

Boundary value problems on a weighted path

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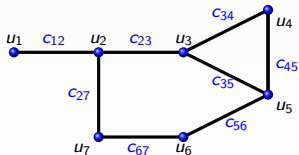
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Outline of the talk

- Notations and definitions
 - Weighted graphs and matrices
 - Schrödinger equations
 - Boundary value problems on weighted graphs
 - Green matrix of the BVP
- Boundary Value Problems on paths
 - Paths with constant potential
 - Orthogonal polynomials
 - Schrödinger matrix of the weighted path associated to orthogonal polynomials
 - Two-side Boundary Value Problems in weighted paths

Weighted graphs

- A **weighted graph** $\Gamma = (V, E, c)$ is composed by:
 - V is a set of elements called **vertices**.
 - E is a set of elements called **edges**.
 - $c : V \times V \rightarrow [0, \infty)$ is an application named **conductance** associated to the edges.
- u, v are **adjacent**, $u \sim v$ iff $c(u, v) = c_{uv} \neq 0$.
- The **degree of a vertex** u is $d_u = \sum_{v \in V} c_{uv}$.

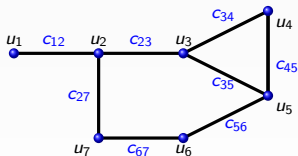


Matrices associated with graphs

Definition

The **weighted Laplacian** matrix of a weighted graph Γ is defined as

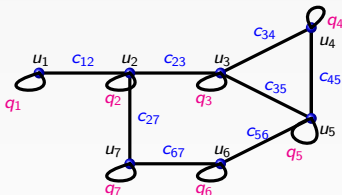
$$(\mathcal{L})_{ij} = \begin{cases} d_i & \text{if } i = j, \\ -c_{ij} & \text{if } i \neq j. \end{cases}$$



$$\mathcal{L} = \begin{pmatrix} d_1 & -c_{12} & 0 & 0 & 0 & 0 & 0 \\ -c_{12} & d_2 & -c_{23} & 0 & 0 & 0 & -c_{27} \\ 0 & -c_{23} & d_3 & -c_{34} & -c_{35} & 0 & 0 \\ 0 & 0 & -c_{34} & d_4 & -c_{45} & 0 & 0 \\ 0 & 0 & -c_{35} & -c_{45} & d_5 & -c_{56} & 0 \\ 0 & 0 & 0 & 0 & -c_{56} & d_6 & -c_{67} \\ 0 & -c_{27} & 0 & 0 & 0 & -c_{67} & d_7 \end{pmatrix}$$

Matrices associated with graphs

Now consider a weighted graph with weighted vertices



Definition

A **Schrödinger matrix** \mathcal{L}_Q on Γ with **potential** Q is defined as the generalization of the weighted Laplacian matrix, that is:

$$\mathcal{L}_q = \mathcal{L} + Q,$$

where $Q = \text{diag}[q_0, \dots, q_{n+1}]$ is called the **potential matrix**.

Schrödinger equations

- ✓ We call the **Homogeneous Schrödinger equation on F** to

$$[HSE] \quad \mathcal{L}_q u = 0$$

- ✓ The **Wronskian of x and $y \in \mathbb{R}^{n+2}$** is:

$$(w[x, y])_k = x_k y_{k+1} - x_{k+1} y_k, \quad \text{for } k = 0, \dots, n$$

$$(w[x, y])_{n+1} = (w[x, y])_n.$$

- ✓ Two solutions x and y of the HSE are **linearly independent** iff

$$(w[x, y])_k \neq 0, \quad k = 0, \dots, n+1$$

- ✓ It is well-known that the product $c_{kk+1}(w[x, y])_k = c$ for any $k = 1, \dots, n+1$ is constant iff \mathcal{L}_q is a symmetric matrix.

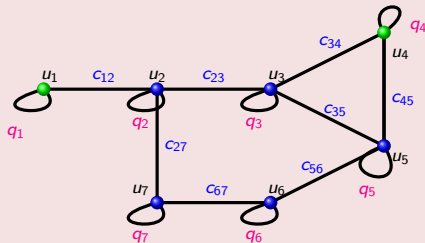
Definition of BVP

✓ Considering a subset of vertices $F \subset V(\Gamma)$, its **boundary** is defined as

$$\delta(F) = \{u \in V(\Gamma) : u \sim v, v \in F\},$$

and its **inner boundary** is defined as $\partial(F) = \delta(F) \cup \delta(F^c)$.

Example:



$$F = \{u_2, u_3, u_5, u_6, u_7\}$$

$$\delta(F) = \{u_1, u_4\}$$

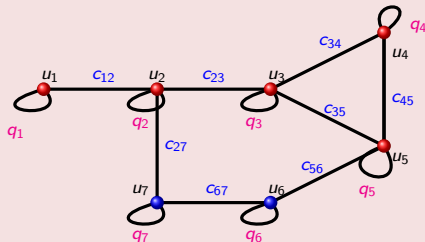
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$$\delta(F) = \{u_1, u_4\}$$

$$\partial(F) = \{u_1, u_2, u_4, u_3, u_5\}$$

Definition of BVP

Definition

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

$$\mathcal{L}_q u = f \text{ on } F, \quad \mathcal{B}_1 u = g_1, \quad \dots, \quad \mathcal{B}_p u = g_p,$$

for a given $f \in \mathbb{R}^{n+2}$ and $\mathcal{B}_i u = \sum_{j \in \partial(F)} b_{ij} u_j$, $g_i \in \mathbb{R}$, $i = 1, \dots, p$.

Examples of application:

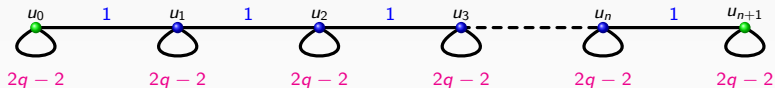
- Chip-firing games [Chung, Lovász]: $\mathcal{L}f = c_i - c_e$ on F .
- Hitting-time [Markov chains]: $\mathcal{L}H_k = \delta_j$ on $V - \{k\}$.

Open questions:

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

Paths with constant potential

In a preliminar work E. Bendito, A. Carmona, A.M. Encinas, [Eigenvalues, Eigenfunctions and Green's Functions on a Path via Chebyshev Polynomials](#), *Appl. Anal. Discrete Math.*, **3**, (2009), 182-302, study BVP in a path P_{n+2} with constant potential $2q - 2$



$$\begin{aligned}
 F &= \{u_1, \dots, u_n\} \\
 \delta(F) &= \{u_0, u_{n+1}\} \\
 \partial(F) &= \{u_0, u_1, u_n, u_{n+1}\}
 \end{aligned}
 \quad
 \mathcal{L}_q = \begin{pmatrix}
 2q & -1 & 0 & \dots & 0 \\
 -1 & 2q & -1 & \dots & 0 \\
 0 & -1 & 2q & \dots & 0 \\
 \vdots & \vdots & \vdots & \ddots & \vdots \\
 0 & 0 & & \dots & 2q
 \end{pmatrix}$$

A **linear boundary condition of F** in the path is given by

$$\mathcal{B}_i u = c_{i,1} u_0 + c_{i,1} u_1 + c_{i,n} u_n + c_{i,n+1} u_{n+1}, \text{ for any } u \in \mathbb{R}^{n+2}.$$

Paths with constant potential

So the BVP with two-side conditions is given by:

$$\begin{cases} \mathcal{L}_q u = f, \\ c_{10}u_0 + c_{11}u_1 + c_{1n}u_n + c_{1n+1}u_{n+1} = g_1, \\ c_{20}u_0 + c_{21}u_1 + c_{2n}u_n + c_{2n+1}u_{n+1} = g_2. \end{cases}$$

- A base of independent solutions of the HSE is $\{u, v\}$, where $x_k = \mathcal{U}_{k-1}(q)$, $y_k = \mathcal{U}_{k-2}(q)$, $1 \leq k \leq n$.
- They obtain the solution of the two-side BVP problem in terms of linear combinations of the second-order Chebyshev polynomials $\{\mathcal{U}_k\}$.

BVP in weighted paths

GOAL: To generalize this result for a path with non-constant potential

Families of Orthogonal Polynomials

- Given $\{\mathcal{A}_n\}_{n=0}^{\infty}$ a real positive sequence and $\{\mathcal{B}_n\}_{n=0}^{\infty}$ a real sequence of numbers, consider $\{\mathcal{R}_n(x)\}_{n=0}^{\infty}$ a sequence of real orthogonal polynomials satisfying the recurrence relation

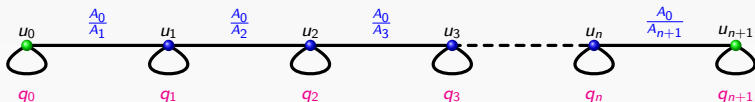
$$\mathcal{R}_n(x) = (\mathcal{A}_n x + \mathcal{B}_n) \mathcal{R}_{n-1}(x) - \mathcal{C}_n \mathcal{R}_{n-2}(x), \quad n \geq 2. \quad (1)$$

with $\mathcal{C}_n = \mathcal{A}_n / \mathcal{A}_{n-1}$.

- Choosing a pair of initial polynomials $\mathcal{R}_0(x)$ and $\mathcal{R}_1(x)$ we obtain a family of orthogonal polynomials satisfying the recurrence relation.
- If we consider the two families such that:
 - First kind OP:** $\{\mathcal{P}_n\}_{n=0}^{\infty}$ with $\mathcal{P}_0(x) = 1$, $\mathcal{P}_1(x) = ax + b$,
 - Second kind OP:** $\{\mathcal{Q}_n\}_{n=0}^{\infty}$, with $\mathcal{Q}_0(x) = 1$, $\mathcal{Q}_1(x) = \frac{A_0 + A_1}{A_0} \mathcal{P}_1(x)$.they verify that $\mathcal{P}_{-1}(x) = \mathcal{P}_1(x)$ and $\mathcal{Q}_{-1}(x) = 0$.

Schrödinger equations on weighted Paths

Now consider the weighted path



With $q_k = \frac{A_0(A_{k+1}x+B_{k+1})}{A_{k+1}} - \frac{A_0}{A_k}$, $k = 1, \dots, n$ and Schrödinger matrix:

$$\mathcal{L}_q = \begin{pmatrix} \frac{A_0(A_1x+B_1)}{A_1} - 1 & -\frac{A_0}{A_1} & 0 & \dots & 0 \\ -\frac{A_0}{A_1} & \frac{A_0(A_2x+B_2)}{A_2} & -\frac{A_0}{A_2} & \dots & 0 \\ 0 & -\frac{A_0}{A_2} & \frac{A_0(A_3x+B_3)}{A_3} & \dots & -\frac{A_0}{A_{n+1}} \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \dots & -\frac{A_0}{A_{n+1}} & \frac{A_0(A_{n+2}x+B_{n+2}-1)}{A_{n+2}} \end{pmatrix}$$

Green matrix of the Homogeneous Schrödinger Equation

Definition

The **Green matrix of the Schrödinger equation** is the matrix $g_q \in \mathcal{M}_{n+2, n+2}$ defined as the unique solution of the initial value problem with conditions

$$\mathcal{L}_q \cdot (g_q)_{\cdot, s} = \varepsilon_s \text{ on } F, \quad (g_q)_{s, s} = 0, \quad (g_q)_{s+1, s} = -\frac{1}{c_{s, s+1}}, \quad s \in F.$$

Lema

If x, y are two linearly independent solutions of the HSE on F , then

$$(g_q)_{k, s} = \frac{1}{c_{k, k+1}(\omega(x, y))_k} (x_k y_s - x_s y_k), \quad 0 \leq k, s \leq n+1$$

Proposition

Given $f \in \mathbb{R}^{n+2}$, the vector y such that $y_0 = 0$, and $y_k = \sum_{s=1}^k (g_q)_{k, s} f_s$, for $0 \leq k, s \leq n+1$ is the unique solution of the semi-homogeneous BVP.

Homogeneous Schrödinger Equation

Lemma

The vectors $x, y \in \mathbb{R}^{n+2}$ such that $x_k = \mathcal{P}_k(x)$ and $y_k = \mathcal{Q}_k(x)$ for any $k \in V$, form a basis $\{u, v\}$ of the solution space of the HSE on F , as

$$(w[x, y])_k = \frac{A_{k+1}}{A_0} P_1(x), \quad \text{for any } k \in V, P_1(x) \neq 0.$$

Moreover, the Green matrix of the HSE is

$$(g_q(x))_{k,s} = \frac{1}{\mathcal{P}_1(x)} [\mathcal{P}_k(x) \mathcal{Q}_s(x) - \mathcal{P}_s(x) \mathcal{Q}_k(x)], \quad k, s \in V.$$

Therefore, the general solution of the Schrödinger equation on F with data $f \in \mathcal{C}$ is determined by

$$u_k = \alpha \mathcal{P}_k(x) + \beta \mathcal{Q}_k(x) + \sum_{s=1}^k (g_q(x))_{k,s} f_s,$$

where $\alpha, \beta \in \mathbb{R}$.

Homogeneous Schrödinger Equation

- A solution $y \in \mathbb{R}^{n+2}$ is a solution of the HBVP iff $y = \alpha u + \beta v$, where $\alpha, \beta \in \mathbb{R}$ and $\{u, v\}$ is a basis of the HSE on V , satisfies

$$\begin{pmatrix} \mathcal{B}_1 u & \mathcal{B}_1 v \\ \mathcal{B}_2 u & \mathcal{B}_2 v \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

- Thus the BVP is regular iff $P_B(x) = \mathcal{B}_1 u \mathcal{B}_2 v - \mathcal{B}_2 u \mathcal{B}_1 v \neq 0$ and hence iff for any data $f \in \mathbb{R}^{n+2}$, $g_1, g_2 \in \mathbb{R}$ it has a unique solution.
- For $u_k = \mathcal{P}_k(x)$ and $v_k = \mathcal{Q}_k(x)$, $k \in V$,

$$P_B(x) = \sum_{i,j \in \partial F} d_{ij} u_i v_j = \mathcal{P}_1(x) \sum_{\substack{i < j \\ i,j \in \partial F}} d_{i,j} (g_q(x))_{i,j},$$

where $d_{ij} = c_{1i} c_{2j} - c_{2i} c_{1j}$ for all $i, j \in \partial F$ and $g_q(x)$ is the Green matrix of the HSE.

Semi-homogeneous BVP

The two side boundary problems can be restricted to the study of the semi-homogeneous ones:

Lemma

Consider $\alpha, \beta, \gamma, \delta \in \mathbb{R}$ such that $c_{j1}\alpha + c_{j2}\beta + c_{j3}\gamma + c_{j4}\delta = g_j$, for $j = 1, 2$, then $u \in \mathbb{R}^{n+2}$ verifies the general BVP, iff the vector $v = u - \alpha\varepsilon_0 - \beta\varepsilon_1 - \gamma\varepsilon_n - \delta\varepsilon_{n+1}$ verifies

$$\begin{aligned} \mathcal{L}_q v &= f + \left(\frac{A_0}{A_1} \alpha - \frac{A_0}{A_2} (A_2 x + B_2) \beta \right) \varepsilon_1 + \frac{A_0}{A_2} \beta \varepsilon_2 + \frac{A_0}{A_n} \gamma \varepsilon_{n-1} \\ &\quad + \left(\frac{A_0}{A_{n+1}} \delta - \frac{A_0}{A_{n+1}} (A_{n+1} x + B_{n+1}) \gamma \right) \varepsilon_n \end{aligned}$$

on F and $\mathcal{B}_1 u = \mathcal{B}_2 u = 0$.

Two-side boundary value problems

The solution of any regular semi-homogeneous BVP can be obtained through the so-called Green matrix:

Definition

The **Green matrix for the two-side boundary problem** is $\mathcal{G}_q \in \mathcal{M}_{n+2, n+2}$ such that

$$\mathcal{L}_q \cdot (\mathcal{G}_q)_{\cdot, s} = \varepsilon_s \text{ on } F, \quad \mathcal{B}_1(\mathcal{G}_q)_{\cdot, s} = \mathcal{B}_2(\mathcal{G}_q)_{\cdot, s} = 0, \quad s \in F.$$

Lema

For any $f \in \mathbb{R}^{n+2}$ the unique solution of the semi-homogeneous BVP with data f is the vector

$$u_k = \sum_{s=1}^n (\mathcal{G}_q)_{k, s} f_s.$$

Green matrix of the BVP

Theorem

The BVP is regular iff $P_B(x) \neq 0$. In this case, the Green matrix is given, for any $1 \leq s \leq n$ and $0 \leq k \leq n+1$, by

$$\begin{aligned}
 (\mathcal{G}_q)_{k,s} = & \frac{P_1(x)}{P_B(x)} \left[d_{n,n+1} \frac{A_{n+1}}{A_0} (g_q(x))_{s,k} + \sum_{i=0}^1 \sum_{j=n}^{n+1} d_{i,j} (g_q(x))_{k,i} (g_q(x))_{j,s} \right] \\
 & + \begin{cases} 0, & k \leq s \\ (g_q(x))_{k,s}, & k \geq s. \end{cases}
 \end{aligned}$$

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

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

- 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 boundary polynomial for both problems is:

$$P_B(x) = \frac{\mathcal{P}_1(x)}{A_0} (A_1 d_{0,1} + A_{n+1} d_{n,n+1}).$$

The Green matrix for the initial boundary value problem is given by

$$(\mathcal{G}_q)_{k,s} = \begin{cases} 0, & k \leq s, \\ (g_q(x))_{k,s}, & k \geq s. \end{cases}$$

Whereas the Green function for the final boundary value problem is

$$(\mathcal{G}_q)_{k,s} = \begin{cases} (g_q(x))_{k,s}, & k \leq s, \\ 0, & k \geq s, \end{cases}$$

for any $1 \leq s \leq n$, $0 \leq k \leq n+1$.

Sturm-Liouville BVP

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

Corollary

The boundary polynomial for the Sturm-Liouville BVP is

$$P_B(x) = a \left[d(Q_{n+1}(x) - P_{n+1}(x)) + c(Q_n(x) - P_n(x)) \right] + b \left[P_1(x)(dQ_{n+1}(x) + cQ_n(x)) - Q_1(x)(dP_{n+1}(x) + cP_n(x)) \right]$$

and the Green matrix for the Sturm-Liouville boundary value problem is

$$(g_q(x))_{k,s} = \frac{1}{P_1(x)P_B(x)} \left[a(P_k(x) - Q_k(x)) + b(Q_1(x)P_k(x) - Q_k(x)P_1(x)) \right] \times \left[c(P_s(x)Q_n(x) - P_n(x)Q_s(x)) + d(P_s(x)Q_{n+1}(x) - P_{n+1}(x)Q_s(x)) \right]$$

for any $0 \leq k \leq s \leq n$ and $1 \leq s$; whereas

$$(g_q(x))_{k,s} = \frac{1}{P_1(x)P_B(x)} \left[a(P_s(x) - Q_s(x)) + b(Q_1(x)P_s(x) - Q_s(x)P_1(x)) \right] \times \left[c(P_k(x)Q_n(x) - P_n(x)Q_k(x)) + d(P_k(x)Q_{n+1}(x) - P_{n+1}(x)Q_k(x)) \right]$$

for any $n+1 \geq k \geq s \geq 1$ and $s \leq n$.

Some References

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Thanks for your attention

Děkuji za pozornost

Gracias por su atención