Two-Side Boundary Value Problems in Distance-Regular Graphs

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Outline

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  - Networks and matrices
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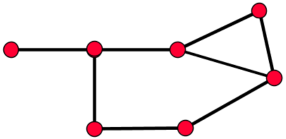
Networks

- A network $\Gamma = (V, E, c)$ is composed by
  - V is a set of elements called vertices
  - E is a set of elements called edges
  - $c : V \times V \longrightarrow [0, \infty)$ is an application named conductance associated to the edges
- Two vertices i, j are adjacent, $i \sim j$ iff $c(i,j) \neq 0$
- The degree of a vertex is $\omega_i = \sum_{j \in V} c(i,j)$



Matrices associated with networks

Definition

The Laplacian matrix of the network Γ is defined as

$$(\mathcal{L})_{ij} = \begin{cases} \omega_i & if \quad i = j, \\ -c(i,j) & if \quad i \neq j, \\ 0 & otherwise. \end{cases}$$

Definition

A Schrödinger matrix $\mathcal{L}_Q$ on Γ with potential Q is defined as a generalization of the weighted Laplacian matrix as

$$\mathcal{L}_Q = \mathcal{L} + Q$$

where $Q = diag[q_0, \dots, q_d]$ is the potential matrix.

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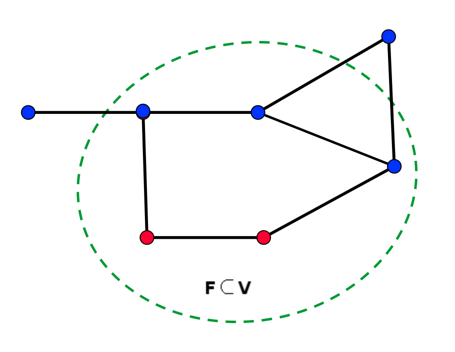
Schrödinger equations

Consider a subset of vertices $F \subset \Gamma(V)$



The Schrödinger equation on F with data $\vec{f}$ is the equation

$$(\mathcal{L}_Q \vec{u}^{\,T})_i = \vec{f}_i^{\,T}, \; i \in F, \; \vec{u}, \vec{f} \in \mathbb{R}^{n+1}$$

The homogenoeus Schrödinger equation on F is the equation

$$(\mathcal{L}_Q \vec{u}^{\,T})_i = 0, \; i \in F, \; \vec{u} \in \mathbb{R}^{n+1}$$

Green's matrix of the Schrödinger equation

✓ Any solution u of the homogeneous Schrödinger equation (HSE) satisfies the recurrence relation:

$$xu_i(x) = a_i u_i(x) + b_{i-1} u_{i-1}(x) + c_{i+1} u_{i+1}(x), \quad 0 \le i \le d,$$

✓ The Wronskian of u and $v \in \mathbb{R}^{n+1}$ is

$$w[u,v](k) = \begin{vmatrix} u_k & v_k \\ u_{k+1} & v_{k+1} \end{vmatrix}, \quad k = 0, \dots, n,$$

$$w[u,v](n+1) = w[u,v](n)$$

✓ Two solutions u, v of the homogeneous Schrödinger equation are lin. independent iff $w[u,v](k) \neq 0$ for all $0 \le k \le n$.

Green's matrix of the Schrödinger equation

Definition

The Green's matrix of the Schrödinger equation, $\mathcal{G}_Q$, is either the inverse matrix of $\mathcal{L}_Q$ iff $\mathcal{L}_Q$ is invertible, or the Moore-Penrose inverse of $\mathcal{L}_Q$.

- For any $\vec{f} \in \mathbb{R}^{n+1}$ the unique solution of the Schrödinger equation with data $\vec{f}$ is

$$\boxed{\vec{u} = \mathcal{G}_Q \vec{f}.}$$

Application of Schrödinger equations

We are interested in solving

- The Schrödinger equation on F with data $f \in \mathbb{R}^{d+1}$:

$$\boxed{\mathcal{L}_Q u = f}$$

- The Homogeneous Schrödinger equation on F:

$$\boxed{\mathcal{L}_Q u = 0}$$

With certain linear conditions on the boundary

$$\mathcal{B}u = c_0 u_0 + c_1 u_1 + \cdots + c_d u_d = g \quad u \in \mathbb{R}^{d+1}.$$

Boundary value problems

Definition

A boundary value problem on F consists in finding $u \in \mathbb{R}^{d+1}$ such that

$$\mathcal{L}_Q u = f \text{ on } F, \quad \mathcal{B}_1 u = g_1, \quad \mathcal{B}_2 u = g_2,$$

for a given $f \in \mathbb{R}^{d+1}$ and $g_1, g_2 \in \mathbb{R}$.

Examples of application:

- $\mathcal{L} f = c_i - c_e$ on F (Chip-firing games)
- $\mathcal{L} H_k = \delta_j$ on $V - \{k\}$ (Hitting-time)

Schrödinger equations

Questions:

- Which kind of Schrödinger equations can we solve?
- Which kind of boundary value problems can we solve?
- In which kind of networks can we solve them?

Schrödinger matrices on Paths

- Let P_{n+2} be a finite path on $n+2$ vertices, $V(P_{n+2}) = \overline{F}$

Definition

The Schrödinger matrix on P_{n+2} associated to $\{p_i\}_{i=0}^{n+1}$ is

$$\mathcal{L}_Q(x) = \begin{pmatrix} \frac{x-a_0}{k_0} & -\frac{b_0}{k_1} & 0 & \dots & \dots & 0 \\ -\frac{b_0}{k_1} & \frac{x-a_1}{k_1} & -\frac{b_1}{k_2} & 0 & \dots & 0 \\ 0 & -\frac{b_1}{k_2} & \frac{x-a_2}{k_2} & -\frac{b_2}{k_3} & \dots & 0 \\ \vdots & \vdots & & \ddots & & \vdots \\ 0 & 0 & \dots & & -\frac{b_n}{k_n} & \frac{x-a_{n+1}}{k_n} \end{pmatrix}$$

where $q_i(x) = \frac{x-a_i-b_{i-1}}{k_i} - \frac{b_i}{k_{i+1}}$ is the potential for any $0 \le i \le n+1$.

Distance-regular graphs

- For two vertices $u, v \in \Gamma$, the distance from u to v, $d(u,v)$, is the least number of edges in a path from u to v.
- The maximum distance between two vertices of Γ is the diameter d of Γ.
- Let

$$(A_k)_{i,j} = \begin{cases} 1 & \textit{if} \quad d(i,j) = k, \\ 0 & \quad\quad \textit{otherwise}. \end{cases}$$

  be the distance matrices of Γ, for $0 \le k \le d$. Observe that $A_1 = A$ is the adjacency matrix of Γ.
- A graph $G = (V, E)$ is distance-regular iff there exists $a_i, b_i, c_i \in \mathbb{R}$ such that

$$AA_i = a_i A_i + b_{i-1} A_{i-1} + c_{i+1} A_{i+1}, \quad 0 \le i \le d,$$

  where $b_{-1} = c_{d+1} = 0$.

Distance-regular graphs

- The distance-matrices of a distance-regular are a polynomial of degree i in A, that is, $A_i = p_i(A), \quad 0 \le i \le d$,. These polynomials are called the distance-polynomials, and they are a family of orthogonal polynomials satisfying the recurrence

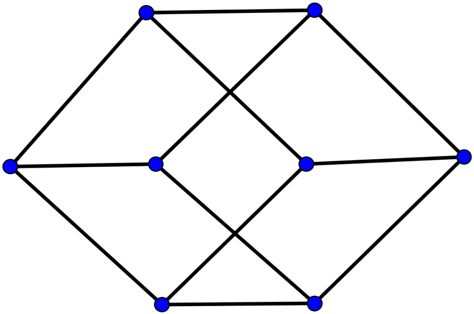
$$xp_i(x) = a_i p_i(x) + b_{i-1} p_{i-1}(x) + c_{i+1} p_{i+1}(x), \quad 0 \le i \le d,$$

- The associated matrix is a Jacobi matrix

$$J_d = \begin{pmatrix} a_0 & c_1 & 0 & \dots & \dots & 0 \\ b_0 & a_1 & c_2 & 0 & \dots & 0 \\ 0 & b_1 & a_2 & c_3 & \dots & 0 \\ \vdots & \vdots & & \ddots & & \vdots \\ 0 & 0 & \dots & & & a_d \end{pmatrix}$$

Distance-regular graphs

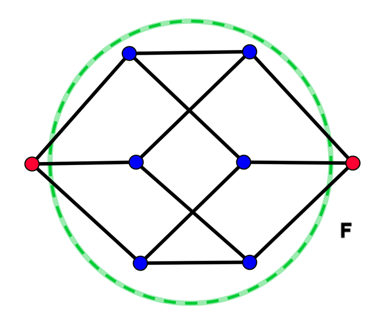
Example: the cube

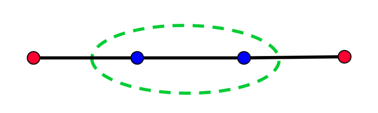


$$J_2 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 3 & 0 & 2 & 0 \\ 0 & 2 & 0 & 3 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Distance-regular graphs

A boundary value problem on F in Γ is equivalent to a boundary value problem in a weighted path P_{n+2}





$$J_2 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 3 & 0 & 2 & 0 \\ 0 & 2 & 0 & 3 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Solving Schrödinger Equations

Lemma 1

For any $k \in V$, the vectors $\vec{p} = (p_0(x), \dots, p_d(x))$, $\vec{r} = (r_0(x), \dots, r_d(x)) \in \mathbb{R}^{d+1}$ are a basis of the solution space of the HSE on F, as the wronskian is $w[\vec{p}, \vec{r}](n) = x/2$ for any $0 \leq n \leq d-1$.

The Green matrix of the HSE is:

$$(\mathcal{G}_H)_{ij} = \frac{2}{x}[p_i(x)r_j(x) - p_j(x)r_i(x)], \quad 0 \leq i,j \leq d, \quad x \in \mathbb{R}. \quad (1)$$

Thus, the general solution $\vec{y}$ of the Schrödinger equation on F with data $\vec{f} \in \mathbb{R}^{d+1}$ is given for any $0 \leq i \leq d$ by

$$(\vec{y})_i = \alpha p_i(x) + \beta r_i(x) + \sum_{k=1}^{i} (\mathcal{G}_H)_{ij} f_j, \quad \alpha, \beta \in \mathbb{R}.$$

Two-side boundary value problems on a Path

✓ A two-side boundary condition on a P_{n+2} is

$$\mathcal{B}u = au_0 + bu_1 + cu_n + du_{n+1}, \text{for any } u \in \mathbb{R}^{n+2}.$$

✓ A two-side boundary value problem on F consists in finding $u \in \mathbb{R}^{n+2}$ such that

$$\boxed{\mathcal{L}_Q u = f \text{ on } F, \quad \mathcal{B}_1 u = g_1, \quad \mathcal{B}_2 u = g_2,}$$

for a given $f \in \mathbb{R}^{n+2}$ and $g_1, g_2 \in \mathbb{R}$.

✓ The problem is semi-homogeneous when $g_1 = g_2 = 0$, and homogeneous if besides $f = 0$ and $g_1 = g_2 = 0$.

Two-side boundary value problems

- The boundary conditions in a matricial form:

$$\begin{bmatrix} \mathcal{B}_1 u \\ \mathcal{B}_2 u \end{bmatrix} = \begin{bmatrix} c_{1,0} & c_{1,1} \\ c_{2,0} & c_{2,1} \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \end{bmatrix} + \begin{bmatrix} c_{1,n} & c_{1,n+1} \\ c_{2,n} & c_{2,n+1} \end{bmatrix} \begin{bmatrix} u_n \\ u_{n+1} \end{bmatrix}$$

- Let μ_{ij} be the determinant of

$$\mu_{ij} = \begin{vmatrix} c_{1i} & c_{1j} \\ c_{2i} & c_{2j} \end{vmatrix}, \quad j \in B = \{0, 1, n, n+1\}$$

- The BVP is regular iff it has a unique solution iff the boundary polynomial

$$P_c(x) = \sum_{i \in B} \sum_{j \in B} d_{ij} u_i v_j \neq 0,$$

Two-side boundary value problems

By the classical theory of differential equations

✓ Any general BVP can be solved by solving the semihomogeneous BVP associated.

Definition

The Green's matrix of the boundary value problem, G_Q, is the matrix such that

$$\mathcal{L}_Q G_Q = I, \quad \mathcal{B}_1 G_Q = 0, \quad \mathcal{B}_2 G_Q = 0$$

- For any $f \in \mathbb{R}^{n+2}$ the unique solution of the boundary value problem with data f is

$$u = G_Q f.$$

The Green's function of the two-side BVP

Theorem

The BVP is regular iff

$$P_{\mathcal{B}}(x) = \frac{x}{2} \sum_{\substack{i<j \\ i,j\in\{1,\dots,d-1\}}} \mu_{ij}(\mathcal{G}_H(x))_{ij} \neq 0$$

In this case, the Green matrix of the BVP problem, for any $s \in F$, $k \in V$, is the matrix whose ks-element, $(\mathcal{G}_Q(x))_{ks}$, is given by

$$\frac{x}{2P_{\mathcal{B}}(x)} \left[\frac{k_{d-1}}{c_d} \mu_{d-1d}(\mathcal{G}_H(x))_{sk} + \sum_{i=0}^{1} (\mathcal{G}_H(x))_{ik} \left(\sum_{j=d-1}^{d} \mu_{ij}(\mathcal{G}_H(x))_{sj} \right) \right] + \begin{cases} 0 & k \leq s, \\ (\mathcal{G}_H(x))_{ks} & k \geq s. \end{cases}$$

Two-side boundary value problems

Typical two-side boundary value problems:

- Unilateral BVP
  - Initial value problem: $c_{2,j} = 0$ for $j \in B = \{0, 1, n, n+1\}$
  - Final value problem $c_{1,i} = 0$ for $i \in B = \{0, 1, n, n+1\}$
- Sturm-Liouville BVP

$$\begin{aligned} &\mathcal{L}_Q u = f \ \text{ on } F, \\ &c_{1,0} u_0 + c_{1,1} u_1 = g_1, \\ &c_{2,n} u_n + c_{2,n+1} u_{n+1} = g_2. \end{aligned}$$

  - outer-Dirichlet Problem $c_{1,0} c_{1,1} = c_{2,n} c_{2,n+1} = 0$.
  - Neumann Problem $c_{1,0} + c_{1,1} = c_{2,n} + c_{2,n+1} = 0$.
  - Dirichlet-Neumann Problem $c_{1,0} c_{1,1} = 0$, $c_{2,n} = -c_{2,n+1} \neq 0$.

Unilateral BVP

Initial value problem: $c_{2,j} = 0$ Final value problem $c_{1,i} = 0$

Corollary 1

The Green's function for the initial value problem is

$$(G_Q)_{k,s} = \begin{cases} 0 & \text{if } k \le s, \\ \frac{1+c_1}{\mathcal{Q}_1(x)}\widetilde{g}_x[k,s] & \text{if } k \ge s, \end{cases}$$

and the Green's function for the final value problem is

$$(G_Q)_{k,s} = \frac{1+c_1}{\mathcal{Q}_1(x)}\widetilde{g}_x[k,s] + \begin{cases} 0 & \text{if } k \le s, \\ \frac{1+c_1}{\mathcal{Q}_1(x)}\widetilde{g}_x[k,s] & \text{if } k \ge s, \end{cases}$$

where $\widetilde{g}_x[i,j] = [p_i(x)r_j(x) - p_j(x)r_i(x)]$, for $i,j \in \overline{F}$.

Sturm-Liouville BVP

$au_0 + bu_1 = g_1,\ cu_n + du_{n+1} = g_2$ if $(|a| + |b|)(|c| + |d|) > 0$

Corollary 2

For the Sturm-Liouville conditions the boundary polynomial is

$$P_c(x) = ac\widetilde{g}_x[0,n] + ad\widetilde{g}_x[0,n+1] + bc\widetilde{g}_x[1,n] + bd\widetilde{g}_x[1,n+1],$$

and the corresponding Green's function for the Sturm-Liouville BVP is

$$\begin{aligned}(G_Q)_{k,s} &= \frac{1+c_1}{\mathcal{Q}_1(x)P_c(x)}\Big((a+xb)\big(c\widetilde{g}_x[n,s] \\ &+ d\widetilde{g}_x[n+1,s]\big)\widetilde{g}_x[k,0]\Big) + \begin{cases} 0 & \text{if } k \le s, \\ g_x[k,s] & \text{if } k \ge s, \end{cases}\end{aligned}$$

where $\widetilde{g}_x[i,j] = \mathcal{P}_i(x)\mathcal{Q}_j(x) - \mathcal{P}_j(x)\mathcal{Q}_i(x)$, for $i,j \in \overline{F}$.

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Gracias

por su atención