Topological Derivatives for Control of Gas Networks

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Outline

Background

- Application of Distributed Parameter Networks:
    - Modeling and control of gas or water transportation
    - Structural optimization for beam networks
- Applications of Optimal Control:
    - Minimizing travel time via accelerator control
    - Trajectory management in aviation and space technology
- Distributed Parameters: Temperature, pressure, flow velocity

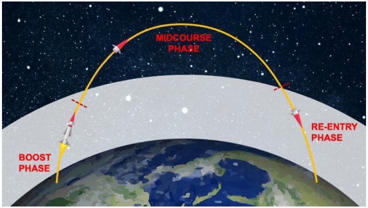


Fig. 1: Illustration of pipeline (left) and hypersonic glide vehicle trajectory (right).

Control and Design for Nonlinear Systems on Networks

- Optimal control of nonlinear system for the specific cost which admits the turnpike property leads to the optimum design of nonlinear steady state optimal control problem with bounded or estimated *loss of optimality*;
- Linearization of nonlinear system results in the optimal control problem for linear state equation. Then for the cost with turnpike property the optimum design problem is considered for optimal control problem of steady state model.
- In the first case the *Maximum Principle* is applied for the necessary and sufficient optimality conditions of the nonlinear steady state optimal control problem (Nikolai Osmolovskii, Meizhi Qian, J.S. Control and Cybernetics, 2023).

Definition of Networks

- Graph $G = (V, E)$; V: the set of nodes; E: the set of edges
- Multiple nodes: $v_M \in V_M \subset V$; single nodes: $\partial V = V \backslash V_M$
- Neumann (free) nodes $v_N \in V_N := \{v_j \in \partial V \mid v_j \text{ is free } \} \subset V$
- Controlled nodes: $v_C \in V_C = \{v_j \in \partial V \mid v_j \text{ is controlled } \} \subset V$
- $\epsilon_{i,j}$ the orientation of the outer normal vector on the boundary, i.e.,

$$\epsilon_{i,j} := \begin{cases} -1 & \text{if the } i\text{-th edge starts at node } v_{\mathrm{j}}, \\ +1 & \text{if the } i\text{-th edge ends at node } v_{\mathrm{j}}, \\ 0 & \text{otherwise} . \end{cases}$$

- $\mathcal{E}_J$: the index set of all edges adjacent at node v_J
- Continuity: $y_i(v_J) = y_j(v_J), \ \forall i, j \in \mathcal{E}_J, \ v_J \in V_M$
- Kirchhoff: $\sum\limits_{i \in \mathcal{E}_J} \epsilon_{i,J} y_i'(v_J) = 0, \ v_J \in V_M \cup V_N$

Shape Optimization

- Minimization problem:

$$J(\Omega) = I(\Omega, u_\Omega) \longrightarrow \inf_{\Omega}$$

- $\Omega \subset \mathbb{R}^n$ is an open set
- u_Ω stands for the solution of the state equation
- Two methods to determine the descent direction:
  1. Boundary variations and shape gradients;
  2. Topological derivatives and the level set method.
- The convergence of the shape gradient flow method for the second order regularization of the Kohn-Vogelius functional is shown in two spatial dimensions (P.I. Plotnikov, J.S., JGEA, 2023).

Topological Derivative

- To minimize the shape functionals under PDEs constraints.
- Given the shape functional $\Omega \to J(\Omega)$, the topological derivative at the interior vertex $P_0 \in V$ is defined by the following limit, if the limit exists,

$$\mathcal{J}(P_0) := \lim_{\varepsilon \to 0} \frac{1}{\varepsilon}(J(\Omega_\varepsilon) - J(\Omega))\,. \tag{1}$$

The existence of limit in Eq. (1) implies the expansion of the shape functional

$$J(\Omega_\varepsilon) = J(\Omega) + \varepsilon \mathcal{J}(P_0) + o(\varepsilon)\,. \tag{2}$$

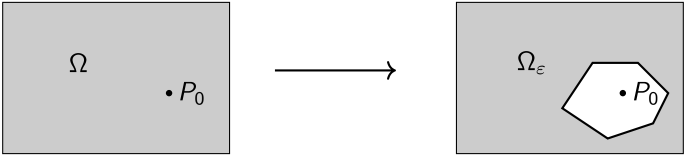
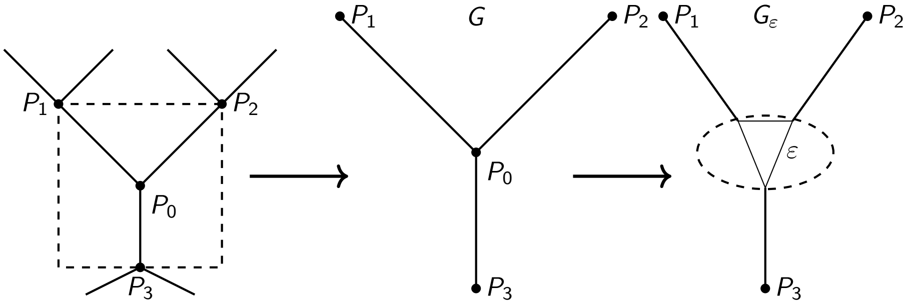


Fig. 2: Topology change by creation of a hole (continuum).

Design of Networks



(a) Network (b) Star (c) Star with cycle

Fig. 3: Topology change by creation of a small cycle .

Turnpike Definition

- Dynamic optimal control problem: (optimal solution $(x(t), u(t))$)

$$\min_{u \in L_2(0,T;U)} \int_0^T J(x(t), u(t))dt$$

$$\text{s.t. } \dot{x}(t) = \mathcal{A}x(t) + \mathcal{B}u(t) + f(x(t), u(t)), \; x(0) = x_0$$

- Corresponding steady state system: (optimal solution $(\bar{x}, \bar{u})$)

$$\min_{u \in U} J(x, u) \quad \text{s.t.} \, 0 = \mathcal{A}x + \mathcal{B}u + f(x, u)$$

- $(x, u) \in C(0, T; X) \times L_2(0, T; U)$ satisfies the **exponential turnpike property**, if there is a constant $c > 0$ and a decay parameter $\mu > 0$, both independent of T such that

$$\|x(t) - \bar{x}\|_X + \|u(t) - \bar{u}\|_U \leq c \left(e^{-\mu t} + e^{-\mu(T-t)} \right)$$

- For long time horizons, in the interior of the time interval, the solutions to the dynamic optimal control problems are approximated by the solutions to the corresponding static optimal control problem.

Turnpike Property

If the turnpike property occurs for the optimal control problem for evolution state equation and the tracking type cost, then the optimum design of control systems can be performed for the steady state equation.
See the references in the linear case:

- Gugat, Martin; Sokolowski, Jan. *An aspect of the turnpike property. Long time horizon behavior.* Serdica Math. J. 49 (2023), no. 1-3, 127-154.
- Gugat, Martin; Qian, Meizhi; Sokolowski, Jan. *Network Design and Control: Shape and Topology Optimization for the Turnpike Property for the Wave Equation.* J. Geom. Anal. 34 (2024), no. 9, Paper No. 273.

See the references in the nonlinear case:

- Emmanuel Trélat, Enrique Zuazua *The turnpike property in finite-dimensional nonlinear optimal control.* J. Differential Equations, 258.1 (2015): 81-114.
- Noboru Sakamoto, Enrique Zuazua *The turnpike property in nonlinear optimal control - a geometric approach.* Automatica 134 (2021), Paper No. 109939, 11 pp.

Graph

- Optimum design: selection of geometry of the graph
- Shape optimization: selection of the length of edges
- Topology optimization: nucleation of small cycles at central nodes of tree

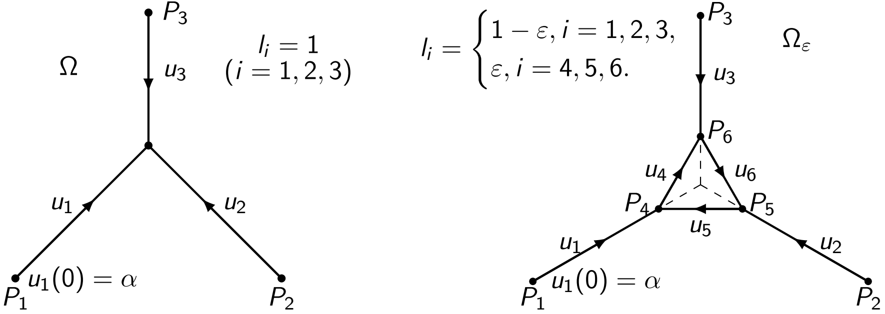


Fig. 4: The three-star graph (left) and tripod-directed network with a cycle (right)

Statement of the problem for three-star graph

- Tracking type cost functional:

$$J := \sum_{i=1}^{3} \int_0^1 F_i(x, u_i(x), f_i(x))\mathrm{d}x, \tag{3}$$

where

$$F_i(x, u_i, f_i) = \frac{1}{2}(u_i - u_i^*(x))^2 + \frac{1}{2}(f_i - f_i^*(x))^2,$$

$u_i^*(\cdot)$, $f_i^*(\cdot)$ are given (**desired**) smooth functions.

- State equation:

$$-u_i''(x) = \varphi_i\left(u_i\left(x\right)\right) + f_i(x),\ x \in [0,1],\ i = 1,2,3 \tag{4}$$

- Boundary condition: $u_1(0) = \alpha,\ u_2(0) = 0,\ u_3(0) = 0$
- Continuity condition: $u_1(1) = u_2(1) = u_3(1)$
- Kirchhoff condition: $u_1'(1) + u_2'(1) + u_3'(1) = 0$
- $u_i : [0,1] \to \mathbb{R}$, twice continuously differentiable functions (**state variables**)
- $f_i : [0,1] \to \mathbb{R}$, continuous functions (**controls**)
- φ_i: a **nonlinear operator** that described the behavior

Local Minimum Principle

- First-order differential equations introducing additional variables $v_i(x)$:

$$
\begin{aligned}
u_i'(x) &= v_i(x), \\
-v_i'(x) &= \varphi_i\left(u_i\left(x\right)\right) + f_i(x),\ x \in [0,1],\ i = 1,2,3
\end{aligned}
$$

with the boundary and transmission conditions

$$
\begin{aligned}
&u_1(0) = \alpha,\ u_2(0) = 0,\ u_3(0) = 0, \\
&u_1(1) = u_2(1) = u_3(1),\ v_1(1) + v_2(1) + v_3(1) = 0.
\end{aligned}
$$

- Hamiltonian formula:

$$
H = \sum_{i=1}^{3} p_i v_i - \sum_{i=1}^{3} q_i(\varphi_i(u_i) + f_i) + \lambda_0 \sum_{i=1}^{3} F_i(x, u_i, f_i),
$$

where p_i, q_i are adjoint variables and $\lambda_0 \geq 0$ is the Lagrange cost multiplier.

- Partial derivatives H_{u_i}, H_{v_i}, H_{f_i} are as follows

$$
\begin{aligned}
H_{u_i} &= -q_i \varphi_i'(u_i) + \lambda_0(u_i - u_i^*(x)), \quad H_{v_i} = p_i, \\
H_{f_i} &= -q_i + \lambda_0(f_i - f_i^*(x)).
\end{aligned}
$$

Local Minimum Principle

- Adjoint equation: $-p_i' = H_{u_i}$, $-q_i' = H_{v_i}$
- Optimality conditions: $H_{f_i} = 0$
- Optimality System:

$$
\begin{aligned}
-p_i'(x) &= -q_i(x)\varphi_i'(u_i(x)) + u_i(x) - u_i^*(x), \\
-q_i'(x) &= p_i(x), \\
-q_i(x) &+ f_i(x) - f_i^*(x) = 0, \; i = 1, 2, 3
\end{aligned} \tag{5}
$$

with the transversality conditions

$$
\begin{aligned}
& p_1(1) + p_2(1) + p_3(1) = 0, \\
& q_1(0) = 0, \; q_2(0) = 0, \; q_3(0) = 0, \\
& q_1(1) = q_2(1) = q_3(1).
\end{aligned} \tag{6}
$$

Statement of Problem for Tripod-directed with a Cycle

- State equation:

$$-u_i''(x_i) = \varphi_i\left(u_i\left(x_i\right)\right) + f_i\left(x_i\right),\ x_i \in [0, l_i], \tag{7}$$

where $l_i = 1 - \varepsilon$ $(i = 1, 2, 3)$ and $l_i = \varepsilon$ $(i = 4, 5, 6)$

- Boundary condition:

$$u_1(0) = \alpha,\ \ u_2(0) = 0,\ \ u_3(0) = 0$$

- Continuity and Kirchhoff condition:

$$\begin{aligned}
&\text{at } P_4 : u_1(1-\varepsilon) = u_4(0) = u_5(\varepsilon),\ u_1'(1-\varepsilon) - u_4'(0) + u_5'(\varepsilon) = 0\\
&\text{at } P_5 : u_2(1-\varepsilon) = u_5(0) = u_6(\varepsilon),\ u_2'(1-\varepsilon) - u_5'(0) + u_6'(\varepsilon) = 0\\
&\text{at } P_6 : u_3(1-\varepsilon) = u_6(0) = u_4(\varepsilon),\ u_3'(1-\varepsilon) - u_6'(0) + u_4'(\varepsilon) = 0
\end{aligned}$$

- Tracking cost function:

$$J = \sum_{i=1}^{6} \int_0^{l_i} F_i\left(x_i, u_i\left(x_i\right), f_i\left(x_i\right)\right) \mathrm{d}x_i$$

Optimality conditions

- State equation:

$$u_i'(x) = v_i(x), -v_i'(x) = \varphi_i(u_i(x)) + f_i(x), \; x \in [0, l_i], \; i = 1, \cdots, 6 \quad (8)$$

- Endpoint conditions:

$$\begin{aligned} u_1(0) &= \alpha, \; u_2(0) = 0, \; u_3(0) = 0, \\ u_1(1-\varepsilon) &= u_4(0) = u_5(\varepsilon), \;\; v_1(1-\varepsilon) - v_4(0) + v_5(\varepsilon) = 0, \\ u_2(1-\varepsilon) &= u_5(0) = u_6(\varepsilon), \;\; v_2(1-\varepsilon) - v_5(0) + v_6(\varepsilon) = 0, \\ u_3(1-\varepsilon) &= u_4(\varepsilon) = u_6(0), \;\; v_3(1-\varepsilon) + v_4(\varepsilon) - v_6(0) = 0. \end{aligned} \quad (9)$$

- Adjoint equations:

$$\begin{aligned} -p_i'(x) &= -q_i(x)\varphi_i'(u_i(x)) + u_i(x) - u_i^*(x), \\ -q_i'(x) &= p_i(x), \; i = 1, \ldots, 6. \end{aligned} \quad (10)$$

- Stationarity condition of the Hamiltonian with respect to the control

$$-q_i(x) + f_i(x) - f_i^*(x) = 0, \quad i = 1, \ldots, 6. \quad (11)$$

Optimality conditions

- Transversality condition:

$$\begin{aligned}
&q_1(0) = 0,\ q_2(0) = 0,\ q_3(0) = 0,\\
&p_4(0) = \quad p_1(1-\varepsilon) + p_5(\varepsilon),\ \ q_2(1-\varepsilon) = q_5(0) = q_6(\varepsilon),\\
&p_6(\varepsilon) = -p_2(1-\varepsilon) + p_5(0),\ \ q_3(1-\varepsilon) = q_6(0) = q_4(\varepsilon),\\
&p_4(\varepsilon) = -p_3(1-\varepsilon) + p_6(0),\ \ q_1(1-\varepsilon) = q_4(0) = q_5(\varepsilon).
\end{aligned} \tag{12}$$

- Optimality system:

$$\begin{cases}
\text{State equation Eq.(8)}\\
\text{Adjoint equation Eq.(10)}\\
\text{Stationarity conditions Eq.(11)}\\
\text{Endpoint conditions for } u_i \text{ Eq.(9)}\\
\text{Transversality conditions for } q_i \text{ Eq.(12)}
\end{cases}$$

Numerical Example

- The behavior is described by the function
$$\varphi_i(u_i) = u_i - u_i^2. \tag{13}$$
- Set $\varepsilon_0 = 0.2$, $\varepsilon_{\max} = 0.5$, $\varepsilon \in (0, \varepsilon_{\max})$, $l_i^* = l_i(\varepsilon_0)$
- $u_i^* = \begin{cases} x^3 - 2\,(1-\varepsilon_{\max})x^2 + (1-\varepsilon_{\max})^2 x, \ \ x \in (0, 1-\varepsilon_{\max}) \\ 0, \ x \in (1-\varepsilon_{\max}, 1-\varepsilon_0), i = 1, 2, 3 \end{cases}$
  $u_i^* = 0, \ i = 4, 5, 6,$
- $f_i^* = -(u_i^*)'' - \varphi(u_i^*), \ i = 1, \cdots, 6.$
- $J = \sum_{i=1}^{6} \int_0^{l_i} \left((u_i(x) - u_i^*(x))^2 + (f_i(x) - f_i^*(x))^2 \right) \mathrm{d}x_i + \frac{1}{2}\,(l_i - l_i^*)^2 \to \min$

Numerical Discretization

- The optimality system of equations can be written as

$$\begin{cases} -u''(x) = u_i(x) - u_i^2(x) + f_i^*(x) + q_i(x), \\ q_i''(x) = -q_i(x) + 2q_i(x)u_i(x) + u_i(x) - u_i^*(x), \\ \text{Endpoint constraints and transversality conditions for } u_i, q_i,\ i = 1, \dots, 6 \end{cases}$$

- The weak form:

$$\sum_{i=1}^{6} \int_0^{l_i} \left(u_i'\psi_i' - u_i\psi_i + u_i^2\psi_i + q_i\psi_i \right) = \sum_{i=1}^{6} \int_0^{l_i} f_i^*\psi_i,$$

$$\sum_{i=1}^{6} \int_0^{l_i} \left(q_i'\psi_i' - q_i\psi_i + 2u_iq_i\psi_i + u_i\psi_i \right) = \sum_{i=1}^{3} \int_0^{l_i} u_i^*\psi_i,$$

- Space discretize: $\mathbb{P}_2$ (quadratic) finite element method
- Handle the nonlinear component: Newton method

Numerical Results

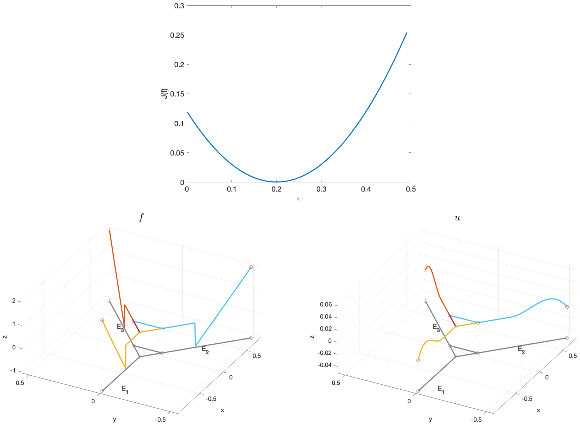


Fig. 5: The shape functional for $\varepsilon \in (0, 0.5)$ (top), optimal control f and state u for $\varepsilon = \varepsilon_0$ (bottom left and right).

Topological derivatives for networks

In the above example the topological derivative is given by the derivative of optimal cost for control problem at $\varepsilon = 0^+$.

1. Introduced in linear case for the energy functional by G. Leugering and J.S.
2. For Timoshenko beams and the elastic energy obtained by Ogiermann in his dissertation
3. For Control problems introduced by J.S. and A. Zochowski
4. For Control problems on networks developped by Meizhi Qian in her dissertation

Conclusion and Future

- Conclusion
  - Using the *Turnpike Property* for dynamic control problem, the control problem is solved for the steady state equations
  - Optimal control problem combined with the optimum design problem in one optimization problem on 3-star metric graph
  - The necessary and sufficient optimality conditions are established for static control problems
  - Numerical example for the nonlinear static state equation on networks
- Future
  - Topological derivatives for network of geometrically exact beams in the static setting
  - Shape optimum design of networks with geometrically exact beams for optimal control problems

Thanks for your attention!