

This must also be done quickly for various applications.



# SPECTRAL SPARSIFICATION

Spectral sparsification is a stronger notion than cut sparsification, and plays an important role in the construction of Laplacian solvers.

**Definition 5.1:** Given an undirected graph  $G = (V, E)$  and a parameter  $\varepsilon > 0$ , a weighted graph  $H = (V, E')$  is said to be an  $\varepsilon$ -spectral sparsifier of  $G$  if

$$\frac{1}{(1 + \varepsilon)} \leq \frac{\mathbf{x}^T L_H \mathbf{x}}{\mathbf{x}^T L_G \mathbf{x}} \leq (1 + \varepsilon), \forall \mathbf{x} \in \mathbb{R}^n$$

Where  $L_G$  and  $L_H$  are the graph Laplacians for  $G$  and  $H$ .

# SPECTRAL SPARSIFICATION (CONTD.)

The goal is then to minimize the number of edges in  $H$ , while constructing it as quickly as possible. In particular, we want to construct a spectral sparsifier with  $\tilde{O}(n/\text{poly}(\varepsilon))$  edges in  $\tilde{O}(m)$  time.

Note that an  $\varepsilon$ -spectral sparsifier is also a  $\varepsilon$ -cut sparsifier as for any cut, we can plug in  $\mathbf{1}_S$ , the indicator for the cut, into the equation.

We shall soon prove the following theorem:

**Theorem 5.1:** There exists a randomized algorithm that, given a graph  $G = (V, E)$  and a parameter  $\varepsilon > 0$ , constructs a spectral sparsifier  $H$  of size  $O(n \log n / \varepsilon^2)$  (edges) with probability  $1 - 1/n$

# USING EFFECTIVE RESISTANCES

The algorithm we use is an edge sampling algorithm – we repeatedly sample (with replacement) edges from the graph  $G$  according to a carefully chosen probability distribution, and then weight these sampled edges proportionally to the inverse of their probability of their being selected.

Formally, let  $p_e$  be the probability that edge  $e$  is selected, and let  $Y$  be the random variable such that  $\mathbb{P}[Y = e] = p_e$ . Let  $T$  be the number of samples. Finally let  $Y_1, Y_2, \dots, Y_T$  be i.i.d. copies of  $Y$ . Then the weighted multiset of edges is:

$$\left\{ \left( Y_1, \frac{1}{T \cdot p_{Y_1}} \right), \left( Y_2, \frac{1}{T \cdot p_{Y_2}} \right), \dots, \left( Y_T, \frac{1}{T \cdot p_{Y_T}} \right) \right\}$$

# PROPERTIES OF ITS LAPLACIAN

Let  $B$  be some incidence matrix for  $G$  and  $\mathbf{b}_e$  be the column vector corresponding to edge  $e$  in  $B^T$ . Then  $L_G = B^T B$ . Now define  $\mathbf{u}_e \stackrel{\text{def}}{=} \mathbf{b}_e / \sqrt{p_e}$ . Then, by the definition, we have:

$$L_H = \sum_{i=1}^T \frac{\mathbf{b}_{Y_i} \mathbf{b}_{Y_i}^T}{T \cdot p_{Y_i}} = \frac{1}{T} \sum_{i=1}^T \mathbf{u}_{Y_i} \mathbf{u}_{Y_i}^T$$

Now note that:

$$\mathbb{E}[\mathbf{u}_Y \mathbf{u}_Y^T] = \sum_{e \in E} \mathbb{P}[Y = e] \cdot \mathbf{u}_e \mathbf{u}_e^T = L_G$$

From this, it is obvious that  $\mathbb{E}[L_H] = L_G$

# CHOOSING THE PROBABILITY DISTRIBUTION

We have to now specify the probability distribution. To do this, we use the intuition from **Theorem 4.5** where we found that effective resistances are related to the probability of an edge being present in a randomly chosen minimum spanning tree.

We let  $p_e \stackrel{\text{def}}{=} \frac{R_e}{n-1}$ , where  $R_e = R_{\text{eff}}(e)$ . The  $n - 1$  normalization factor is present as  $\sum_e R_e = n - 1$ .

While this intuition behind choosing this distribution is not very clear, the idea is to choose edges proportional to  $R_e$  as picking a few random minimum spanning trees for  $G$  seems like a good strategy to help in building a spectral sparsifier for it.

# PROOF OF THEOREM 5.1

Recall the matrix  $\Pi \stackrel{\text{def}}{=} BL_G^+ B^T$ , which satisfies:

- $\Pi^2 = \Pi$
- If  $\Pi_e$  is the column of  $\Pi$  corresponding to edge  $e$ , then  $R_e = \|\Pi_e\|^2$
- $\sum_e R_e = n - 1$
- $\Pi$  is unitarily equivalent to  $\sum_{j=1}^{n-1} \mathbf{e}_j \mathbf{e}_j^T$ , where  $\mathbf{e}_j$  is the  $j^{\text{th}}$  standard basis vector for  $\mathbb{R}^m$ . This is because  $\Pi$  is symmetric (thus normal), and has only two eigenvalues: 1 with multiplicity  $n - 1$  and 0 with multiplicity  $m - n + 1$ , same as  $\sum_{j=1}^{n-1} \mathbf{e}_j \mathbf{e}_j^T$ .

Next we shall state an important theorem (without proof).

# MATRIX CHERNOFF BOUND

**Theorem 5.2**<sup>[1]</sup>: Let  $\varepsilon > 0$  be a small constant. Let  $M^{d \times d}$  be a random, symmetric PSD matrix such that  $\mathbb{E}[M] = I_d$ , where  $I_d$  is the  $d$ -dimensional identity matrix. Let  $\rho = \sup_M \|M\|$ . Let  $T$  be a non-negative integer and let  $M_1, M_2, \dots, M_T$  be i.i.d. copies of  $M$ . Then,

$$\mathbb{P} \left[ \left\| \frac{1}{T} \sum_{i=1}^T M_i - \mathbb{E}[M] \right\| > \varepsilon \right] \leq 2d \cdot \exp \left( -\frac{T\varepsilon^2}{2\rho} \right)$$

This theorem also holds under various other conditions, the one we are interested in being when  $\mathbb{E}[M]$  is unitarily equivalent to  $\sum_{j=1}^{d'} \mathbf{e}_j \mathbf{e}_j^T$ , for some  $0 < d' \leq d$ , in which case  $d'$  replaces  $d$  in the bound.

[1] R. AHLWEDE AND A. WINTER, "STRONG CONVERSE FOR IDENTIFICATION VIA QUANTUM CHANNELS," IN IEEE TRANSACTIONS ON INFORMATION THEORY, MARCH 2002

# CONDITIONS FOR USING THEOREM 5.2

To use **Theorem 5.2**, we define  $\mathbf{v}_e \stackrel{\text{def}}{=} \Pi_e / \sqrt{p_e}$ ,  $M \stackrel{\text{def}}{=} \mathbf{v}_Y \mathbf{v}_Y^T$  and  $M_i \stackrel{\text{def}}{=} \mathbf{v}_{Y_i} \mathbf{v}_{Y_i}^T$  for  $i = 1, 2, \dots, T$ . Now note that:

$$\mathbb{E}[M] = \mathbb{E}[\mathbf{v}_e \mathbf{v}_e^T] = \sum_{e \in E} \Pi_e \Pi_e^T = \Pi$$

Thus  $\mathbb{E}[M]$  is unitarily equivalent to  $\sum_{j=1}^{n-1} \mathbf{e}_j \mathbf{e}_j^T$ . Also note that:

$$\|\mathbf{v}_e\|^2 = \frac{\|\Pi_e\|^2}{p_e} = \frac{R_e}{p_e} = n - 1$$

From this we have  $\|M\| \leq n - 1$ , so we can apply **Theorem 5.2**



## USING THEOREM 5.2

Define  $\tilde{\Pi} \stackrel{\text{def}}{=} \frac{1}{T} \sum_{i=1}^T M_i$

We now use **Theorem 5.2** to get:

$$\mathbb{P}[\|\tilde{\Pi} - \Pi\| > \varepsilon] \leq 2(n-1) \cdot \exp\left(-\frac{T\varepsilon^2}{2(n-1)}\right)$$

By setting  $T = O(n \log n / \varepsilon^2)$  we can ensure that this probability of failure is  $n^{-\Omega(1)}$ .  
Since  $\Pi = BL_G^+ B^\top$ , we have that, for any edge  $e$ :

$$\mathbf{v}_e = \frac{\Pi_e}{\sqrt{p_e}} = \frac{BL_G^+ \mathbf{b}_e}{\sqrt{p_e}} = BL_G^+ \mathbf{u}_e$$

## PROOF OF THEOREM 5.1 (CONTD.)

Thus, we have:

$$\tilde{\Pi} = \frac{1}{T} \sum_{i=1}^T \mathbf{v}_{Y_i} \mathbf{v}_{Y_i}^T = \frac{1}{T} \sum_{i=1}^T BL_G^+ \mathbf{u}_{Y_i} \mathbf{u}_{Y_i}^T L_G^+ B^T = BL_G^+ L_H L_G^+ B^T$$

and,

$$\Pi = BL_G^+ B^T = BL_G^+ L_G L_G^+ B^T$$

Thus,

$$\|\tilde{\Pi} - \Pi\| = \sup_{\mathbf{x} \neq \mathbf{0}} \left| \frac{\mathbf{x}^T (\tilde{\Pi} - \Pi) \mathbf{x}}{\mathbf{x}^T \mathbf{x}} \right| = \sup_{\mathbf{x} \neq \mathbf{0}} \left| \frac{\mathbf{x}^T BL_G^+ (L_H - L_G) L_G^+ B^T \mathbf{x}}{\mathbf{x}^T \mathbf{x}} \right|$$

## PROOF OF THEOREM 5.1 (CONTD.)

Now note that as  $G$  is connected, for any  $\mathbf{z}$ , if  $B\mathbf{z} = \mathbf{0}$ , then  $\mathbf{z}$  is parallel to  $\mathbf{1}$ . Thus is we consider only  $\mathbf{z} \neq \mathbf{0}$  such that  $\langle \mathbf{z}, \mathbf{1} \rangle = 0$ , then  $B\mathbf{z} \neq \mathbf{0}$ .

So we substitute  $\mathbf{x} = B\mathbf{z}$  in the equation to get:

$$\begin{aligned}\|\tilde{\Pi} - \Pi\| &\geq \sup_{\mathbf{z} \neq \mathbf{0}, \langle \mathbf{z}, \mathbf{1} \rangle = 0} \left| \frac{\mathbf{z}^T B^T B L_G^+ (L_H - L_G) L_G^+ B^T B \mathbf{z}}{\mathbf{z}^T B^T B \mathbf{z}} \right| \\ \|\tilde{\Pi} - \Pi\| &\geq \sup_{\mathbf{z} \neq \mathbf{0}, \langle \mathbf{z}, \mathbf{1} \rangle = 0} \left| \frac{\mathbf{z}^T L_G L_G^+ (L_H - L_G) L_G^+ L_G \mathbf{z}}{\mathbf{z}^T L_G \mathbf{z}} \right| \\ \|\tilde{\Pi} - \Pi\| &\geq \sup_{\mathbf{z} \neq \mathbf{0}, \langle \mathbf{z}, \mathbf{1} \rangle = 0} \left| \frac{\mathbf{z}^T L_H \mathbf{z}}{\mathbf{z}^T L_G \mathbf{z}} - 1 \right|\end{aligned}$$

## PROOF OF THEOREM 5.1 (CONTD.)

Thus we have

$$\mathbb{P} \left[ \sup_{\mathbf{z} \neq \mathbf{0}, \langle \mathbf{z}, \mathbf{1} \rangle = 0} \left| \frac{\mathbf{z}^T L_H \mathbf{z}}{\mathbf{z}^T L_G \mathbf{z}} - 1 \right| > \varepsilon \right] \leq \mathbb{P} [\| \tilde{\Pi} - \Pi \| > \varepsilon] = n^{-\Omega(1)}$$

This completes the proof of **Theorem 5.1**.

The theorem can be extended to include a running time bound of  $\tilde{O}(m \log 1/\varepsilon)$ , however we shall not be proving that here.

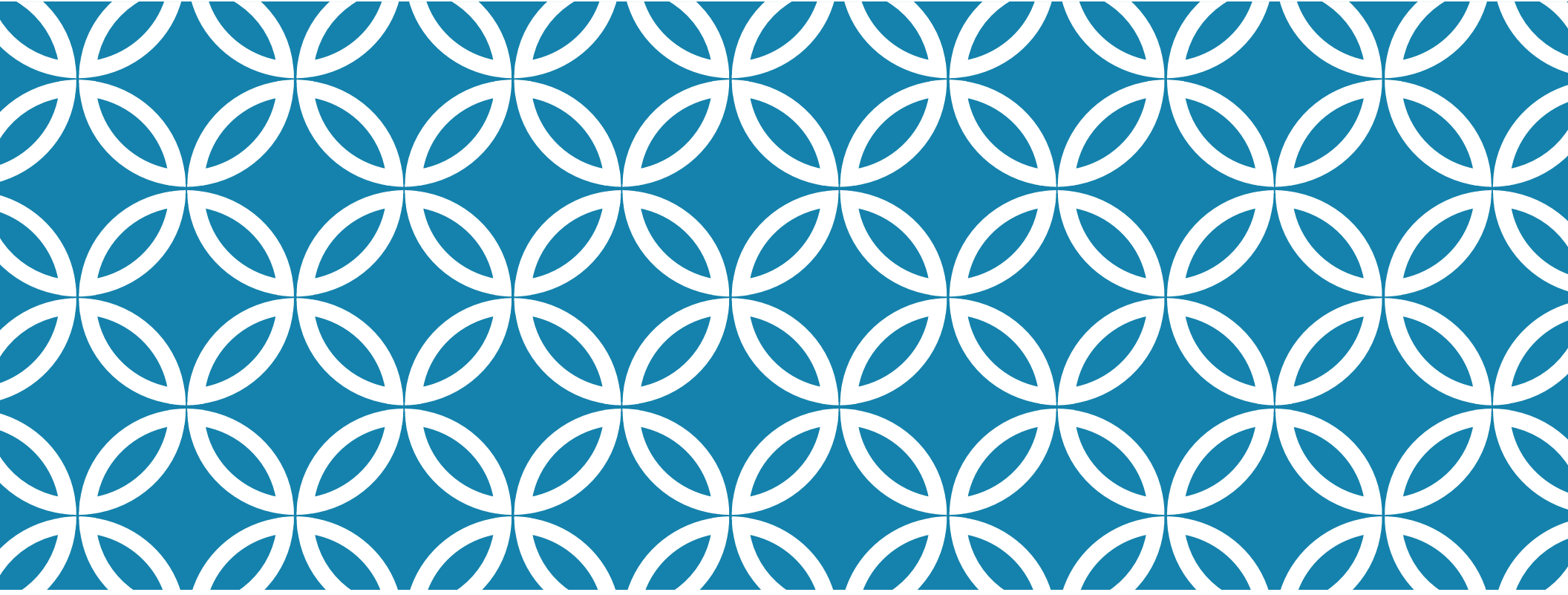
# CRUDE SPECTRAL SPARSIFICATION

Instead of requiring knowledge of  $R_e$ , we can work with the knowledge of  $q_e \geq R_e$  for all  $e$ . This is a crude spectral sparsifier, and can be easily shown to work with  $W \stackrel{\text{def}}{=} \sum_e q_e$  random samples. Thus we have a new theorem:

**Theorem 5.3:** Consider a graph  $G = (V, E)$  with edge weights  $w_G$ ,  $\gamma > 0$ , and numbers  $q_e \geq w_G(e)R_e$  for all  $e$ . If  $W \stackrel{\text{def}}{=} \sum_e q_e$ , then the spectral sparsifier in **Theorem 5.1** upon taking  $O(W \log W \log 1/\gamma)$  samples from the probability distribution induced by the  $q_e$ s produces a graph  $H$  that satisfies

$$G \preceq 2H \preceq 3G$$

With a probability of at least  $1 - \gamma$ .



# CHOLESKY DECOMPOSITION

Solving Laplacians for Trees

# INTRODUCTION

Cholesky Decomposition is a way to solve  $A\mathbf{x} = \mathbf{b}$  where  $A$  is symmetric and PD. However, the same method still works for the Laplacian of a connected graph, as  $\langle \mathbf{b}, \mathbf{1} \rangle = 0$ , i.e., we are working in the subspace orthogonal to  $\mathbf{1}$ . Here,  $L^+ \succ 0$ .

**Lemma 6.1:** *Schur's Lemma:*  $A = \begin{pmatrix} d_1 & \mathbf{u}_1^T \\ \mathbf{u}_1 & B_1 \end{pmatrix} \succ 0$  iff

$$d_1 > 0 \text{ and } B_1 - \frac{\mathbf{u}_1 \mathbf{u}_1^T}{d_1} \succ 0.$$

# PROOF OF SCHUR'S LEMMA

As  $A > 0$ ,  $d_1 > 0$  (consider  $\mathbf{e}_1^T A \mathbf{e}_1 = d_1$ ). Now, consider minimising the quadratic expression  $z^2 d + 2z \mathbf{u}_1^T \mathbf{y} + \mathbf{y}^T B_1 \mathbf{y}$  over  $z$ , for any (fixed)  $\mathbf{y}$ . The minima is at  $z = -\mathbf{u}_1^T \mathbf{y} / d_1$ . Thus, the minima is  $\mathbf{y}^T \left( B_1 - \mathbf{u}_1 \mathbf{u}_1^T / d_1 \right) \mathbf{y}$ . As this is true for all  $\mathbf{y}$ ,  $B_1 - \mathbf{u}_1 \mathbf{u}_1^T / d_1$  must be PD.

The other direction is trivial.



# CHOLESKY DECOMPOSITION

**Theorem 6.2: Cholesky Decomposition:** If  $A \succ 0$  and symmetric, then there exists a lower triangular matrix  $\Lambda$ , such that  $A = \Lambda\Lambda^T$ .

Proof:

The theorem is trivially true for a  $1 \times 1$  matrix. Now, say it was true for all  $(n - 1) \times (n - 1)$  matrices.

Since  $A \succ 0$ , it is sufficient to express  $A = \Lambda\Delta\Lambda^T$ . This is because the positive definiteness implies that  $\Delta_{ii} > 0$ , which means we can write  $A = (\Lambda\Delta^{1/2})(\Lambda\Delta^{1/2})^T$ .

We can now write  $A$  as

$$\begin{pmatrix} d_1 & \mathbf{u}_1^T \\ \mathbf{u}_1 & B_1 \end{pmatrix} = \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{u}_1/d_1 & I_{n-1} \end{pmatrix} \begin{pmatrix} d_1 & \mathbf{0}^T \\ \mathbf{0} & B_1 - \mathbf{u}_1\mathbf{u}_1^T/d_1 \end{pmatrix} \begin{pmatrix} 1 & \mathbf{u}_1^T/d_1 \\ \mathbf{0} & I_{n-1} \end{pmatrix}$$

# PROOF OF CHOLESKY DECOMPOSITION

Let the matrix in the middle in the middle be  $A_1$ . Now let  $B = B_1 - \mathbf{u}_1\mathbf{u}_1^T/d_1$ . Now, by Schur's Lemma,  $B \succ 0$ .

Using the induction hypothesis, we have  $B = \Lambda'\Delta'\Lambda'^T$ , and

$$A_1 = \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & \Lambda' \end{pmatrix} \begin{pmatrix} d_1 & \mathbf{0}^T \\ \mathbf{0} & \Delta' \end{pmatrix} \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & \Lambda'^T \end{pmatrix} \stackrel{\text{def}}{=} \Lambda''\Delta\Lambda''^T$$

Thus, we have  $A = \Lambda_1\Lambda''\Delta\Lambda''^T\Lambda_1^T$ . Now, as the product of lower triangular matrices is lower triangular, we are done.

# USING CHOLESKY DECOMPOSITION

Given a decomposition, we can solve  $A\mathbf{x} = \mathbf{b}$  quickly.

We can evaluate  $\mathbf{b}' = \Lambda^+ \mathbf{b}$  and then  $\mathbf{x} = (\Lambda^T)^+ \mathbf{b}'$ . Due to the triangular nature of  $\Lambda$ , the time taken to calculate the pseudoinverse is of the order of the number of non-zero elements of  $\Lambda$ .

If we first permute the rows by a permutation matrix  $Q$  and then find the decomposition, we might find a decomposition with fewer non-zero elements (known as the *fill-in*). However, finding the minimum fill-in is NP-hard.

# FAST SOLVERS FOR TREES

We try to find a fast solver for  $L_T \mathbf{x} = \mathbf{b}$ , where  $T$  is a tree.

We can associate every symmetric matrix  $A$  with a weighted graph (potentially with self loops), where  $A(i, j)$  is the weight of the edge connecting  $ij$ .

- Note: This is not the Laplacian of the graph.

**Theorem 6.3:** Given a symmetric, PSD matrix  $A$  and a vector  $\mathbf{b}$  such that the graph of  $A$  corresponds to a tree, one can find in  $O(n)$  time a permutation matrix  $Q$  such that the Cholesky decomposition of  $Q^T A Q$  has at most  $O(n)$  nonzero entries.

# PROOF OF THEOREM 6.3

We can view the proof of 6.2 as one that modifies the graph. When we recursively process row  $i$ , the resulting graph (corresponding to  $A_1$ ) has the following changes:

- a. All edges  $ij, i \neq j$  are deleted. This corresponds to setting  $A_1(i, j) = 0$ .
- b. For every pair  $jk$  neighbouring to  $i$ , a (potentially new) edge is modified. This corresponds to

$$\text{setting } A_1(j, k) = B_1(j, k) - \frac{\frac{u_1 u_1^T}{A(i, j)A(i, k)}}{\frac{A(i, i)}{d_1}}.$$

Suppose the graph corresponds to the system is a tree, potentially with self loops. Then in each iteration, we can choose a leaf node, by choosing an appropriate permutation matrix.

## PROOF OF THEOREM 6.3

Since there is a single node adjacent to  $i$ , the graph associated with  $A_1$  is a tree.

This implies, we can write  $A = \Lambda \Delta \Lambda^T$  where  $\Lambda = \Lambda_1 \Lambda_2 \dots \Lambda_n$ , where each  $\Lambda_i$  is lower triangular, and has at most one nonzero off-diagonal element.

This gives a Cholesky decomposition with at most  $O(n)$  nonzero entries, where in each iteration  $O(1)$  operations are done, which implies the process takes  $O(n)$  time.

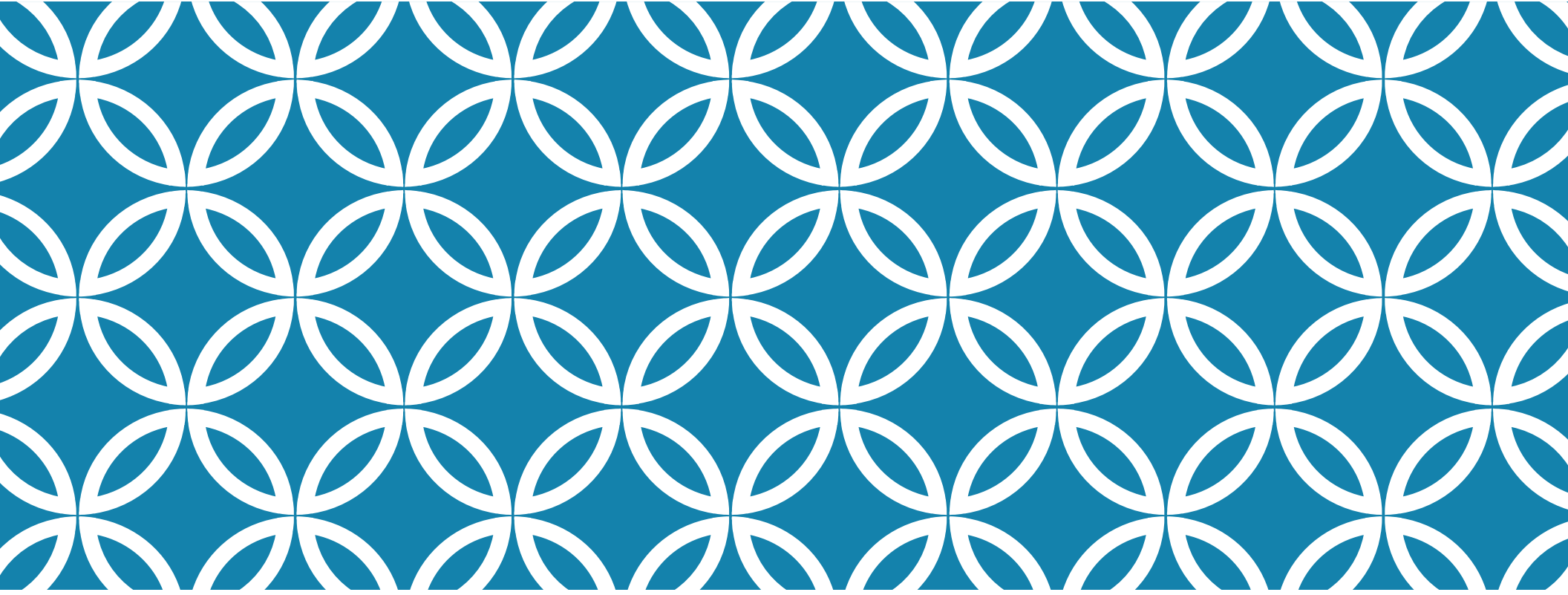
# AN IMPORTANT COROLLARY

**Corollary 6.4:** If  $L_T$  is the Laplacian of a tree  $T$  and  $\mathbf{b}$  is a vector such that  $\langle \mathbf{b}, \mathbf{1} \rangle = 0$ , then the solution of  $L_T \mathbf{x} = \mathbf{b}$  can be found in  $O(n)$  time.

Proof: We can see the graph associated with the Laplacian of a tree is a tree. Hence, by 6.3, we can find the Cholesky Decomposition of the permuted Laplacian to get  $\Lambda \Lambda^T Q^T \mathbf{x} = Q^T \mathbf{b}$  in  $O(n)$  time.

This is possible despite  $\Lambda$  not being full rank (as  $L_T$ ) is not full rank, as  $\langle \mathbf{b}, \mathbf{1} \rangle = 0$ , and thus  $\mathbf{b}$  is in the column space of  $L_T Q$ .

Therefore, this solution can be calculated in the number of nonzero entries of  $L_T$ , i.e., in  $O(n)$  time



# ITERATIVE LINEAR SOLVERS

The Gradient Method



# THE OPTIMIZATION VIEW

We shall formulate solving the equation  $A\mathbf{x} = \mathbf{b}$  as a convex optimization problem. For this, we assume that  $A$  is symmetric and positive-definite.

Solving  $A\mathbf{x} = \mathbf{b}$  is equivalent to finding the minimum of  $f(\mathbf{x})$  –

$$f(\mathbf{x}) \stackrel{\text{def}}{=} \frac{1}{2} \mathbf{x}^T A \mathbf{x} - \mathbf{b}^T \mathbf{x}$$

Since  $A$  is PD,  $\nabla^2 f = A > 0$ , so  $f$  is strictly convex and thus has a unique minimum  $\mathbf{x}^*$ . As we already know, this  $\mathbf{x}^*$  must satisfy –

$$\nabla f(\mathbf{x}^*) = A\mathbf{x}^* - \mathbf{b} = \mathbf{0}$$

# GRADIENT DESCENT-BASED SOLVER

Since  $f$  is convex, we can use the well known gradient descent algorithm to solve for  $\mathbf{x}^*$ . Typically in gradient descent, we start at  $\mathbf{x}_0$  and iterative move from  $\mathbf{x}_t$  to  $\mathbf{x}_{t+1}$  by moving opposite the direction of the gradient of  $f$ , which can (here) be calculated with a single multiplication of a matrix and a vector, which takes time  $t_A$  (say).

**Theorem 7.1:** There is an algorithm GDSOLVE that, given an  $n \times n$  matrix  $A \succ 0$ , a vector  $\mathbf{b}$  and  $\varepsilon > 0$ , finds a vector  $\mathbf{x}$  such that

$$\|\mathbf{x} - A^+\mathbf{b}\|_A \leq \varepsilon \|A^+\mathbf{b}\|_A$$

in time  $O(t_A \cdot \kappa(A) \log 1/\varepsilon)$ , where the condition number of  $A$  is defined as  $\kappa(A) \stackrel{\text{def}}{=} \lambda_n(A)/\lambda_1(A)$ . For a vector  $\mathbf{v}$ ,  $\|\mathbf{v}\|_A \stackrel{\text{def}}{=} \sqrt{\mathbf{v}^T A \mathbf{v}}$ .

# THE STEP SIZE

First we define  $\mathbf{d}_t \stackrel{\text{def}}{=} \mathbf{x}^* - \mathbf{x}_t$  and  $\mathbf{r}_t \stackrel{\text{def}}{=} -\nabla f(\mathbf{x}_t) = \mathbf{b} - A\mathbf{x}_t = A\mathbf{d}_t$ .

The step size  $\eta_t$  is a parameter which determines how much to move towards  $\mathbf{r}_t$ , and we have  $\mathbf{x}_{t+1} \stackrel{\text{def}}{=} \mathbf{x}_t + \eta_t \mathbf{r}_t$ .

We can choose  $\eta_t$  greedily, to minimize  $f(\mathbf{x}_{t+1})$ . Define  $g$  as:

$$g(\eta) \stackrel{\text{def}}{=} f(\mathbf{x}_t + \eta \mathbf{r}_t) = \frac{1}{2} (\mathbf{x}_t + \eta \mathbf{r}_t)^T A (\mathbf{x}_t + \eta \mathbf{r}_t) - \mathbf{b}^T (\mathbf{x}_t + \eta \mathbf{r}_t)$$

It is easy to see that  $g$  attains its minimum at  $\eta_t = \frac{\mathbf{r}_t^T \mathbf{r}_t}{\mathbf{r}_t^T A \mathbf{r}_t}$

# ALGORITHM 7.1: GDSOLVE

**Input:** Symmetric, PD matrix  $A \in \mathbb{R}^{n \times n}$ , vector  $\mathbf{b} \in \mathbb{R}^n$  and  $T$ .

**Output:**  $\mathbf{x}_T \in \mathbb{R}^n$

1.  $\mathbf{x}_0 \leftarrow \mathbf{0}$
2. **for**  $t = 0 \rightarrow T - 1$  **do**
  1. Set  $\mathbf{r}_t = \mathbf{b} - A\mathbf{x}_t$
  2. Set  $\eta_t = \frac{\mathbf{r}_t^T \mathbf{r}_t}{\mathbf{r}_t^T A \mathbf{r}_t}$
  3. Set  $\mathbf{x}_{t+1} = \mathbf{x}_t + \eta_t \mathbf{r}_t$
3. **end for**
4. **return**  $\mathbf{x}_T$

**LEMMA 7.2:**  $\|\mathbf{d}_{t+1}\|_A^2 \leq \left(1 - \frac{1}{\kappa(A)}\right) \cdot \|\mathbf{d}_t\|_A^2$ .

Note two things:  $\mathbf{d}_{t+1} = \mathbf{d}_t - \eta_t \mathbf{r}_t$  and  $\mathbf{r}_{t+1} = \mathbf{r}_t - \eta_t A \mathbf{r}_t$ . This gives  $\mathbf{r}_t^T \mathbf{r}_{t+1} = \mathbf{r}_t^T \mathbf{r}_t - \frac{\mathbf{r}_t^T \mathbf{r}_t}{\mathbf{r}_t^T A \mathbf{r}_t} \mathbf{r}_t^T A \mathbf{r}_t = 0$ , so  $\mathbf{r}_t$  and  $\mathbf{r}_{t+1}$  are orthogonal.

Thus,  $\|\mathbf{d}_{t+1}\|_A^2 = \mathbf{d}_{t+1}^T A \mathbf{d}_{t+1} = (\mathbf{d}_t - \eta_t \mathbf{r}_t)^T \mathbf{r}_{t+1} = \mathbf{d}_t^T \mathbf{r}_{t+1}$  since  $\mathbf{r}_t$  and  $\mathbf{r}_{t+1}$  are orthogonal. Thus,  $\|\mathbf{d}_{t+1}\|_A^2 = \mathbf{d}_t^T \mathbf{r}_{t+1} = \mathbf{d}_t^T A (\mathbf{d}_t - \eta_t \mathbf{r}_t)$

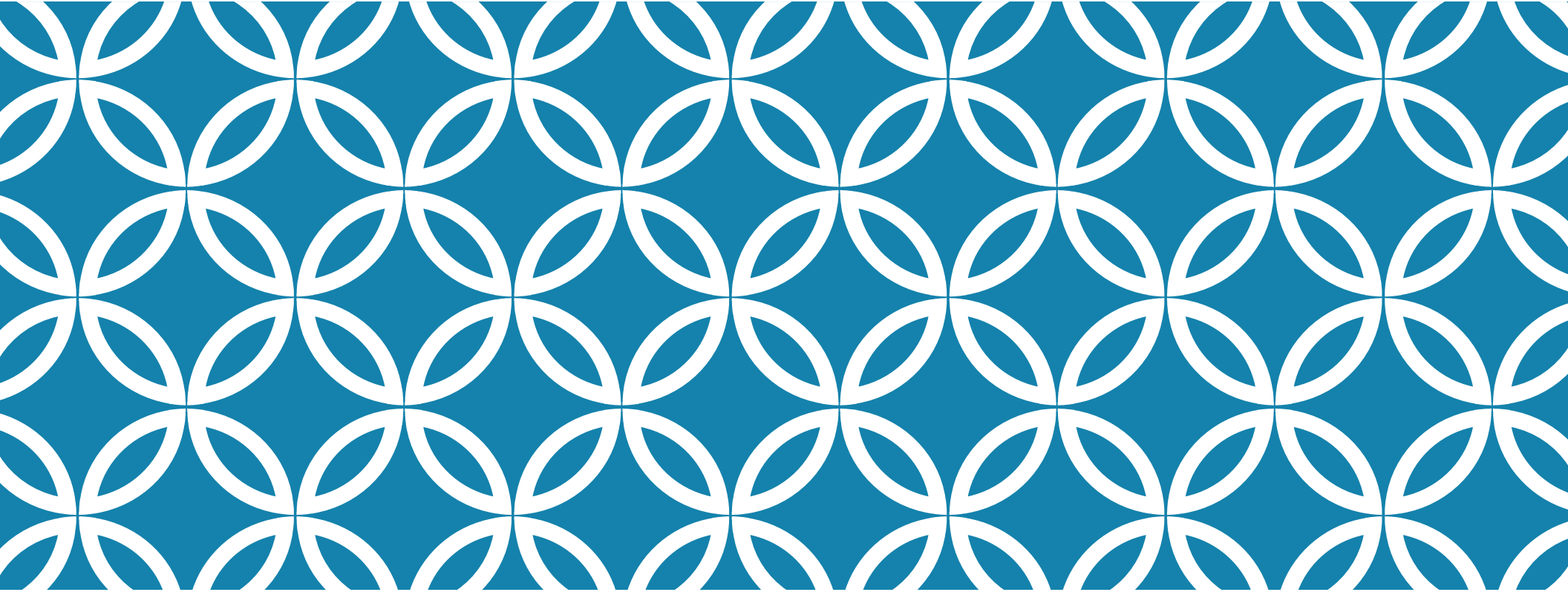
Now we factor out the  $\|\mathbf{d}_t\|_A^2$  to get

$$\|\mathbf{d}_t\|_A^2 \cdot \left(1 - \eta_t \frac{\mathbf{d}_t^T A \mathbf{r}_t}{\mathbf{d}_t^T A \mathbf{d}_t}\right) = \|\mathbf{d}_t\|_A^2 \cdot \left(1 - \frac{\mathbf{r}_t^T \mathbf{r}_t}{\mathbf{r}_t^T A \mathbf{r}_t} \cdot \frac{\mathbf{d}_t^T A^2 \mathbf{d}_t}{\mathbf{d}_t^T A \mathbf{d}_t}\right)$$

# PROOF OF LEMMA 7.2 AND THEOREM 7.1

Now recall the min-max characterization of eigenvalues (**Theorem 1.5**). Thus, the first factor (in the product inside the brackets) is at most  $1/\lambda_n(A)$  while the second factor is at least  $\lambda_1(A)$  [since  $A \succ 0$ ,  $A^{1/2}\mathbf{d}_t \neq 0$  so we can shift one of the  $A$ s around in the product]. Thus,  $\|\mathbf{d}_{t+1}\|_A^2 \leq (1 - 1/\kappa(A))\|\mathbf{d}_t\|_A^2$

Simply take  $T = 2\kappa(A) \log 1/\varepsilon$  to get  $\|\mathbf{d}_T\|_A \leq \varepsilon\|\mathbf{d}_0\|_A$ , which completes the proof of **Theorem 7.1**



# ITERATIVE LINEAR SOLVERS

The Conjugate Gradient Method

# THE KRYLOV SUBSPACE

Consider the same problem as before, i.e.,

$$\min_{\mathbf{x}} f(\mathbf{x}) \stackrel{\text{def}}{=} \frac{1}{2} \mathbf{x}^T A \mathbf{x} - \mathbf{b}^T \mathbf{x}$$

In the previous algorithm, we generated, which generated:

$$\begin{aligned} \mathbf{x}_1 &= \mathbf{x}_0 + \eta_0 \mathbf{r}_0 \\ \mathbf{x}_2 &= \mathbf{x}_1 + \eta_1 \mathbf{r}_1 = \mathbf{x}_1 + \eta_1 (\mathbf{r}_0 - \eta_0 A \mathbf{r}_0) = \mathbf{x}_0 + \eta_1 \mathbf{r}_0 - \eta_1 \eta_0 A \mathbf{r}_0, \end{aligned}$$

and so on, with  $\mathbf{r}_0 = \mathbf{b}$  and  $\mathbf{r}_i = \mathbf{b} - A \mathbf{x}_i$ .

This implies  $\mathbf{x}_t \in \mathbf{x}_0 + \mathcal{K}_t$ , where  $\mathcal{K}_t$  is the subspace spanned by  $\{A^i \mathbf{b} : i \in \{0, 1, \dots, t-1\}\}$ . This is known as the Krylov Subspace of order  $t$  generated by  $A$  and  $\mathbf{b}$ .



# IDEA BEHIND CONJUGATE GRADIENT

In the previous algorithm, the point we move to might not be the minimizer of  $f$  over the affine space  $\mathbf{x}_0 + \mathcal{K}_t$ . This is what we will do in this algorithm.

**Theorem 8.1:** There is an algorithm that, given an  $n \times n$  symmetric matrix  $A \succ 0$ , a vector  $\mathbf{b}$ , and  $\varepsilon > 0$ , finds a vector  $\mathbf{x}$  such that

$$\|\mathbf{x} - A^+\mathbf{b}\|_A \leq \varepsilon \|A^+\mathbf{b}\|_A$$

in time  $O\left(t\sqrt{\kappa(A)}\log\frac{1}{\varepsilon}\right)$ .

We shall find this algorithm and prove the theorem in the following section.

# MOTIVATION FOR PROOF

We could find the minimizer of  $f$  over  $\mathbf{x} + \mathcal{K}_t$  quickly, if we had a basis of  $\mathcal{K}_t$ ,  $\{\mathbf{p}_0, \mathbf{p}_1, \dots, \mathbf{p}_{t-1}\}$  such that:

$$f\left(\mathbf{x}_0 + \sum_{i=0}^{t-1} \beta_i \mathbf{p}_i\right) - f(\mathbf{x}_0) = \sum_{i=0}^{t-1} (f(\mathbf{x}_0 + \beta_i \mathbf{p}_i) - f(\mathbf{x}_0))$$

We could find the minimiser over each  $\beta_i$  separately.

If  $f$  is linear, this is trivially true. Thus, we only consider the quadratic portion. For brevity, let  $\mathbf{v}_i = \beta_i \mathbf{p}_i$ . Then, evaluating the LHS:

$$\frac{1}{2} \left(\mathbf{x} + \sum_i \mathbf{v}_i\right)^T A \left(\mathbf{x} + \sum_i \mathbf{v}_i\right) - \frac{1}{2} \mathbf{x}^T A \mathbf{x} = \mathbf{x}^T A \sum_i \mathbf{v}_i + \frac{1}{2} \left(\sum_i \mathbf{v}_i\right)^T A \left(\sum_i \mathbf{v}_i\right)$$

The RHS evaluates to  $\sum_i \left(\mathbf{x}^T A \mathbf{v}_i + \frac{1}{2} \mathbf{v}_i^T A \mathbf{v}_i\right)$ . The two are equal iff the cross terms  $\mathbf{v}_i^T A \mathbf{v}_j = 0$ , whenever  $i \neq j$ .

# A-ORTHOGONAL VECTORS

**Definition 8.1:** Given a symmetric matrix  $A$ , two vectors  $\mathbf{x}, \mathbf{y}$  are  $A$ -orthogonal iff  $\mathbf{x}^T A \mathbf{y} = 0$ .

Thus, we can see that our choices for  $\{\mathbf{p}_0, \dots, \mathbf{p}_{t-1}\}$  must be  $A$ -orthogonal.

With this orthogonal basis, we can calculate  $\alpha_t$  to be the vectors that minimise  $f(\mathbf{x}_0 + \alpha \mathbf{p}_t) - f(\mathbf{x}_0)$ . Then,  $\alpha_t = \frac{\mathbf{p}_t^T \mathbf{r}_0}{\mathbf{p}_t^T A \mathbf{r}_0}$ .

# COMPUTING THE $A$ -ORTHONORMAL BASIS

Gram-Schmidt orthogonalization would take  $O(t)$  matrix-vector computations to calculate  $\mathbf{p}_{t+1}$ .

We use the symmetry of  $A$  to reduce this to  $O(1)$  computations.

We start with  $\mathbf{p}_0 = \mathbf{r}_0$ . Suppose that  $\{\mathbf{p}_0, \dots, \mathbf{p}_i\}$  spans  $\mathcal{K}_{i+1}$ , and  $A\mathbf{p}_i \in \mathcal{K}_{i+2}$ , for some  $i$ . This is true for  $i = 0$ .

Consider  $A\mathbf{p}_i$ . If  $A\mathbf{p}_i \in \mathcal{K}_{i+1}$ ,  $\mathcal{K}_j = \mathcal{K}_{i+1}, \forall j \geq i + 1$ , and we would be done, as this would span the entire space. Now assume that  $A\mathbf{p}_i \notin \mathcal{K}_{i+1}$ . Now, we construct  $\mathbf{p}_{i+1}$  as follows:

$$\mathbf{p}_{i+1} \stackrel{\text{def}}{=} A\mathbf{p}_i - \sum_{j \leq i} \frac{(A\mathbf{p}_j)^T A\mathbf{p}_j}{\mathbf{p}_j^T A\mathbf{p}_j} \mathbf{p}_j$$

# COMPUTING THE $A$ -ORTHONORMAL BASIS

This implies that

$$\mathcal{K}_{i+2} = \text{span}\{\mathbf{r}_0, A\mathbf{r}_0, \dots, A^{i+1}\mathbf{r}_0\} = \text{span}\{\mathbf{p}_0, \dots, \mathbf{p}_{i+1}\}$$

This completes the induction.

Now, this implies that  $A\mathbf{p}_i$  can be written as a linear combination of  $\mathbf{p}_j$ , for  $j \leq i + 1$ . Thus, for all  $j \leq i$ ,

$$(A\mathbf{p}_i)^T(A\mathbf{p}_j) = \mathbf{p}_i^T A(A\mathbf{p}_j) = \sum_{k \leq j+1} c_j \mathbf{p}_i^T A \mathbf{p}_k$$

Thus,  $\forall j < i - 1$ ,  $(A\mathbf{p}_i)^T(A\mathbf{p}_j) = 0$ . Thus, we can write  $\mathbf{p}_{t+1}$  as:

$$\mathbf{p}_{t+1} = A\mathbf{p}_t - \frac{\mathbf{p}_t^T A^2 \mathbf{p}_t}{\mathbf{p}_t^T A \mathbf{p}_t} \mathbf{p}_t - \frac{\mathbf{p}_t^T A^2 \mathbf{p}_{t-1}}{\mathbf{p}_{t-1}^T A \mathbf{p}_{t-1}} \mathbf{p}_{t-1}$$

# THE COMPLETE CONJUGATE GRADIENT ALGORITHM

Algorithm 8.1: CGSolve

Input: Symmetric, PD matrix  $A \in \mathbb{R}^{n \times n}$ ,  $\mathbf{b} \in \mathbb{R}^n$ , and  $T$

Output:  $\mathbf{x}_T \in \mathbb{R}^n$

1.  $\mathbf{x}_0 \leftarrow \mathbf{0}, \mathbf{r}_0 \leftarrow \mathbf{b}, \mathbf{p}_0 \leftarrow \mathbf{r}_0$
2. for  $t = 0 \rightarrow T - 1$  do:
  1.  $\alpha_t \leftarrow \frac{\mathbf{p}_t^T \mathbf{r}_0}{\mathbf{p}_t^T A \mathbf{p}_t}$
  2.  $\mathbf{r}_t \leftarrow \mathbf{b} - A \mathbf{x}_t$
  3.  $\mathbf{x}_{t+1} \leftarrow \mathbf{x}_t + \alpha_t \mathbf{p}_t$
  4.  $\mathbf{p}_{t+1} \leftarrow A \mathbf{p}_t - \frac{\mathbf{p}_t^T A^2 \mathbf{p}_t}{\mathbf{p}_t^T A \mathbf{p}_t} \mathbf{p}_t - \frac{\mathbf{p}_t^T A^2 \mathbf{p}_{t-1}}{\mathbf{p}_{t-1}^T A \mathbf{p}_{t-1}} \mathbf{p}_{t-1}$
3. end for
4. return  $\mathbf{x}_T$

# ANALYSIS OF THE ALGORITHM

We can see in  $n$  steps,  $\mathbf{x}_n = \mathbf{x}^*$ , as  $\mathbf{x}^* \in \mathbf{x}_0 + \mathcal{K}_n$ .

What if we want an  $\varepsilon$ -approximate solution?

Since  $\mathbf{x}_t \in \mathbf{x}_0 + \mathcal{K}_t$ ,  $\mathbf{x}_t = \mathbf{x}_0 + \sum_{i=0}^{t-1} \gamma_i A^i \mathbf{r}_0$ . This motivates the definition of  $p(x) = \sum_{i=0}^{t-1} \gamma_i x^i$ . Thus,  $\mathbf{x}_t = \mathbf{x}_0 + p(A)\mathbf{r}_0$ .

Now, as  $\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0 = A(\mathbf{x}^* - \mathbf{x}_0)$ ,  $\mathbf{x}_t = \mathbf{x}_0 + p(A)A(\mathbf{x}^* - \mathbf{x}_0)$ . Therefore,  
$$\mathbf{x}_t - \mathbf{x}^* = (I - p(A)A)(\mathbf{x}_0 - \mathbf{x}^*) = q(A)(\mathbf{x}_0 - \mathbf{x}^*)$$

Where  $q(x) = 1 - xp(x)$ .

Now, there is a one-to-one correspondence between points in  $\mathbf{x}_0 + \mathcal{K}_n$  and degree  $t - 1$  polynomials, which has a one-to-one correspondence to degree  $t$  polynomials that evaluate to 1 at 0. Let this set of polynomials be  $\mathcal{Q}_t$ .

# ANALYSIS OF THE ALGORITHM

Since  $\mathbf{x}_t$  minimises  $\|\mathbf{x}_t - \mathbf{x}^*\|_A^2$  over  $\mathcal{K}_t$ , we get:

$$f(\mathbf{x}_t) - f(\mathbf{x}^*) = \frac{1}{2} \|\mathbf{x}_t - \mathbf{x}^*\|_A^2 = \min_{q \in \mathcal{Q}_t} (q(A)(\mathbf{x}_t - \mathbf{x}^*))^T A (q(A)(\mathbf{x}_t - \mathbf{x}^*))$$

**Lemma 8.2:** Let  $A$  be a symmetric matrix with eigenvalues  $\lambda_1, \dots, \lambda_n$ . Then, for a polynomial  $p(\cdot)$  and vector  $\mathbf{v}$ :

$$(p(A)\mathbf{v})^T A (p(A)\mathbf{v}) \leq \mathbf{v}^T A \mathbf{v} \cdot \max_{i \in [n]} |p(\lambda_i)|^2$$



## PROOF OF 8.2

We can write  $A = U\Gamma U^T$ , which is the eigendecomposition of  $A$ . Now  $p(A) = Up(\Gamma)U^T$ , giving us:

$$p(\Gamma)^T Ap(\Gamma) = Up(\Gamma)\Gamma p(\Gamma)U^T = U\Gamma p^2(\Gamma)U^T$$

Now, we can write any vector  $\mathbf{v} = \sum_i \zeta_i \mathbf{u}_i$ . Therefore,  $\mathbf{v}^T p(\Gamma)^T Ap(\Gamma) \mathbf{v} = \sum_i \zeta_i^2 \lambda_i p^2(\lambda_i)$ , and  $\mathbf{v}^T A \mathbf{v} = \sum_i \zeta_i^2 \lambda_i$ . The lemma follows trivially.

## USING LEMMA 8.2

Using Lemma 8.2, we have:

$$f(\mathbf{x}_t) - f(\mathbf{x}^*) \leq \min_{q \in \mathcal{Q}_t} \max_{i \in [n]} |q(\lambda_i)|^2 f(\mathbf{x}_0) - f(\mathbf{x}^*)$$

Now, as  $\lambda_1 \leq \dots \leq \lambda_n$ ,

$$f(\mathbf{x}_t) - f(\mathbf{x}^*) \leq \min_{q \in \mathcal{Q}_t} \max_{x \in [\lambda_1, \lambda_n]} |q(x)|^2 f(\mathbf{x}_0) - f(\mathbf{x}^*)$$

As  $f(\mathbf{x}^*) = -\frac{1}{2} \|\mathbf{x}^*\|_A^2$ , and  $f(\mathbf{0}) = 0$ , we have proved:

**Lemma 8.3:** Let  $A > 0$ ,  $\lambda_1, \lambda_n$  be the smallest and largest eigenvalues of  $A$ , and  $\mathcal{Q}_t$  be the set of polynomials of degree at most  $t$  which take value 1 at 0. Then:

$$\|\mathbf{x}_t - \mathbf{x}^*\|_A^2 \leq \|\mathbf{x}^*\|_A^2 \min_{q \in \mathcal{Q}_t} \max_{x \in [\lambda_1, \lambda_n]} |q(x)|^2$$

Thus, any polynomial  $q \in \mathcal{Q}_t$  can be used to give an upper bound.

# Chebyshev Polynomials

We recursively define the Chebyshev polynomials (of the first kind) as follows:

$$\begin{aligned} T_0(x) &\stackrel{\text{def}}{=} 1, T_1(x) \stackrel{\text{def}}{=} x \\ T_t(x) &\stackrel{\text{def}}{=} 2xT_{t-1}(x) - T_{t-2}(x) \end{aligned}$$

**Lemma 8.5:**  $T_t(\cos \theta) = \cos t\theta$ . Specifically,  $T_t([-1,1]) \subseteq [-1,1]$ .

- Proof: This is true for the base case. Now,  $\cos(t+1)\theta - \cos(t-1)\theta = 2\cos\theta\cos t\theta$ , and thus we are done.

Now, for  $0 < a < b$ , we define:

$$Q_{a,b,t}(x) \stackrel{\text{def}}{=} \frac{T_t\left(\frac{a+b-2x}{b-a}\right)}{T_t\left(\frac{a+b}{b-a}\right)}$$

# PROOF OF 8.1

We can see that  $Q_{a,b,t} \in Q_t$  and for  $x \in [a, b]$ , the numerator is at most 1, by lemma 8.5. Now, taking  $a = \lambda_1, b = \lambda_n$  we have,  $\forall x \in [\lambda_1, \lambda_n]$

$$Q_{\lambda_1, \lambda_n, t}(x) \leq T_t \left( \frac{\lambda_n + \lambda_1}{\lambda_n - \lambda_1} \right)^{-1} = T_t \left( \frac{\kappa(A) + 1}{\kappa(A) - 1} \right)^{-1}$$

One can show, using cosh that

$$T_t \left( \frac{\kappa(A) + 1}{\kappa(A) - 1} \right) = \frac{1}{2} \left( \left( \frac{\sqrt{\kappa(A)} + 1}{\sqrt{\kappa(A)} - 1} \right)^t + \left( \frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \right)^t \right)$$

This gives us:

$$Q_{\lambda_1, \lambda_n, t}(x) \leq 2 \left( \frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \right)^t$$

Thus, by Lemma 8.3, for any  $t > \Omega \left( \sqrt{\kappa(A)} \log \varepsilon^{-1} \right)$ , after  $t$  steps of CGSolve, we get:

$$f(\mathbf{x}_t) - f(\mathbf{x}^*) \leq \varepsilon^2 (f(\mathbf{x}_0) - f(\mathbf{x}^*)) \Rightarrow \|\mathbf{x} - A^+ \mathbf{b}\|_A \leq \varepsilon \|A^+ \mathbf{b}\|_A$$

# Chebyshev Iteration

In CGSolve, the output is not linear in the input, i.e., we want sequence of polynomials such that  $\mathbf{x}_t = p_t(A)\mathbf{b}$ .

As in the proof of 8.3, it is sufficient to define  $p_t$ s such that:

$$\max_{x \in [\lambda_1, \lambda_n]} |xp_t(x) - 1| \leq O\left(1 - \sqrt{\lambda_1/\lambda_2}\right)^t$$

Which gives us:

$$\|\mathbf{x}_t - A^+\mathbf{b}\|_A \leq O\left(1 - \sqrt{\lambda_1/\lambda_2}\right)^t \|A^+\mathbf{b}\|_A^2$$

We can set  $p_t = Q_{\lambda_1, \lambda_n, t}$  to get this bound. Further, we can see that if  $0 < \lambda_l \leq \lambda_1$  is used in place of  $\lambda_1$  and  $\lambda_u \geq \lambda_n$  is used in place of  $\lambda_n$ , we get a similar bound.

# CHEBYSHEV ITERATION

We can calculate the polynomial  $Q_{\lambda_1, \lambda_n, t}$  using recursion, using the definitions shown before.

The iteration proceeds as follows:

$$\begin{aligned}\mathbf{x}_0 &= \mathbf{0}, \mathbf{x}_1 = \mathbf{b} \\ \mathbf{x}_t &= \alpha_2 A \mathbf{x}_{t-1} + \alpha_1 \mathbf{x}_{t-2} + \alpha_0 \mathbf{b}\end{aligned}$$

The values of  $\alpha_i$  depend on  $\lambda_l$  and  $\lambda_u$ .

**Theorem 8.6**<sup>[1]</sup>: There is an algorithm, which takes a  $n \times n$  symmetric PD matrix  $A$ , a vector  $\mathbf{b}$ , numbers  $0 < \lambda_l \leq \lambda_1$  and  $\lambda_u \geq \lambda_n$ , and an error parameter  $\varepsilon > 0$  and returns  $\mathbf{x}$  such that:

- a)  $\|\mathbf{x} - A^+ \mathbf{b}\|_A \leq \varepsilon \|A^+ \mathbf{b}\|_A$
- b)  $\mathbf{x} = Z \mathbf{b}$ , where  $Z$  only depends on  $A$  and  $\varepsilon$ .
- c)  $\|Z - A^+\| \leq \varepsilon$

This algorithm runs in  $O\left(t_A \sqrt{\lambda_u / \lambda_l} \log(\varepsilon^{-1} \lambda_l^{-1})\right)$  time.

[1] BARRETT, RICHARD; MICHAEL, BERRY; TONY, CHAN; DEMMEL, JAMES; DONATO, JUNE; DONGARRA, JACK; EIJKHOUT, VICTOR; POZO, ROLDAN; ROMINE, CHARLES; VAN DER VORST, HENK (1993). "TEMPLATES FOR THE SOLUTION OF LINEAR SYSTEMS: BUILDING BLOCKS FOR ITERATIVE METHODS"