A non-standard numerical method for variational data assimilation for a convection-diffusion equation

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   Forward Data Assimilation

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   Well-posedness
   Reconstruction Method

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   POD Reconstruction Algorithm

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Data Assimilation

Given

- Parabolic state equation (with boundary conditions)
  \[ \mathcal{Y}_t + A\mathcal{Y} = \mathcal{F} \]
- Distributed measurements \( \overline{\mathcal{Y}} \) on (subset) \( \omega \)

Find

Initial conditions \( \mathcal{Y}_0 \), s. t. solution \( \mathcal{Y} \) of IBVP satisfies \( \mathcal{Y}|_{\omega} = \overline{\mathcal{Y}} \)

Ill-posed problem!
Applications

Application

Weather prediction (Navier-Stokes), Geophysics (Boussinesq)

1. Given observations in $[0, T_0]$, compute initial state $Y_0$ (assimilation)
2. Solve IBVP in $[0, T_1], T_1 > T_0$ (prediction)

Current methods

Tikhonov-regularised optimal control (4DVAR)
Statistical methods (Ensemble Kalman filter)
Forward Data Assimilation

**Idea**

1. Given observations in $[0, T_0]$, compute final state $Y_{T_0}$ (assimilation)
2. Solve IBVP in $[T_0, T_1]$ (prediction)

$\Rightarrow$ Replace
- ill-posed control problem for state equation with
  - well-posed control problem for adjoint equation
Problem Formulation

$\Omega \subset \mathbb{R}^n$ domain, boundary $\Gamma$, $c : \Omega \to \mathbb{R}$, $b : \Omega \times [0, T] \to \mathbb{R}^n$

**Convection-Diffusion equation**

\[
\begin{cases}
y_t - c^2 \Delta y + b^T \nabla y = f, & \Omega \times [0, T] \\
y = 0, & \Gamma \times [0, T]
\end{cases}
\]

$\omega \subset \Omega$ nonempty: **Given** $y|_{\omega}(x, t)$, **find** $y(T)$!

**Adjoint equation**

\[
\begin{cases}
-\varphi_t - c^2 \Delta \varphi - \text{div}(b \varphi) = v \chi_\omega, & \Omega \times [0, T] \\
\varphi = 0, & \Gamma \times [0, T] \\
\varphi(x, T) = \varphi_T(x), & x \in \Omega
\end{cases}
\]

$\chi_\omega$ characteristic function of $\omega \subset \Omega$, control $v : \Omega \times [0, T] \to \mathbb{R}$
Problem Formulation

Ω ⊂ \mathbb{R}^n\text{ domain, boundary } \Gamma, \, c : \Omega \to \mathbb{R}, \, b : \Omega \times [0, \, T] \to \mathbb{R}^n

Convection-Diffusion equation

\begin{align*}
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\(\omega \subset \Omega\) nonempty: \text{Given } y|_{\omega}(x, \, t), \text{ find } y(T)!

Adjoint equation

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\end{align*}

\(\chi_{\omega}\) characteristic function of \(\omega \subset \Omega\), control \(v : \Omega \times [0, \, T] \to \mathbb{R}\)
Well-posedness

**Theorem (Puel 2002)**

\[ \Gamma \text{ class } C^2, \ f \in L^2(0, T; L^2(\Omega)), \ c \in C^1(\bar{\Omega}), \ b \in L^2(0, T; H^1(\Omega)^n) \]

Then: For all \( T > 0, \omega \subset \Omega \) nonempty, for any \( \varphi_T \in L^2(\Omega) \)
- there exists \( v = v(\varphi_T) \in L^2(0, T; L^2(\Omega)) \), s. t. solution of adjoint equation satisfies:
  \[ \varphi(0) = 0 \]
- there exists \( C(\Omega, \omega, T) > 0: \)
  \[ \| y(T) \|_{L^2(\Omega)} \leq C \left( \int_0^T \int_\omega |y|^2 \, dx \, dt + \int_0^T \int_\Omega |f|^2 \, dx \, dt \right) \]

Proof relies on Carleman estimate for 2nd order parabolic equation
Reconstruction Method

Under conditions of last theorem, the following identity holds:

\[
\int_{\Omega} y(T) \varphi_T \, dx = \int_0^T \int_{\Omega} f \varphi \, dx dt - \int_0^T \int_{\omega} yv(\varphi_T) \, dx dt
\]

for all \( \varphi_T \in L^2(\Omega) \) with null controlled (by \( v \)) adjoint solution \( \varphi \)

⇒ Reconstruction method for \( y(T) \):

Algorithm

Given measurement \( y|_{\omega} \), Hilbert basis \( \{ \varphi_n \} \) of \( L^2(\Omega) \):

1. Calculate null controls \( v(\varphi_n) \), adjoint solution \( \varphi \)
2. Calculate coefficients \( c_n := \langle y(T), \varphi_n \rangle_{L^2(\Omega)} \)
3. Then: \( y(T) = \sum_n c_n \varphi_n \)
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3. Then: \( y(T) = \sum_n c_n \varphi_n \)
Exact Distributed Control: Glowinski/Lions

**Biadjoint equation**

\[
\begin{cases}
\psi_t - c^2 \Delta \psi + b^T \nabla \psi = 0, & \Omega \times [0, T] \\
\psi = 0, & \Gamma \times [0, T] \\
\psi(0) = \psi_0, & \Omega
\end{cases}
\]

Let \( \varphi(0; \nu) \) solution of adjoint equation controlled by \( \nu \) at \( t = 0 \)

**Operator formulation**

\[\Lambda : \psi_0 \mapsto \varphi(0; \psi(x, T - t)\chi_\omega)\]

Then: Solution \( \psi^*_0 \) of \( \Lambda \psi_0 = 0 \) yields null control \( \nu(\varphi_T) := \psi^* \chi_\omega \)

\[\Rightarrow \text{Use CG method to compute } \psi^*_0\]
Exact Distributed Control: Glowinski/Lions

Biadjoint equation

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\begin{aligned}
\psi_t - c^2 \Delta \psi + b^T \nabla \psi &= 0, & \Omega \times [0, T] \\
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⇒ Use CG method to compute \( \psi^*_0 \)
Finite Dimensional Approximation

Solve problem in finite dimensional subspace $V_h \subset L^2(\Omega)$:

Algorithm (finite dimensional)

Given discrete measurement $y^h|_\omega$, basis $\{\varphi^h_n\}$ of $V_h$:

1. Calculate null controls $v^h(\varphi^h_n)$
2. Calculate coefficients

$$c_n := \left\langle f, \varphi^h_n \right\rangle_{V_h \times L^2([0,T])} - \left\langle y^h|_\omega, v^h(\varphi^h_n) \right\rangle_{V_h \times L^2([0,T])}$$

3. Set $y^h_T := \sum_n c_n \varphi^h_n$
Choice of basis

Use Finite Element Space:

- $V_h$ space of piecewise polynomials on mesh
- $\{\varphi_n^h\}$ nodal basis (hat functions)
- Weighted inner product for $x, y \in V_h$

\[
\langle x, y \rangle_{V_h} := \xi^T M \eta
\]

with $x = \sum \xi_i \varphi_i$, $y = \sum \eta_i \varphi_i$, and

\[
M_{ij} := \int_{\Omega} \varphi_i^h \varphi_j^h
\]

Efficient calculation of coefficients, but curse of dimensions!

$\Rightarrow$ Use model reduction
**Proper Orthogonal Decomposition (POD)**

Given set \( \{ \varphi_i \}_{i=1}^{N} \subset V_h \), find \( l < N \) elements \( u_i \in \text{span}\{ \varphi_n \} \) solving

\[
\max_{u_i \in V_h} \left\{ \sum_{k=1}^{l} \sum_{i=1}^{N} \langle \varphi_i, u_k \rangle_{V_h}^2 \quad \text{s. t.} \quad \langle u_i, u_j \rangle_{V_h} = \delta_{ij}, \ 1 \leq i, j \leq l \right\}
\]

Matrix representation \( \Phi := (\varphi_1 | \cdots | \varphi_N) \), \( \varphi_i \in \mathbb{R}^{\dim V_h} \):

**Optimality conditions**

\[
\Phi^T M \Phi v_i = \lambda_i v_i
\]

\[
u_i := \frac{1}{\sqrt{\lambda_i}} \Phi v_i
\]

⇒ Solve symmetric eigenvalue problem
Proper Orthogonal Decomposition (POD)

Given set \{\varphi_i\}_{i=1}^N \subset V_h, find \( l < N \) elements \( u_i \in \text{span}\{\varphi_n\} \) solving

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\max_{u_i \in V_h} \left\{ \sum_{k=1}^{l} \sum_{i=1}^{N} \langle \varphi_i, u_k \rangle_{V_h}^2 \right\} \text{ s. t. } \langle u_i, u_j \rangle_{V_h} = \delta_{ij}, \quad 1 \leq i, j \leq l
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\( \Rightarrow \) Solve symmetric eigenvalue problem
POD Approximation Error

POD basis \( \{u_i\}_{i=1}^{l} \) singular vectors of \( M^{1/2} \Phi \)

\[ \Rightarrow \{u_i\}_{i=1}^{l} \text{ best rank } l \text{-approximation of } \{\varphi_i\}_{i=1}^{N} \text{ (in mean)} \]

Error estimate

\( V_h \) Finite Element space, \( h \) mesh size, \( P^h \) projector on \( V_h \)

\( \{u_i\}_{i=1}^{m} \) POD Basis, eigenvalues \( \lambda_i, m = \dim V_h \)

\[ w_l := \sum_{i=1}^{l} \left\langle P^h y(T), u_i \right\rangle_{V_h} u_i, \quad 1 \leq l \leq m \]

Then there exists \( C(\Omega, V_h) > 0 \), s. t.

\[ \|y(T) - w_l\|_{L^2(\Omega)}^2 \leq C \left( \sum_{i=l+1}^{m} \lambda_i + h \|y(T)\|_{H^1(\Omega)} \right) \]
 POD Approximation Error

POD basis \( \{u_i\}_{i=1}^l \) singular vectors of \( M^{1/2}\Phi \)

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**Error estimate**

\( V_h \) Finite Element space, \( h \) mesh size, \( P^h \) projector on \( V_h \)
\( \{u_i\}_{i=1}^m \) POD Basis, eigenvalues \( \lambda_i \), \( m = \text{dim } V_h \)

\[
w_l := \sum_{i=1}^l \left\langle P^h y(T), u_i \right\rangle_{V_h} u_i, \quad 1 \leq l \leq m
\]

Then there exists \( C(\Omega, V_h) > 0 \), s. t.

\[
\|y(T) - w_l\|_{L^2(\Omega)}^2 \leq C \left( \sum_{i=l+1}^m \lambda_i + h \|y(T)\|_{H^1(\Omega)} \right)
\]
Problem specific POD basis

POD basis depends only on Finite Element space:

- Can be precalculated (in parallel)
- But not most efficient: less basis elements sufficient?

⇒ Use optimal problem specific subset
Problem specific POD basis

Iterative POD basis \((\tilde{u}_1, \ldots, \tilde{u}_l)\)

1. Calculate FE-POD basis \(u_i, \ i = 1, \ldots, N_0 \leq N\)
2. Estimate (e.g. by interpolation) error function

\[
e_n := y^h(T) - \sum_{i=1}^{n-1} c_i \tilde{u}_i
\]

3. Pick

\[
\tilde{u}_n := \arg\max_{u_k \notin \{\tilde{u}_1, \ldots, \tilde{u}_{n-1}\}} \langle e_n, u_k \rangle_{V_h}
\]

4. Calculate \(c_n\) using exact control

5. Repeat from step 2 while \(\| e_n \|_{V_h} > \text{tolerance}\)
Test Problem

- Domain $\Omega = [0, 1]^2$, $T = 1$
- $c^2 = 0.1$, $b = (1, 1)^T$
- Right hand side: $O = \left\{ \sqrt{(x_1 - 0.5)^2 - (x_2 - 0.5)^2} \leq 0.2 \right\}$,
  
  $$f(x, t) = 10 \cos(3\pi t) \sqrt{r^2 - (x_1 - 0.5)^2 - (x_2 - 0.5)^2} \chi_O$$

- Initial value
  $$y(x, 0) = 10 \sin(3x_1\pi) \left[ \sin(2x_2\pi) + \sin(3x_2\pi) + \sin(4x_2\pi) \right]$$

- Discretisation: rectangular grid $h_1 = h_2 = \frac{1}{128}$, $h_t = \frac{1}{256}$
- Piecewise bilinear finite elements
- Implementation in deal.II
Measurement area

Plot of measurement area $\omega$ (blue), $|\omega| \approx 0.087|\Omega|$
POD Basis

Plot of two POD basis elements $\varphi_5, \varphi_{12}$
Quality of Reconstruction

Comparison of exact solution (left) and reconstruction from 10 POD elements (right)
Quality of Reconstruction

Comparison of exact solution (left) and reconstruction from 100 POD elements (right)
Quality of Reconstruction

Cut of exact solution $y(T)$ and reconstruction from 10 POD elements
Quality of Reconstruction

Cut of exact solution $y(T)$ and reconstruction from 100 POD elements
Quality of Reconstruction

Cut of exact solution $y(T)$ and reconstruction from sorted POD elements
Convergence

Convergence of approximation using unsorted POD elements
Convergence of approximation using sorted POD elements
Conclusion

Summary:

- Reconstructing final conditions is well-posed problem
- Efficiently computable using proper orthogonal decomposition
- Strategies exist for good choice of components
- Fast alternative to 4DVAR

Perspective:

- Adaptive grid refinement: Adaptive POD
- Rates of convergence
Thank you for your attention!
Influence of noise

Reconstruction from noisy measurement

\[ y^\delta(T) = y^h(T) + \delta \| y^h(T) \| \]