Optimal State and Parameter Estimation Algorithms

Applications to Biomedical Problems

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Agenda

- Optimal Benchmarks for State Estimation
- A near-optimal, implementable piecewise affine algorithm
- Illustration on an academic example
- Application to biomedical problems
Part I

Optimal Reconstruction Benchmarks for State Estimation

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

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

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

Solution manifold:

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

is the set of all admissible solutions.
Forward problem/Model Order Reduction:

Given (many) \( y \in Y \), compute \( u(y) \).

Inverse problem: For an unknown \( u = u(y) \) with unknown \( y \in Y \), 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 \( \ell_i \) model the sensor response:

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

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

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

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 \( p > m \).
Running Assumptions: No noise, no model error.

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

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

Defining the observation space

$$W := \text{span}\{\omega_1, \ldots, \omega_m\} \subset V$$

we have the equivalence

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

Our task is to find a reconstruction algorithm

$$A : W \rightarrow V$$

such that $A(P_W u)$ approximates the state $u$. 
Quality of $A : W \rightarrow V$: 

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

Optimal performance among all algorithms:

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

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

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

$$A^*_{wc}(w) = \text{cen} (\mathcal{M}_w)$$
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

\[
A : W \rightarrow V
\]

\[
\omega \mapsto A(\omega) := \arg \min_{\nu \in \omega + W^\perp} \text{dist}(\nu, \overline{V}_n)
\]

is an affine algorithm in the sense that

\[
A(\cdot - P_{W\bar{u}}) \in \mathcal{L}(W, V).
\]

Performance:

\[
E(A, \mathcal{M}) \leq \beta_{n,m}^{-1} \varepsilon_n
\]

\[
\varepsilon_n := \max_{u \in \mathcal{M}} \text{dist}(u, \overline{V}_n), \quad \beta_{n,m} := \inf_{\nu \in V_n} \frac{\|P_{W_m} \nu\|}{\|\nu\|} = \cos(\theta_{V_n, W_m}) \in (0, 1]
\]
Choice of $\overline{V}_n$ and $W$

Choice of $\overline{V}_n$:

- **Optimal** $\overline{V}_n$ (see [CDD$^+$20])
  \[ \rightsquigarrow \text{“Optimize over } \beta_{n,m} \epsilon_n”. \]

- **Reduced Order Models** (PBDW, GEIM, see [MPPY15, MM13])
  \[ \rightsquigarrow \text{Conceived for forward problem} \]
  \[ \rightsquigarrow \text{Build } \overline{V}_n \text{ with good } \epsilon_n \]
  \[ \rightsquigarrow \epsilon_n \text{ decays fast with } n \text{ in elliptic/parabolic problems.} \]

- **“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].
We have that

$$E^*(\mathcal{M}) = \min_{A:W \rightarrow V} E(A, \mathcal{M}) \leq d_{m+1}(\mathcal{M}) \leq \min_{A:W \rightarrow V} E(A, \mathcal{M}),$$

where

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

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)
Consider a partition of the parameter domain

\[ Y = Y_1 \cup \cdots \cup Y_K \quad \leadsto \quad M = M_1 \cup \cdots \cup M_K. \]

For each \( M_k \), 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

\[ u_k = A_k(\omega), \quad k = 1, \ldots, K. \]
Model selection

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

$$k^* = k(\omega) = \arg\min_{k=1,\ldots,K} \text{dist}(A_k(\omega), \mathcal{M}),$$

but

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

is not easily computable.
We would like to select the reconstruction that is closest to $M$

$$k^* = k(\omega) = \arg\min_{k=1,...,K} \text{dist}(A_k(\omega), M),$$

but

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

$\sigma$ can also account for noise and model error in the analysis.
Theorem 1 (Cohen, Dahmen, Mula, Nichols, 2021)

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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

\[- \text{div}(a(x, y) \nabla u(x, y)) = 1 \text{ on } \Omega = [0, 1]^2, \text{ (well-posed in } V = H_0^1(\Omega))\]

\[a = a(x, y) = 1 + \sum_j c_j y_j \chi_{D_j}(x), \ y = (y_j) \in [-1, 1]^{16}, \ell_i(u) = \int_\Omega e^{-\frac{|x-x_j|^2}{\sigma^2}} u(x) \, dx\]
Numerical example

$K$ = Number of local reduced bases in the nonlinear family

Error bounds $\sigma_K$ w/ $\dim(W_m) = 16$, $\dim(Y) = 4$

Error bounds $\sigma_K$ w/ $\dim(W_m) = 4$, $\dim(Y) = 4$

$c_1 = 0.99 t^{-1}$
$c_2 = 0.9 t^{-1}$
$c_3 = 0.99 t^{-2}$
$c_4 = 0.9 t^{-2}$

$c = 0.99$
$c = 0.9$

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Optimal schemes for inverse problems
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 $\Omega$, reconstruct quickly the 3D velocity and pressure fields from Doppler US velocity measurements.

**Strategy:** (see [GGLM21, GLM21a])
- Parametric Navier Stokes equations $\rightarrow M \approx V_n$.
- 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 $\Omega$, provide a fast reconstruction.

**Roadmap:**
- Direct computation of $V_n^\Omega$ 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.


