Optimal State and Parameter Estimation Algorithms

Applications to Biomedical Problems

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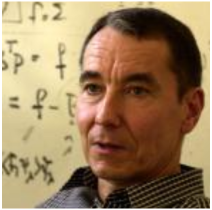
Methodology:

(a) A. Cohen



(b) W. Dahmen

(c) J. Nichols

Biomedical Applications:

(d) F. Galarce

(e) J.F. Gerbeau

(f) Lombardi

Agenda

1. Optimal Benchmarks for State Estimation
2. A near-optimal, implementable piecewise affine algorithm
3. Illustration on an academic example
4. Application to biomedical problems

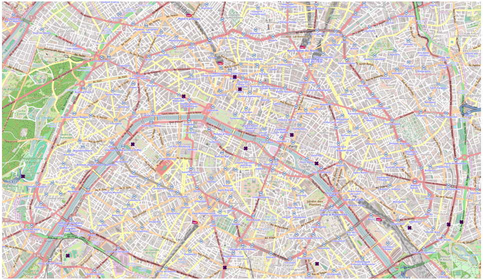
Part I

Optimal Reconstruction Benchmarks for State Estimation

Ref: [Mul21] **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:

$$\mathcal{B}(y)u = f(y)$$

where

$$y = (y_1, \dots, y_p) \in \mathrm{Y} \subset \mathbb{R}^p$$

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

Solution manifold:

$$\mathcal{M} := \{u(y) \,:\, y \in \mathrm{Y}\} \subset V$$

is the set of all admissible solutions.

Forward problem/Model Order Reduction:

$$\text{Given (many) } y \in \mathrm{Y}, \text{ compute } u(y).$$

Inverse problem: For an unknown $u = u(y)$ with unknown $y \in \mathrm{Y}$, we observe a vector of linear measurements

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

where

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

The ℓ_i model the sensor response:

- $\ell_i \in V'$ are indep. linear functionals. Riesz representers: $\omega_i \in V$.
- Examples:
  - $\ell_i(u) = \delta_{x_i}(u) = u(x_i)$
  - $\ell_i(u) = \int_\Omega e^{-\frac{||x-x_i||^2}{\sigma^2}} u(x)\mathrm{d}x$

Mathematical setting

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

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

Types of inverse problems:

- **State Estimation:**

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

- **Parameter Estimation:**

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

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

- 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.

Optimal reconstruction algorithms

Quality of $A : W \to V$:

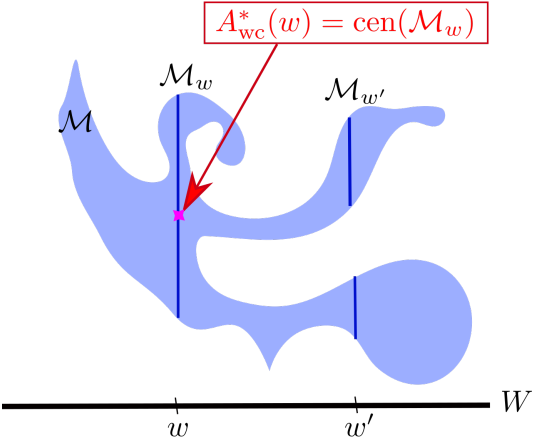
$$E(A, \mathcal{M}) = \max_{u \in \mathcal{M}} ||u - A(P_W u)||$$

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^*.

An optimal algorithm A^*. Not feasible in practice.



Practical issue: A^*_{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 $1 \le n \le m$. The mapping

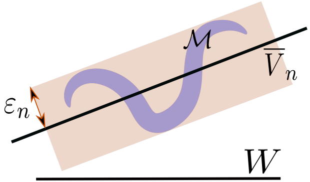
$$A : W \to V$$
$$\omega \mapsto A(\omega) := \underset{v \in \omega + W^\perp}{\arg\min}\ \mathrm{dist}(v, \overline{V}_n)$$

is an affine algorithm in the sense that

$$A(\cdot - P_W \bar{u}) \in \mathcal{L}(W, V).$$

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

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



Choice of $\overline{V}_n$ and W

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].

Limitations of Affine Algorithms

We have that

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

where

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

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.

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)

Piecewise-affine algorithms

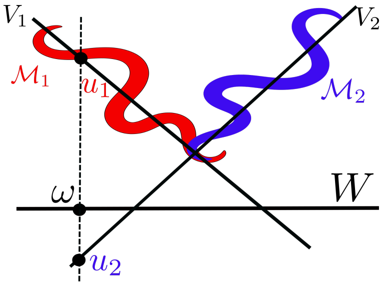
Consider a partition of the parameter domain

$$\mathrm{Y} = \mathrm{Y}_1 \cup \cdots \cup \mathrm{Y}_K \quad \rightsquigarrow \mathcal{M} = \mathcal{M}_1 \cup \cdots \cup \mathcal{M}_K.$$

For each $\mathcal{M}_k$, we may find an appropriate $\overline{V}_k$, and define A_k.

From the given data $\omega = P_W u$, we need to select between the reconstructions

$$u_k = A_k(\omega), \quad k = 1, \dots, K.$$



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

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

is not easily computable.

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is not easily computable.

In uniformly coercive problems, we have that the residual

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

is uniformly equivalent to the ambient norm

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

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

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

This is a convex problem in affinely parametrized PDEs.

Model selection

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

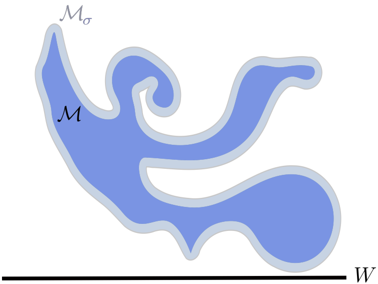
For a given target tolerance $\sigma > 0$, we can find a partition of $\mathcal{M}$ s.t.

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

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

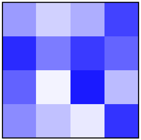
Numerical illustration on an academic example

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

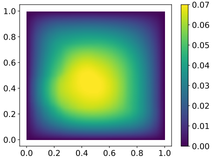
Elliptic PDE with piecewise constant diffusion field

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

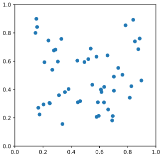
$$a = a(x,y) = 1 + \sum_j c_j y_j \chi_{D_j}(x),\; y = (y_j) \in [-1,1]^{16},\; \ell_i(u) = \int_\Omega e^{-\frac{||x-x_i||^2}{\sigma^2}} u(x)\mathrm{d}x$$



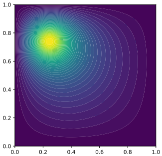
$a(x,y)$



$u(y)$



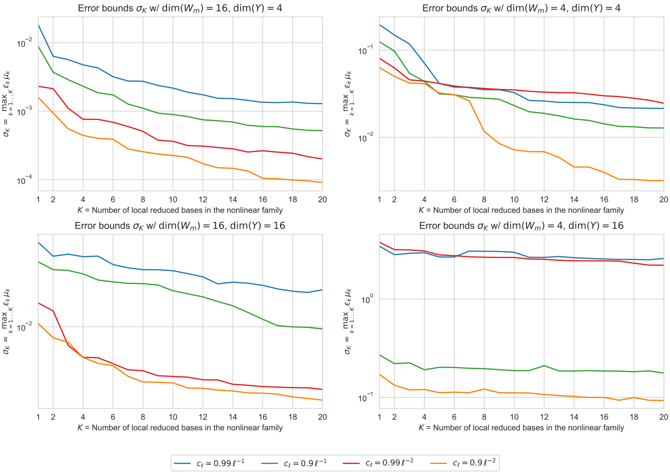
Pos. Sensors



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



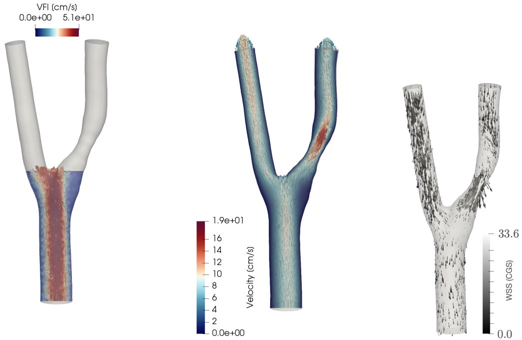
Part IV

Application to biomedical problems

Ref: [GLM21b] **State Estimation with Shape Variability. Application to biomedical problems.** (SISC, 2022)

Motivation: 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.

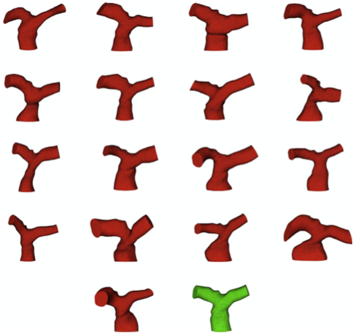


Strategy: (see [GGLM21, GLM21a])

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

Motivation: 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.

Conclusions

- Theoretical foundations for state estimation with reduced models.
- Some results on parameter estimation.
- Alternative to bayesian inversion using more deterministic notions of accuracy quantification.
- Extension to problems with shape variability.

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