Optimal State and Parameter Estimation Algorithms

Theory and Applications

Olga Mula (TU Eindhoven)

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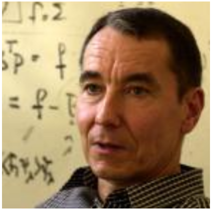
Agenda

1. Optimal Benchmarks for State Estimation
2. A near-optimal, implementable piecewise affine algorithm
3. Applications and current developments:
    - Biomedical Problems
    - Shape recovery [Agustin Somacal]
    - Hamiltonian Problems [Federico Vismara]
    - Conservation Laws and Wasserstein Gradient Flows [Pratik Rai]
    - Wasserstein PDE-G-CNN [Daan Bon]

Methodology:

(a) A. Cohen



(b) W. Dahmen

(c) J. Nichols

Biomedical Applications:

(d) F. Galarce

(e) J.F. Gerbeau

(f) Lombardi

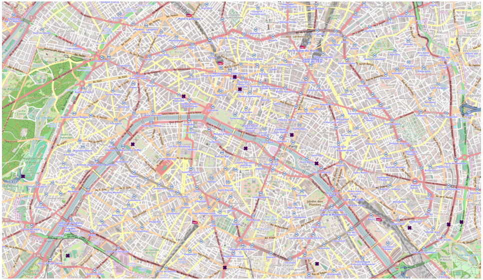
Part I

Optimal Reconstruction Benchmarks for State Estimation

Ref: [Mul23] **Inverse Problems: A Deterministic Approach using Physics-Based Reduced Models**. O. Mula (Lecture Notes, submitted, 2021)

What is an Inverse Problem?

In *Inverse Problems*, we aim to find the cause of an observed effect.



Priors:

- Regularity/Sparsity
- PDE
  - Bayesian
  - **Deterministic**

Mathematical setting

Ambient space V:

- Hilbert space over a domain $\Omega \subset \mathbb{R}^d$.
- Potentially very high or infinite dimension.

Parametrized PDE to model physical system:

$$\mathcal{B}(u, \theta) = f(\theta)$$

where

$$\theta = (\theta_1, \dots, \theta_p) \in \Theta \subset \mathbb{R}^p$$

is a vector of parameters ranging in some domain $\Theta \subset \mathbb{R}^p$.

Solution manifold:

$$\mathcal{M} := \{u(\theta) \, : \, \theta \in \Theta\} \subset V$$

is the set of all admissible solutions.

Mathematical setting

Forward problem/Model Order Reduction:

Given (many) $\theta \in \Theta$, compute $u(\theta)$.

Inverse problem: For an unknown $u = u(\theta)$ with unknown $\theta \in \Theta$, we observe a vector of linear measurements

$$z = (z_1, \dots, z_m) \in \mathbb{R}^m$$

where

$$z_i = \ell_i(u) = \langle \omega_i, u \rangle, \quad i = 1, \dots, m.$$

and $\ell_i \in V'$ are indep. linear functionals. Riesz representers: $\omega_i \in V$.

We want to invert the cascade of forward mappings:

$$\theta \in \Theta \subset \mathbb{R}^p \quad \mapsto \quad u(\theta) \in \mathcal{M} \quad \mapsto \quad z = \ell(u) \in \mathbb{R}^m$$

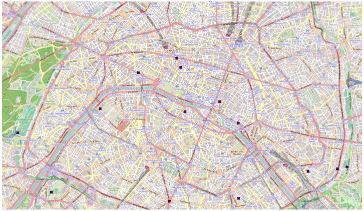
The $\ell_i \leftrightarrow \omega_i$ model the sensor response.

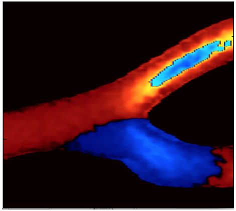
Their form is a given data of the problem.

Some examples:

Type	V	$\ell_i(u)$	ω_i
Pointwise	RKHS	$\delta_{x_i}(u) = u(x_i)$	k_{x_i}
Local average	$L^2(\Omega)$	$\int_\Omega e^{-\frac{\|\|x-x_i\|\|^2}{\sigma^2}} u(x)\mathrm{d}x$	$e^{-\frac{\|\|x-x_i\|\|^2}{\sigma^2}}$
Local average	$H^1_0(\Omega)$	$\int_\Omega e^{-\frac{\|\|x-x_i\|\|^2}{\sigma^2}} u(x)\mathrm{d}x$	(*)

$$\langle \omega_i, v(x) \rangle_{H^1_0(\Omega)} = \int_\Omega \nabla \omega_i \cdot \nabla v(x)\mathrm{d}x = \ell_i(v), \forall v \in H^1_0(\Omega) \qquad (*)$$





Mathematical setting

In inverse problems, we want to invert the cascade of forward mappings:

$$\theta \in \Theta \subset \mathbb{R}^p \quad \mapsto \quad u(\theta) \in \mathcal{M} \quad \mapsto \quad z = \ell(u) \in \mathbb{R}^m$$

Types of inverse problems:

- **State Estimation:**

$$z \mapsto u^*(z) \approx u$$

- **Parameter Estimation:**

$$z \mapsto y^*(z) \approx y$$

  when $z = \ell(u(\theta))$.

- In time-dependent problems: find initial condition, forecast of u...

Severely ill-posed problems when $p > m$.

State Estimation

Running Assumptions: No noise, no model error.

Goal: From the unknown $u \in \mathcal{M}$, we are given

$$\ell_i(u) = \langle \omega_i, u \rangle, \quad i = 1, \dots, m,$$

Defining the *observation space*

$$W := \mathrm{span}\{\omega_1, \dots, \omega_m\} \subset V$$

we have the equivalence

$$\ell_i(u), i = 1, \dots, m \quad \Leftrightarrow \quad \omega = P_W u.$$

Our task is to find a reconstruction algorithm

$$A : W \to V$$

such that $A(P_W u)$ approximates the state u.

Remark: A is a decoder.

Optimal reconstruction algorithms

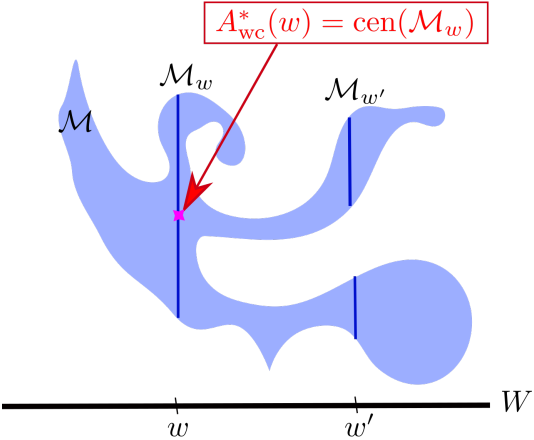
Quality of $A : W \to V$:

$$E(A, \mathcal{M}) = \max_{u \in \mathcal{M}} ||u - A(P_W u)||$$

Optimal performance among all algorithms:

$$E^*(\mathcal{M}) = \min_{A: W \to V} E(A, \mathcal{M}).$$

There is a simple mathematical description of an optimal map A^*.



Practical issue: $A^*_{\rm wc}$ is not easily computable since $\mathcal{M}$ may have a complicated geometry which is in general not given explicitly.

Part II

An implementable piecewise affine algorithm that meets the benchmark

▷ Linear/Affine algorithms

- Nonlinear piecewise affine algorithms

Ref: [CDD$^+$20] **Optimal Affine reduced model algorithms for data-based state estimation** (SINUM, 2020)

Affine reconstruction algorithms

Definition:

Let $\overline{V}_n = \bar{u} + V_n$ be an affine subspace with $1 \leq n \leq m$. The mapping

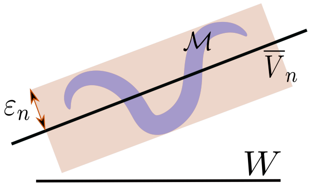
$$A : W \to V$$
$$\omega \mapsto A(\omega) := \underset{v \in \omega + W^\perp}{\arg\min}\ \mathrm{dist}(v, \overline{V}_n)$$

is an affine algorithm in the sense that

$$A(\cdot - P_W \bar{u}) \in V_n \oplus (W \cap V_n^\perp).$$

Performance: $E(A, \mathcal{M}) \leq \beta_{n,m}^{-1} \varepsilon_n$

$$\varepsilon_n := \max_{u \in \mathcal{M}} \mathrm{dist}(u, \overline{V}_n), \quad \beta_{n,m} := \inf_{v \in V_n} \frac{\|P_{W_m} v\|}{\|v\|} = \cos(\theta_{V_n, W_m}) \in (0, 1]$$



Choice of $\overline{V}_n$:

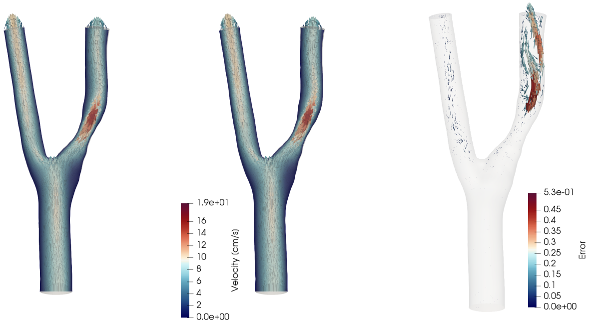
- **Optimal** $\overline{V}_n$ (see [CDD+20])
  $\rightsquigarrow$ "Optimize over $\beta_{n,m}\varepsilon_n$".
- **Reduced Order Models** (PBDW, GEIM, see [MPPY15, MM13])
  $\rightsquigarrow$ Conceived for forward problem
  $\rightsquigarrow$ Build $\overline{V}_n$ with good ε_n
  $\rightsquigarrow$ ε_n decays fast with n in elliptic/parabolic problems.
- **"Multi-purpose" spaces** such as Fourier expansions (Compressed Sensing literature, see [AHP13])

Sensor placement:

Fix $\overline{V}_n$, build W from a dictionary $\mathcal{D}$, see [BCMN18].

Setting:

- Parametric Navier Stokes equations
  $\rightarrow \mathcal{M} \approx V_n = \text{span}\{(v_i, p_i)\}_{i=1}^n$.
- W_m: Doppler velocity observations.
- State estimation of (v, p), and quantities of interest.



u $\quad$ u^* $\quad$ $u - u^*$

Example 2: Flow past a cylinder

VIDEO

An implementable piecewise affine algorithm that meets the benchmark

- Linear/Affine algorithms
- ▷ Piecewise affine algorithms

Ref: [CDMN22] **Nonlinear reduced models for state and parameter estimation** (SIAM JUQ, 2022)

Limitations of Affine Algorithms

We have that

$$E^*(\mathcal{M}) = \min_{\substack{A:W\to V \\ A \text{ any mapping}}} E(A,\mathcal{M}) \le d_{m+1}(\mathcal{M}) \le \min_{\substack{A:W\to V \\ A \text{ affine}}} E(A,\mathcal{M}),$$

where

$$d_{m+1}(\mathcal{M}) := \min_{\substack{Z\subseteq V \\ \dim(Z)\le m+1}} \max_{u\in\mathcal{M}} \|u - P_Z u\|$$

is the Kolmogorov $m+1$-width.

Depending on $\mathcal{M}$ and W, we may have

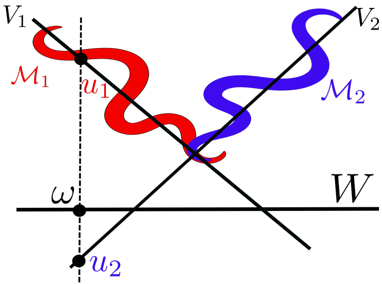
$$E^*(\mathcal{M}) \ll d_{m+1}(\mathcal{M}).$$

This problem typically arises in elliptic PDEs with loss of coercivity and in hyperbolic PDEs.

Piecewise-affine algorithms

Consider a partition of the parameter domain

$$\Theta = \Theta_1 \cup \cdots \cup \Theta_K \quad \rightsquigarrow \mathcal{M} = \mathcal{M}_1 \cup \cdots \cup \mathcal{M}_K.$$



Model selection

We would like to select the reconstruction that is closest to $\mathcal{M}$

$$k^* = k(\omega) = \mathrm{argmin}_{k=1,\dots,K} \mathrm{dist}(A_k(\omega), \mathcal{M}),$$

but

$$\mathrm{dist}(A_k(\omega), \mathcal{M}) := \min_{\theta\in\Theta} \|u(\theta) - A_k(\omega)\|.$$

is not easily computable.

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but

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is not easily computable.

In uniformly coercive problems, we have that the residual

$$\mathcal{R}(v, \theta) := \| \mathcal{B}(\theta) v - f(\theta) \|^2_{V'}, \quad \forall (v, \theta) \in V \times \Theta$$

is uniformly equivalent to the ambient norm

$$r \| v - u(\theta) \|_V \le \mathcal{R}(v, \theta) \le R \| v - u(\theta) \|_V, \quad \forall v \in V.$$

We can thus equivalently compute for all $k = 1, \dots, K$

$$\min_{\theta \in \Theta} \mathcal{R}(A_k(\omega), \theta) \quad \xrightarrow[\min_{k=1,\dots,K}]{} \quad \hat{k}(\omega),\ \hat{y}(\omega)$$

This is a convex problem in affinely parametrized PDEs.

Model selection

Theorem 1 (Cohen, Dahmen, Mula, Nichols, 2021)

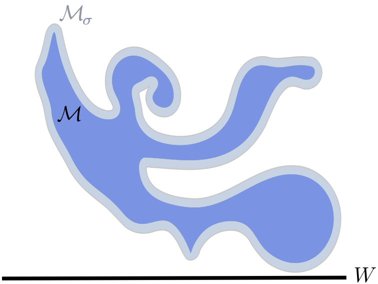
For a given target tolerance $\sigma > 0$, we can find a partition of $\mathcal{M}$ s.t.

$$E^*(\mathcal{M}) \leq E(A_{\hat{k}}, \mathcal{M}) \leq E^*(\mathcal{M}_\sigma)$$

where $\hat{k}$ comes from our model selection on the residual.

We can make $\sigma \to 0$ by increasing K (with dyadic splittings).

σ can also account for noise and model error in the analysis.



Model selection

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Merits and Limitations:

- ✓ General algorithm.
- ✓ Good efficiency if few partitions (elliptic, parabolic pbs with possibly weak coercivity)
- ✗ In transport-dominated problems, for a given target $\sigma > 0$ too many partitions may be required.

Part III

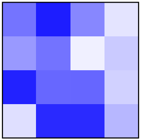
Numerical illustration on an academic example

Ref: [CDMN22] **Nonlinear reduced models for state and parameter estimation** (SIAM JUQ, 2022)

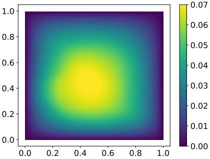
Elliptic PDE with piecewise constant diffusion field

$$-\operatorname{div}(a(x,\theta)\nabla u(x,\theta)) = 1 \text{ on } \Omega = [0,1]^2, \ (\text{well-posed in } V = H^1_0(\Omega))$$

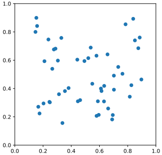
$$a = a(x,\theta) = 1 + \sum_j c_j \theta_j \chi_{D_j}(x), \ \theta = (\theta_j) \in [-1,1]^{16}, \ \ell_i(u) = \int_\Omega e^{-\frac{||x-x_i||^2}{\sigma^2}} u(x)\mathrm{d}x$$



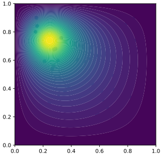
$a(x,\theta)$



$u(\theta)$



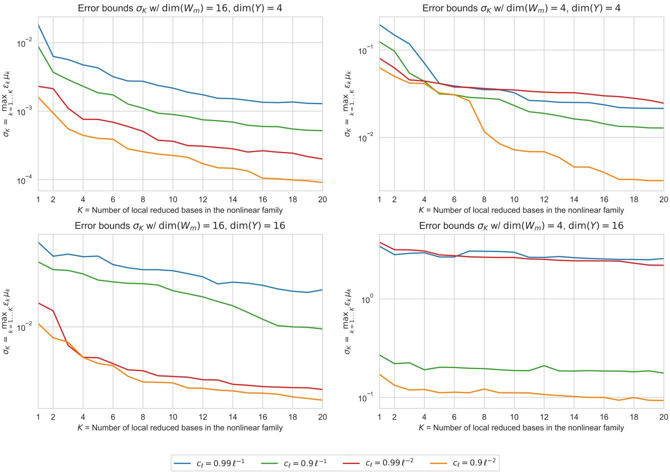
Pos. Sensors



w_i

$$c_j = \begin{cases} 0.9 j^{-2} & \text{elliptic ++} \\ 0.99 j^{-2} & \text{elliptic +} \\ 0.9 j^{-1} & \text{elliptic -} \\ 0.99 j^{-1} & \text{elliptic - -} \end{cases}$$

Numerical example



Part IV

Application to biomedical problems

(g) F. Galarce

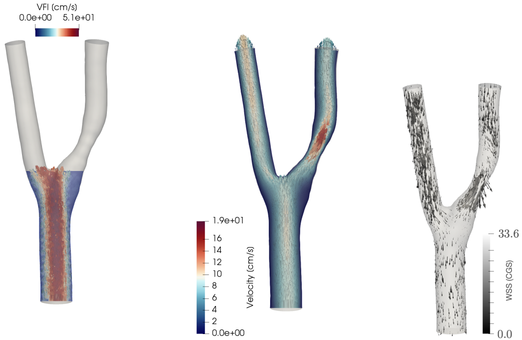
(h) J.F. Gerbeau

(i) Lombardi

Ref: [GLM22] **State Estimation with Shape Variability. Application to biomedical problems.** (SISC, 2022)

State Estimation on Carotid Arteries

Problem 1: Given a carotid artery Ω, reconstruct quickly the 3D velocity and pressure fields from Doppler US velocity measurements.

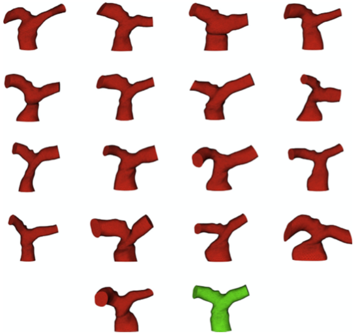


Strategy: (see [GGLM21, GLM21])

- Parametric Navier Stokes equations $\rightarrow \mathcal{M} \approx V_n.$
- Affine Algorithm for State estimation $\rightarrow V_n,\ W_m.$

State Estimation on Carotid Arteries

Problem 2: The morphology of the carotid varies for each patient.



Goal: Given a new target carotid Ω, provide a fast reconstruction.

Roadmap:

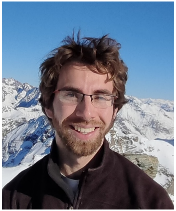
- Direct computation of V_n^Ω would take too long.
- Use pre-computations on a database of carotids.

Part V

Shape reconstruction with nonlinear V_n

(j) A. Somacal (Sorbonne)

(k) A. Cohen (Sorbonne)

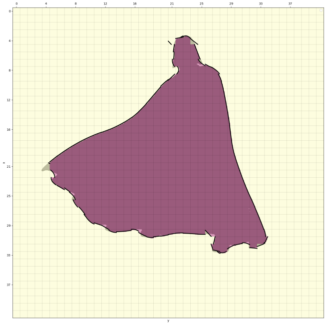


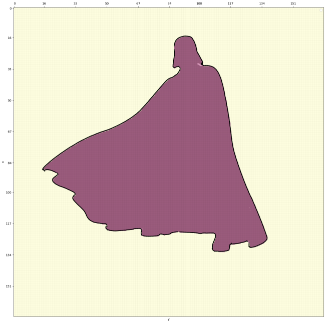
(l) M. Dolbeault (Sorbonne)

Ref: [CDMS22] **Nonlinear approximation spaces for inverse problems.** Analysis and Applications (2023).

Shape reconstruction to subcell resolution

- $\ell_i(u)$ = "cell averages"
- V_n = "Indicator functions of a family of curves on each cell"





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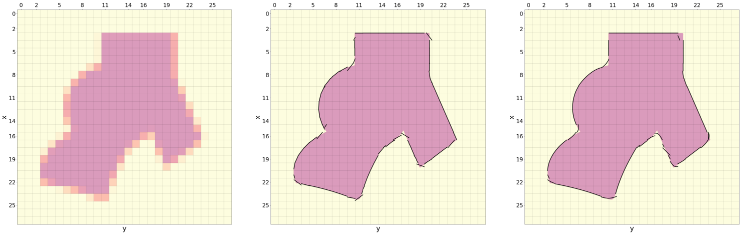

Figure: 28×28 grid

Shape reconstruction to subcell resolution

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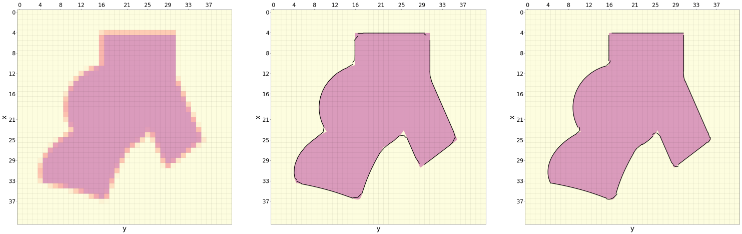


Figure: 42×42 grid

Part VI

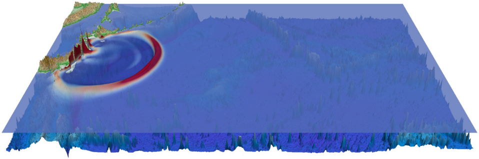
Hamiltonian problems

(a) F. Vismara (TU/e)

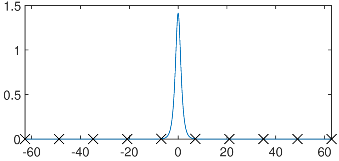
(b) C. Pagliantini (U. Pisa)

Ref: [MPV] **State Estimation of Hamiltonian systems with dynamical low rank reduced models.** In preparation.

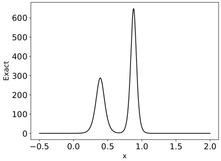
Difficulty: Transport of local features



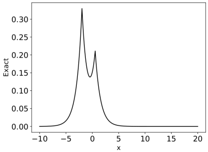
Shallow-water



Schrödinger



KdV



Camassa-Holm

- Transport effects are challenging for state estimation.
- Exploit geometry, and group structure.

State Estimation

Goal: Approximate an unknown function $u = u(\cdot, \theta^\dagger) \in \mathcal{M} \subset \mathcal{C}^1(\mathbb{T}, V)$.

Data: We do not know $\theta^\dagger$ but instead we are given m observations

$$z_i(t) = \ell_i(u(t)) = \langle \omega_i, u(t) \rangle_V \,, \quad i = 1, \dots, m,$$

where $\ell_i \in V'$ are given indep. linear functionals.

Defining the observation space

$$W_m := \mathrm{span}\{\omega_1, \dots, \omega_m\} \subset V$$

we have the equivalence

$$z_i(t) = \ell_i(u), i = 1, \dots, m \quad \Leftrightarrow \quad \omega(t) = P_{W_m} u(t).$$

Task: Build $A : \mathbb{T} \to \mathcal{F}(W_m, V)$ such that for all $t \in \mathbb{T}$

$$A(t)(\omega(t)) = A\left(t, \omega(t)\right) \approx u(t) \in V.$$

A must respect the Hamiltonian structure.

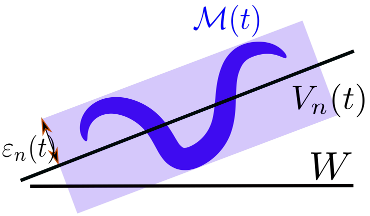
Dynamical linear reconstruction algorithms

Definition:
For a given $t \in \mathbb{T}$, let $V_n(t)$ be a linear subspace ($1 \leq n \leq m$).
The mapping

$$\begin{aligned} A(t) : W_m &\to V_n(t) \oplus (W_m \cap V_n^\perp(t)) \subset V \\ \omega &\mapsto A(\omega) := \underset{v \in \omega + W_m^\perp}{\arg\min}\ \mathrm{dist}(v, V_n(t)) \end{aligned}$$

is a linear algorithm in the sense that $A(t) \in \mathcal{L}(W_m, V)$.

Performance: $E(A(t), \mathcal{M}(t)) \leq \beta_{n,m}^{-1}(t)\, \varepsilon_n(t)$

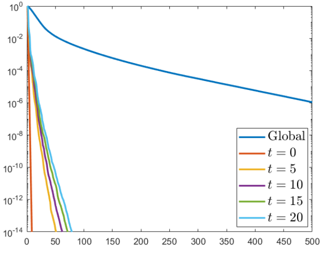


$$\varepsilon_n(t) := \max_{u(t) \in \mathcal{M}(t)} \mathrm{dist}(u(t), V_n(t)),$$

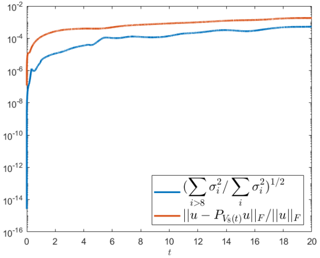
$$\beta_{n,m}(t) := \inf_{v \in V_n(t)} \frac{\|P_{W_m} v\|}{\|v\|} = \cos(\theta_{V_n(t), W_m}) \in (0, 1]$$

Choice of $V_n(t)$:

- **Optimal** $V_n(t)$ (see [CDD+20])
  - ✗ Computationally demanding.
- **Dynamical low-rank Reduced Order Models** [HP21, Pag21, HPR22]
  - ✓ $\varepsilon_n(t) \to_{n\to\infty} 0$ fast.
  - ✗ No control on $\beta_{n,m}(t)$.



SVD of $\mathcal{M}(t)$ and $\cup_{t\in\mathbb{T}}\mathcal{M}(t)$



$V_8(t)$ vs SVD of $\mathcal{M}(t)$

Choice of W_m:
If measurements give **local** information and we keep W_m constant:

$$\beta_{n,m}(t) \to 0 \text{ as } t \text{ grows}$$

We thus take:

$$W_m = W_m(t) \quad \Rightarrow \quad \beta_{n,m}(t) := \inf_{v \in V_n(t)} \frac{\|P_{W_m(t)} v\|}{\|v\|} = \cos(\theta_{V_n(t), W_m(t)})$$

Strategy: Move sensor locations to maximize $\beta_{n,m}(t)$ for a given $V_n(t)$.

Choice of W_m (Sensor placement)

Choice of W_m:

If measurements give **global** information, we can in principle keep W_m constant and select good ω_i from a dictionary $\mathcal{D}$ with, e.g., a greedy algorithm. [BCMN18]

Dynamical sensor placement

Suppose $V = L^2(\Omega)$. For a given t,

$$\ell_i(u(t)) := \int_\Omega exp\left(-\frac{||x_i(t)-x||^2}{\sigma^2}\right) u(t,x)\mathrm{d}x = \langle \omega_i(t), u(t,\cdot)\rangle_{L^2(\Omega)}\,.$$

Gathering the sensor locations in

$$x(t) = \{x_i(t)\}_{i=1}^m \in \left(\mathbb{R}^d\right)^m,$$

we thus have

$$W_m(x(t)) := \{\omega_i(x_i(t))\}_{i=1}^m$$

with

$$\omega_i(x_i(t)) = \exp\left(-\frac{||x_i(t)-x||^2}{\sigma^2}\right)$$

Dynamical sensor placement

Suppose we know $V_n(t)$ for $[t, t+\Delta t]$.

We search for the sensors' optimal path

$$x : [t, t+\Delta t] \to \mathbb{R}^m$$

which maximizes stability in $[t, t+\Delta t]$

$$\max_{\substack{x:[t,t+\Delta t]\to\mathbb{R}^m \\ x(t)=a \\ \dot{x}(t)=b}} \int_t^{t+\Delta t} \left(\beta(V_n(t), W_m(x(t))) - \frac{\lambda}{2} \|\dot{x}(t)\|^2 \right) \mathrm{d}\tau,$$

where $\lambda > 0$ penalizes unphysically large velocities.

Dynamical sensor placement

Denoting

$$z(t) = (x(t), \dot{x}(t))^T,$$

the Euler-Lagrange equations yield:

$$\dot{z}(t) = \begin{bmatrix} z_2(t) \\ -\frac{1}{\lambda}\nabla_x \beta(z_1(\tau)) \end{bmatrix}$$

and a time integration scheme yields the evolution of the sensor locations.

Any scheme requires knowing how to compute

$$\nabla_x \beta(x).$$

Computing $\nabla_x \beta(x)$

We can prove that

$$\beta(x) = \lambda_{\min}(x)$$

where $\lambda_{\min}$ is the smallest eigenvalue of

$$\mathbb{M}(x) = \left(\left\langle P_{W_m(x)} v_i(t), P_{W_m(x)} v_j(t) \right\rangle_{L^2(\Omega)} \right)_{1 \le i,j \le 2n}$$

So there exists an eigenvector $q(x)$ such that

$$\begin{aligned} & \mathbb{M}(x) q(x) = \beta(x) q(x) \\ \Rightarrow \quad & \beta(x) = q^T(x) \mathbb{M}(x) q(x), \quad q^T(x) q(x) = 1. \end{aligned}$$

It follows that

$$\frac{\partial \beta}{\partial x_i}(x) = q^T(x) \frac{\partial \mathbb{M}}{\partial x_i}(x) q(x).$$

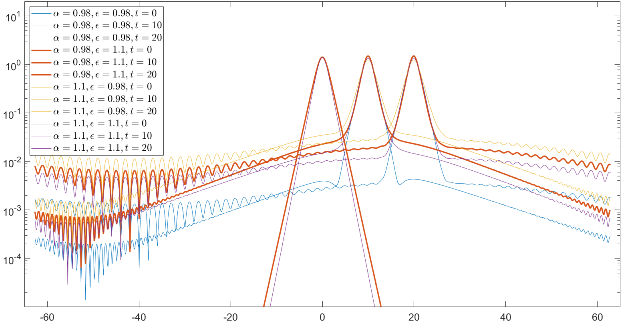
and a tedious calculation yields $\frac{\partial \mathbb{M}}{\partial x_i}(x)$.

Schrödinger problem in 1D:

$$\begin{cases} iu_t(t,x,\theta) - u_{xx} + \varepsilon |u|^2 u = 0, & \forall (t,x) \in (0,T] \times [-L,L] \\ u(0,x,\theta) = \dfrac{\sqrt{2}}{\cosh(\alpha x)} e^{i\frac{x}{2}} & \end{cases}$$

and

$$\theta = (\varepsilon, \alpha) \in \Theta := [0.98, 1.1]^2, \qquad V = L^2([-L,L]).$$



Static placement

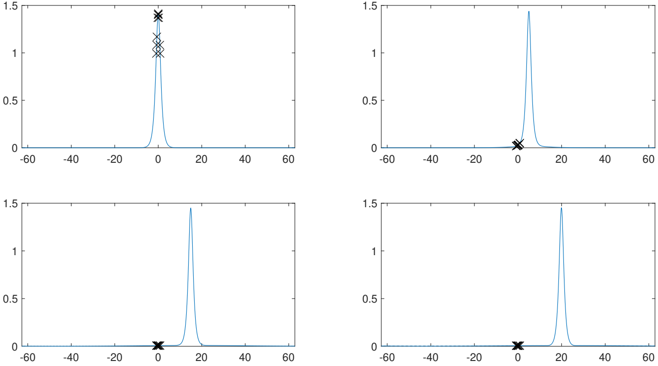


Figure: Static placement, $m = 10$.

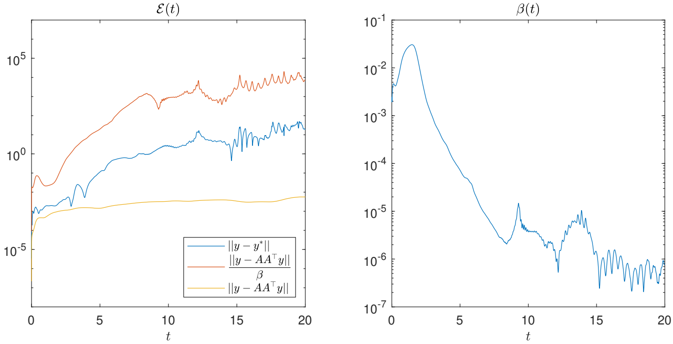


Figure: Left: Reconstruction errors with $n = 8$, $m = 10$. Right: $\beta(t)$.

Dynamical sensor placement

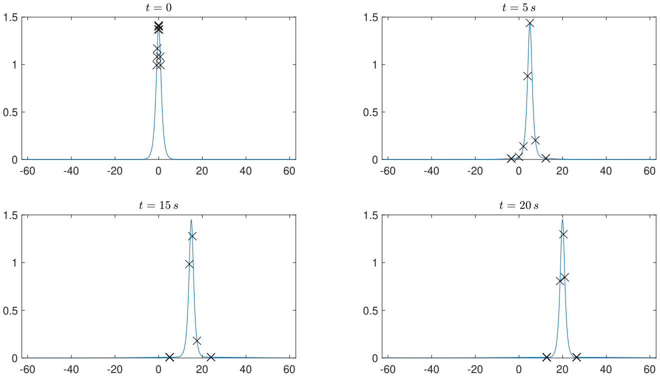


Figure: Dynamical placement of sensors, $m = 10$.

Dynamical sensor placement

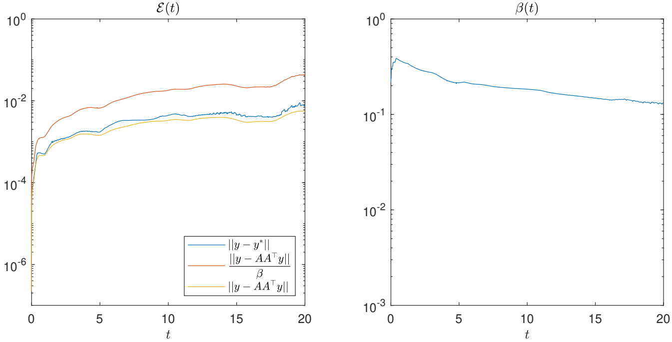
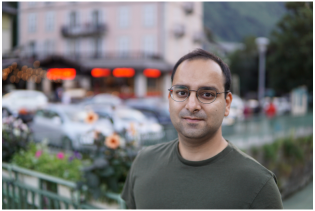


Figure: Left: Reconstruction errors with $n = 8$, $m = 10$. Right: $\beta(t)$.

Part VII

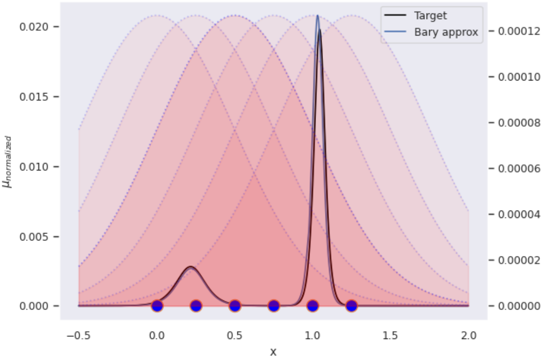
Conservation Laws and Gradient Flows



(a) P. Rai (TU/e)

Ref: [MR23] **State Estimation in Wasserstein spaces.** In preparation.

By extending the formulation to general metric spaces, we can use the Wasserstein model reduction approach for inverse problems in W_2.



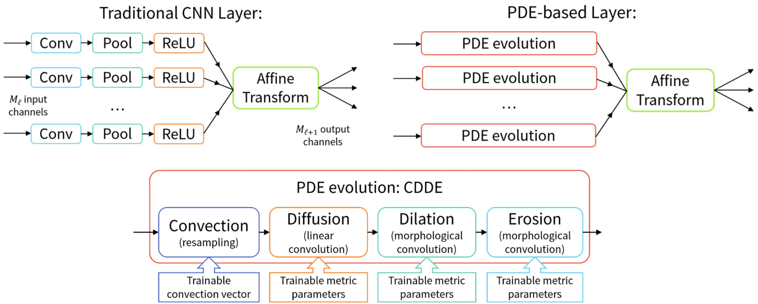
Part VIII

Wasserstein PDE-G-CNN

(b) D. Bon (TU/e)

(c) R. Duits (TU/e)

Ref: [BDM] **Wasserstein PDE-G-CNNs.** In preparation.



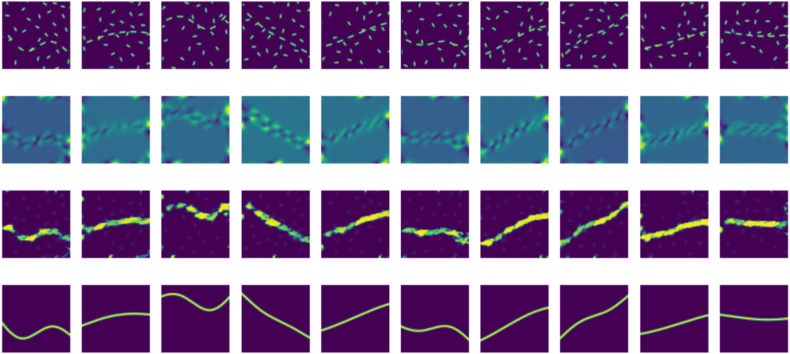
$$\begin{cases} \frac{\partial W}{\partial t}(\boldsymbol{p}, t) & = -\, \boldsymbol{c} W(\boldsymbol{p}, t) - \left(-\Delta_{\mathcal{G}_1}\right)^{\alpha} W(\boldsymbol{p}, t) + \|\nabla_{\mathcal{G}_2^+} W(\boldsymbol{p}, t)\|_{\mathcal{G}_2^+}^{2\alpha} - \|\nabla_{\mathcal{G}_2^-} W(\boldsymbol{p}, t)\|_{\mathcal{G}_2^-}^{2\alpha} \\ W(\boldsymbol{p}, 0) & = f(\boldsymbol{p}) \end{cases} \tag{1}$$

1

Source: B. Smets, J. Portegies, E. Bekkers, and R. Duits. PDE-based group equivariant convolutional neural networks, 2020.

Wasserstein PDE-G-CNN

How to define PDE-G-CNNs for measures? As a first step, we can add the learning of Optimal Transport maps as an extra layer.



Conclusions

- Theoretical foundations for optimal algorithms for state estimation
- Reduced Models are crucial to develop viable algorithms.
- Still plenty of room to develop nonlinear approaches.
- Alternative to bayesian inversion using more deterministic notions of accuracy quantification.
- Extension to problems with shape variability.
- Current works on Hamiltonian systems, conservation laws, Wasserstein gradient flows, and imaging problems.

Material

- Slides: `www.olgamula.com`
- Notebook:

  `https://`
  `//github.com/agussomacal/ROMHighContrast/tree/NonLinearROM`
- Lecture Notes: **Inverse Problems: A Deterministic Approach using Physics-Based Reduced Models**, OM.

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