Inverse Problems for the Schrödinger Operator on Metric Graphs

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Graphs

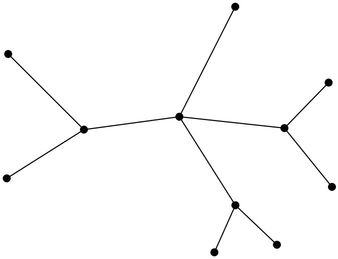


Fig. 1: A tree graph

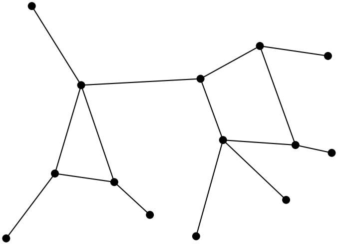


Fig. 2: A graph with cycles

Metric graphs

Let $\Omega = \{V, E\}$ be a finite compact graph, where $E = \{e_j\}_{j=1}^N$ is a set of edges and $V = \{v_j\}_{j=1}^M$ is a set of vertices.

A graph is a tree if it has no cycles.

We recall that a graph is called a *metric graph* if every edge $e_j \in E$ is identified with an interval of the real line with a positive length l_j.

Let $\{\gamma_1, \dots, \gamma_m\} =: \Gamma \subset V$ be the boundary vertices, $\Gamma = \{v \in V | \, \mathrm{degree}\,(\mathrm{v}) = 1\}$, where the degree of a vertex is the number of edges incident to it.

Quantum graphs

By quantum graphs we understand metric graphs with differential equations defined on the edges coupled by certain vertex matching (compatibility) conditions.

Control and inverse theories for PDEs on graphs constitute an important part of the rapidly developing area of applied mathematics — analysis on graphs.

Network-like structures play a fundamental role in many problems of science and engineering. The classical problem is the problem of oscillations of the flexible structures of strings, beams, cables.

Recently, quantum graphs were applied to description of nanostructured materials like ceramic or metallic foams, percolation networks and carbon and graphene nano-tubes.

Outline

- Spectral and dynamical inverse problems on an interval
- The boundary control (BC) method
- Control and inverse problems on tree graphs
- Control and inverse problems on graphs with cycles

Inverse spectral problems

Let $\{\lambda_n, \varphi_n\}$, $n = 0, 1, \ldots$ be the eigenvalues and eigenfunctions of the Sturm–Liouville problem:

$$-\varphi''(x,\lambda) + q(x)\varphi(x,\lambda) = \lambda\varphi(x,\lambda); \quad x \in (0, l)$$

$$\varphi(0,\lambda) = \varphi(l,\lambda) = 0.$$

Inverse spectral problem: recover unknown $q(x)$ from the spectral data: $\{\lambda_n, \varphi_n'(0)\}$.

Borg, Levinson, Gel'fand, Levitan, Krein, Marchenko

Weyl solution:

$$-\phi''(x,\lambda) + q(x)\phi(x,\lambda) = \lambda\phi(x,\lambda); \quad \phi(0,\lambda) = 1, \ \phi(l,\lambda) = 0.$$

Weyl function: $m(\lambda) := \phi'(0,\lambda), \ \Im\lambda > 0.$

Inverse dynamical problems

A. Blagoveschenskii (1971)

The Boundary Control method in inverse theory was proposed in the end of 80-ies (M. Belishev, A. Kachalov, Ya. Kurylev, S. Ivanov, S. A.)

It is based on deep connections between inverse (identification) problems and controllability of dynamical systems.

It was successfully applied to the wave, heat, beam, Maxwell, Schrödinger, and Dirac equations.

Wave Equation

Let us consider the 1D wave equation

$$w_{tt}(x,t) - w_{xx}(x,t) + q(x)w(x,t) = 0, \quad x \in (0,l), \ t > 0, \quad (1)$$

with the boundary conditions

$$w(0,t) = f(t), \ w(l,t) = 0, \ t > 0, \quad (2)$$

and zero initial conditions

$$w(x,0) = w_t(x,0) = 0, \ x \in (0,l). \quad (3)$$

The potential q is a real valued integrable function; function f is referred to as *boundary control*; $w = w^f(x,t)$.
Nonseladjoint version of the BC method was proposed in S.A. and Belishev (1996).

Representation of the Solution

For $t \leq l$,

$$w^f(x,t) = \begin{cases} f(t-x) + \int_x^t h(x,s)\, f(t-s)\, ds & \text{for } x < t\,, \\ 0 & \text{for } x \geq t\,. \end{cases} \quad (4)$$

Here h is a solution of the Goursat problem:

$$h_{tt} - h_{xx} + q(x)h = 0, \quad 0 < x < t\,, \quad (5)$$

$$h(0,t) = 0\,, \quad h(x,x) = -\frac{1}{2}\int_0^x q(s)\, ds\,. \quad (6)$$

For $t \leq 2l$, we set $q(2l-x) := q(x)$, solve (5), (6) and get

$$u(x,t) = f(t-x) + \int_x^t h(x,s)f(t-s)ds - f(t+x-2l)$$

$$-\int_{2l-x}^t h(2l-x,s)f(t-s)ds.$$

Inverse Problem and Controllability

The **response operator** $R^T : \mathcal{F}^T \mapsto \mathcal{F}^T := L^2(0,T)$,

$$(R^T f)(t) := w_x^f(0,t) \ \left(= f'(t) + \int_0^t r(t)\, f(t-s)\, ds \right).$$

Inverse problem: given R^{2T} recover $q(x)$, $x \in [0,T]$.

Controllability: For any function $z \in \mathcal{H}^T := \{u \in L^2(0,\infty) : \ \text{supp}\ u \subset [0,T]\}$, there exists a unique control $f \in \mathcal{F}^T$ such that

$$(W^T f)(x) := w^f(x,T) = z(x) \ \text{ in } \mathcal{H}^T.$$

Really, this problem reduces to the equation

$$z(x) = f(T-x) + \int_x^T h(x,s)\, f(T-s)\, ds.$$

Krein's type equation

Dual to the control problem is the observation problem, and the connecting operator $C^T := (W^T)^* W^T$ plays a central role in the BC method.

$$(C^T f)(t) = f(t) + \int_0^T [p(2T - t - s) - p(|t - s|)]\, f(s)\, ds, \quad t \in [0, T],$$

$$p(t) := \frac{1}{2} \int_0^t r(s)\, ds\,.$$

Let $y(x)$ be a solution to the boundary value problem

$$y''(x) - q(x)y(x) = 0,\ \ y(0) = 0,\ \ y'(0) = 1,\ \ x > 0, \qquad (7)$$

and consider the problem: find a control $f^T \in \mathcal{F}^T$ such that

$$w^{f^T}(x, T) = \begin{cases} y(x), & x \le T, \\ 0, & x > T. \end{cases} \qquad (8)$$

Solution of the inverse problem

Function f^T satisfies the equation

$$(C^T f)(t) = T - t, \quad t \in [0, T],$$

Applying the propagation of singularities property, we obtain

$$w^{f^T}(T - 0, T) = f^T(+0) := \mu(T).$$

From (8), $w^{f^T}(T - 0, T) = y(T)$, thus (7) gives

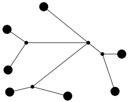
$$q(T) = \frac{y''(T)}{y(T)} = \frac{\mu''(T)}{\mu(T)}.$$

By varying T in $(0, l)$, we obtain $q(\cdot)$ in that interval.

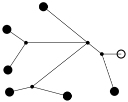
Operator R^T and the Weyl function $m(\lambda)$ are connected with each other through the Fourier–Laplace transform.

Controllability and inverse problems for trees

It is known that the IBVP for the wave equation on a tree graph is exactly controllable/observable/identifiable if the controls/observations act at all or at all but one of the boundary vertices.



or



The wave equation on graphs with cycles is never exactly controllable from the boundary. The similar statement is true for inverse problems.

Inverse spectral problems for trees

Spectral problem on graph:

$$-\varphi''(x,\lambda)+q(x)\varphi(x,\lambda)=\lambda\varphi(x,\lambda);\ x\in\Omega\setminus V;\ \varphi(v,\lambda)=0,\ v\in\Gamma$$

$$\varphi_i(v,\lambda)=\varphi_j(v,\lambda),\ e_i,e_j\in E(v);\ \sum_{e_i\in E(v)}\partial\varphi_i(v,\lambda)=0;\ \ v\in V\setminus\Gamma$$

Inverse problem 1: recover the topology of Ω, lengths of the edges and $q(x)$ from $\{\lambda_n,\partial\varphi_n|_\Gamma\}$.

Weyl solution:

$\phi_i(x,\lambda):\ \phi_i(v_i,\lambda)=1,\ \phi_i(v_j,\lambda)=0,\ j\neq i,\ v_i,v_j\in\Gamma.$

Weyl matrix function: $\mathbf{M}(\lambda):\mathbf{M}_{ij}(\lambda)=\partial\phi_i(v_j,\lambda).$

Inverse problem 2: recover the graph from $\mathbf{M}(\lambda):\Im\lambda>0.$

Brief review

- First papers concerning inverse problems on general metric trees were: Belishev 2004, Brown and Weikard 2005, Yurko 2005, S.A. and Kurasov 2008. Extensive lists of references can be found in books: Berkolaiko and Kuchment 2013, Kurasov 2023 and survey Yurko 2016.
- As inverse data, Belishev used $\{\lambda_n, \partial\varphi_n|_\Gamma\}$, Brown and Weikard – $\mathbf{M}(\lambda)$, Yurko – $\{M_{ii}(\lambda)\}, i = 1, ..., N-1$, S.A. and Kurasov – $\{M_{ij(\lambda)}\}, i, j = 1, ..., N-1$.
- Brown–Weikard and Yurko assumed that the topology of the graph and the lengths of edges are given and recovered $q(x)$.
- S.A. and Kurasov considered also dynamical inverse problem and introduced the Leaf Peeling (LP) method. Pure dynamical version of the LP method was considereded in S.A., Mikhaylov and Nurtazina (2017); S.A and Zhao (2021).

Dynamical inverse problem on trees

$$u_{tt} - u_{xx} + q(x)u = 0 \ \text{ in } \{\Omega \setminus V\} \times (0, T) \tag{9}$$

$$\begin{array}{l} \sum_{e_j \in E(v)} \partial u_j(v, t) = 0, \ u_i(v, t) = u_j(v, t) \\ e_i, e_j \in E(v), \ v \in V \setminus \Gamma, \ t \in [0, T] \end{array} \tag{10}$$

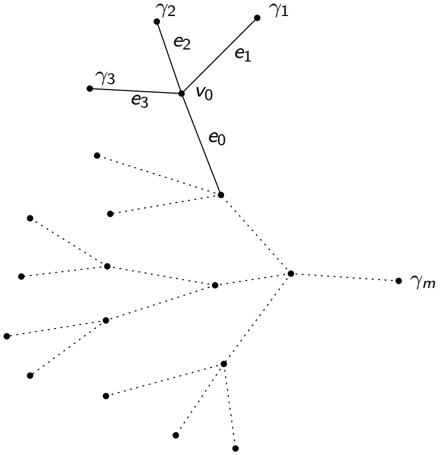
$$\begin{array}{c} u = f \quad \text{on} \quad \Gamma_1 \times [0, T], \quad u = 0 \quad \text{on} \quad \Gamma_0 \times [0, T] \\ u|_{t=0} = u_t|_{t=0} = 0 \ \text{ in } \ \Omega \end{array} \tag{11}$$

The *response operator*, $R^T = \{R_{ij}^T\}_{i,j=1}^m$, on $L^2(0, T; \mathbb{R}^{|\Gamma_1|})$:

$$(R^T f)(t) := \partial u^f(\cdot, t)|_{\Gamma_1} , \qquad 0 < t < T . \tag{12}$$

If Γ_1 contains all or all but one of the boundary vertices, the operator R^T known for $T > T_*$ uniquely determines the graph.

Leaf peeling method: sheaf and reduced tree



A sheaf on a tree graph rooted at γ_m (the sheaf is in solid lines), in which v_0 is the abscission vertex and e_0 is the stem edge.

Locality of the BC method

$$(R_{11}f_1)(t) = -f_1'(t) - \frac{2}{deg\ v_0}\, f_1'(t-2l_1) + \int_0^t r_1(s)\, f_1(t-s)\, ds + \dots$$

Numerical experiments

The method of NSBF was successfully combined with the LP method for solving spectral inverse problems on metric trees in S.A., Khmelnitskaya and Kravchenko (2023, 2024).

Controllability on trees

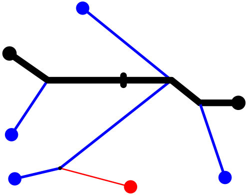
Control problems for the wave equations on metric graphs (mostly trees) were studied in many papers, see books: Lagnese, Leugering, Schmidt (1994); S.A. and Ivanov ()1995); Dáger and Zuazua (2006); and surveys S.A. (2008); Zuazua (2013).
The sharp estimate of controllability time and the and efficient control algorithm were proposed in S.A. and Zhao 2021:

Let Γ_1 contain all or all but one of the boundary vertices and U be a union of disjoint paths (except for the end points) from a controlled vertex to a point in a finite tree graph Ω such that $\cup_{P\in U} P = \Omega$. We put

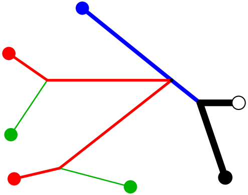
$$T_0 = \min_U \max_{P\in U} \text{ length } P.$$

If $T \geq T_0$ then for any $y \in L^2(\Omega)$, there exists $f \in L^2(0, T; \mathbb{R}^{|\Gamma_1|})$ such that $u^f(\cdot, T) = y$.

Union path representation of a tree



Controls act at all boundary vertices



Controls act at all but one boundary vertices

Minimal control time

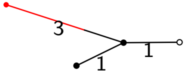
The time T required for either shape or velocity controllability is

$$T \geq T_0 := \min_{U} \max_{P \in U} \text{length } P(\gamma, a).$$

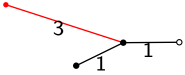
Let $T_f := \inf \left[T : \cup_{f \in \mathcal{F}^T} \{ \text{supp } u^f(\cdot, T) = \Omega \} \right]$
$T_m := \max_{j=1,2} \{ \text{dist}(v_j, v_3) \}$, then

$$\boxed{T_f \leq T_0 \leq T_m}$$

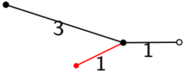
Example:



$T_f = 2$

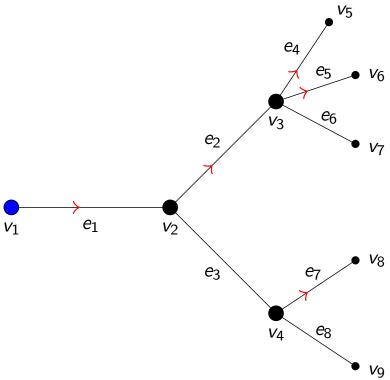


$T_0 = 3$



$T_m = 4$

Another inverse problem (S.A. and Edward 2021)



$u_1(v_1,t) = f(t)$, $(Rf)(t) = \{\partial u_1^f(v_1,t), \partial u_2^f(v_2,t), \partial u_4^f(v_3,t), \partial u_5^f(v_3,t), \partial u_7^f(v_4,t)\}$.

Schrödinger operator

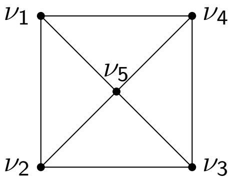
We set $\mathcal{H} := L^2(\Omega)$ and define the space $\mathcal{H}^1$ of continuous functions y on Ω such that $y_j := y|_{e_j} \in H^1(e_j)\ \forall e_j \in E$ and $y|_\Gamma = 0$. The space $\mathcal{H}^2$ consists of functions $y \in \mathcal{H}^1$ such that $y_j \in H^2(e_j)\ \forall e_j \in E$, satisfying the KN conditions.

Let q be a real valued function (potential) such that $q|_{e_j} \in C[0, l_j]$. We define the Schrödinger operator on the graph Ω as the operator $L = -\frac{d^2}{dx^2} + q$ in $\mathcal{H}$ with the domain $\mathcal{H}^2$.

Changing q we change the operator L and, therefore, its spectrum and its multiplicity $\sigma(\Omega, q)$. **The maximal possible multiplicity of an eigenvalue of** L, **denoted by** $\sigma(\Omega)$, is important for control and inverse problems on graphs. Formula for this graph invariant was obtained by Kac and Pivovarchik (2011).

Cyclically connected graphs

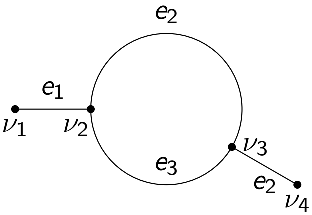
A graph Γ is said to be **cyclically connected** if, for each pair of vertices $v, v' \in \Omega$, a finite set of cycles $C_1, C_2, \ldots, C_n$ in Ω exist such that $v \in C_1$, $v' \in C_n$ and each neighboring pair of cycles possesses at least one common vertex.



For cyclically connected graphs $\sigma(\Omega) = \mu + 1$, where μ is the cyclomatic number of the graph (the number of independent cycles). We recall that $\mu = |E| - |V| + 1$.

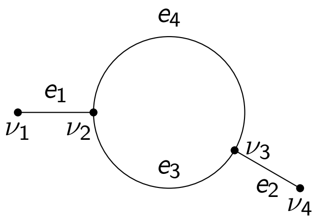
Quasi-trees

A graph is a **quasi-tree** if it is not cyclically connected and each (if any) cyclically connected subgraph of it has more than one vertex in common with the complement of this subgraph. For quasi-trees $\sigma(\Omega) = \mu + |\Gamma| - 1$, in particular, for trees it is $|\Gamma| - 1$.



$\sigma(\Omega) = \mu + p^t - 1$, where p^t be the numbers of boundary vertices for the tree obtained by contracting all the cycles of the graph into vertices.

Inverse problem for a graph with cycle



$\phi : \phi(v_1, \lambda) = 1,\ \phi(v_4, \lambda) = 0,$ KN on $v_2,\ v_3$;
$M(\lambda) := \{\partial\phi_1(v_1, \lambda),\ \partial\phi_2(v_2, \lambda)\}.$

Observation problem

Now we discuss controllability and observability results for graphs with cycles obtained in S.A. and Zhao 2022.
We consider the following IBVP:

$$w_{tt} - w_{xx} + q(x)w = 0 \quad \text{in} \ \ \{\Omega \setminus V\} \times (0, T), \tag{13}$$

$$w_j(v, t) = w_k(v, t) \text{ for } e_j, e_k \in E(v_i), v_i \in V \setminus \Gamma, \tag{14}$$

$$\sum_{e_j \in E(v)} \partial w_j(v, t) = 0 \ \text{ at each vertex } \ v \in V \setminus \Gamma, \tag{15}$$

$$w|_{\Gamma} = 0, \ \ w|_{t=0} = w^0, \ w_t|_{t=0} = w^1 \quad \text{in} \ \ \Omega. \tag{16}$$

Here $T > 0$, $w^0 \in \mathcal{H}^1$, $w^1 \in \mathcal{H}$. Using the Fourier method, one can show, similarly to (S.A. and Nicaise 2015), that for any v, j

$$w(v, \cdot) \in H^1(0, T), \ \partial w_j(v, \cdot) \in L^2(0, T). \tag{17}$$

Observability

We define a set of active vertices $V^* \subset V$, where we put observers for the trace $w(v,\cdot)$. For each vertex v we define a set of active edges $E^*(v) \subset E(v)$, where we put observers for directional derivatives $\partial w_j(v,\cdot)$, $e_j \in E^*(v)$. Note that $E^*(v)$ may be empty.

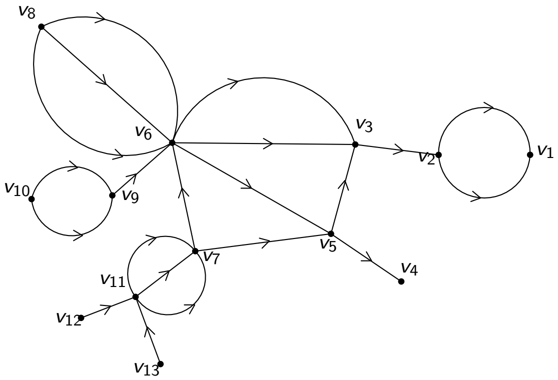
Let $E^* := \cup_{v\in V} E^*(v)$. We call $\{V^*, E^*\}$ the **active set**. We say that the system (13)–(16) with the active set $\{V^*, E^*\}$ is (exactly) **observable** in time T if there is a positive constant C, independent of w_0, w_1, such that

$$\sum_{v\in V^*} \|w(v,\cdot)\|^2_{H^1(0,T)} + \sum_{e_j\in E^*} \|\partial w_j(v,\cdot)\|^2_{L^2(0,T)} \geq C\left\{\|w^0\|^2_{\mathcal{H}^1} + \|w^1\|^2_{\mathcal{H}}\right\}$$

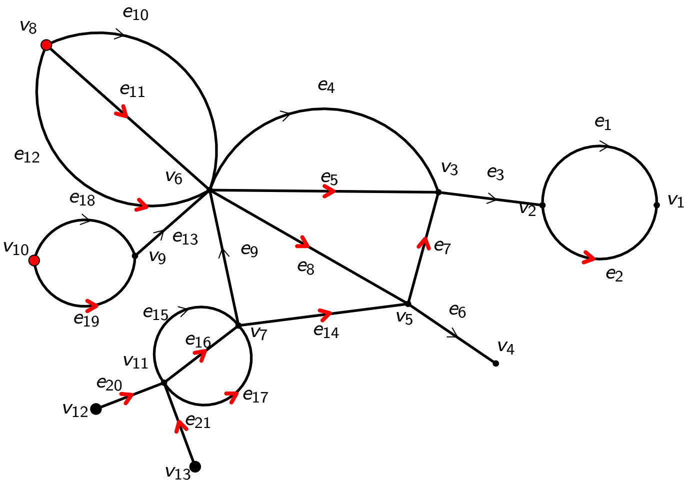
for every $w^0 \in \mathcal{H}^1,\ w^1 \in \mathcal{H}$.

Acyclic orientation

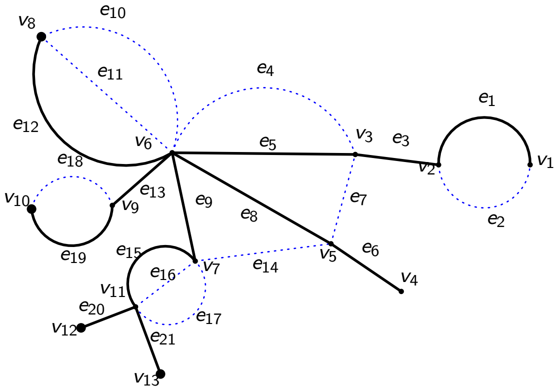
Start with an acyclic orientation



Placing observers on $\vec{\Omega}$

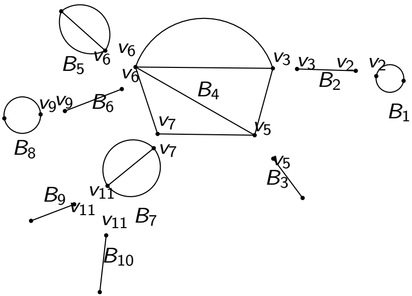


Minimal number of controllers



minimal number of controllers= number of controllers needed on the spanning tree + number of cycles

The minimal number of controllers as a graph invariant



Cutpoints separate Ω into blocks. Denote $|B_\Gamma|$ as the number of blocks that only share one common vertex with the rest of the graph. The the minimal number of controllers is

$$\kappa(\Omega) = \begin{cases} \mu + 1, & \Omega \text{ has one block;} \\ \mu - 1 + |B_\Gamma|, & \Omega \text{ has two or more blocks.} \end{cases}$$

Comparing $\kappa(\Omega)$ with $\sigma(\Omega)$

For all graphs $\kappa(\Omega) \geq \sigma(\Omega)$.

$\kappa(\Omega) = \sigma(\Omega)$ for trees, for a ring, the lasso graph, quasi-trees, and in many other cases.

For a chamomile flower like graph $\sigma(\Omega) = \mu + 1, \ \kappa(\Omega) = 2\mu - 1$.

If we have $\kappa(\Omega)$ or more observers, we can guarantee exact controllability, observability and stable indentifiability of our system.

If we have less than $\sigma(\Omega)$ we do not generally have even approximate controllability, or uniqueness property of observation/identification.