Physical models and Hormone Functions on Graphs

\( G = (V, E, \omega) \) connected. \( B \subset V, B \neq \emptyset \). Boundary

\[ S = V - B. \]

\( x : V \to \mathbb{R} \) is harmonic on \( S \) if

\[ \forall a \in S \quad x(a) = \frac{1}{\deg(a)} \sum_{b \in \delta(a)} \omega_{ab} x(b) \]

weighted average of its neighbors.

**Examples** Random walk. Distinguishing \( s, t, \in V \)

\( B = \{ s, t \} \). Consider a random walk that stops whenever it hits \( s \) or \( t \).

\[ x(a) = \Pr \left[ \text{walk that starts at a stops at } s \right] \]

\( x(s) = 1, \quad x(t) = 0 \), because stops there.

Claim \( x \) is harmonic on \( S \).

For \( a \notin \{ s, t \} \)

\[ \Pr x \text{ stops at } a = \sum_{b \in \delta(a)} \Pr \left[ \text{walks to } b \right] \cdot \Pr \left( b \rightarrow a \right) \]

\[ x(a) = \sum_{b \in \delta(a)} \frac{\omega_{ab}}{\deg(a)} x(b) \]
Consider path on \( \{1, \ldots, n\} \) \( t = 1, s = 0 \)

\[ x(a) = \frac{a-1}{n-1} \]

will show that solution to these equations is unique, given values at \( t = 0 \) on \( B \).

First, more intuition

View each edge as a spring. \( w_{ab} = \text{spring constant} \)
\[ \text{higher} = \text{stronger connection}. \]

Fix values on boundary \( B \), let Hooke's law determine the rest.

Hooke: force spring \((a,b)\) exerts on \( a \) is \( (x(b) - x(a))w_{ab} \)

Equilibrium: all forces zero, except on \( B \).

\[ \sum_{b \sim a} (x(b) - x(a))w_{ab} = 0 \iff \sum_{b \sim a} x(b)w_{ab} = \sum_{b \sim a} x(a) \]

\[ x(a) = \frac{1}{d(a)} \sum_{b \sim a} x(b) \]

Hence on \( S \)

Path again: \( x(1) = 1, x(n) = n \),
\[ \text{must have } x(0) = 0 \]
Uniqueness of solutions, and how to find them.

Harmonic equation is \( a \in S \Rightarrow \delta(a) x(a) = \sum_{b \in S} \omega_{ab} x(b) = 0 \)

That is \( \delta(a)^T \mathbf{L} x = 0 \), a row of \( \mathbf{L} \) for each \( a \in S \).

Now \( x(a) \) for \( b \in S \) to \( x(b) \).

\[
\delta(a) x(a) - \sum_{b \in S} \omega_{ab} x(b) = \sum_{b \in S} \omega_{ab} x(b)
\]

Becomes \( \mathbf{L}(s,s) x(s) = \mathbf{M}(s,b) x(b) \)

So, \( x(s) = \mathbf{L}(s,s)^{-1} \mathbf{M}(s,b) x(b) \)

Need to show \( \mathbf{L}(s,s) \) exists. True if \( G \) connected & \( B \neq \emptyset \).

Because \( \mathbf{L}(s,s) \) is nice.

Claim \( \mathbf{L}(s,s) = \mathbf{L} \mathbf{G}(s) + X S \)

where \( X S \) diagonal \( X S(a,a) = \sum_{b \in S} \omega_{ab} \)

Lem. Let \( H \) be connected and \( X \) be non-nes, non-zero diagonal.

Then \( LH + X \) is pos def.
Proof} need to show \( U \times 0 \times^T (L_H + X)x > 0 \)

If \( x \) is non-constant, \( x^T L_H x > 0 \).

If \( x \) is constant = \( c1 \), \( c \neq 0 \) so,
\[
 x^T X x = c^2 \sum a^T X(a,a) > 0
\]

As \( L_H \) and \( X \) psd, \( x^T (L_H + X)x = \min \{ x^T L_H x, x^T X x \} > 0 \).

Almost proves \( L(\delta, \delta) \) psd def, but \( G(\delta) \) could be disconnected.

**Lemma** \( \text{If } G \text{ connected, } B \neq \emptyset, S = V - B, \)

Then \( L(S, S) \) is psd def.

Let \( S_1, \ldots, S_k \) be connected components of \( G(S) \).

Then \( L(S, S) \) has form
\[
\begin{pmatrix}
 L(S_1, S_1) &  &  \\
 & \ddots & \\
 &  & L(S_k, S_k)
\end{pmatrix}
\]

Each \( G(S_i) \) is connected.

And, \( 3a \in S_i \text{ st. } X(a,a) > 0 \), because
\( G \to \) is an edge of \( G \) connecting some verkt of \( S_i \) to \( B \).

\[
 L(S, S) = \sum_{i=1}^k \left( L(S_i, S_i) + X(S_i, S_i) \right) \text{ each psd def.}
\]
Energy - last term to identify.

Energy in spring with constant $w$ when stretched to length $L$ is $\frac{1}{2} w L^2$

So, energy in network is

$$\frac{1}{2} \sum_{\langle a,b \rangle \in E} w_{ab}(x(a) - x(b))^2 = \frac{1}{2} x^T J x$$

Physics says energy minimized at equilibrium, so,

$$\nabla E = \frac{\partial}{\partial x(a)} \left( \frac{1}{2} x^T J x \right) = 0$$

$$\frac{\partial}{\partial x(a)} \left[ \frac{1}{2} \sum_{b,a} w_{ab}(x(a) - x(b))^2 \right] = \frac{1}{2} \sum_{b,a} w_{ab} 2(x(a) - x(b))$$

$$= \sum_{b,a} w_{ab}(x(a) - x(b)) = 0$$

$$\Leftarrow \Rightarrow \text{homogeneous at } a$$
Resistor Networks

Resistance of edge \( ab \) is \( R_{ab} = \frac{1}{W_{ab}} \)

Associate voltages with vertices, and flows on edges.

\[ U = I R \]

Ohm's law: voltage difference = current \( \times \) resistance

\( i(a,b) = \text{current flow from } a \text{ to } b \)

\( i(b,a) = -i(a,b) \)

\( U(a) - U(b) = i(a,b) R_{ab} \)

\( i(a,b) = W_{ab} (U(b) - U(a)) \quad \text{current flow high to low.} \)

\( U = \text{signed edge-vertex adjacency matrix} \text{ is } E \times V \)

\[ U((a,b), c) = \begin{cases} 1 & a=c \\ -1 & b=c \\ 0 & \text{o.w.} \end{cases} \]

are picking an arbitrary orientation for each edge.

\( W = E \times E \) diagonal edge weight matrix.

\( i = W U \)

\( i_{\text{ext}} = \text{current entering. } i_{\text{ext}}(a) = \text{current entering at } a. \)
\[ \tilde{\text{ext}}(a) = \sum_{b,a} \tilde{i}(a|b) \quad \text{no current stored at a node.} \]

\[ \tilde{\text{ext}} = U^T i \]

Check signs:

\[ U = \begin{pmatrix} c_{ia} & -1 & 0 & 1 \\ b_{ia} & 0 & 1 & -1 \end{pmatrix} \]

\[ U^T i = \begin{pmatrix} -1 & 0 \\ 0 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 2 \\ -1 \end{pmatrix} = \begin{pmatrix} -2 \\ -1 \\ 3 \end{pmatrix} \]

\[ L = U^T W U \quad \tilde{\text{ext}} = L v \]

\[ = \sum_{(a,b) \in E} \omega_{a,b} (\delta_a - \delta_b)(\delta_a - \delta_b)^T \]

\[ B = \{ a : \tilde{\text{ext}}(a) \neq 0 \} \]
For $a \in S$, $\delta(a) = 0$

\[ \Rightarrow \sum_{a} L_{a} v = 0 \]

\[ \Rightarrow \Delta(a) v(a) = \sum_{b \sim a} \omega_{ab} v(b) \]

$\nu$ is harmonic at $a$.

As $i(a(b)) = \omega_{ab} (v(b) - v(a))$

\[ \Rightarrow \sum_{b \sim a} i(a(b)) = \sum_{b \sim a} \omega_{ab} (v(b) - v(a)) = 0 \]

\[ \Rightarrow \text{zero net flow at } a. \]
Given \( \mathbf{v} \), how solve for \( \mathbf{u} \)?

\[ \mathbf{b} = \mathbf{L}\mathbf{v}, \quad \mathbf{u} = \mathbf{L}^{-1}\mathbf{b} \]

But there is no \( \mathbf{L}^{-1} \)?

There is a solution if \( \sum_{a} \mathbf{b}_{\mathbf{a}}(a) = 0 \), and \( \mathbf{G} \) connected.

Called the pseudo-inverse \( \mathbf{L}^+ \)

\[ \mathbf{L}^+\mathbf{L} = \mathbf{L}\mathbf{L}^+ = \mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}^T = \frac{1}{n}\mathbf{L}\mathbf{L}^T \]

projection onto span \( \mathbf{L} \)

\( \mathbf{L}^+ \) is identity on the span.

\[ \mathbf{L} = \sum_{i} \lambda_{i} \mathbf{\Psi}_{i}\mathbf{\Psi}_{i}^T, \quad \mathbf{L}^+ = \sum_{i=\lambda_{i} \neq 0} \frac{1}{\lambda_{i}} \mathbf{\Psi}_{i}\mathbf{\Psi}_{i}^T \]