Boundary value problems
on a weighted path

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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
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 $d_u = \sum_{v \in V} c_{uv}$.
The weighted Laplacian matrix of a weighted graph $\Gamma$ is defined as

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

Now consider a weighted graph with weighted vertices

Definition

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

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

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

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

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

Two solutions \( x \) and \( y \) of the HSE are **linearly independent** iff

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

It is well-known that the product \( c_{kk+1}(w[x,y])_k = c \) for any \( k = 1, \ldots , n + 1 \) is constant iff \( \mathcal{L}_q \) is a symmetric matrix.
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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$$\partial(F) = \{ u_1, u_2, u_4, u_3, u_5 \}$$
Definition of BVP

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

$\mathcal{L}_q u = f$ on $F, \quad B_1 u = g_1, \quad \ldots, \quad B_p u = g_p,$

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

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 $V - \{k\}$. 

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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?

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

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

**Diagram:**

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

$$
\mathcal{B}_i u = c_{i,1} u_0 + c_{i,1} u_1 + c_{i,n} u_n + c_{i,n+1} u_{n+1}, \text{ for any } u \in \mathbb{R}^{n+2}.
$$
So the BVP with two-side conditions is given by:

\[
\begin{align*}
\mathcal{L}_q u &= f, \\
\sum_{i=0}^{n+1} c_{1i} u_i &= g_1, \\
\sum_{i=0}^{n+1} c_{2i} u_i &= g_2.
\end{align*}
\]

- A base of independent solutions of the HSE is \( \{ u, v \} \), where \( x_k = U_{k-1}(q), \ y_k = U_{k-2}(q), \ 1 \leq k \leq n \).
- They obtain the solution of the two-side BVP problem in terms of linear combinations of the second-order Chebyshev polynomials \( \{ U_k \} \).
GOAL: To generalize this result for a path with non-constant potential
Families of Orthogonal Polynomials

- Given \( \{A_n\}_{n=0}^{\infty} \) a real positive sequence and \( \{B_n\}_{n=0}^{\infty} \) a real sequence of numbers, consider \( \{R_n(x)\}_{n=0}^{\infty} \) a sequence of real orthogonal polynomials satisfying the recurrence relation

\[
R_n(x) = (A_n x + B_n)R_{n-1}(x) - C_n R_{n-2}(x), \quad n \geq 2. \tag{1}
\]

with \( C_n = A_n / A_{n-1} \).

- Choosing a pair of initial polynomials \( R_0(x) \) and \( R_1(x) \) we obtain a family of orthogonal polynomials satisfying the recurrence relation.

- If we consider the two families such that:
  - First kind OP: \( \{P_n\}_{n=0}^{\infty} \) with \( P_0(x) = 1 \), \( P_1(x) = ax + b \),
  - Second kind OP: \( \{Q_n\}_{n=0}^{\infty} \), with \( Q_0(x) = 1 \), \( Q_1(x) = \frac{A_0 + A_1}{A_0} P_1(x) \).

they verify that \( P_{-1}(x) = P_1(x) \) and \( Q_{-1}(x) = 0 \).
Now consider the weighted path

\[
\begin{array}{cccccccc}
& & & & & & & \\
u_0 & A_0 & A_1 & A_0 & A_2 & A_0 & A_3 & A_0 & \cdots & A_0 & A_{n+1} & u_{n+1} \\
& q_0 & & q_1 & & q_2 & & q_3 & & q_n & q_{n+1} & \\
& & & & & & & \\
u_n & & & & & & & & & & & \\
\end{array}
\]

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

\[
\mathcal{L}_q = \\
\begin{pmatrix}
\frac{A_0(A_1x + B_1)}{A_1} - 1 & -\frac{A_0}{A_1} & 0 & \cdots & 0 \\
-\frac{A_0}{A_1} & \frac{A_0}{A_2} - \frac{A_0}{A_1} & -\frac{A_0}{A_2} & \cdots & 0 \\
0 & -\frac{A_0}{A_2} & \frac{A_0}{A_3} & \cdots & -\frac{A_0}{A_{n+1}} \\
& \vdots & & \ddots & \vdots \\
0 & 0 & \cdots & -\frac{A_0}{A_{n+1}} & \frac{A_0}{A_{n+2}} - 1
\end{pmatrix}
\]
**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

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

**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.
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 \(\alpha, \beta \in \mathbb{R}\).
• 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

$$\begin{pmatrix} B_1u & B_1v \\ B_2u & B_2v \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$  

• Thus the BVP is regular iff $P_B(x) = B_1uB_2v - B_2uB_1v \neq 0$ 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 $u_k = P_k(x)$ and $v_k = Q_k(x)$, $k \in V$,

$$P_B(x) = \sum_{i,j \in \partial F} d_{ij} u_i v_j = P_1(x) \sum_{i<j \atop i,j \in \partial F} d_{i,j} (g_q(x))_{i,j},$$

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

$$L_q v = f + \left( \frac{A_0}{A_1} \alpha - \frac{A_0}{A_2} (A_2 x + B_2) \beta \right) \varepsilon_1 + \frac{A_0}{A_2} \beta \varepsilon_2 + \frac{A_0}{A_n} \gamma \varepsilon_{n-1}$$

$$+ \left( \frac{A_0}{A_{n+1}} \delta - \frac{A_0}{A_{n+1}} (A_{n+1} x + B_{n+1}) \gamma \right) \varepsilon_n$$

on $F$ and $B_1 u = B_2 u = 0$. 
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 $G_q \in \mathcal{M}_{n+2,n+2}$ such that

$$L_q \cdot (G_q)_{:,s} = \varepsilon_s \text{ on } F, \quad B_1(G_q)_{:,s} = B_2(G_q)_{:,s} = 0, \quad s \in F.$$

**Lema**

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

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

$$(G_q)_{k,s} = \frac{P_1(x)}{P_B(x)} \left[ d_{n,n+1} \frac{A_{n+1}}{A_0} (g_q(x))_{s,k} + \sum_{i=0}^{1} \sum_{j=n}^{n+1} d_{i,j} (g_q(x))_{k,i} (g_q(x))_{j,s} \right]$$

$$+ \begin{cases} 0, & k \leq s \\ (g_q(x))_{k,s}, & k \geq s. \end{cases}$$
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**

\[
\mathcal{L}_q(u) = f \quad \text{on } F,
\]

\[
c_{1,0} u_0 + c_{1,1} u_1 = g_1,
\]

\[
c_{2,n} u_n + c_{2,n+1} u_{n+1} = g_2.
\]

- **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:

$$P_B(x) = \frac{P_1(x)}{A_0}(A_{1d_0,1} + A_{n+1d_{n,n+1}}).$$

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

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

Whereas the Green function for the final boundary value problem is

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

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

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Boundary value problems on a weighted path
Sturm-Liouville BVP

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

**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

Thanks for your attention
Děkuji za pozornost
Gracias por su atención