Notes I: Network Laplacian and Green's Functions

Shivam Kogar

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To study our 2D network, we flatten our indices $(x, y) \to x + ny$ as captured below in a 3×3 square lattice:

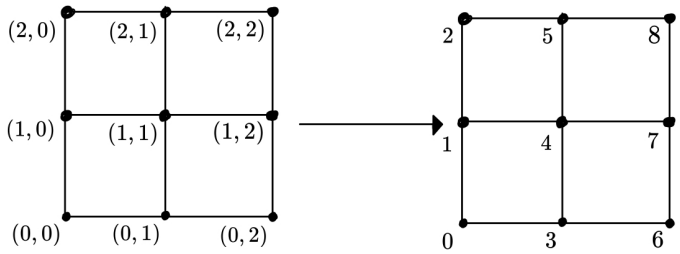

Figure 1: Flattening of Indices for 3×3 Lattice

The local connectivity and conductance properties are captured by the *Laplacian matrix* of the network, defined as follows:

$$L_{ij} = \begin{cases} \deg(i), & i = j \\ -1, & (i, j) \in E \\ 0, & \text{else} \end{cases}$$

For example, consider the following networks and their Laplacian matrices:

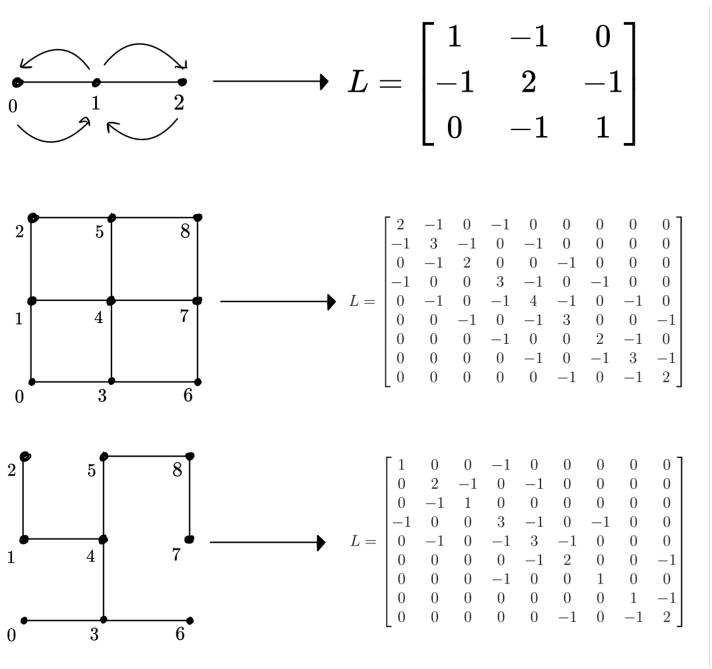

Figure 2: Laplacian matrices of 2D lattices

Our 'flattening' scheme means that our $n \times n$ lattice is encapsulated by a $n^2 \times n^2$ Laplacian matrix. Hereafter, we will use the convention $N = n^2$; the network Laplacian is thus an $N \times N$ matrix. Observe that these Laplacian matrices are *symmetric* ($L_{ij} = L_{ji}$) and *sparse* (as $N \to \infty$, most entries are zero entries). See the Appendix for a discussion of these properties. Our goal is to use this encapsulation of *local* conductance to capture *global* conductance properties between distant sites i, j. We define the *resistance distance* between i and j as the net resistance between the two sites, encompassing all paths interpolating the two sites. Since L captures local conductances, we should expect $\text{inv}(L)$ to capture local resistances. However, L is not invertible as it has a zero eigenvalue with eigenvector $\mathbf{1}^\top = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \end{bmatrix}^\top$. Therefore, we use the Moore-Penrose pseudoinverse L^+ that inverts L on $\text{null}(T)^\perp$. Ohm's law gives us the relationship $V = L^+ I$. Now suppose we inject one unit of current at site i and extract one unit of current at site j so that $I = e_i - e_j$. The voltage drop $v_i - v_j = R_{ij}(e_i - e_j) = L^+(e_i - e_j)$. L^+ now defines our system's behavior in response to a unit impulse, and therefore we denote it as a Green's function $\mathcal{G}_{ij}$ with matrix elements L_{ij} denoted G_{ij}. The resistance distance is given by

$$\begin{aligned} R_{ij} &= (e_i - e_j)^\top \mathcal{G}_{ij}(e_i - e_j) \\ &= G_{ii} + G_{jj} - G_{ij} - G_{ji} \end{aligned}$$

However, for computational reasons (see Appendix), it is often easier to work in the Laplace domain and compute

$$\mathcal{G}_{ij} = \lim_{s \to 0}(\hat{G}_{ii}(s) + \hat{G}_{jj}(s) - \hat{G}_{ij}(s) - \hat{G}_{ji}(s))$$

$$= \lim_{s \to 0} (\text{inv}(L + sI)_{ii} + \text{inv}(L + sI)_{jj} - \text{inv}(L + sI)_{ij} - \text{inv}(L + sI)_{ji})$$

which gives us our net conductance between i and j as $\Sigma_{ij} = \mathcal{G}_{ij}^{-1}$. This formulation allows us to simulate random resistor networks with large lattice size n using Monte Carlo methods.

Appendix: Sparseness and Symmetry
In this appendix, we address why we care that the Laplacian is sparse or symmetric.

Theorem. (Real Spectral Theorem).
Let $T \in \mathcal{L}(V)$, where V is a finite-dimensional inner product space over $\mathbb{F} = \mathbb{R}$ (an analogous version of the theorem exists for $\mathbb{F} = \mathbb{C}$). Then the following are equivalent:

1. T is symmetric,
2. There exists an orthonormal basis $e_1, ..., e_n$ of V, where e_i is an eigenvector of T $\forall i \in 1, ..., n$
3. $\mathcal{M}(T)$ is diagonal with respect to this orthonormal basis.

A weaker statement than the Spectral Theorem is also useful to us:

Theorem. (Eigenvalues of symmetric matrices are real).
I will include the proof since it's short and elegant. Let $(V, \langle \cdot, \cdot \rangle)$ be an inner product space over $\mathbb{R}$, and let $T \in \mathcal{L}(V)$ such that $T = T^\top$. Recall that the inner product is linear in the first slot and conjugate-linear in the second slot. If $v, w \in V$

$$\langle Tv, w \rangle = \langle v, Tw \rangle$$

So if $Tv = \lambda v$,

$$\begin{aligned} \lambda \langle v, v \rangle &= \langle \lambda v, v \rangle \\ &= \langle Tv, v \rangle \\ &= \langle v, Tv \rangle \\ &= \langle v, \lambda v \rangle \\ &= \overline{\lambda} \langle v, v \rangle \\ \Rightarrow \lambda = \overline{\lambda} &\Rightarrow \lambda \in \mathbb{R} \end{aligned}$$

We show in the next set of notes that this orthonormal basis of eigenvectors assumes a natural form involving simple trigonometric functions like sin and cos, because of the natural correspondence between our discrete model and continuous oscillatory phenomena.

Now we address sparseness. A $n \times n$ matrix is *sparse* if the number of nonzero entries is $O(n)$, i.e., roughly linear in n. In Fig. 2, we see that most of the nonzero entries lie on or near the matrix diagonal, and we can think of the length of the diagonal as roughly on the order of n. Furthermore, if we carefully inspect the second and third Laplacian in Fig. 2, the third Laplacian is sparser than the second. This makes sense; when the network has less bonds, there are more zero entries in the Laplacian matrix. Hence, our characterization of the matrix as sparse makes even more sense given that we are working with sparsely connected lattices.

Recall that our Green's function can be described as the Moore-Penrose pseudoinverse L^+ of the Laplacian matrix L. While L is sparse, L^+ is not; and

operations involving L^+ therefore require $O(n^2)$ time complexity and space complexity. Computing and using the Moore-Penrose pseudoinverse is both time-intensive and memory-intensive. In my computational experiments, I found that it was more efficient to consider the true inverse of $L + sI$ at the $s \to 0$ limit in the Laplace domain, as we can tune our choice of s to balance accurate results and tractible computation.