

Implicit Sampling for Data Assimilation in Geophysics

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Data assimilation

Uncertain model

$$\mathbf{X}_m = \mathbf{X}_{m-1} + \tau f(\mathbf{X}_{m-1}, \theta, t_{m-1}) + \sqrt{\tau} G(\mathbf{X}_{m-1}, \theta, t_{m-1}) \mathbf{E}_m$$

+

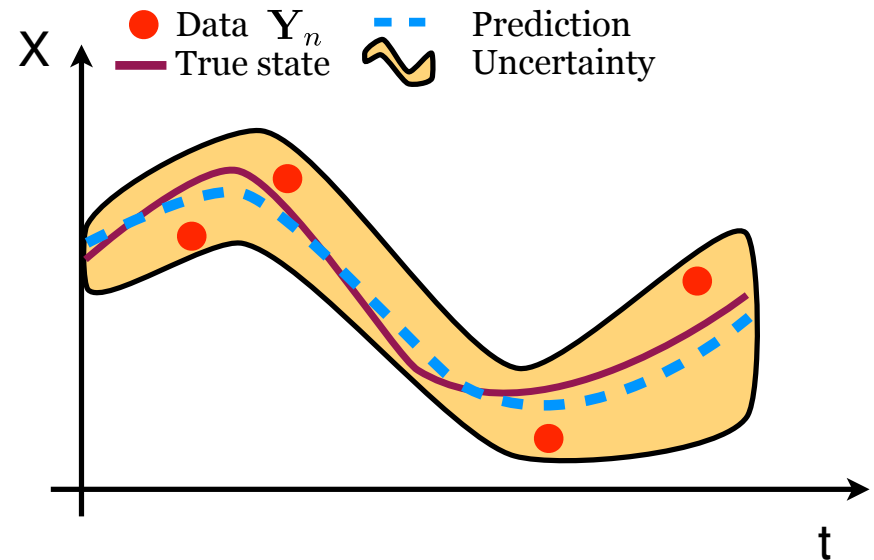
Incomplete, noisy
observations

$$\mathbf{Y}_n = h(\mathbf{X}_{m(n)}, \theta, t_n) + \sqrt{R} \mathbf{D}_n$$

↓

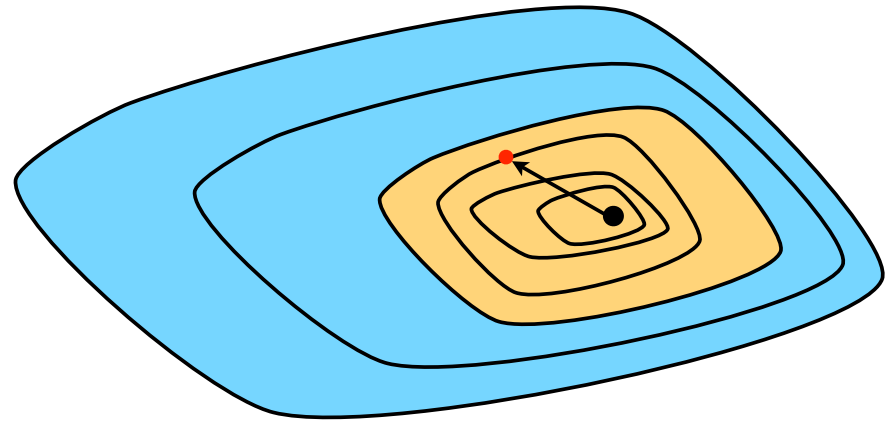
Prediction + uncertainty

$p(\mathbf{x}_{0:m(k)}, \theta | \mathbf{y}_{1:k})$, the target



Implicit sampling

- ▶ Monte Carlo method for importance sampling
- ▶ No forecast distribution, work directly with target
- ▶ Apply particle by particle
- ▶ Use numerical optimization to identify high probability regions based on model and observations
- ▶ Focus the sampling within these regions



- Black dot: mode
- Red dot: sample
- Yellow area: < 3 std. devs.
- Blue area: > 3 std. devs.

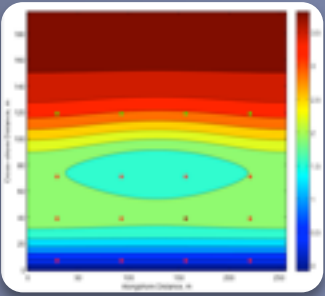


What makes this a good idea?

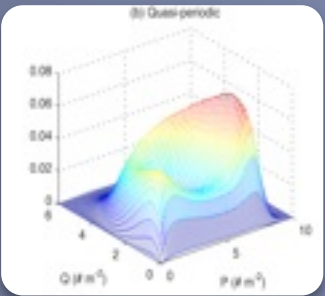
- ▶ **Nonparametric**
 - ▶ Strong theoretical basis for nonlinear/non-Gaussian problems
- ▶ **Sequential/on-line**
 - ▶ Can assimilate any number of observations with each application and discard them thereafter
- ▶ **Optimized for observations**
 - ▶ Computational resources are directed toward important regions of sample space
 - ▶ Avoids sampling “blindly” like many particle filters, i.e., produces samples with non-negligible information
- ▶ **Many implementations, tuned for application ...**



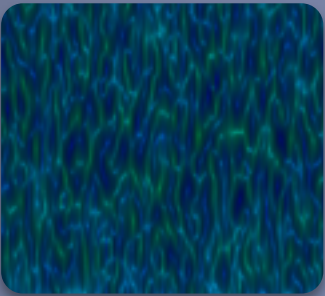
Twin experiments



Shallow water



Predator-prey



Geomagnetism

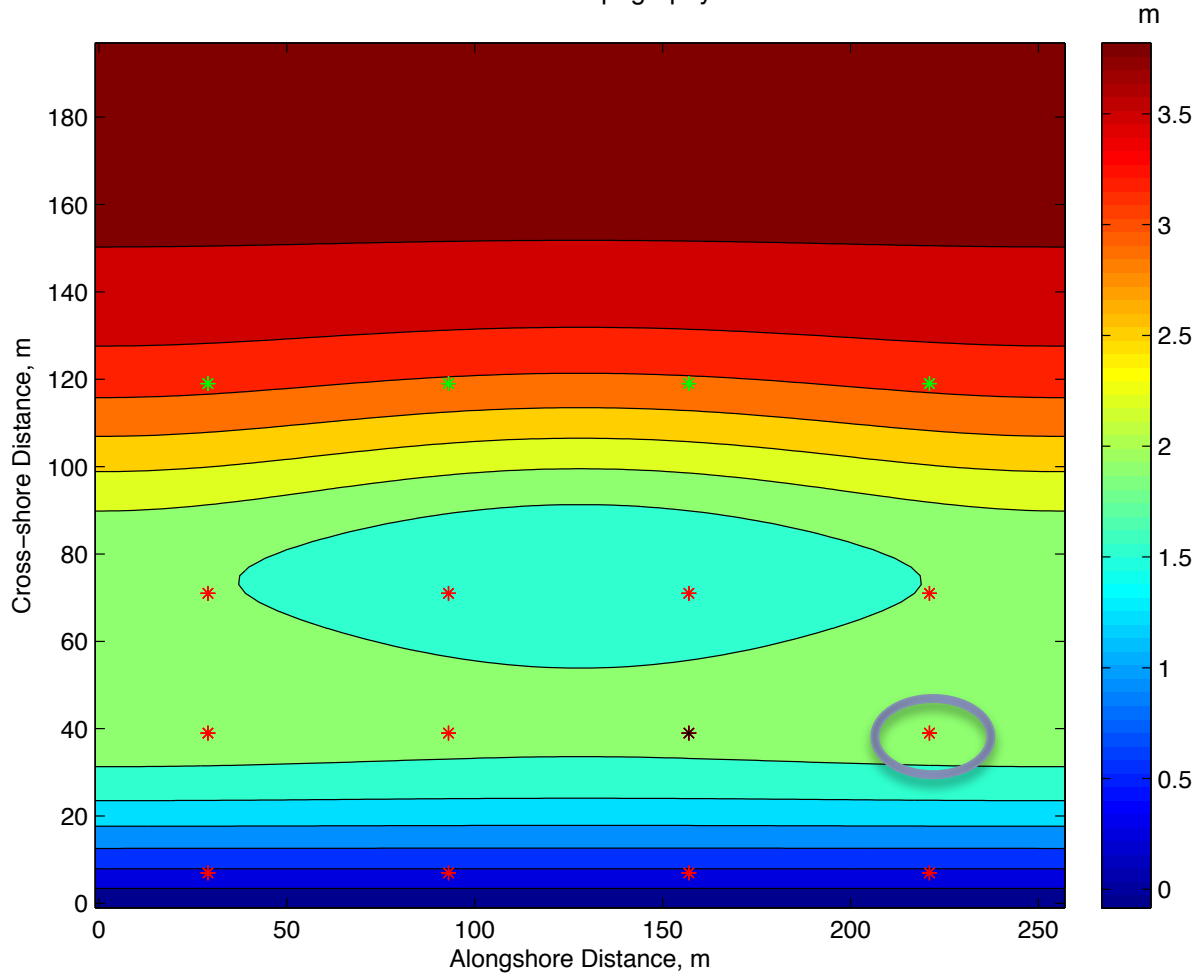


1. Shallow water

- ▶ State dimension $O(30k)$: height and 2 velocity components on a 100×100 horizontal grid
 - ▶ Weak dissipation + strong advection + forcing by wave breaking = strong nonlinearity
 - ▶ Assimilate velocity data every time step at 16 points using 10 particles
 - ▶ Cost fcn.,
$$\mathcal{J}^{(i)} = -\log \left[p(\mathbf{x}_{k+1} | \mathbf{y}_{1:k+1}, \mathbf{x}_k^{(i)}) \right]$$
$$= \frac{1}{2} (\mathbf{x}_{k+1} - \mathbf{x}^*)^T H (\mathbf{x}_{k+1} - \mathbf{x}^*)$$
 - ▶ Target is Gaussian, find \mathbf{x}^* and H from Kalman filter algebra
-



Bottom topography



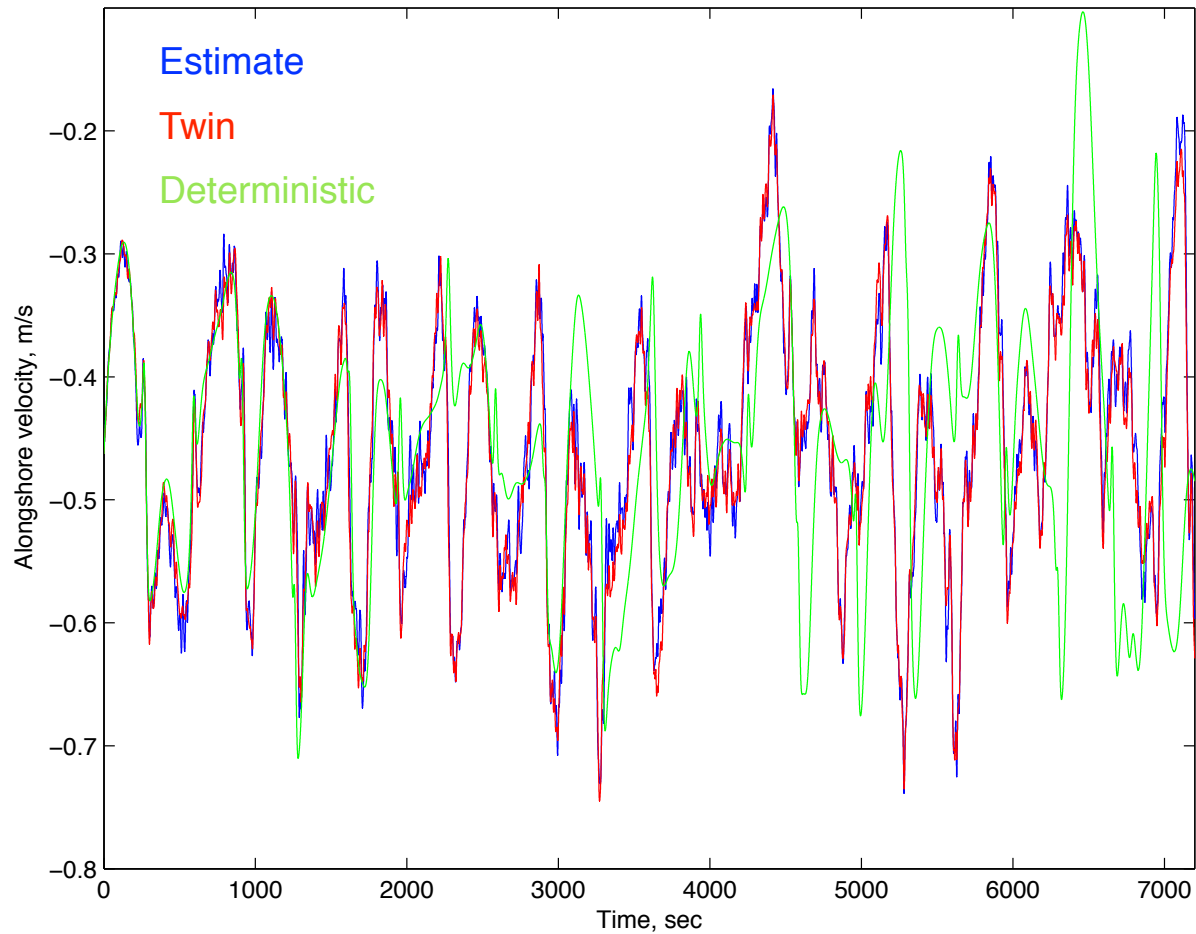
Shallow water

Bottom topography contours

Very shallow = strong forcing by breaking

Observation points indicated with asterisk

Comparison to follow indicated at the circled point



Shallow water

Good agreement between estimate and twin

Assimilation necessary: noticeable phase shift from deterministic and twin solutions after 5000 secs



2. Predator-prey

- ▶ Estimate 2 state variables P (prey) and Q (predator) and 7 unknown parameters $\theta = (\theta_1, \dots, \theta_7)$.

$$\begin{aligned}\frac{dP}{dt} &= (\theta_1 + \theta_2 P)P + \theta_3 \frac{PQ}{1 + \theta_7 P} \\ \frac{dQ}{dt} &= (\theta_4 + \theta_5 Q)Q + \theta_6 \frac{PQ}{1 + \theta_7 P}\end{aligned}$$

- ▶ State and parameters have only one sign
- ▶ Transform (anamorphosis) to variables that are more nearly Gaussian, e.g., $\zeta = (\log P, \log Q, \log \theta)$



Predator-prey

- ▶ **Assimilate 50 observations every 50 times steps:**
 - ▶ all at once (smoother), cost function is

$$\mathcal{J} = -\log [p(\mathbf{x}_{0:m(k)}, \theta | \mathbf{y}_{1:k})]$$

- ▶ or sequentially (filter), cost function is

$$\mathcal{J}^{(i)} = -\log [p(\mathbf{x}_{m(k)+1:m(k+1)}, \theta | \mathbf{y}_{1:k+1}, \mathbf{x}_{m(k)}^{(i)}, \theta^{(i)})]$$

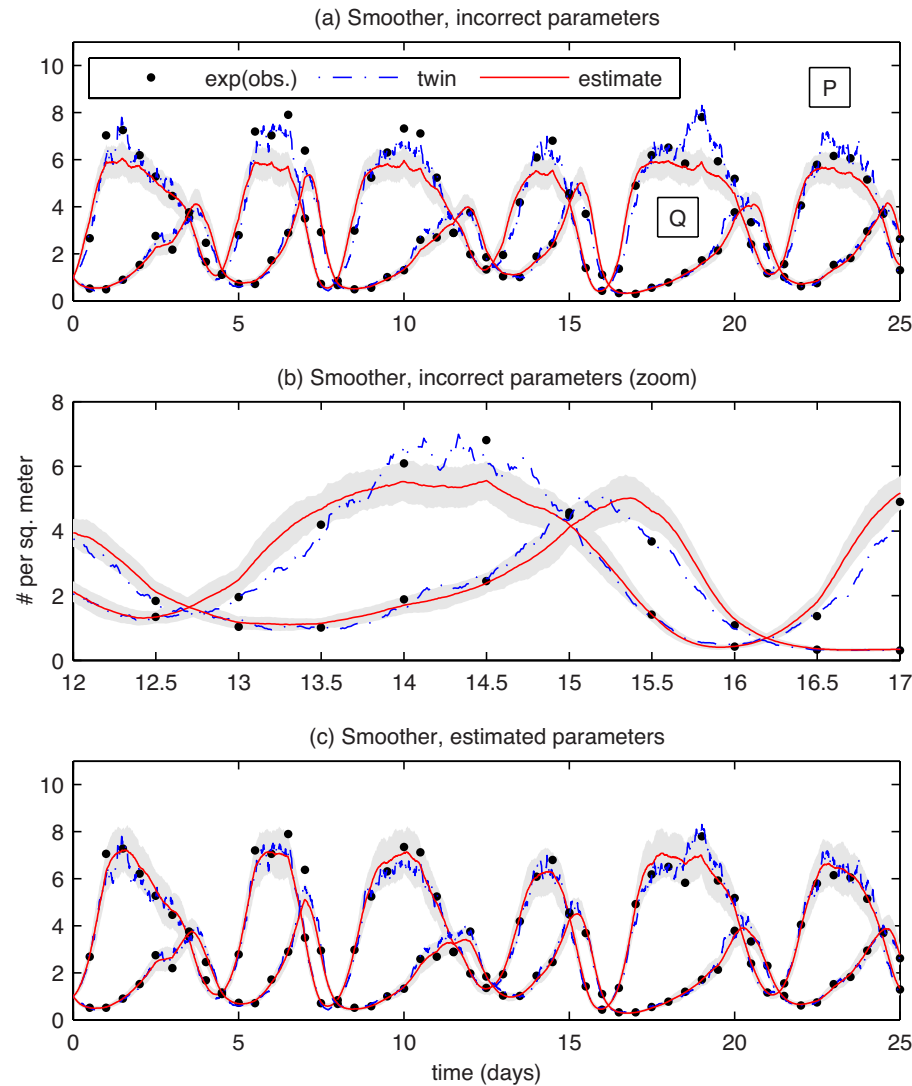
- ▶ **In transformed variable ζ , cost is nearly, but not exactly quadratic:**
 - ▶ optimize to find its min ζ^* , and Hessian H at ζ^*
 - ▶ use Gaussian importance sampling



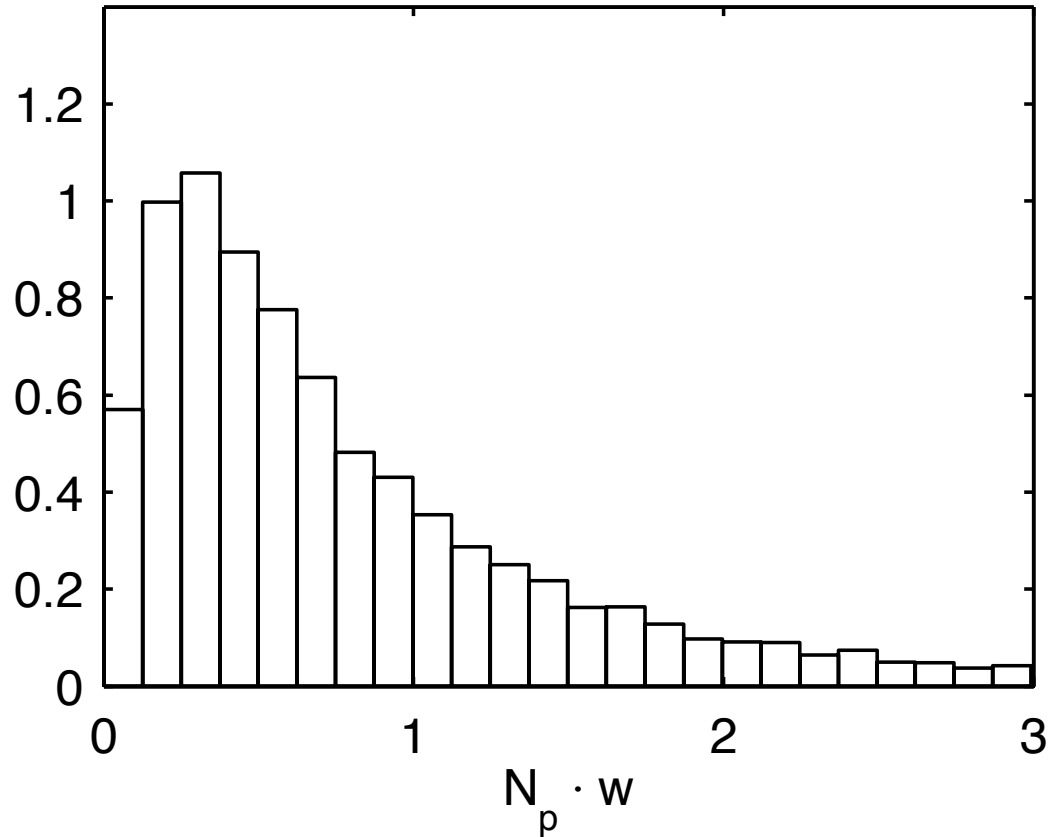
Predator-prey (smoother)

Comparison of state estimate in two cases: (a,b) parameters fixed at incorrect values, (c) estimated parameters

240 particles



Rank histogram / Talagrand diagram



Predator-prey (smoother)

Rank histogram computed
with 240,000 particles

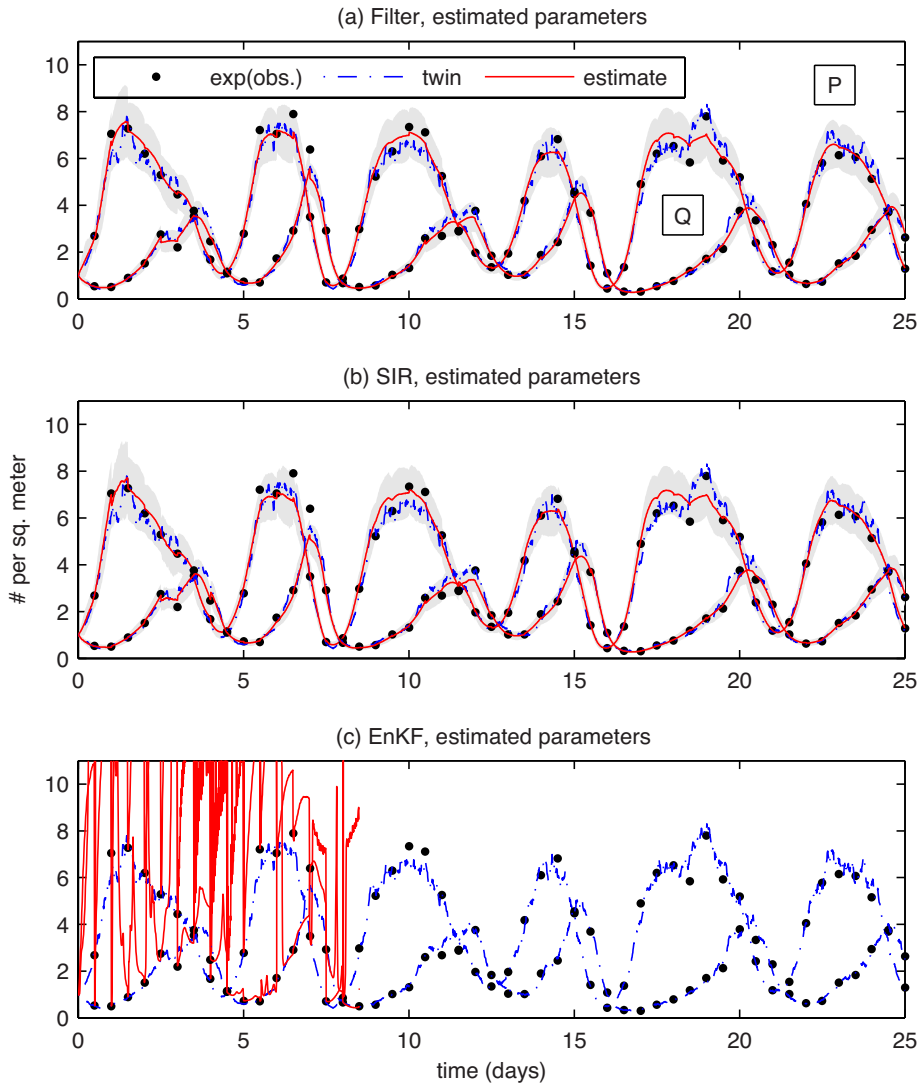
Noticeable drop-off in
distribution before zero



Predator-prey (filter)

2400 particles for implicit and SIR filters and 240,000 for EnKF

EnKF covariance blows up, works with denser observations

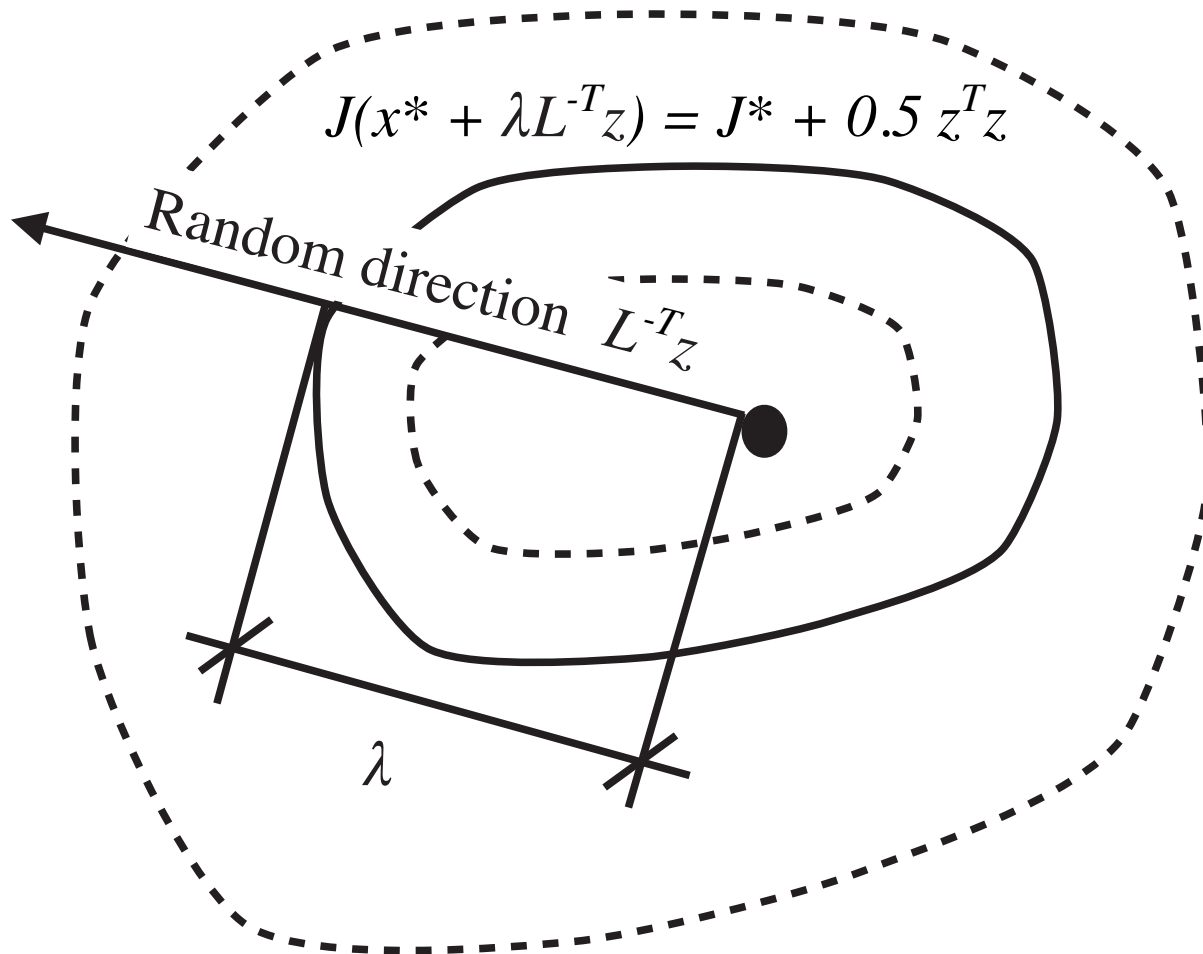


3. Geomagnetism

- ▶ SPDEs for velocity and magnetic field
- ▶ Legendre spectral elements to transform to system of very stiff SDEs
- ▶ Observations of magnetic field only at 200 equally spaced locations
- ▶ Cost is far from quadratic: many steps between observations

$$\mathcal{J}^{(i)} = -\log \left[p(\mathbf{x}_{m(k)+1:m(k+1)}, |\mathbf{y}_{1:k+1}, \mathbf{x}_{m(k)}^{(i)}) \right]$$

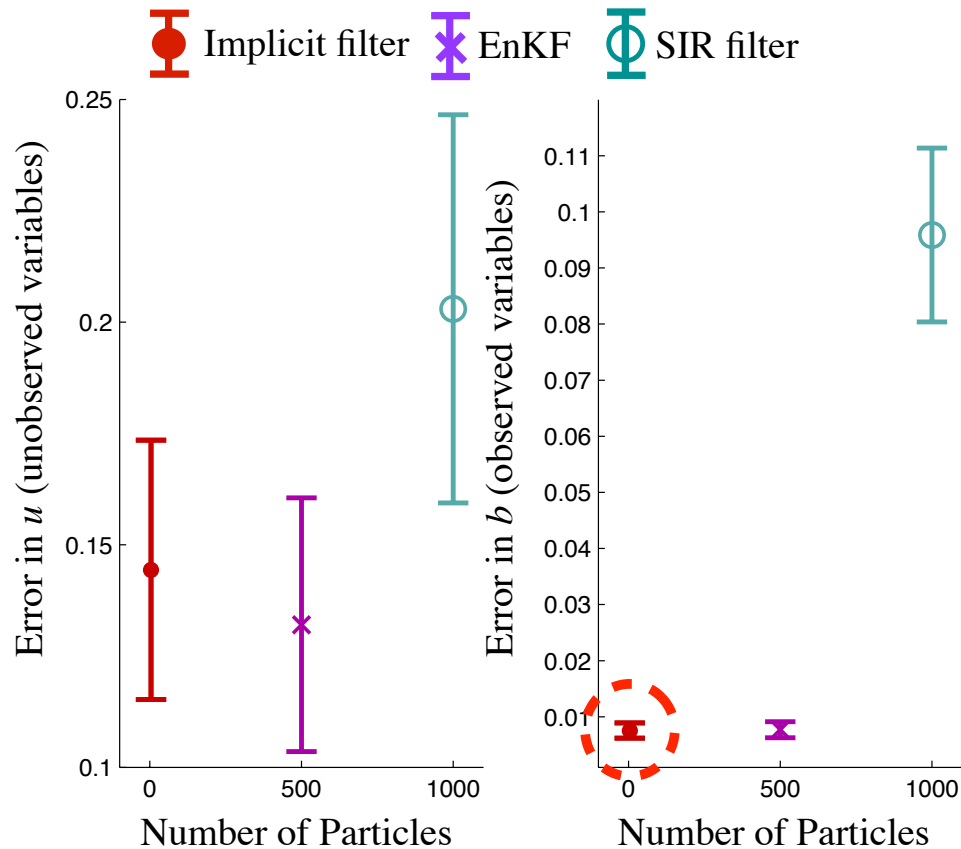




Geomagnetism

If target is far from Gaussian (skew, kurtosis, etc.), use random maps to sample:

1. Draw $z \sim N(0, I)$
2. Cholesky factor $H = LL^T$
3. Search along $L^{-T}z$ until proposal and target have the same level set



Geomagnetism

Comparable errors for implicit filter $O(10)$ particles, EnKF $O(100)$ particles, and SIR $O(1000)$ particles

Fig. 5. Filtering results for data collected at a high spatial resolution (200 measurement locations). The errors at $t = 0.2$ of the implicit particle filter (red), EnKF (purple) and SIR filter (green) are plotted as a function of the number of particles. The error bars represent the mean of the errors and mean of the standard deviations of the errors.

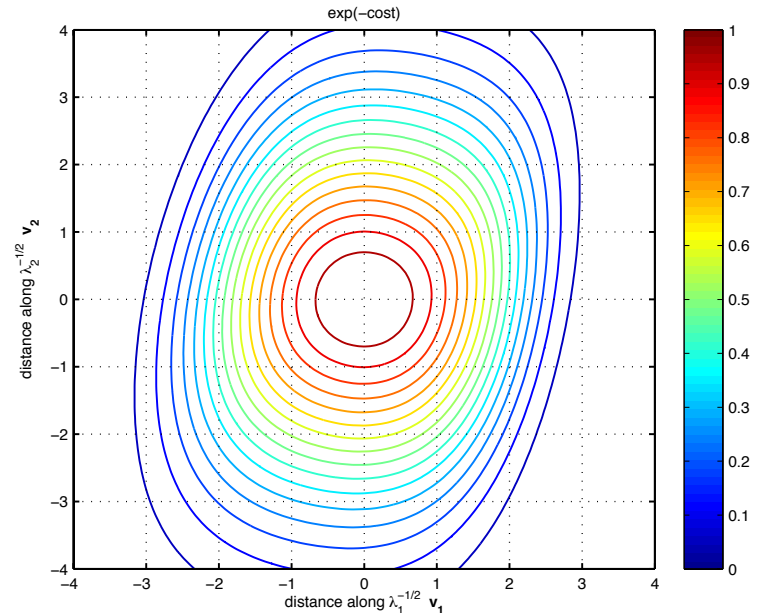
References

- ▶ Lorenz '63, Geomagnetism, and Kuramoto-Sivashinsky (KS)
 - ▶ Morzfeld et al., JCP (2012)
 - ▶ Morzfeld and Chorin, NPG (2012)
 - ▶ Atkins et al., MWR (to appear)
- ▶ Predator-prey
 - ▶ Weir et al., BMB (to appear)
- ▶ KS and shallow water
 - ▶ Jardak et al., JNMF (2009)
 - ▶ Jardak et al., JGR (2010)
- ▶ High dimensional scaling
 - ▶ Bengtsson et al., IMS (2008)
 - ▶ Bickel et al., IMS (2008)
 - ▶ Snyder et al., MWR (2008)
- ▶ ... many more
 - ▶ Miller, van Leeuwen (state estimation)
 - ▶ Kivman, Losa, Dowd, Fennel, Mattern (parameter estimation)



Conclusions

- ▶ Implicit sampling is successful in 3 applications to nonlinear models in $O(10)$ to $O(10k)$ dimensions
- ▶ Able to estimate state and parameters; handles constraints and multiplicative noise
- ▶ Can improve results with adaptive refinements of importance density*



*see poster: Estimation of Ecological Model Parameters by Implicit Sampling, Session 1 (today)



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