Green matrices associated with Generalized Linear Polyominoes

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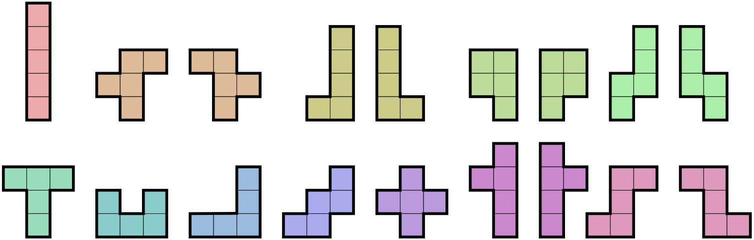
- Polyominoes
- Organic Chemistry: Kirchhoff Index
- Generalized Linear Polyominoes
- Perturbation of a path
- Combinatorial Laplacian
- Inverse M–matrix problem. Green matrices.

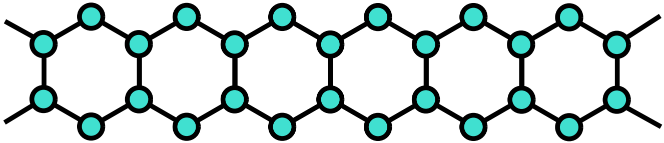
Polyominoes

Pentaminoes

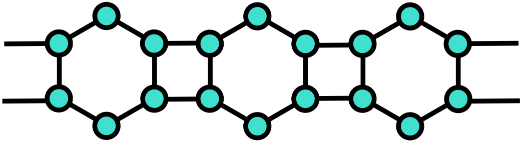


Organic Chemistry

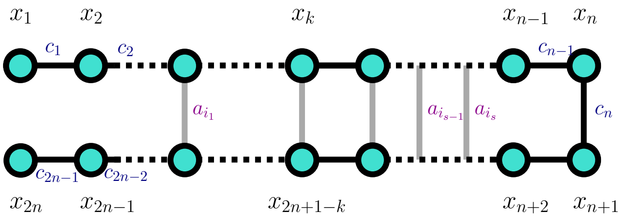
Hexagonal Chain (benzene, naphtalene)



Phenylene



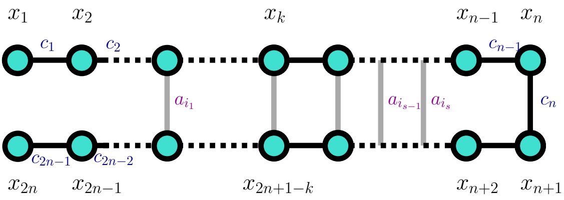
Generalized Linear Polyominoes $\mathbb{L}_n$



A path P_{2n} with vertices $V = \{x_1, \dots, x_{2n}\}$ and conductances

- $c(x_i, x_{i+1}) > 0$, for $i = 1, \dots, 2n-1$,
- $c(x_i, x_{2n+1-i}) \geq 0$ for any $i = 1, \dots, n-1$
- $c(x_i, x_j) = 0$ otherwise.

A Generalized Linear Polyomino $\Gamma \in \mathbb{L}_n$



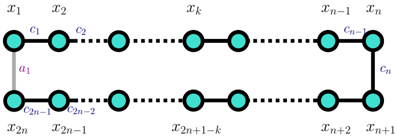
- The weight ω on the vertex set V : $\omega_j = \omega(x_j)$, $j = 1, \dots, 2n$
- $c_j = c(x_j, x_{j+1})$, $j = 1, \dots, 2n-1$
- $a_j = c(x_j, x_{2n+1-j})$, $j = 1, \dots, n-1$.

Definition

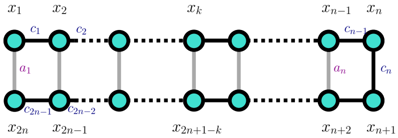
The *link number* of Γ is $s = |\{i = 1, \dots, n-1 : a_i > 0\}|$.

Some Generalized Linear Polyominoes

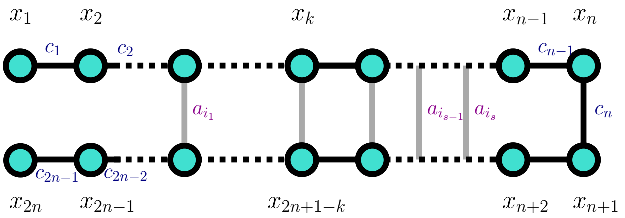
Cycle. Link number $s = 1$



Ladder. Link number $s = n - 1$



A Generalized Linear Polyominoes $\Gamma \in \mathbb{L}_n$



- We focus in obtaining the Green function of Γ as a perturbation of a path.
- Polyominoes Green function $\leftrightarrow$ Green matrices.

Type D matrices

Definition

A $s \times s$ matrix $\Sigma = (\sigma_{ij})$ is of (*weak*) *type D* if there exist real numbers $\{\sigma_i\}_{i=1}^n$, with $\sigma_n > \sigma_{n-1} > \ldots > \sigma_1$ (*no restrict.*), *such that* $\sigma_{ij} = \sigma_{\min\{i,j\}}$.

Theorem

If Σ *is a type* D *matrix,* $\sigma_1 > 0$*, then* Σ^{-1} *is a tridiagonal* *M–matrix*

Example

$$\Sigma = \begin{bmatrix} 3 & 3 & 3 & 3 \\ 3 & 5 & 5 & 5 \\ 3 & 5 & 7 & 7 \\ 3 & 5 & 7 & 9 \end{bmatrix} \qquad \Sigma^{-1} = \begin{bmatrix} \frac{5}{6} & -\frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 1 & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 1 & -\frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

Flipped (weak) type D matrices

Definition

$\Sigma = (\sigma_{ij})$ is a *flipped (weak) type D* matrix with parameters $\{\sigma_i\}_{k=1}^{s}$ if $\sigma_{ij} = \sigma_{\max\{i,j\}}$.

Theorem

$$\Sigma \text{ is invertible iff } \sigma_j \neq \sigma_{j+1},\ \gamma_j = \frac{1}{\sigma_j - \sigma_{j+1}},\ \text{and } j = 1, \dots, s.$$

$$\Sigma^{-1} = \begin{bmatrix} \gamma_1 & -\gamma_1 & 0 & \cdots & 0 & 0 \\ -\gamma_1 & \gamma_1+\gamma_2 & -\gamma_2 & \cdots & 0 & 0 \\ 0 & -\gamma_2 & \gamma_2+\gamma_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \gamma_{s-2}+\gamma_{s-1} & -\gamma_{s-1} \\ 0 & 0 & 0 & \cdots & -\gamma_{s-1} & \gamma_{s-1}+\gamma_s \end{bmatrix}$$

Green matrix

Definition

If A is a weak type D matrix, and B is a flipped weak type D matrix, then

$$G = A \circ B$$

is a *Green* matrix

Theorem

G *is a nonsingular Green matrix iff* G^{-1} *is an irreducible tridiagonal matrix.*

Combinatorial Laplacian of a network

- The *Laplacian Operator* of a network $\Gamma = (V, E, c)$

$$\mathcal{L}(u)(x) = \sum_{y \in V} c(x,y)\big(u(x) - u(y)\big)$$

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- The *Combinatorial Laplacian* of the network Γ

$$\mathsf{L} = \begin{bmatrix} k(x_1) & \cdots & -c(x_1,x_n) \\ \vdots & \ddots & \vdots \\ -c(x_n,x_1) & \cdots & k(x_n) \end{bmatrix}, \qquad k(x_i) = \sum_{j=1}^{n} c(x_i,x_j)$$

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- $\mathcal{L}$ is singular, positive semidefinite and $\mathcal{L}(v) = 0$ iff $v =$ const.

Green operator $\mathcal{G}$. Green function $G(x,y)$

- If $\langle f, 1 \rangle = 0$, then $u = \mathcal{G}(f)$ is the only solution of the Poisson's equation $\mathcal{L}(u) = f$ such that $\langle u, 1 \rangle = 0$

Green operator $\mathcal{G}$. Green function $G(x, y)$

- Given f, $u = \mathcal{G}(f)$ is the only solution of the Poisson's equation $\mathcal{L}(u) = f - \frac{1}{n}\langle f, 1\rangle$ such that $\langle u, 1\rangle = 0$

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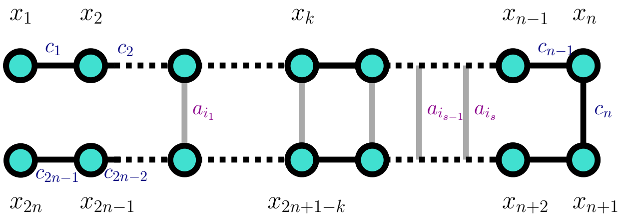
The Polyomino as a perturbation of a Path



- Polyomino: add s edges to a weighted path P_{2n}

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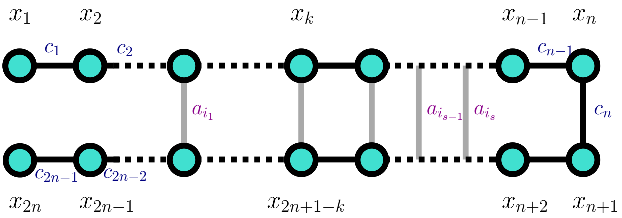

- Polyomino: add s edges to a weighted path P_{2n}
- Dipole: $\sigma_k = \rho_k \left(\dfrac{\varepsilon_{x_{2n+1-i_k}}}{\omega_{2n+1-i_k}} - \dfrac{\varepsilon_{x_{i_k}}}{\omega_{i_k}} \right), \qquad k = 1\dots, s$

with $\rho_k = \sqrt{a_{i_k}\omega_{i_k}\omega_{2n+1-i_k}}$

Effective resistance

Definition

The *effective resistance* $R(x, y)$ is the only solution of $\mathcal{L}(u) = \sigma_{xy}$

The *total resistance* at x_j is $r(x_j) = \dfrac{G(x_j, x_j)}{\omega_j^2}$

Properties

- $R(x_i, x_j) = \frac{G(x_i,x_i)}{\omega_i^2} + \frac{G(x_j,x_j)}{\omega_j^2} - 2\frac{G(x_i,x_j)}{\omega_i \omega_j}$
- R defines a distance.
- $R(x_i, x_k) + R(x_k, x_j) = R(x_i, x_j)$, when $1 \leq i \leq k \leq j \leq 2n$, and x_k disconnects Γ

Operators associated with a perturbation

$$\Lambda = \big(\langle \mathcal{G}(\sigma_j), \sigma_k \rangle\big); \ \mathsf{I} + \Lambda \text{ is non singular}$$

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Green function

- $G^{\Gamma}(x_i, x_j) = G(x_i, x_j) - \dfrac{\omega_i \omega_j}{4} \langle \big(\mathsf{I} + \Lambda\big)^{-1} (\mathsf{r} - \mathsf{v}_i), (\mathsf{r} - \mathsf{v}_j) \rangle$

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Effective resistance

- $R^\Gamma(x_i, x_j) = R(x_i, x_j) - \dfrac{1}{4} \langle \big(\mathsf{I} + \Lambda\big)^{-1} (\mathsf{v}_j - \mathsf{v}_i), (\mathsf{v}_j - \mathsf{v}_i) \rangle$

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Kirchhoff Index

- $\mathsf{k}^{\Gamma} = \mathsf{k} + \frac{1}{4}\langle \big(\mathsf{I} + \Lambda\big)^{-1}\mathsf{r}, \mathsf{r}\rangle - \frac{1}{4}\sum_{j=1}^{2n} \omega_j^2 \langle \big(\mathsf{I} + \Lambda\big)^{-1}\mathsf{v}_j, \mathsf{v}_j\rangle$

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▶ $G^{\Gamma}(x_i, x_j) = G(x_i, x_j) - \dfrac{\omega_i \omega_j}{4} \langle \big(\mathsf{I} + \Lambda\big)^{-1}(\mathsf{r} - \mathsf{v}_i), (\mathsf{r} - \mathsf{v}_j)$

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$\mathsf{r} = \big(\rho_k \big[r(x_{2n+1-i_k}) - r(x_{i_k})\big]\big)_{k=1}^{s}$, $\mathsf{v}_j = \big(\rho_k \big[R(x_{2n+1-i_k}, x_j) - R(x_{i_k}, x_j)\big]\big)_{k=1}^{s}$,

On a weighted path P_{2n}

- Green function

$$G(x_i, x_j) = \omega_i\omega_j \left[\sum_{k=1}^{\min\{i,j\}-1} \frac{W_k^2}{c_k\omega_k\omega_{k+1}} + \sum_{k=\max\{i,j\}}^{2n-1} \frac{(1-W_k)^2}{c_k\omega_k\omega_{k+1}} - \sum_{k=\min\{i,j\}}^{\max\{i,j\}-1} \frac{W_k(1-W_k)}{c_k\omega_k\omega_{k+1}} \right]$$

where $W_j = \sum_{i=1}^{j} \omega_i^2$, $j = 1, \ldots, 2n$

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- Total resistance and Effective resistance

$$r(x_i) = \sum_{k=1}^{i-1} \frac{W_k^2}{c_k \omega_k \omega_{k+1}} + \sum_{k=i}^{2n-1} \frac{(1-W_k)^2}{c_k \omega_k \omega_{k+1}}, \qquad R(x_i, x_j) = \sum_{k=\min\{i,j\}}^{\max\{i,j\}-1} \frac{1}{c_k \omega_k \omega_{k+1}}$$

Computing $(I+\Lambda)^{-1}$

- $\langle \mathcal{G}\big(\sigma_k\big), \sigma_m\rangle = \rho_k\rho_m R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}})$

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- $\mathsf{D}^{-1}(\mathsf{I}+\Lambda)\mathsf{D}^{-1} = \mathsf{D}^{-2} + \mathsf{R},$ $\mathsf{D} = (\rho_1, \dots, \rho_s)$ diagonal matrix

$$\mathsf{R} = \begin{bmatrix} R(x_{i_1}, x_{2n+1-i_1}) & R(x_{i_2}, x_{2n+1-i_2}) & \cdots & R(x_{i_s}, x_{2n+1-i_s}) \\ R(x_{i_2}, x_{2n+1-i_2}) & R(x_{i_2}, x_{2n+1-i_2}) & \cdots & R(x_{i_s}, x_{2n+1-i_s}) \\ \vdots & \vdots & \ddots & \vdots \\ R(x_{i_s}, x_{2n+1-i_s}) & R(x_{i_s}, x_{2n+1-i_s}) & \cdots & R(x_{i_s}, x_{2n+1-i_s}) \end{bmatrix}.$$

$R(x_1, x_{2n+1-1}) > \cdots > R(x_{n-1}, x_{n+1}) \Rightarrow$ R is a flypped type D-matrix

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$\Rightarrow \mathrm{R}^{-1}$ is a tridiagonal and invertible M–matrix