Polyominos lineales generalizados, funciones de Green y matrices de Green

A. Carmona[1], A.M. Encinas[1] and M. Mitjana[2]

[1]Dept. Matemàtica Aplicada III

[2]Dept. Matemàtica Aplicada I

UNIVERSITAT POLITÈCNICA DE CATALUNYA

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Polyominos

- Presentación de los poliominos

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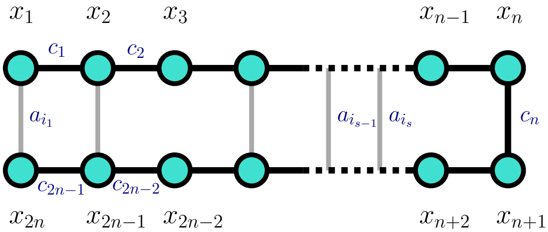
- Presentación de los poliominos
- Presentación de los poliominos lineales

Polyominos

- Presentación de los poliominos
- Presentación de los poliominos lineales
- Interés en Química Orgánica

Polyominos lineales generalizados: $\mathbb{L}_n$

- $V = \{x_1, \dots, x_{2n}\}$



- $c_i = c(x_i, x_{i+1}) > 0,\ i = 1, \dots, 2n-1$

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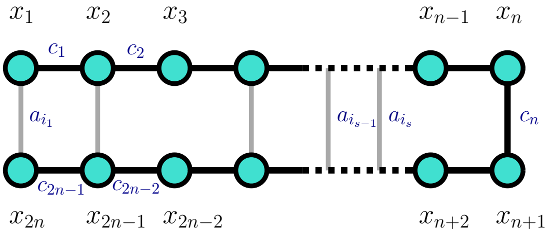

- $c_i = c(x_i, x_{i+1}) > 0,\ i = 1, \ldots, 2n-1$
- $a_i = c(x_i, x_{2n+1-i}) \geq 0,\ i = 1, \ldots, n-1$

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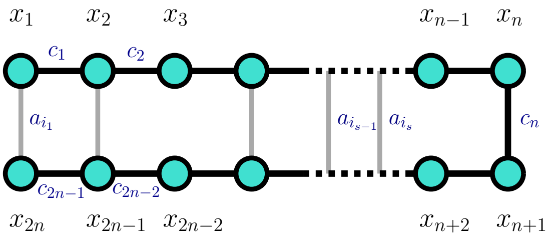

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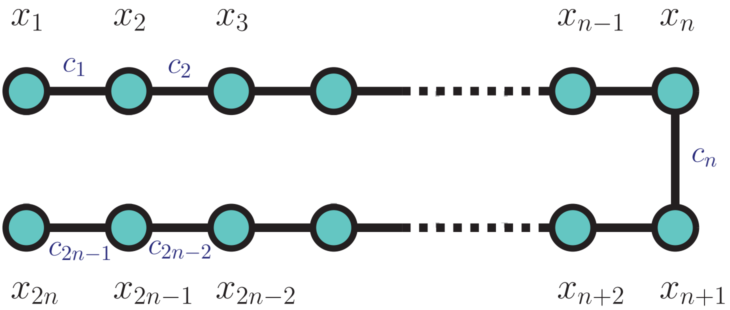
- $a_i = c(x_i, x_{2n+1-i}) \geq 0,\ i = 1, \ldots, n-1$
- Encadenamiento de $\mathcal{P} \in \mathbb{L}_n$: $s = \#\{i : a_i > 0\}$

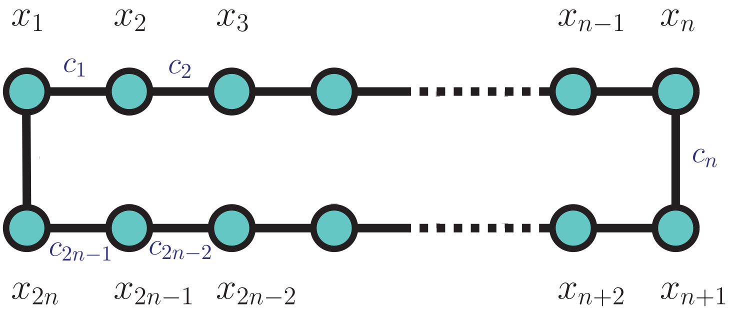
Polyominos lineales generalizados: $\mathbb{L}_n$

- Camino



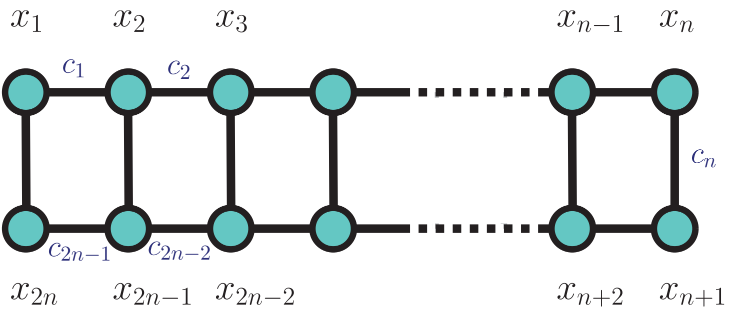
Polyominos lineales generalizados: $\mathbb{L}_n$

- Ciclo



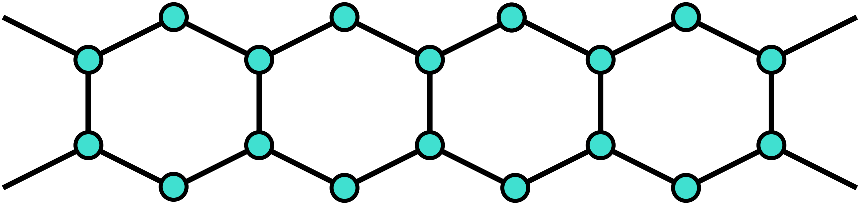
Polyominos lineales generalizados: $\mathbb{L}_n$

- Cadena Lineal



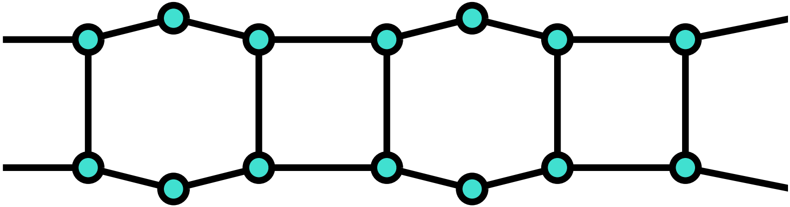
Polyominos lineales generalizados: $\mathbb{L}_n$

- Cadena Hexagonal

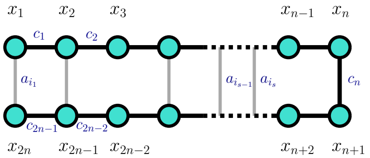


Polyominos lineales generalizados: $\mathbb{L}_n$

- Phenyleno

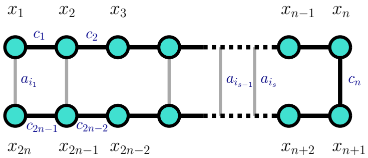


Laplaciano combinatorio



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

Laplaciano combinatorio



Laplaciano Combinatorio: L

- $$\mathsf{L} = \begin{bmatrix} c_1 + a_{i_1} & -c_1 & & & -a_{i_1} \\ -c_1 & c_1 + c_2 + a_{i_2} & -c_2 & -a_{i_2} & \\ & \ddots & \ddots & \ddots & \\ & -a_{i_2} & -c_{2n-2} & c_{2n-2} + c_{2n-1} + a_{i_2} & -c_{2n-1} \\ -a_{i_1} & & & -c_{2n-1} & c_{2n-1} + a_{i_1} \end{bmatrix}$$

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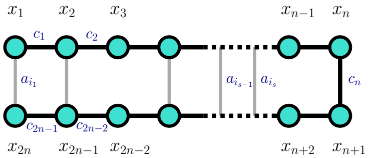

- $\boxed{\mathcal{L} \text{ es semidefinido positivo, singular y } \mathcal{L}(v) = 0 \text{ iff } v = \text{cte}}$

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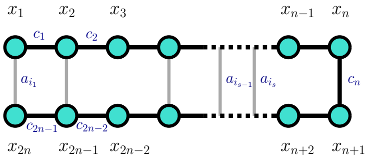

- $\mathcal{L}$ es semidefinido positivo, singular y $\mathcal{L}(v) = 0$ iff $v = $ cte
- *Operador y función de Green*: $\mathcal{G}$ y $G(x, y)$
- Si $\langle f, 1\rangle = 0$, entonces $u = \mathcal{G}(f)$ es la única solución de la ecuación de Poisson $\mathcal{L}(u) = f$ tal que $\langle u, 1\rangle = 0$

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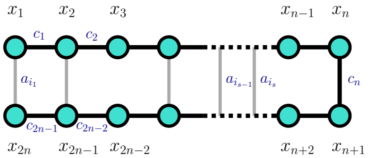

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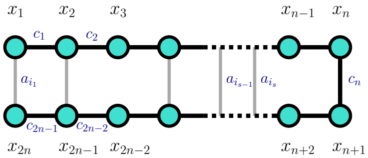
- Operador y función de Green: $\mathcal{G}$ y $G(x, y)$
- Dada f, entonces $u = \mathcal{G}(f)$ es la única solución de la ecuación de Poisson $\mathcal{L}(u) = f - \frac{1}{n}\langle f, 1\rangle$ tal que $\langle u, 1\rangle = 0$

Laplaciano combinatorio



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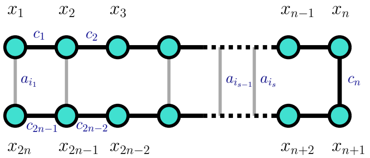

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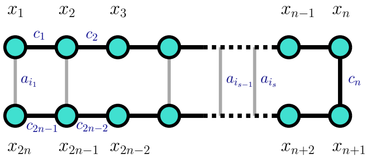
Perturbación con dipolos



- Obtenemos el *Polyomino*, **añadiendo** s **ramas**

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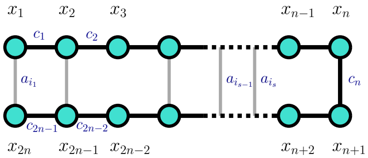

- Obtenemos el *Polyomino*, **añadiendo s ramas**
- Consideremos el *Dipolo*, $\sigma_j = \sqrt{a_{i_j}}\left(\varepsilon_{x_{i_j}} - \varepsilon_{x_{n+1-i_j}}\right)$

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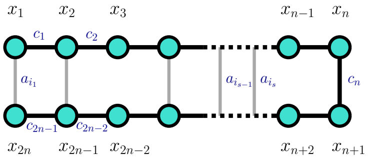

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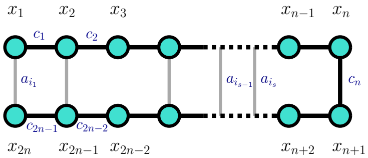
- $$\boxed{\mathcal{L} = \mathcal{L}^{\text{path}} + \sum_{j=1}^{s} \mathcal{P}_{\sigma_j}, \text{ donde } \mathcal{P}_{\sigma_j}(u) = \sigma_j \langle \sigma_j, u \rangle}$$

Perturbación con dipolos



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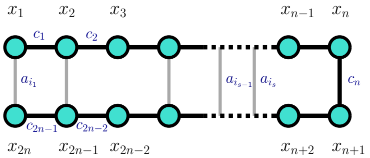

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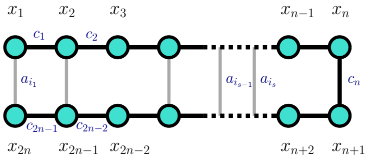

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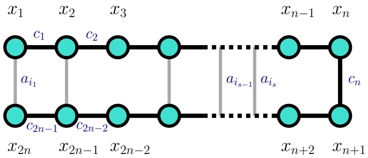
- $$\boxed{\mathcal{G} = \mathcal{G}^{\text{path}} - \sum_{k,m=1}^{s} b_{km}\mathcal{P}_{\mathcal{G}^{\text{path}}(\sigma_m)\mathcal{G}^{\text{path}}(\sigma_k)},\ \mathcal{P}_{\sigma\tau}(u) = \sigma\langle \tau, u\rangle}$$

Perturbación con dipolos



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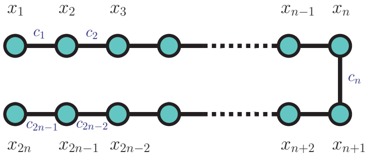
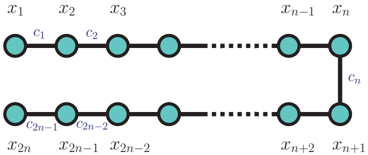
- $$\boxed{G(x,y) = G^{\text{path}}(x,y) - \sum_{k,m=1}^{s} b_{km} G^{\text{path}}(\sigma_m)(x) G^{\text{path}}(\sigma_k)(y)}$$

Función de Green y resistencia efectiva



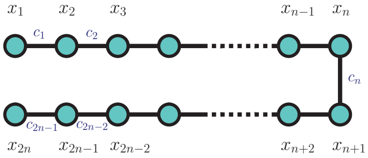
- La función de Green del camino sobre $2n$ vértices es
- $$G^{\text{path}}(x_i,x_j)=\frac{1}{4n^2}\left[\sum_{\ell=1}^{\min\{i,j\}-1}\frac{\ell^2}{c_\ell}+\sum_{\ell=\max\{i,j\}}^{2n-1}\frac{(2n-\ell)}{c_\ell}-\sum_{\ell=\min\{i,j\}}^{\max\{i,j\}-1}\frac{k(2n-\ell)}{c_\ell}\right]$$

Función de Green y resistencia efectiva



- La *Resistencia Efectiva* es $$\boxed{R(x_i,x_j) = 2n \sum_{\ell=\min\{i,j\}}^{\max\{i,j\}-1} \frac{1}{c_\ell}}$$

Función de Green y resistencia efectiva



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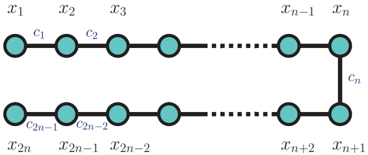
- $$\boxed{\mathcal{G}^{\text{path}}(\sigma_k)(x_j) = 2n\sqrt{a_{i_k}}\left[\sum_{\ell=\max\{j,i_k\}}^{2n-i_k} \frac{1}{c_\ell} - \sum_{\ell=i_k}^{2n-i_k} \frac{1}{c_\ell}\right]}$$

Función de Green y resistencia efectiva



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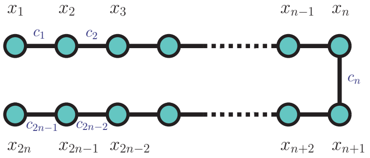
- $\boxed{\langle \mathcal{G}^{\text{path}}(\sigma_k), \sigma_m \rangle = \sqrt{a_{i_k} a_{i_m}}\, R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}})}$

Función de Green y resistencia efectiva



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- **OBJETIVO:** Determinar $\left(\mathsf{I} + \Lambda\right)^{-1}$, $\Lambda = \left(\langle \mathcal{G}^{\text{path}}(\sigma_m), \sigma_k \rangle\right)$

Inversión de la matriz $\mathsf{I} + \Lambda$

- $\Lambda = \left(\sqrt{a_{i_k} a_{i_m}}\, R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}})\right)$

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- $\mathsf{I} + \Lambda = \mathsf{D}^{\frac{1}{2}} \left[\mathsf{D}^{-1} + \mathsf{A}\right] \mathsf{D}^{\frac{1}{2}}$, donde

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

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- Si $\alpha_j = R(x_{i_j}, x_{2n+1-i_j}) = 2n \sum_{\ell=i_j}^{2n-i_j} \frac{1}{c_\ell}$

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- Si $\alpha_j = R(x_{i_j}, x_{2n+1-i_j}) = 2n \sum_{\ell=i_j}^{2n-i_j} \frac{1}{c_\ell} \Longrightarrow \mathsf{A} = \left(\alpha_{\max\{k,m\}}\right)$

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- $$\boxed{\left(\mathsf{I}+\Lambda\right)^{-1} = \mathsf{I} - \mathsf{D}^{\frac{1}{2}}(\mathsf{A}^{-1}+\mathsf{D})^{-1}\mathsf{D}^{\frac{1}{2}}}$$

Propiedades de $\mathsf{A} = \left(R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}})\right)$

- *Parámetros* $\alpha_1, \dots, \alpha_s$

Propiedades de $\mathsf{A} = \Big(R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}})\Big)$

- *Parámetros* $\alpha_1, \dots, \alpha_s$
- *Matriz de tipo D débil*: $\Sigma = \big(\alpha_{\min\{k,m\}}\big)$

Propiedades de $\mathsf{A} = \Big(R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}})\Big)$

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- *Matriz de Green*: $\mathsf{G} = \big(\alpha_{\min\{k,m\}}\big) \circ \big(\beta_{\max\{k,m\}}\big)$

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- $$\boxed{g_{km} = \alpha_{\min\{k,m\}}\beta_{\max\{k,m\}} = \begin{cases} \alpha_k\beta_m, & \text{si } k \leq m, \\ \alpha_m\beta_k, & \text{si } k \geq m \end{cases}}$$

Propiedades de $\mathsf{A} = \left(R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}})\right)$

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- G es una matriz de Green no singular sii G^{-1} es una matriz triangular irreducible

Propiedades de $\mathsf{A} = \Big(R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}})\Big)$

- *Parámetros:* $\alpha_1, \dots, \alpha_s$ ($\alpha_{s+1} = 0$)
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Propiedades de A $= \Big(R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}}) \Big)$

- *Parámetros:* $\alpha_1, \dots, \alpha_s$ ($\alpha_{s+1} = 0$)
- *Matriz de tipo D inverso débil*: $\Sigma = \big(\alpha_{\max\{k,m\}}\big)$
- *Matriz de tipo D inverso*: Si además $\alpha_1 > \cdots > \alpha_s$
- Σ es invertible sii $\alpha_i \neq \alpha_{i+1}$. Además, si $\gamma_j = (\sigma_j - \sigma_{j+1})^{-1}$

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

Propiedades de $\mathsf{A} = \Big(R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}}) \Big)$

- *Parámetros:* $\alpha_j = R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}})$
- $\alpha_1 > \cdots > \alpha_s > 0$

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- $$\mathsf{A}^{-1} = \begin{bmatrix} \gamma_1 & -\gamma_1 & 0 & \cdots & 0 \\ -\gamma_1 & \gamma_1+\gamma_2 & -\gamma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \gamma_{s-2}+\gamma_{s-1} & -\gamma_{s-1} \\ 0 & 0 & \cdots & -\gamma_{s-1} & \gamma_{s-1}+\gamma_s \end{bmatrix}$$
  $$\gamma_s = R(x_{i_s}, x_{2n+1-i_s})^{-1},$$
  $$\gamma_k = \left[R(x_{i_k}, x_{i_{k+1}}) + R(x_{2n+1-i_{k+1}}, x_{2n+1-i_k})\right]^{-1}$$

Cálculo de $(b_{km}) = (\mathsf{I} + \Lambda)^{-1}$, $s \geq 3$

- $\big(\mathsf{I} + \Lambda\big)^{-1} = \mathsf{I} - \mathsf{D}^{\frac{1}{2}}(\mathsf{A}^{-1} + \mathsf{D})^{-1}\mathsf{D}^{\frac{1}{2}}$

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- $(a_{i_k}+\gamma_{k-1}+\gamma_k)z_k - \gamma_{k-1}z_{k-1} - \gamma_k z_{k+1} = 0$

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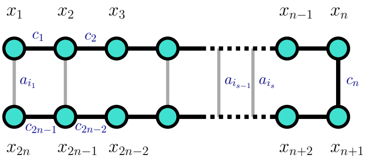
- $(a_{i_k}+\gamma_{k-1}+\gamma_k)z_k - \gamma_{k-1}z_{k-1} - \gamma_k z_{k+1} = 0,\ 2 \leq k \leq s-1$
- Si $\{u_k\}_{k=1}^{s}$, $\{v_k\}_{k=1}^{s}$ son las soluciones que satisfacen

  $u_1 = \gamma_1,\ u_2 = a_{i_1}+\gamma_1,\ \ v_{s-1} = a_{i_s}+\gamma_{s-1}+\gamma_s,\ v_s = \gamma_{s-1},$

  $$b_{km} = \delta_{km} - \frac{\sqrt{a_{i_k}a_{i_m}}}{\gamma_1\big((a_{i_1}+\gamma_1)v_1 - \gamma_1 v_2\big)}u_{\min\{k,m\}}v_{\max\{k,m\}}$$

Cálculo de $(b_{km}) = (\mathsf{I}+\Lambda)^{-1}$, $s \geq 3$



- $\mathcal{P} \in \mathbb{L}_n$ es *autocomplementario* si existen $a, r_1, r_2 > 0$ con

$$a_{i_j} = a,\ R(x_{i_j}, x_{i_{j+1}}) = r_1 \text{ y } R(x_{2n+1-i_{j+1}}, x_{2n+1-i_j}) = r_2$$

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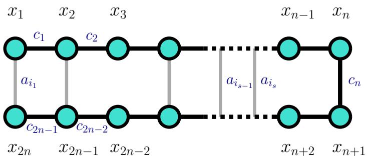

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- $\left(a + 2(r_1 + r_2)^{-1}\right) z_k - (r_1 + r_2)^{-1} z_{k-1} - (r_1 + r_2)^{-1} z_{k+1} = 0$

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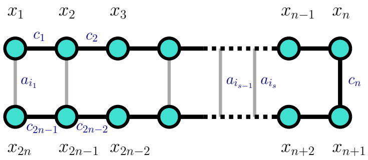

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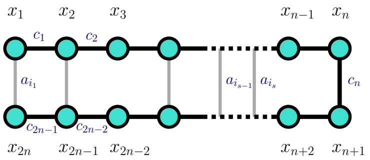
- $\big(a + 2(r_1+r_2)^{-1}\big) z_k - (r_1+r_2)^{-1} z_{k-1} - (r_1+r_2)^{-1} z_{k+1} = 0$
- $2\Big(\dfrac{a(r_1+r_2)}{2} + 1\Big) z_k - z_{k-1} - z_{k+1} = 0$

Cálculo de $(b_{km}) = (\mathsf{I} + \Lambda)^{-1}$, $s \geq 3$



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- $$z_{k+1} = 2qz_k + z_{k-1}, \text{ con } q = 1 + \frac{ar}{2} \text{ y } r = r_1 + r_2$$

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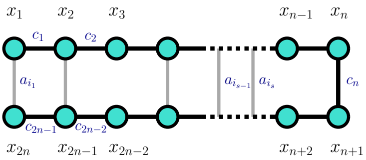

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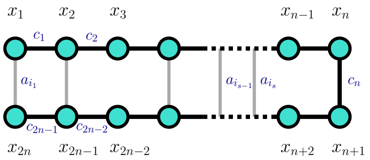
- $$u_i = \frac{1}{r} V_{i-1}(q), \quad v_i = \frac{\left[R(x_{i_s}, x_{2n+1-i_s}) V_{s-i}(q) + rU_{s-1-i}(q)\right]}{rR(x_{i_s}, x_{2n+1-i_s})}$$

Cálculo de $(b_{km}) = (\mathsf{I}+\Lambda)^{-1}$, $s \geq 3$



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- $$b_{km} = \delta_{km} - \frac{aV_{\min\{k,m\}-1}(q)}{R(x_{i_s}, x_{2n+1-i_s})\big[aU_{s-1}(q) + V_{s-1}(q)\big]} \times \Big[R(x_{i_s}, x_{2n+1-i_s})V_{s-\max\{k,m\}}(q) + rU_{s-1-\max\{k,m\}}(q)\Big]$$