Inverse Parameter Estimation
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Motivation

- Parametric PDEs are used to model complex physical systems
- **Uncertainty Quantification:** We may have uncertainty in the parameters (or even the model)
- However we have some information (measurements) of the state (solution to the pde)
- Using this information, what can we say about the parameters giving rise to this state?
- This talk concerns rigorous theory to answer this question
The Setting

- We limit ourselves to the friendly setting of Parametric Elliptic PDEs.

- $D \subset \mathbb{R}^d$ is a Lipschitz domain and $\mathcal{A}$ is the collection of diffusion coefficients $a \in L_\infty(D)$ that satisfy the Uniform Ellipticity Assumption $\text{UEA} : 0 < r \leq a(x) \leq R, \quad x \in D, \quad \text{for all } a \in \mathcal{A}$

- For each $a \in \mathcal{A}$ we are interested in the solution $u_a$ to

$$
-\text{div}(a(x) \nabla u_a(x)) = f(x), \quad x \in D,
$$

$$
u_a(x) = 0, \quad x \in \partial D
$$

- Let $\mathcal{M} := \mathcal{M}(f; \mathcal{A}) = \{u_a : a \in \mathcal{A}\}$ be the solution manifold and $F : a \mapsto u_a$ the solution map.
Usually we work with subsets $\mathcal{A}_0 \subset \mathcal{A}$ which impose additional structure on the diffusion coefficients.

The affine model: $a$ satisfies UEA, i.e. $a \in \mathcal{A}$ and

$$a(x, y) = \bar{a}(x) + \sum_{j=1}^{\infty} y_j \psi_j(x), \ y_j \in [-1, 1], \ j = 1, 2, \ldots$$

Notation: $\mathcal{P} := [-1, 1]^N$ the set of parameters and $u(x, y) := u_a(x)$

We typically impose further restrictions on the affine decomposition such as decay for the $\|\psi_j\|_{L_\infty(D)}$, for example $(\|\psi_j\|_{L_\infty(D)})_{j \geq 1} \in \ell_p$ with $p < 1$

Second example: $\mathcal{A}_s := \mathcal{A}_s(M) := \{a \in \mathcal{A} : \|a\|_{H^s} \leq M\}$

Note in this example we still have the condition that $a \in L_\infty(D)$
Parameter Identification

First Question: Does $u_a$ determine $a$?

We fix $f$ and ask whether the solution map $F : a \rightarrow u_a$ is invertible.

The answer depends on $f$. 
Parameter Identification

- If for some \( a \in \mathcal{A} \) we have \( \nabla u_a \) vanishes on an open subset \( D_0 \subset D \) then for any \( b \) which agrees with \( a \) outside of \( D_0 \), we have \( u_a = u_b \) and therefore there is no uniqueness.

To avoid this, we assume always that \( f \in L_\infty(D) \) and \( f > 0 \) on \( D \).

- Problem 1: Does this guarantee unique invertibility of \( F \)?
The forward map

Before analyzing the inverse map we recall results about the smoothness of the forward map $F$

The usual estimate is
$$\|u_a - u_b\|_{H^1(D)} \leq \frac{\|f\|_{H^{-1}}}{r^2} \|a - b\|_{L^\infty(D)}$$

The above is not useful when $a, b$ have jump discontinuities that do not match

Improved estimates (Bonito-DeVore-Nochetto): If $p \geq 2$ and $q := \frac{2p}{p-2}$ then
$$\|u_a - u_b\|_{H^1(D)} \leq r^{-1} \|\nabla u_a\|_{L^p(D)} \|a - b\|_{L^q(D)}, \quad q = \frac{2p}{p-2}$$

Note that since $a \in L^\infty(D)$, we obtain
$$\|u_a - u_b\|_{H^1(D)} \leq C \|\nabla u_a\|_{L^p(D)} \|a - b\|^\theta_{L^2(D)}, \quad \theta = 2/q$$
Sufficient conditions

- The previous result requires $\nabla u_a \in L_p$

- Sufficient conditions on $a$ which guarantee $\nabla u_a \in L_p$?

  - There is always a range of $p > 2$ (depending only on $D$), i.e. $2 \leq p < P$. where this is true for all $a \in \mathcal{A}$
  
  - Hence there is always a $\theta = \theta(D) > 0$ such that for all $a \in \mathcal{A}$ we have

    $$\|u_a - u_b\|_{H^1(D)} \leq C \|a - b\|_{L^2(D)}^\theta$$

- If $a \in \text{VMO}$ then $\nabla u_a \in L_p(D)$ for all $p < \infty$
  
  - Hence for all $0 < \theta < 1$ and all $a \in \mathcal{A} \cap \text{VMO}$ we have

    $$\|u_a - u_b\|_{H^1(D)} \leq C \|a - b\|_{L^2(D)}^\theta$$

- Here $C$ depends on $p$ and the VMO modulus of $a$
If $D = [0, 1]$ and $f \geq c > 0$ is in $L_\infty(D)$ the analysis is simple.

- For any $a, b \in \mathcal{A}$ we have $\|u_a - u_b\|_{H_1} \leq C\|a - b\|_{L_2[0,1]}$
- For any $a, b \in \mathcal{A}$ we have $\|a - b\|_{L_2[0,1]} \leq C\|u_a - u_b\|_{H_1}^{1/3}$
- The exponent $1/3$ cannot be improved.
- Notice that these results hold with no additional assumptions on $a$ other than UEa, i.e. $a \in \mathcal{A}$
Higher Dimensions

In higher space dimension $d \geq 2$ the situation is more complex and the results are not as complete.

We assume $f \geq c > 0$ and $f \in L_{\infty}(D)$, with $D$ Lipschitz.

In this setting, I do not even know if $u_a$ uniquely determines $a \in A$ (see Problem 1).

We can show unique determination of $a$ and smoothness for the inverse map $u_a \mapsto a$ provided we impose extra conditions on the diffusion coefficients $a$.

In Bonito-Cohen-DeVore-Petrova-Welper we prove results of the type

$$\|a - b\|_{L_2(D)} \leq C\|u_a - u_b\|_{H^1(D)}^\beta$$

In otherwords, we prove that the inverse map is $\text{Lip } \beta$ under additional assumptions on the diffusion coeff.
Values of $\beta$

- Under the additional assumption that the diffusion coefficients are in $A_1(D)$ we have $\beta = 1/6$

- Under the additional assumption that the diffusion coefficients are in $A_s(D) \cap \text{VMO}(\varphi)$ with $s > 1/2$, we can prove that there is $\beta = \beta(s) > 0$

- We can drop the VMO requirement provided $a, b \in A_s(D)$ and $s > s^*$ with $s^* < 1$ depending only on $D$

- These results do not apply if $a, b$ are piecewise constant. However, in this case we have the following:
  - Let $P_n$ be the partition of $D = [0, 1]^d$ into $n^d$ cubes of equal side length $1/n$ and let $A^n$ be the set of diffusion coefficients in $A$ that are piecewise constant subordinate to $P_n$
  - $\|a - b\|_{L^2} \leq Cn\|u_a - u_b\|_{H^1(D)}$, $a, b \in A^n$
Lip $\beta$ smoothness of inverse map
Summary

- Under moderate assumptions on the diffusion coeff.
  \[ \|u_a - u_b\|_{H^1_0(D)} \leq C\|a - b\|_{L^2(D)}^\alpha \] for some \( \alpha > 0 \)
  \[ \|a - b\|_{L^2(D)} \leq C\|u_a - u_b\|_{H^1_0(D)}^\beta \] for some \( \beta > 0 \)

- If we observe the full state \( u_a \) this still does not tell us how to find \( a \). In most settings, we do not observe the full state \( u_a \) but rather just partial information, namely, a finite number of measurements of the state.

- The remainder of this talk will address how well we can expect to recover \( a \) with this partial information. These are difficult questions - results are limited.

- In Uncertainty Quantification one assumes that parameters occur with an underlying probability distribution: the most closely related results are in Schwab-Stuart - IP 2012.
The Numerical Setting

- We assume that we have a finite number of measurements \( l_j(u_a) = w_j, j = 1, \ldots, m \), of the state \( u_a \).
- Since we are in a Hilbert space \( \mathcal{H} := H^1_0(D) \) we can write \( l_j = \langle \cdot, \omega_j \rangle \) with \( \omega_j \in \mathcal{H} \).
- We let \( W := \text{span}\{\omega_1, \ldots, \omega_m\} \).
- Then we can view the information we have as we are given \( w = P_W(u_a) \).
- Let \( A_0 \subset \mathcal{A} \) where membership in \( A_0 \) may impose additional smoothness conditions on \( a \). Once we have \( A_0 \) fixed there is an \( \alpha, \beta \).
- Notice that there are typically many \( a \in A_0 \) for which \( P_W(u_a) = w \) and so we need to clarify our goal.
Non-uniqueness of $\mathcal{M}(u_a) = w$

\[ \mathcal{M}(u_a) = \mathcal{M}(u_b) = w \in \mathbb{R}^m \]
Goals

- Given any $w \in W$ (which may or may not be a measurement of some $u_a$, $a \in A_0$) define the sets $S_w(\eta) := \{b \in A_0 : \|P_W(u_b) - w\|_{L_2(D)} \leq \eta\}, \quad \eta \geq 0$

- Ideal Goal: Describe $S_w(0)$

- This is too demanding for several reasons
  - Noise: If measurements are noisy, say we observe $\hat{w}$ then the $a$ we seek is only in $S_w(\delta)$ for some $\delta > 0$ depending on the noise level
  - Numerical issues: We cannot expect to compute an $a$ in $S_w(\eta)$ only an approximation to such an $a$
  - Computational resources: Decreasing $\eta$ will eat up more and more computational resources eventually becoming unreasonable
Possible Goals: Smallest Ball

- The user provides a tolerance $\eta \geq 0$,

- **Smallest Ball**: Find a ball $B(a^*, R^*)$ in $L_2(D)$ such that $a^* \in A_0$ and $S_w(\eta) \subset B(a^*, R^*)$ with the ball as small as possible:
  - The smallest ball is the Chebyshev ball of $S_w(\eta)$
  - $a^*$ would give a (coarse) approximation to all possible $a$
Smallest ball for $S_w(0)$
Possible Goals: Sketch

- The user provides a tolerance $\eta \geq 0$,

- **Sketch:** Find a small discrete set $\hat{S}$ that gives an $\epsilon$ net for $S_w(\eta)$

- Smallest set is the **entropy cover** of $S_w(\eta)$

- Therefore we would like cardinality of $\hat{S}$ to be comparable to the covering number $N_\epsilon(S_w(\eta))$
Sketch for $S_w(\eta)$
ε net
Covering
Algorithms for finding the **smallest ball** have three components

I. Use $w$ to find $\hat{u} \in H^1(D)$ and $\hat{R}$ such that $B(\hat{u}, \hat{R})$ contains all $u_a, a \in A_0$, such that $M(u_a) = w$

II. Find $b \in A_0$ such that $u_b$ approximates $\hat{u}$ at least to the precision $\hat{R}$

III. Use the smoothness of the inverse map and the knowledge of $u_b$ to find a ball $B(b, \tilde{R})$ which contains all $a \in A_0$ such that $M(u_a) = w$

III. Our inverse theorem gives $\tilde{R} \leq C(2\hat{R})^\beta$. Indeed,

$$\|a - b\|_{L^2(D)} \leq C\|u_a - u_b\|_{H^1_0(D)}^\beta \leq C(2\hat{R})^\beta$$

So **Task III** is easy once the other tasks are complete
I. by Reduced Modeling

- Task I is complicated by the fact that the solution manifold $\mathcal{M} := \{u_a : a \in A_0\}$ is not easy to understand.
- Strategy is to replace $\mathcal{M}$ by a reduced model.
- Such models produce a low dimensional linear space $V \subset H^1(D)$ such that $\text{dist}(\mathcal{M}, V)$ is small enough to complete Task I.
- Two strategies for doing this:
  - Greedy Algorithms
  - High dimensional polynomial expansions
Greedy algorithms

- These algorithms choose (through greedy selection) snapshots $v_1 = u_{a_1}, \ldots, v_n := u_{a_n}$ so that $V_n := \text{span}\{v_1, \ldots, v_n\}$ is a good approximation to $\mathcal{M}$

- Greedy strategy introduced by Buffa-Maday-Patera-Prud’homme-Turinici chooses the $k$-th snapshot which is furthest from $V_{k-1}$

- Theorem (Binev-Cohen-Dahmen-DeVore-Petrova-Wojtaszczyk)
  - If there exist $n$ dimensional spaces $Y_n \subset \mathcal{H}_0^1(D)$ such that $\text{dist}(\mathcal{M}, Y_n) \leq C'n^{-\alpha}, \ n = 1, \ldots, N$ then $\text{dist}(\mathcal{M}, V_n) \leq C'n^{-\alpha}, \ n = 1, \ldots, N$
  - Almost optimal in terms of $n$ widths
  - These algorithms have a very costly off-line implementation
Polynomial Expansions

Cohen-DeVore-Schwab I,II, Chkifa-Cohen-DeVore-Schwab, +

If the $a$ have an affine expansion with
$$(\|\psi_j\|_{L_\infty(D)})_{j\geq 1} \in \ell_p, \quad p < 1$$

Then $u(x, y) = \sum_\nu u_\nu(x)y^\nu$ with $(\|u_\nu\|_{H_0^1(D)}) \in \ell_p$

It follows that for each $n \geq 1$, there is a set $\Lambda_n$ such that
- $\#(\Lambda_n) = n$
- $\sup_{y \in \mathcal{P}} \|u(\cdot, y) - \sum_{\nu \in \Lambda_n} u_\nu y^\nu\|_{H_0^1(D)} \leq Cn^{-1/p+1}$

This gives certifiable decay of $n$ widths of $M$

$u_\nu$ found by recursively solving PDEs

Finding $\Lambda_n$ costly
Assimilating Data

- Take a reduced space $V = V_n$: what is a good choice for $V$ will be uncovered as we proceed
- Let $\mathcal{N}$ be the null space of the measurement map $M$
- Define $\mu(\mathcal{N}, V) := \sup_{\eta \in \mathcal{N}} \frac{\|\eta\|_{H^1}}{\text{dist}(\eta, V)_{H^1}}$
  - $\mu$ is the reciprocal of the angle between $V$ and $W$
- Let $v^*(w) = \text{Argmin}_{v \in V} \|w - M(v)\|_{\ell^2}$
- Then, Maday-Patera -Penn-Yano show that the ball $B(v^*(w), \hat{R})$, with $\hat{R} := 2\mu(\mathcal{N}, V^*)\text{dist}(M, V^*)_{H^1}$, contains all $u_a \in M$ such that $M(u_a) = w$. So we take $\hat{u} := v^*(w)$
- The best choice $V^*$ is one which minimizes $\mu(\mathcal{N}, V)\text{dist}(M, V)_{H^1}$ over all $V \subset H^1_0$. This would complete Task I with $\hat{R} = 2\mu(\mathcal{N}, V^*)\text{dist}(M, V^*)_{H^1}$
Task II

- We know $\hat{u} := v^*(w)$ and we want to find $b \in A_0$ such that $\|v^*(w) - u_b\|_{H^1_0(D)} \leq C\hat{R}$

- As long as $C \geq 2$ we know there are such $b$

- One way to find such a $b$ is to search over a (minimal) set $A^n \subset A_0$ such that $A^n = \{a_j\}$ is an $\epsilon$ net for $A_0$ with $\epsilon := (\hat{R}/C)^{1/\alpha}$

- Indeed, we know from our results on the forward map that $\|u_a - u_{a'}\|_{H^1} \leq C_0\|a - b\|^\alpha$

- Hence, the $u_{a_j}$ are an $\epsilon'$ net for $A_0$ with $\epsilon' = C_0\hat{R}/C$

- We use $C$ so that we only have to approximately solve for $u_a$ using the reduced space $V^*$

- In fact, we never solve for $u_a$ but rather use surrogate error estimators based on residuals- these are fast!
Post Mortem

- The bottlenecks in the above algorithm for finding a ball are
  - Finding the space $V^*$
  - Can we do this via greedy selection?
  - The usual greedy algorithms do not take into account $\mu(\mathcal{N}, V)$
  - The discretization of $\mathcal{A}^n$ - this manifests itself when the number of parameters is large
  - For an affine model of the parameters, we quantize the $y_j$ with fine quantization when $\|\psi_j\|_{L_\infty(D)}$ is large and coarse quantization when it is small
Finding a sketch of $\mathcal{S}_w(\eta)$

A dream algorithm for sketching would be one which identifies an $\epsilon$ net for $\mathcal{S}_w(\eta)$ whose size and computational costs are proportional to $N_\epsilon(\mathcal{S}_w(\eta))$

We proceed to describe the main ingredients of such algorithms in the case of the affine model

One constructs recursively

- Discretizations $\mathcal{A}^1, \mathcal{A}^2, \ldots$ of $\mathcal{A}_0$ using quantization of the $y_j$ as described earlier
- Reduced model spaces $V_1, V_2, \ldots$ with control on $\mu(N, V_n)\text{dist}(\mathcal{M}, V_n)$
- Using residual error estimators one can define cheap surrogates for computing $\|w - M(u_a)\|_{\ell_2}$
Testing points in $A^n$

Points in $A^n$ can then be tested, i.e., one computes an approximation to $\|w - M(u_a)\|_{\ell_2}$ at the needed accuracy and thereby $A^n$ can be decomposed into subsets $A^n(\text{out})$: These are points in $A^n$ which one can not only say these points can not be in $S_w(\eta)$ but also regions of $A_0$ near these points can be eliminated from further consideration because the residual error is too large. Here one uses the direct and inverse estimates.

$A^n(\text{in})$: These are points in $A^n$ that cannot be eliminated because the residual error estimate is not large enough.

The sets $A^n(\text{in})$ give finer and finer nets for $S_w(\eta)$.
Bottlenecks

- As before finding good educated model spaces
  \( \mu(N, V) \text{dist}(M, V) \)
- The usual greedy algorithms or polynomial basis selections do not pay attention to \( \mu \) - naturally because they were not formulated with measurements in mind
- Greedy algorithms are numerically intensive
- The cardinality of the sets \( \mathcal{A}_n^{(in)} \) grow exponentially in \( n \) limiting how large one can choose \( n \)
- This may lie in the nature of the problem since \( \epsilon \) nets typically grow like \( \epsilon^{-\tau} \) with \( \tau \) moderately large
- It would be good to have a priori theoretical bounds for \( N_{\epsilon}(\mathcal{S}_w(\eta)) \)