Evaluating Data Assimilation Algorithms with MCMC: Two Case studies

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Data Assimilation Shortcourse
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Collaboration with Andrew Stuart and Marco Iglesias (Warwick).

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Center for Uncertainty Quantification

Outline

1. NSE
   - INVERSE PROBLEM
   - ALGORITHMS
   - RESULTS
   - STABILITY
2. SUBSURFACE
   - INVERSE PROBLEM
   - ALGORITHMS
   - RESULTS
3. CONCLUSIONS

Outline

Navier Stokes Equations and Data

Write NSE as ODE in $H = \{u \in L^2(\mathbb{T}^2) \big| \nabla \cdot u = 0, \int_{\mathbb{T}^2} u\, dx = 0\}$:

$$\frac{dv}{dt} + \nu A v + B(v, v) = f, \qquad v(0) = u$$

$$v(t) = \Psi(u; t), \quad \Psi^{(j)}(u) := \Psi(u; j\tau)$$

Find u given noisy observations y_j:

$$y_j = H\Psi^{(j)}(u) + \eta_j,$$

$$\eta_j \sim \mathcal{N}(0, \Gamma)$$

$$Y_j = \{y_i\}_{i=1}^{j}.$$

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Bayesian Formulation

- Prior $\mathbb{P}_0$ on u:

$$\mathbb{P}_0 = \mathcal{N}(m_0, C_0).$$

- Bayes formula:

$$\frac{\mathbb{P}(du|Y_J)}{\mathbb{P}_0(du)} \propto \mathbb{P}(Y_J|u).$$

- Here

$$\mathbb{P}(Y_J|u) \propto \exp\left(-\Phi(u; Y_J)\right)$$

$$\Phi(u; Y_J) = \frac{1}{2}\sum_{j=1}^{J}\left\|\Gamma^{-\frac{1}{2}}\left(y_j - \Psi^{(j)}(u)\right)\right\|^2$$

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Posterior Distribution

- pCN MCMC - Gold standard :

Propose $u^* = m_0 + (1-2\beta)^{\frac{1}{2}}(u^{(n-1)} - m_0) + \sqrt{2\beta}\mathcal{N}(0, C_0)$

$$u^{(n)} = \left\{ \begin{array}{cc} u^* & \text{with probability } 1 \wedge \exp\{\Phi(u^{(n-1)}) - \Phi(u^*)\} \\ u^{(n-1)} & else. \end{array} \right\}$$

- 4DVAR - Gaussian at MAP Estimator :

$$u \approx \mathcal{N}(m_0', C_0'), \qquad C_0' = \left(D^2\Phi(m_0') + \hat{C}_0^{-1}\right)^{-1}$$

$$m_0' = \mathrm{argmin}_u \left(\Phi(u) + \tfrac{1}{2}\|\hat{C}_0^{-\frac{1}{2}}(u - m_0)\|^2\right).$$

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Approximate Gaussian Filters I

- Impose the Gaussian approximation:

$$\mathbb{P}(v_{j-1}|Y_{j-1}) = \Psi^{j-1} \star \mathbb{P}(u|Y_{j-1}) \approx N(m_{j-1}, C_{j-1})$$
$$\mathbb{P}(v_j|Y_{j-1}) = \Psi^{j} \star \mathbb{P}(u|Y_{j}) \approx N(\Psi(m_{j-1}), \widehat{C}_j).$$

- Find update rule: $(m_{j-1}, C_{j-1}) \mapsto (m_j, C_j)$.

$$m_j = (I - K_j H)\Psi(m_{j-1}) + K_j y_j,$$
$$K_j = \widehat{C}_j H^\top (H \widehat{C}_j H^\top + \Gamma)^{-1},$$
$$C_j = (I - K_j H)\widehat{C}_j.$$

Approximate Gaussian Filters I

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Approximate Gaussian Filters II

In all cases

$$C_j^{-1} = \widehat{C}_j^{-1} + H^\top \Gamma^{-1} H$$

- **3DVAR** :

$$C_j \equiv C_0.$$

- **FDF**: For C chosen from Gaussian SPDE parameter fit:

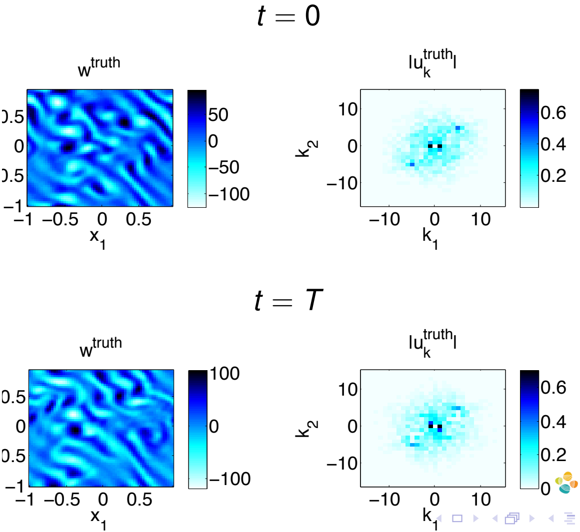
$$C_j \equiv C.$$

- **(LR)ExKF**: (Low rank approximation of):

$$\widehat{C}_j = D\Psi(m_{j-1}) C_{j-1} D\Psi(m_{j-1})^\top.$$

- **EnKF**: Particle approximations for m_j and C_j.

Truth



Relative Error in Mean c/w Posterior

Mean

method	e_{mean}
4DVAR($t = 0$)	0.000731491
4DVAR($t = T$)	0.00130112
3DVAR	0.0634553
FDF	0.165732
LRExKF	0.00614573
EnKF	0.035271

Relative Error in Variance c/w Posterior

Variance

method	$e_{variance}$
4DVAR($t = 0$)	0.0932748
4DVAR($t = T$)	0.220154
3DVAR	6.34057
FDF	28.9155
LRExKF	0.195101
EnKF	0.274428

Accuracy Theorem (3DVAR)

- Recall true signal $v_j = \Psi^{(j)}(u) = v(j\tau)$.
- Define $\sup_{j\geq 1} \|\xi_j\| = \epsilon$.

Theorem (BLLMSS11)

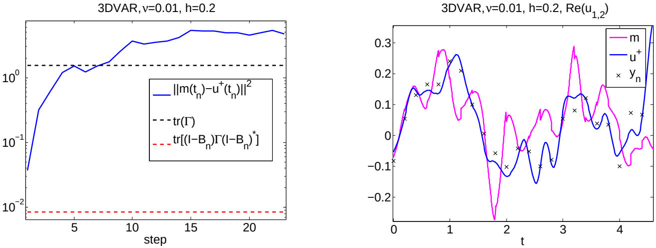
Assume that:

- $m_0 \in B_{\mathrm{V}}(0, R)$;
- *Enough low wavenumbers observed, and τ small enough.*
- $\Gamma = \eta \widehat{C}$;

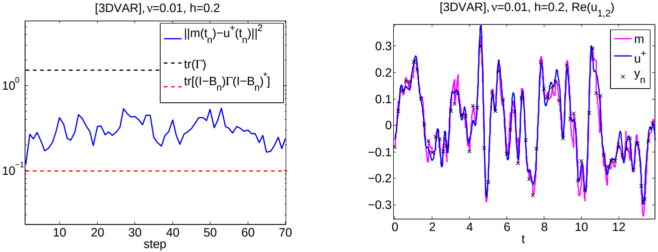
Then $\exists\ \eta_c = \eta_c(r)$, $r \in (0,1)$, and $c \in (0, \infty)$ such that, for all $\eta < \eta_c$,

$$\|\hat{m}_j - v_j\| \leq r^j \|\hat{m}_0 - v_0\| + c\epsilon.$$

Inaccurate


3DVAR, ν=0.01, h=0.2
10^0
10^−1
10^−2
5
10
15
20
step
||m(t_n)−u^+(t_n)||^2
tr(Γ)
tr[(I−B_n)Γ(I−B_n)^*]
3DVAR, ν=0.01, h=0.2, Re(u_1,2)
0.3
0.2
0.1
0
−0.1
−0.2
0
1
2
3
4
t
m
u^+
y_n

Accurate


[3DVAR], ν=0.01, h=0.2
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10^0
10^−1
10
20
30
40
50
60
70
step
[3DVAR], ν=0.01, h=0.2, Re(u_1,2)
m
u^+
y_n
0.3
0.2
0.1
0
−0.1
−0.2
−0.3
0
2
4
6
8
10
12
t

Evaluation wrt gold standard, fixed Interval ($T = J\tau$): Relative Error c/w Posterior: stabilized

From [LS11]:

method	e_{mean}	$e_{variance}$
3DVAR	0.458527	1.8214
[3DVAR]	0.27185	6.62328
LRExKF	0.632448	0.4042
[LRExKF]	0.201327	11.2449
EnKF	0.901703	0.554611
[EnKF]	0.169262	4.07238
FDF	0.189832	11.4573

Outline

Two-phase incompressible flow and Data

$$-\nabla \cdot \left[\lambda(s) e^{u} \nabla p\right] = f_1(p, s) \quad \text{in } D \times [0, T],$$
$$\psi \frac{\partial s}{\partial t} - \nabla \cdot \left[\lambda_w(s) e^{u} \nabla p\right] = f_2(p, s) \quad \text{in } D \times [0, T].$$

h pointwise measurements of total flow rate at production wells and bottom-hold pressure at injection wells.

$$y_j = h_0(p(j\tau), s(j\tau)) + \eta_j,$$
$$\eta_j \sim \mathcal{N}(0, \Gamma)$$
$$Y_j = \{y_i\}_{i=1}^{j}.$$

ertainty

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Filtering

Augmented System Dynamics

Define

$$z = \begin{pmatrix} u \\ p \\ s \end{pmatrix}, \qquad \Psi(z) = \begin{pmatrix} u \\ \psi_p(u,p,s) \\ \psi_s(u,p,s) \end{pmatrix}, \qquad z_{j+1} = \Psi(z_j),$$

and then data is, for $h(\cdot) = (0, h_0(\cdot))$,

$$y_j = h(z_j) + \eta_j \qquad \text{where } \eta_j \sim N(0, \Gamma).$$

State Estimation

Aim to recover posterior distribution on z_j given $Y_j = \{y_i\}_{i=1}^{j}$. In particular $u_j | Y_j$.

Posterior Distribution

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Approximate Gaussian Filters

- EnKF (with and without localization)
- Square-root EnKF (with and without localization)
- Randomized Maximum Likelihood (RML)

The posterior distribution is approximated by an ensemble $\{\hat{u}^n\}_{n=1}^N$ generated by solving

$$\hat{u}^{(n)} = \operatorname{argmin}_u \Big(\Phi(u; Y_J^{(n)}) + \frac{1}{2}||C^{-1/2}(u - u^{(n)})||^2 \Big)$$

where

$$\begin{aligned} u^{(n)} &\sim \mathbb{P}_0, \\ Y_J^{(n)} &= Y_J + \eta_J^{(n)}, \qquad \eta_J^{(n)} \sim \mathcal{N}(0, \oplus_{j=1}^J \Gamma) \end{aligned} \tag{1}$$

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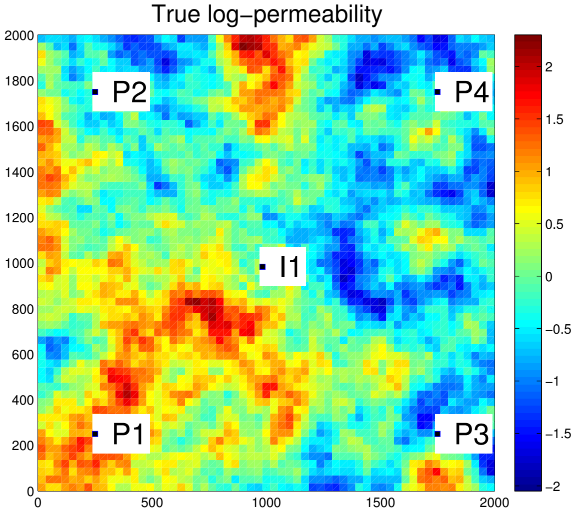
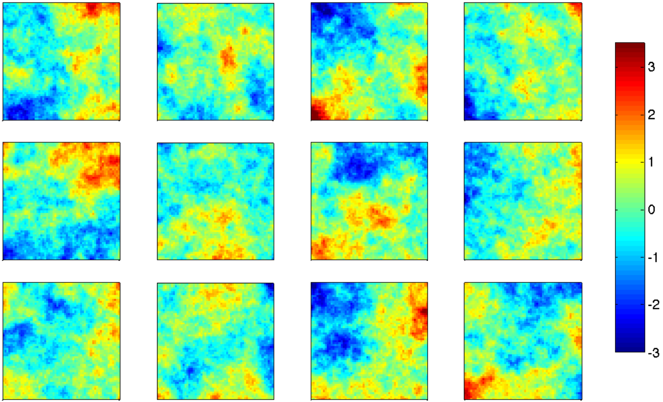
The Truth


True log−permeability
P1
P2
P3
P4
I1
0
200
400
600
800
1000
1200
1400
1600
1800
2000
500
1000
1500
2000
2
1.5
1
0.5
0
−0.5
−1
−1.5
−2

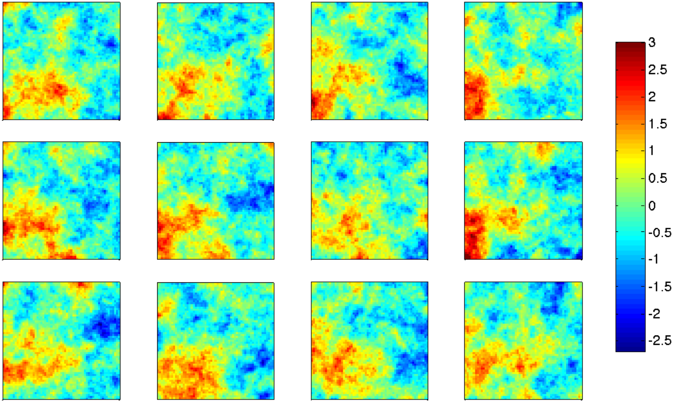
Prior Geology

Monte Carlo samples of the prior distribution $\mathbb{P}_0$ look like:



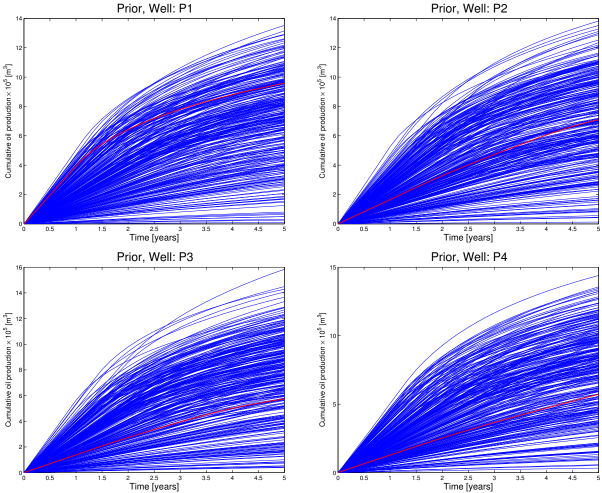
Posterior Geology

MCMC samples of the posterior $\mathbb{P}(\cdot|y)$ look like:



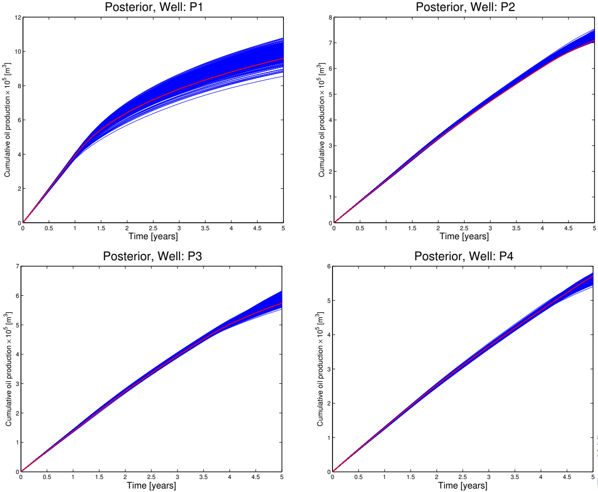
Uncertainty Under The Prior

Large uncertainty in cumulative oil production:



Uncertainty Under The Posterior

Reduction of the uncertainty via data:



Evaluation wrt gold standard, fixed interval

From [ILS13]:

Method	e_{mean}	$e_{variance}$	Cost (FM)
MCMC	0.000	0.000	5.5×10^7
MAP	0.277	0.143	6.0×10^1
RML ($N_e = 50$)	0.235	0.415	3.0×10^3
EnKF ($N_e = 50$)	0.834	0.391	5.0×10^1
EnKF (loc, $N_e = 50$)	0.563	0.252	5.0×10^1
EnKF ($N_e = 8000$)	0.337	0.216	8.0×10^3

FM: Forward Model evaluations.

Outline

Conclusions

- Approximate filters:
  - can reproduce the posterior mean accurately;
  - may not reproduce covariance accurately;
  - can exhibit instability (e.g. on longer time-intervals).
- This instability can cause loss of accuracy in even mean prediction;
- Filter stabilization, via variance inflation can be used to ameliorate instability. Intrusive: changes the covariance.
- Spatial localization techniques can improve accuracy of ensemble method, hence ameliorate instability: mean-field EnKF more stable than finite ensemble.

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Extensions

- Use this technique to assess other algorithms, e.g. particle filters.
- Develop better/more efficient MCMC algorithms.
- Challenge: improve estimates of variance or, more optimistically, general observables.
- Decompose state-space: use e.g. ExKF in the (changing) stable subspace, and a more accurate method in the unstable subspace.

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References 1

- **[LS12]**: K.J.H.Law and A.M.Stuart. "Evaluating Data Assimilation Algorithms." Monthly Weather Review 140, 3757-3782 (2012)
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