The Kirchhoff index of some molecular graphs

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In honor of Dragos Cvetković

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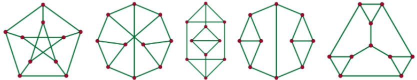
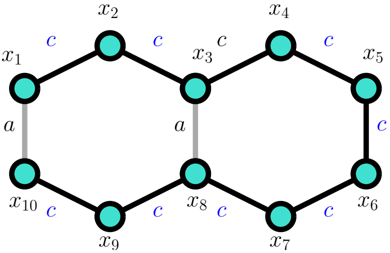
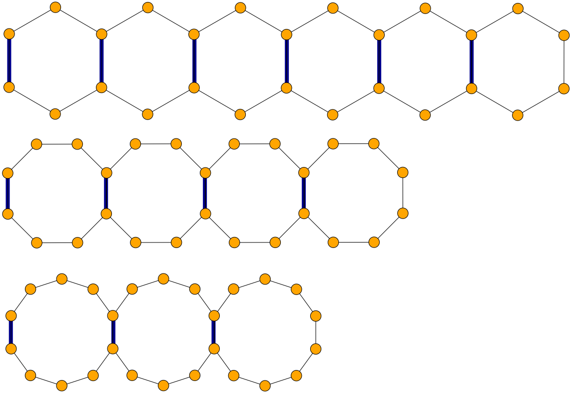


Molecular graphs



Naphtalene

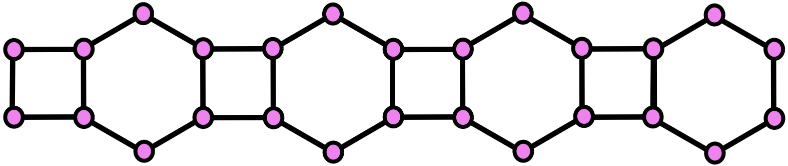
Molecular graphs



Periodic Chains

Molecular graphs

Biperiodic Chains



Linear Phenylene

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

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

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

- 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 $\langle u, 1\rangle = 0$

- For a given f, then $u = \mathcal{G}(f)$ is the only solution of the Poisson's equation

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Effective resistance

Definition

Let $\sigma_{xy} = \varepsilon_x - \varepsilon_y$ be a dipole.
The *effective resistance* $R(x,y)$ is the only solution of

$$\mathcal{L}(u) = \sigma_{xy}$$

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Properties

- $R(x_i, x_j) = G(x_i, x_i) + G(x_j, x_j) - 2G(x_i, x_j)$
- R defines a distance
- $R(x_i, x_k) + R(x_k, x_j) = R(x_i, x_j), \qquad$ if x_k disconnects x_i and x_j
- $R(x_i, x_j) \leq d_c(x_i, x_j)$

Kirchhoff index

Definition

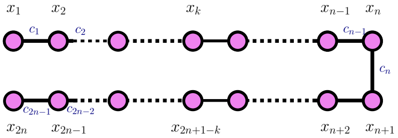
The *Kirchhoff index* of Γ is

$$\mathsf{k} = \frac{1}{2}\sum_{x,y\in V} R(x,y) = n\sum_{x\in V} G(x,x)$$

If $V = \{x_1,\dots,x_n\}$ and $0=\lambda_1<\lambda_2\le\dots\le\lambda_n$ eigenvalues of L

$$\mathsf{k} = n\sum_{i=2}^{n}\frac{1}{\lambda_i}$$

$2n$–path P



- The Green function

$$\boxed{G(x_i,x_j)=\frac{1}{4n^2}\left[\sum_{k=1}^{\min\{i,j\}-1}\frac{k^2}{c_k}+\sum_{k=\max\{i,j\}}^{2n-1}\frac{(2n-k)^2}{c_k}-\sum_{k=\min\{i,j\}}^{\max\{i,j\}-1}\frac{k(2n-k)}{c_k}\right]}$$

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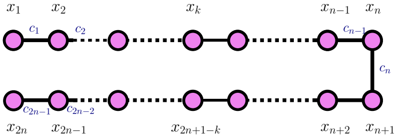

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- The Effective resistance.

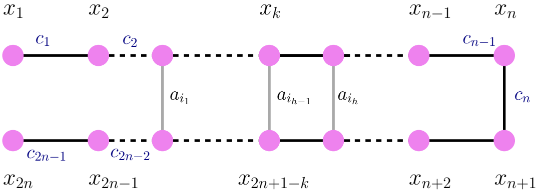
$$\boxed{R(x_i,x_j)=\sum_{k=\min\{i,j\}}^{\max\{i,j\}-1}\frac{1}{c_k}}$$

- The Kirchhoff index

$$\boxed{\mathsf{k}=\sum_{k=1}^{2n-1}\frac{k(2n-k)}{c_k}}$$

Linear Chains

The class of *linear chains* supported by the $2n$–path P consists of all connected networks whose conductance satisfies $\mathbf{c_i} = c(x_i, x_{i+1}) > 0$ for $i = 1, \dots, 2n-1$, $\mathbf{a_i} = c(x_i, x_{2n+1-i}) \geq 0$ for any $i = 1, \dots, n-1$ and $c(x_i, x_j) = 0$ otherwise.



Linear Chains

Theorem

$$G^\Gamma_{ij} = G_{ij} - \langle \mathsf{M}(\mathsf{r}-\mathsf{v}_i),(\mathsf{r}-\mathsf{v}_j)\rangle;$$

$$R^\Gamma_{ij} = R_{ij} - \langle (\mathsf{u}_i-\mathsf{u}_j),(\mathsf{v}_i-\mathsf{v}_j)\rangle;$$

$$\mathsf{k}^\Gamma = \mathsf{k} + 4n^2\langle \mathsf{M}\mathsf{r},\mathsf{r}\rangle - 2n\sum_{j=1}^{2n}\langle \mathsf{u}_j,\mathsf{v}_j\rangle.$$

where,

- $\mathbf{M} = (\mathsf{I}+\Lambda)^{-1}$ and $\Lambda_{jk} = \sqrt{a_j}\sqrt{a_k}R(x_{\max\{i_j,i_k\}}\, x_{2n+1-\max\{i_j,i_k\}})$.
- $\mathbf{v}_{jk} = \dfrac{\sqrt{a_k}}{2}\left[R_{2n+1-i_k\,j} - R_{i_k\,j}\right], \qquad k=1,\dots,s, \;\; j=1,\dots,2n$
- $\mathbf{u}_j = \mathsf{M}\mathsf{v}_j.$
- $\mathsf{r} = \dfrac{1}{2n}\displaystyle\sum_{j=1}^{2n}\mathsf{v}_j.$

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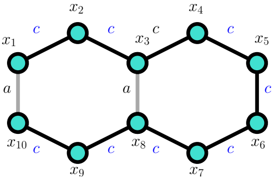
Naphtalene. $s = 2$

$$\mathbf{M} = (\mathsf{I} + \Lambda)^{-1} = \begin{bmatrix} 1 + \frac{9a}{c} & \frac{5a}{c} \\ \frac{5a}{c} & 1 + \frac{5a}{c} \end{bmatrix}^{-1}$$



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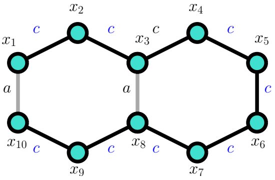

$$\mathsf{k}^{\Gamma} = \frac{33}{2c} - \frac{5a(44a + 25c)}{c(c^2 + 14ca + 20a^2)}$$

Computing $\mathsf{M} = (I + \Lambda)^{-1}, s \geq 3$

- $\Lambda = \langle \mathcal{G}\big(\sigma_k\big), \sigma_m \rangle = \sqrt{a_k}\sqrt{a_m}\, R\big(x_{\max\{i_k, i_m\}}, x_{2n+1-\max\{i_k, i_m\}}\big)$
- $\mathsf{D}^{-1}(\mathsf{I} + \Lambda)\mathsf{D}^{-1} = \mathsf{D}^{-2} + \mathsf{R}$, $\quad \mathsf{D} = (\sqrt{a_{i_1}}, \dots, \sqrt{a_{i_s}})$ diagonal matrix

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

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

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- $\mathsf{M} = \mathsf{D}(\mathsf{I} - (\mathsf{R}^{-1}+\mathsf{D}^2)^{-1}\mathsf{D}^2)\mathsf{D}^{-1} = \mathsf{I} - \mathsf{D}(\mathsf{R}^{-1}+\mathsf{D}^2)^{-1}\mathsf{D}$

Computing $(\mathsf{I}+\Lambda)^{-1}$, $s \geq 3$

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$$\begin{bmatrix} \rho_1^2+\gamma_1 & -\gamma_1 & 0 & \cdots & 0 \\ -\gamma_1 & \rho_2^2+\gamma_1+\gamma_2 & -\gamma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \rho_{s-1}^2+\gamma_{s-2}+\gamma_{s-1} & -\gamma_{s-1} \\ 0 & 0 & \cdots & -\gamma_{s-1} & \rho_s^2+\gamma_{s-1}+\gamma_s \end{bmatrix}$$

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$$\boxed{(\rho_k^2+\gamma_{k-1}+\gamma_k)z_k - \gamma_{k-1}z_{k-1} - \gamma_k z_{k+1} = 0}$$

The Difference Equation

Proposition

If $\mathsf{M} = \big(b_{ij}\big)$ *and* $\{\mathbf{u_j}\}_{j=1}^{s}, \{\mathbf{v_j}\}_{j=1}^{s}$ *are the solutions of*

$$\big(\rho_i^2 + \gamma_{i-1} + \gamma_i\big) z_i - \gamma_{i-1} z_{i-1} - \gamma_i z_{i+1} = 0, \quad i = 2, \ldots, s-1$$

- $\mathbf{u_1} = \gamma_1, \quad \mathbf{u_2} = \rho_1^2 + \gamma_1;$
- $\mathbf{v_{s-1}} = \rho_s^2 + \gamma_s + \gamma_{s-1}, \quad \mathbf{v_s} = \gamma_{s-1}.$

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- $\mathbf{v_{s-1}}=\rho_s^2+\gamma_s+\gamma_{s-1},\ \ \mathbf{v_s}=\gamma_{s-1}.$

Then, $\boxed{\mathbf{b_{ij}}=\delta_{ij}-\dfrac{\rho_i\rho_j}{\gamma_1\big((\rho_1^2+\gamma_1)v_1-\gamma_1 v_2\big)}\mathbf{u}_{\min\{\mathbf{i,j}\}}\mathbf{v}_{\max\{\mathbf{i,j}\}}}$

$\rho_j=\sqrt{a_{i_j}},\qquad i,j=1,\dots,s,.$

Periodic Linear Chains

A *periodic linear chain* with *period* p and h *holes* is a linear chain with $n = ph + 1$, and $i_\ell = p(\ell - 1) + 1, \qquad \ell = 1, \dots, h.$

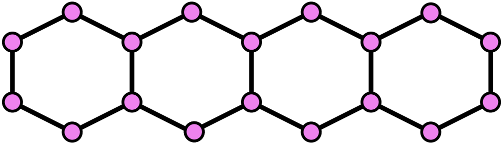

Figure: A periodic linear chain, $n = 9, p = 2$

Homogeneous: $c_i = c > 0$ and $a_{p(\ell-1)+1} = a > 0.$

Effective resistance and Kirchhoff index

$$R^{\Gamma}_{ij} = \frac{|i-j|}{c} - \frac{a}{4c^2}\Big[\langle \mathsf{u}_i, \mathsf{v}_i\rangle + \langle \mathsf{u}_j, \mathsf{v}_j\rangle \mp 2\langle \mathsf{u}_i, \mathsf{v}_j\rangle\Big],$$

$$\mathsf{k}^{\Gamma} = \frac{n(4n^2-1)}{3c} - \frac{na}{c^2}\sum_{j=1}^{n}\langle \mathsf{u}_j, \mathsf{v}_j\rangle.$$

where

- $\mathsf{v}_{i,m} = \begin{cases} 2\big(n-i\big)+1, & 1 \le m \le \ell; \\ 2\Big(n-p(m-1)\Big)-1, & \ell < m \le h, \end{cases}$
- $\mathsf{u}_i = \mathsf{M}\mathsf{v}_\mathsf{i}.$
- $\mathsf{M} = (I+\Lambda)^{-1}.$

$i = p(\ell-1)+1+k; \text{for } 1 \le \ell \le h; 0 \le k \le p-1$

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

$$\Lambda_{ij} = \frac{a}{c}\Big(2\big(n - p\max\{j-1, i-1\}\big) - 1\Big)$$

The difference equation becomes

$$2qz_i - z_{i-1} - z_{i+1} = 0, \qquad i = 2, \dots, h-1$$

$$q = 1 + c^{-1}ap$$

boundary conditions

- $\mathbf{u_1} = \frac{c}{2p}, \mathbf{u_2} = a + \frac{c}{2p}$;
- $\mathbf{v_{h-1}} = a + \frac{(4p+1)c}{2p(2p+1)}, \mathbf{v_h} = \frac{c}{2p}$

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$$\mathbf{u_j} = \frac{c}{2p} V_{j-1}(q); \qquad \mathbf{v_j} = \frac{c}{2p(2p+1)} Q_{h-j}(q).$$

The solution of the difference equation

Proposition

Let $\mathrm{M} = (b_{ij})$, *then*

$$\boxed{b_{ij} = \delta_{ij} - \frac{aV_{\min\{i,j\}-1}(q)Q_{h-\max\{i,j\}}(q)}{cT_h(q) + a(p+1)U_{h-1}(q)},} \qquad i,j = 1,\dots,h.$$

where,

$$\begin{aligned} V_k(q) &= U_k(q) - U_{k-1}(q); \\ Q_k(q) &= (2p+1)U_k(q) - U_{k-1}(q), \end{aligned} \quad k \in \mathbb{Z},$$

$T_k(q), U_k(q)$ are the k–th Chebyshev polynomial of first and second kind.

The Kirchhoff index of a periodic linear chain

Theorem

Given $p, h \in \mathbb{N}^*$ *and* $a, c > 0$,

$$\mathsf{k}^{\Gamma} = \frac{ph(ph+1)(ph+2)}{3c} + \frac{(ph+1)\Big[F_1\,T_h(q) + F_2\,U_{h-1}(q)\Big]}{3c(ap+2c)\big[c\,T_h(q) + a(p+1)\,U_{h-1}(q)\big]}$$

where

$$\begin{aligned} F_1 &= 3c(ap+2c) + hc(p+1)(ap^2+3cp-a),\\ F_2 &= 2a(a-c)p^3 + c(8a-3c)p^2 + \big(a(a-c)+9c^2\big)p\\ &+ \quad ac + hp(ap+2c)(ap^2+3cp-a). \end{aligned}$$

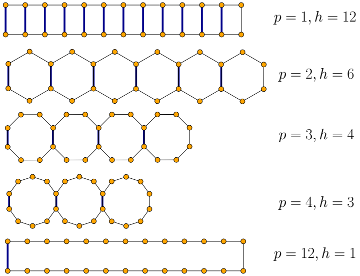
The Kirchhoff index

Corollary

Among all the periodic linear chains with a fixed number of vertices, the Kirchhoff index is minimum when $p = 1$ and maximum for $h = 1$.

Example

h holes	p period	k
12	1	829.9
6	2	907.0
4	3	970.7
3	4	1029.6
2	6	1141.4
1	12	1462.5



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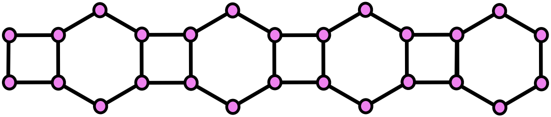

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The difference equation

- Parameters: $\rho = \sqrt{a}$, $\gamma_1 = \dfrac{c}{2p_1}$, $\gamma_2 = \dfrac{c}{2p_2}$

$\gamma_{2i+1} = \gamma_1$; $\gamma_{2i} = \gamma_2$ and $\gamma_{2r} = \dfrac{bc}{2bp_2 + c}$.

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$\gamma_{2i+1} = \gamma_1$; $\gamma_{2i} = \gamma_2$ and $\gamma_{2r} = \dfrac{bc}{2bp_2 + c}$.

- Two type of equations: $\alpha_k = z_{2k}, \beta_k = z_{2k-1}$

$$(\rho^2 + \gamma_1 + \gamma_2)\alpha_k - \gamma_1\beta_k - \gamma_2\beta_{k+1} = 0, \quad k = 1, \dots, r-1$$

$$(\rho^2 + \gamma_1 + \gamma_2)\beta_k - \gamma_2\alpha_{k-1} - \gamma_1\alpha_{k+1} = 0, \quad k = 2, \dots, r-1$$

The difference equation

- Parameters: $\rho = \sqrt{a}$, $\gamma_1 = \dfrac{c}{2p_1}$, $\gamma_2 = \dfrac{c}{2p_2}$

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Become

$$\beta_k = \frac{1}{\rho^2 + \gamma_1 + \gamma_2}\left(\gamma_2\alpha_{k-1} + \gamma_1\alpha_k\right)$$

$$\left((\rho^2 + \gamma_1 + \gamma_2)^2 - \gamma_1^1 - \gamma_2^2\right)\alpha_k - \gamma_1\gamma_2\alpha_{k-1} - \gamma_1\gamma_2\alpha_{k+1} = 0$$

$$2q\alpha_k - \alpha_{k-1} - \alpha_{k+1} = 0,$$

The difference equation

- Boundary conditions
- $\alpha_1 = \rho^2 + \gamma_1; \quad \alpha_2 = 2q(\rho^2 + \gamma_1) - \gamma_1$
- $\alpha_{r-1} = 2q\gamma_1 + \gamma_{2r} + \dfrac{1}{\gamma_2}((\rho^2 + \gamma_1)(\gamma_{2r}) - \gamma_2); \quad \alpha(r) = \gamma_1$

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$$\mathbf{u_j} = (\rho^2 + \gamma_1) U_{j-1}(q) - \gamma_1 U_{j-2}(q)$$

$$\mathbf{v_j} = \gamma_1 U_{r-j}(q) + \Big(\frac{1}{\gamma_2}(\rho^2 + \gamma_1)(\gamma_{2r} - \gamma_2) + \gamma_{2r}\Big) U_{r-j-1}(q)$$

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

$$\beta_k = \frac{1}{\rho^2 + \gamma_1 + \gamma_2}\big(\gamma_2 \alpha_{k-1} + \gamma_1 \alpha_k\big)$$

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

$$\beta_k = \frac{1}{\rho^2 + \gamma_1 + \gamma_2}\big(\gamma_2 \alpha_{k-1} + \gamma_1 \alpha_k\big)$$

$$\overline{\mathbf{u}}_{\mathbf{j}} = \gamma_1 U_{j-1}(q) - (\rho^2 + \gamma_1)\, U_{j-2}(q),$$

$$\overline{\mathbf{v}}_{\mathbf{j}} = (\rho^2 + \gamma_1 + \gamma_{2r}) U_{r-j}(q) + \frac{\gamma_1}{\gamma_2}(\gamma_{2r} - \gamma_2) U_{r-j-1}(q)$$

$\mathrm{M} = (b_{ij})$

$$\mathbf{b_{ij}} = \delta_{ij} - \frac{a}{\gamma_1\big((\rho_1^2+\gamma_1)\overline{\mathbf{v}}_{\mathbf{1}} - \gamma_1\mathbf{v_1}\big)}\,\hat{\mathbf{u}}_{\min\{\mathbf{i},\mathbf{j}\}}\hat{\mathbf{v}}_{\max\{\mathbf{i},\mathbf{j}\}}$$

$$\hat{\mathbf{u}}_{\mathbf{2i}} = u_i, \qquad \hat{\mathbf{u}}_{\mathbf{2i-1}} = \overline{u}_i,$$

$$\hat{\mathbf{v}}_{\mathbf{2i}} = v_i, \qquad \hat{\mathbf{v}}_{\mathbf{2i-1}} = \overline{v}_i.$$