Blending Mathematical Models and Data: Algorithms, Analysis and Applications

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Enabling Quantification of EQUIP Uncertainty for Inverse Problems

THE UNIVERSITY OF WARWICK

Outline

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Current State of Play

Data Everywhere

In every realm of human experience, growing in volume.

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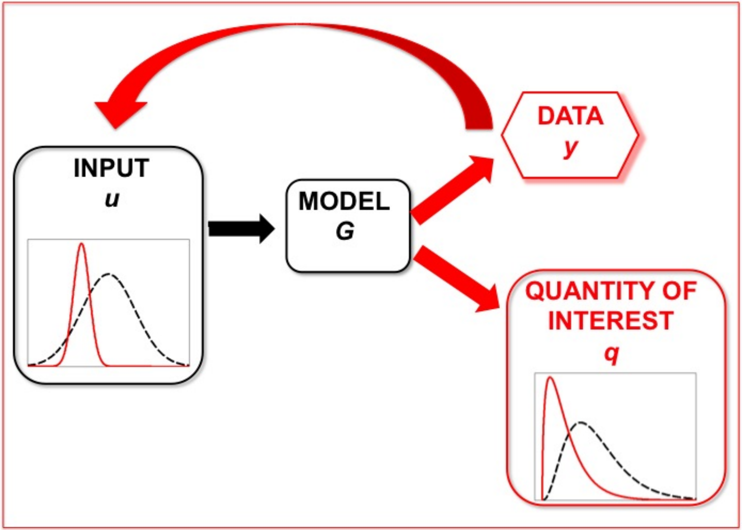
Where Are We Now?

Mathematics in relation to data is in the same state that it was in relation to analysis at the time of Fourier. Interesting times!

Model and Data



Prototypical Problem Areas

- Physics (Newton's Laws, Quantum Mechanics). Strong belief in model.

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All Have Vast Amounts of Data!

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- What extra do we learn from the data?

This Talk

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Challenges in Optimization, Dynamical Systems, Control and High Dimensional Probability

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Numerical Weather Prediction (NWP)

Signal dynamics on separable Hilbert space $(\mathcal{H}, \langle\cdot,\cdot\rangle, |\cdot|)$. For $\Psi : \mathcal{H} \to \mathcal{H}$ and v_j velocity, temperature etc. at time j:

Signal Process

$$v_{j+1} = \Psi(v_j).$$

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Data Assimilation

Blend model and observations to learn $v_0 = u$. *Limit* $\epsilon \to 0$?

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High Dimensional Probability!

Navier-Stokes Equation (all theorems apply)

Incompressible NSE on $\Omega_T = \mathbb{T}^2 \times (0, \infty)$

$$
\begin{aligned}
\partial_t v - \nu \triangle v + v \cdot \nabla v + \nabla p = f \quad & \text{in}\, \Omega_T, \\
\nabla \cdot v = 0 \quad & \text{in}\, \Omega_T, \\
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Discrete-Time Semigroup

- $\mathcal{H} = L^2_{\mathrm{div}}(\mathbb{T}^2; \mathbb{R}^2)$.
- $\Psi : \mathcal{H} \to \mathcal{H}$ defined by:
- $v\big|_{t=h} := \Psi(u)$. Then:
- $v_{j+1} = \Psi(v_j)$.

Observations

- Eulerian:
- $Pv := \{v(x_k)\}_{k=1}^K$.
- (Divergence-Free) Fourier:
- $Pv := \{\int_{\mathbb{T}^2} v(x) e_k(x)\, dx\}_{k=1}^K$.

4DVAR (Talagrand and Courtier [8] Q. J. R. Met. Soc 1987)

(Covariance) Weighted Hilbert Spaces

$$A > 0, |\cdot|_A = |A^{-\frac{1}{2}} \cdot|.$$

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Best Fit to Data and Model

$$m_{\mathrm{post}} = \mathrm{argmin}_{u \in \mathcal{H}} J(u).$$

3DVAR (Lorenc [5] Q. J. R. Met. Soc 1986)

Cycled 3DVAR Filter.

$$m_{j+1} = \mathrm{argmin}_{m \in \mathcal{H}} \{ |m - \Psi(m_j)|_C^2 + \epsilon^{-2} |y_{j+1} - Pm|_\Gamma^2 \}.$$

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Solve Variational Equations (with $C = \epsilon^2(\eta^{-2}\Gamma P + Q)$, Q=I-P)

$$m_{j+1} = (I-K)\Psi(m_j) + Ky_{j+1}, \quad K = (1+\eta^2)^{-1}P,$$

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Variance Inflation (from NWP) $\eta \ll 1$

$$m_{j+1} = Q\Psi(m_j) + P y_{j+1}, \quad \eta = 0. \quad \textit{Synchronization Filter}.$$

The EnKF (Evensen [2] Journal of Geophysical Research 1994.)

Ensemble Kalman Filter. For $n = 1, \ldots, N$:

$$v_{j+1}^{(n)} = \mathrm{argmin}_{v \in \mathcal{H}} \{ |v - \Psi(v_j^{(n)})|_{C_j}^2 + \epsilon^{-2} |y_{j+1} - Pv|_{\Gamma}^2 \}.$$

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Empirical Covariance

$$\bar{v}_j = \frac{1}{N} \sum_{n=1}^{N} v_j^{(n)}, \quad C_j = \frac{1}{N} \sum_{n=1}^{N} (v_j^{(n)} - \bar{v}_j) \otimes (v_j^{(n)} - \bar{v}_j).$$

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Interacting Particles (Coupled Through K_j)

$$v_{j+1}^{(n)} = (I - K_j)\Psi(v_j^{(n)}) + K_j y_{j+1}$$

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$$\mathbb{P}(u) : u \sim \mu^y.$$

Bayes' Formula (to be justified) $\mathbb{P}(u|y) \propto \mathbb{P}(y|u)\mathbb{P}(u)$

$$\mu^y(du) \propto \exp\Big(-\epsilon^{-2}\sum_{j=1}^{J}|y_j - P\Psi^{(j)}(u)|_\Gamma^2\Big)\mu_0(du).$$

Smoothing is Well-Posed (S [7] Acta Numerica 2010.)

Theorem

Assume that prior covariance C is chosen so that $u \in \mathcal{H}$ μ_0 a.s. Then posterior $\mu^y \ll \mu_0$ and

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Hellinger Metric

The metric d_{Hell} is a natural one because, for $f \in L^2_{\mu_0}(\mathcal{H}; S)$,

$$\|\mathbb{E}^{\mu^y} f - \mathbb{E}^{\mu^{y'}} f\|_S \le K\, d_{Hell}(\mu^y, \mu^{y'}).$$

4DVAR is MAP Estimation (Dashti et al [1] Inverse Problems 2013.)

4DVAR

Recall the functional $J : E := \mathrm{Dom}(C^{-\frac{1}{2}}) \to \mathbb{R}^+$ (4DVAR):

$$J(u) := |u - m_{\mathrm{pr}}|_C^2 + \epsilon^{-2} \sum_{j=1}^{J} |y_j - P\Psi^{(j)}(u)|_\Gamma^2.$$

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Theorem

Let $B^\delta(z) := \{v \in \mathcal{H} : |v - z| < \delta\}$. The probability measure μ^y and functional J are related by

$$\lim_{\delta \to 0} \frac{\mu^y\big(B^\delta(z)\big)}{\mu^y\big(B^\delta(0)\big)} = \exp\big(J(0) - J(z)\big).$$

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Thus maximum a posterior (MAP) estimators are minimizers of J.

$\epsilon \to 0$ Asymptotics (Dashti et al [1] Inverse Problems 2013.)

Bayesian Posterior Consistency

Fix $u^\dagger \in \mathcal{H}$, draw $\eta \sim N(0, \Gamma)$, and let J_ϵ be the 4DVAR objective functional corresponding to the data y_ϵ defined by:

$$y_\epsilon = \mathcal{G}(u^\dagger) + \epsilon\eta.$$

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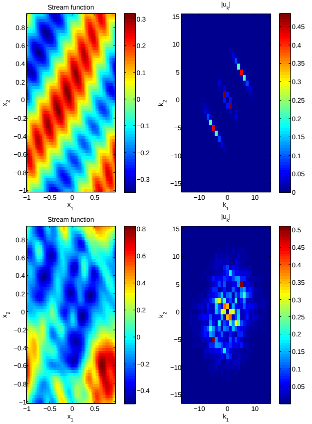
Theorem

There is a $u_\epsilon \in E$:

$$J(u_\epsilon) := \inf\{J_\epsilon(u) : u \in E\}.$$

Furthermore, $\eta-$a.s. there is subsequence $\{u_{\epsilon'}\}$ converging weakly to u_0 in E where $\mathcal{G}(u_0) = \mathcal{G}(u^\dagger)$.

Example: Navier-Stokes Inversion for Initial Condition

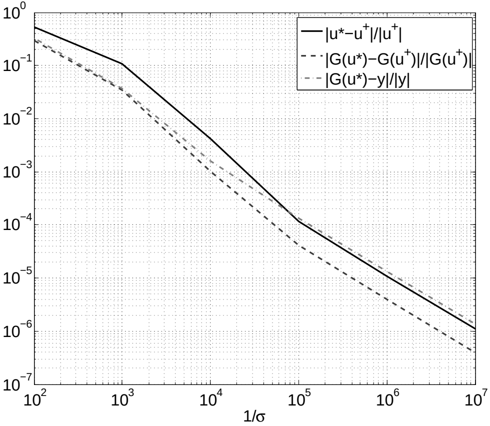


- Incompressible NSE on $\Omega_T = \mathbb{T}^2 \times (0,\infty)$:

$$\begin{aligned} \partial_t v - \nu \triangle v + v\cdot\nabla v + \nabla p = f &\quad \text{in } \Omega_T, \\ \nabla\cdot v = 0 &\quad \text{in } \Omega_T, \\ v\big|_{t=0} = u &\quad \text{in } \mathbb{T}^2. \end{aligned}$$

- $y_{k,\ell} = v(x_k, t_\ell) + \eta_{k,\ell}, \quad \eta_{k,\ell} \sim N(0, \sigma^2 I_{2\times 2})$.
- $y = \mathcal{G}(u) + \eta, \quad \eta \sim N(0, \sigma^2 I)$.
- $C_0 = (-\triangle_{\text{stokes}})^{-2}$; $\Phi = \frac{1}{10^3\sigma^2}|y - \mathcal{G}(u)|^2$.

Example: MAP estimator $u^\star$; Truth $u^\dagger$



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$$\widehat{\mu}_{j+1} = \Psi \star \mu_j.$$

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Observations via Bayes' Theorem

$$\mu_{j+1}(A) = \frac{\int_A \exp\big(-\epsilon^{-2}|y_{j+1} - Pv|_\Gamma^2\big)\widehat{\mu}_{j+1}(dv)}{\int_{\mathcal{H}} \exp\big(-\epsilon^{-2}|y_{j+1} - Pv|_\Gamma^2\big)\widehat{\mu}_{j+1}(dv)}.$$

Filtering is Well-Posed

From the pushforward property

$$\mu_j = \Psi^{(j)}{}_{\star}\mu^{(y_1,\cdots,y_j)}$$

and the well-posedness of the smoothing problem:

Theorem

Assume that prior covariance C is chosen so that $u \in \mathcal{H}$ μ_0 a.s. Then $(y_1, \cdots, y_j) \mapsto \mu_j$ is locally Lipschitz in Hellinger metric.

Detectability

Nonlinear Detectability (Recall $Q = I - P$)

The ball $B(R_0)$ in $\mathcal{H}$ is absorbing for the dynamics and there is a squeezing property: $\alpha(R_0) \in (0,1)$ such that, for all $u, v \in B(R_0)$,

$$\|Q(\Psi(u) - \Psi(v))\|^2 \leq \alpha(\mathbf{R_0}) \|u - v\|^2.$$

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Foais and Prodi '67, Mattingly et al '00s, Olsen, Titi et al '00s.

Consistency of the Filter (Sanz-Alonso and S, 2014, [6] SIAM JUQ.)

Theorem

Assume nonlinear detectability and Fourier observations. Then there is a constant $c > 0$ independent of the noise strength ϵ such that

$$\limsup_{j\to\infty} \mathbb{E}|v_j - \mathbb{E}^{\mu_j} v_j|^2 \leq c\epsilon^2$$

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Idea of proof:

- Let m_j come from synchronization filter (3DVAR variant).
- Prove

$$\limsup_{j\to\infty} \mathbb{E}|v_j - m_j|^2 \leq c\epsilon^2.$$

- Use the L^2 optimality of the filtering distribution.

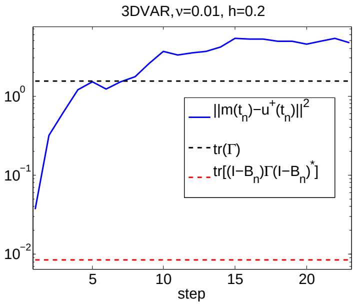
Idea of proof (sketch, Ψ globally Lipschitz):

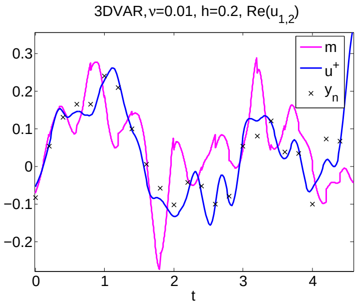
$$\begin{aligned} m_{j+1} &= Q\Psi(m_j) \qquad && + \overbrace{P\Psi(v_j) + \epsilon\eta_{j+1}}^{\mathbf{y_{j+1}}}, \\ v_{j+1} &= Q\Psi(v_j) \qquad && + P\Psi(v_j). \end{aligned}$$

Subtract and use independence plus contractivity of $Q\Psi$:

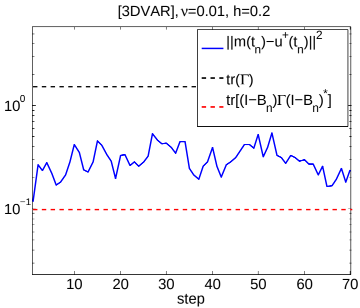
$$\begin{aligned} \mathbb{E}\|v_{j+1} - m_{j+1}\|^2 &= \mathbb{E}\|Q\left(\Psi(v_j) - \Psi(m_j)\right) - \epsilon\eta_{j+1}\|^2 \\ &\le \mathbb{E}\|Q\left(\Psi(v_j) - \Psi(m_j)\right)\|^2 + \epsilon^2\mathbb{E}\|\eta_{j+1}\|^2 \\ &\le \alpha\mathbb{E}\|v_j - m_j\|^2 + \epsilon^2\mathbb{E}\|\eta_{j+1}\|^2. \end{aligned}$$

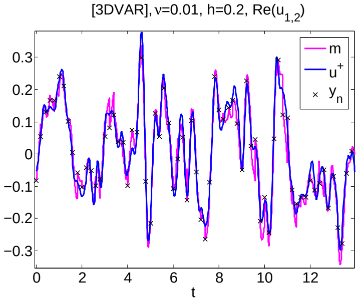
Inaccurate: η too large. (NSE torus) Law and S [4], Monthly Weather Review, 2012





Accurate: smaller η. (NSE torus) Law and S [4], Monthly Weather Review, 2012





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- The ideal probabilistic formulation of the problem is currently beyond computational reach.
- However it provides a benchmark against which to test algorithms like 4DVAR, 3DVAR and EnKF. (Not discussed here).
- It also provides a theoretical framework in which to discuss ability of algorithms to reconstruct the "truth" in the data in small noise or large data volume limits. (Discussed in detail here for 3DVAR and 4DVAR; see Kelly 2014 [3] for EnKF).

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MATLAB files and book chapters freely available:

http://tiny.cc/damat

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