Lecture 2: Introduction to Data Assimilation -Methods

Claudia Schillings

CEMRACS Data Assimilation and Reduced Modeling for High Dimensional Problems



Outline







3 Filtering Approach to the Inverse Problem

Mathematical Formulation of the Problem

We assume a model of the unknown z in the form of

$$z_{n+1} = \Psi(z_n) + \zeta_n, \qquad n \in \mathbb{N}$$

$$z_0 \sim \mathcal{N}(m_0, C_0)$$

with $\Psi \in \mathcal{C}(\mathbb{R}^{n_z}, \mathbb{R}^{n_z})$, $\zeta = (\zeta)_n$ an iid sequence with $\zeta_0 \sim \mathcal{N}(0, \Sigma)$, $\Sigma > 0$, z_0 and ζ are assumed to be independent.

There is a true trajectory of z that produces noisy observations

 $y_{n+1} = Hz_{n+1} + \eta_{n+1}, \qquad n \in \mathbb{N}$

with $H \in \mathcal{L}(\mathbb{R}^{n_z}, \mathbb{R}^{n_y})$ and $\eta = (\eta)_n$ an iid sequence, independent of (z_0, ζ) with $\eta_1 \sim \mathcal{N}(0, \Gamma)$, $\Gamma > 0$.

The aim of **data assimilation** is to characterize the conditional distribution of z_n given the observations.

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Find the signal z on a discrete time interval $\mathfrak{N}_0 = \{0, \dots, N\}$

$$z_{n+1} = \Psi(z_n) + \zeta_n, \qquad j \in \mathfrak{N}_0$$

$$z_0 \sim \mathcal{N}(m_0, C_0) \qquad \zeta_0 \sim \mathcal{N}(0, \Sigma)$$

from given data y on the discrete time interval $\mathfrak{N}=\{1,\ldots,N\}$

$$y_{n+1} = Hz_{n+1} + \eta_{n+1}, \qquad j \in \mathfrak{N}, \qquad \eta_1 \sim \mathcal{N}(0, \Gamma).$$

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$$y_{n+1} = Hz_{n+1} + \eta_{n+1}, \qquad j \in \mathfrak{N}, \qquad \eta_1 \sim \mathcal{N}(0, \Gamma).$$

• Prior $\mathbb{P}(z_0,\ldots,z_N) = \prod_{n=0}^{N-1} \mathbb{P}(z_{n+1}|z_n)\mathbb{P}(z_0)$

with

$$\mathbb{P}(z_0) \propto \exp(\frac{1}{2}|z_0 - m_0|_{C_0}^2)$$

and

$$\mathbb{P}(z_{n+1}|z_n) \propto \exp(\frac{1}{2}|z_{n+1} - \Psi(z_n)|_{\Sigma}^2).$$

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$$y_{n+1} = Hz_{n+1} + \eta_{n+1}, \qquad j \in \mathfrak{N}, \qquad \eta_1 \sim \mathcal{N}(0, \Gamma).$$

• Prior

$$\mathbb{P}(z_0,\ldots,z_N)\propto \exp(-\Theta(z_0,\ldots,z_n))$$

with

$$\Theta(z_0,\ldots,z_N) = \frac{1}{2} |z_0 - m_0|_{C_0}^2 + \sum_{n=0}^{N-1} \frac{1}{2} |z_{n+1} - \Psi(z_n)|_{\Sigma}^2$$

Find the signal z on a discrete time interval $\mathfrak{N}_0=\{0,\ldots,N\}$

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$$y_{n+1} = Hz_{n+1} + \eta_{n+1}, \qquad j \in \mathfrak{N}, \qquad \eta_1 \sim \mathcal{N}(0, \Gamma).$$

• Likelihood

$$\mathbb{P}(y_1,\ldots,y_N|z_0,\ldots,z_N) = \prod_{n=0}^{N-1} \mathbb{P}(y_{n+1}|z_0,\ldots,z_N)$$

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$$\mathbb{P}(y_1, \dots, y_N | z_0, \dots, z_N) = \prod_{n=0}^{N-1} \mathbb{P}(y_{n+1} | z_0, \dots, z_N)$$
$$= \prod_{n=0}^{N-1} \mathbb{P}(y_{n+1} | z_{n+1})$$

N-1

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• Likelihood

$$\mathbb{P}(y_1, \dots, y_N | z_0, \dots, z_N) = \prod_{n=0}^{N-1} \mathbb{P}(y_{n+1} | z_0, \dots, z_N)$$

$$\propto \exp(-\Phi(z_0, \dots, z_n; y_1, \dots, y_n)$$

N-1

with $\Phi(z_0, \dots, z_n; y_1, \dots, y_n) = \sum_{n=0}^{N-1} \frac{1}{2} |y_{n+1} - Hz_{n+1}|_{\Gamma}^2$

Find the signal z on a discrete time interval $\mathfrak{N}_0=\{0,\ldots,N\}$

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Bayes' Theorem

The posterior smoothing distribution on $z_0, \ldots, z_n | y_1, \ldots, y_n$ is given by

 $\mathbb{P}(z_0,\ldots,z_n|y_1,\ldots,y_n)\propto \exp(-\Phi(z_0,\ldots,z_n;y_1,\ldots,y_n)-\Theta(z_0,\ldots,z_n)).$

Find the pdf $\mathbb{P}(z_n|y_1, \ldots, y_n)$ associated with the probability measure on the random variable $z_n|y_1, \ldots, y_n$, i.e. sequentially update the pdf $\mathbb{P}(z_n|y_1, \ldots, y_n)$ as n is incremented.

Update
$$\mathbb{P}(z_{n+1}|y_1, \dots, y_{n+1})$$
 from $\mathbb{P}(z_n|y_1, \dots, y_n)$ via
prediction $\mathbb{P}(z_n|y_1, \dots, y_n) \mapsto \mathbb{P}(z_{n+1}|y_1, \dots, y_n)$ and
analysis $\mathbb{P}(z_{n+1}|y_1, \dots, y_n) \mapsto \mathbb{P}(z_{n+1}|y_1, \dots, y_{n+1}).$

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• Prediction

$$\mathbb{P}(z_{n+1}|y_1,\ldots y_n) = \int_{\mathbb{R}^{n_z}} \mathbb{P}(z_{n+1}|y_1,\ldots y_n,z_n)\mathbb{P}(z_n|y_1,\ldots y_n)\mathrm{d}z_n$$

=
$$\int_{\mathbb{R}^{n_z}} \mathbb{P}(z_{n+1}|z_n)\mathbb{P}(z_n|y_1,\ldots y_n)\mathrm{d}z_n .$$

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• Analysis

$$\mathbb{P}(z_{n+1}|y_1, \dots, y_{n+1}) = \mathbb{P}(z_{n+1}|y_1, \dots, y_n, y_{n+1})$$

$$= \frac{\mathbb{P}(y_{n+1}|z_{n+1}, y_1, \dots, y_n)\mathbb{P}(z_{n+1}|y_1, \dots, y_n)}{\mathbb{P}(y_{n+1}|y_1, \dots, y_n)}$$

$$= \frac{\mathbb{P}(y_{n+1}|z_{n+1})\mathbb{P}(z_{n+1}|y_1, \dots, y_n)}{\mathbb{P}(y_{n+1}|y_1, \dots, y_n)} .$$

Particle Filter

Sequential Importance resampling (SIR) filter, Bootstrap filter

1: Set
$$n = 0$$
 and $\mu_0^J = \mu_0$.

- 2: Draw J independent realizations $z_n^{(j)}$ from μ_n^J and set $w_n^{(j)} = 1/J$ for $j = 1, \ldots, J$.
- 3: Define $\mu_n^J = \sum_{j=1}^J w_n^{(j)} \delta_{z_n^{(j)}}$.
- 4: Forecast ensemble: Draw $\hat{z}_{n+1}^{(j)} \sim p(z_n^{(j)}, \cdot)$ with kernel $p(z_n, z_{n+1}) = \mathbb{P}(z_{n+1}|z_n)$.
- 5: Define $g_n(z_{n+1}) \propto \mathbb{P}(y_{n+1}|z_{n+1})$ and compute

$$w_{n+1}^{(j)} = \tilde{w}_{n+1}^{(j)} / (\sum_{j=1}^{J} \tilde{w}_{n+1}^{(j)}), \qquad \tilde{w}_{n+1}^{(j)} = g_n(\hat{z}_{n+1}^{(j)}) w_n^{(j)}, \quad j = 1, \dots, J.$$

6: Analysis ensemble: Set $\mu_{n+1}^J = \sum_{j=1}^J w_{n+1}^{(j)} \delta_{\hat{z}_{n+1}^{(j)}}$. 7: $n \leftarrow n+1$, goto 2.

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Particle Filter

Convergence

Assume g is bounded from below and above, i.e. $\kappa \leq g_n(z) \leq \kappa^{-1}$ for $\kappa \in (0,1], z \in \mathbb{R}^{n_z}$.

For all $n\geq 0,$ there exists a constant C, independent of J such that for any $\phi\in B(\mathbb{R}^{n_z})$

$$\mathbb{E}[(\mu_n^J(\phi) - \mu_n(\phi))^2] \le C \frac{\|\phi\|^2}{J}.$$

See e.g. D. CRISAN AND A. DOUCET **2002** *A survey of convergence results on particle filtering methods for practitioners IEEE Transactions on Signal Processing* **50** for a convergence proof.

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• The rate of convergence is independent of the state dimension n_z , i.e. particle methods can circumvent the curse of dimensionality.

The constant C depends on the state dimension n_z in general. For the standard setting, the number of particles must increase exponentially as problem sizes increases to avoid degenerary.
 T. BENGTSSON, P. BICKEL AND B. LI 2008 Curse-of-dimensionality revisited: Collapse of the particle filter in very large scale systems IMS Collections 2
 C. SNYDER, T. BENGTSSON, P. BICKEL AND J. ANDERSON 2008 Obstacles to high-dimensional particle filtering Monthly Wea. Rev. 136

Evolution model

 $y_{n+1} = I_d z_{n+1} + \eta_{n+1}, \quad j \in \{1, \dots, 10\}, \quad \eta_1 \sim \mathcal{N}(0, 0.1 \ I_d).$

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Evolution model

$$\begin{split} z_{n+1} &= 1.2 \ I_d \ z_n + \zeta_n \,, \quad j \in \{0, \dots, 10\}, \quad z_0 \sim \mathcal{N}(1, 0.01 \ I_d), \\ \text{bservation model} & \qquad \zeta_0 \sim \mathcal{N}(0, 0.01 \ I_d) \,. \end{split}$$

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Extensions

High-Dimensional Problems

A. BESKOS, D. CRISAN, A. JASRA 2014 On the stability of SMC methods in high dimensions THE ANNALS OF APPLIED PROBABILITY 24 P. REBESCHINI AND R. VAN HANDEL 2015 Can local particle filters beat the curse of dimensionality? The Annals of Applied Probability 25

 Arnaud Doucet's SMC and Particle Filters Resources https://www.stats.ox.ac.uk/ doucet/smc_resources.html

Ensemble Kalman Filter

- 1: Set n = 0. Draw J independent realizations $z_n^{(j)}$ from μ_0 .
- 2: Forecast ensemble: Set $\hat{z}_{n+1}^{(j)} = \Psi(z_n^{(j)}) + \zeta_n^{(j)}$ for $j = 1, \ldots, J$. Use the ensemble $(\hat{z}_{n+1}^{(j)})_{j=1}^J$ to define the empirical mean and covariance

$$\hat{m}_{n+1} = \frac{1}{J} \sum_{j=1}^{J} \hat{z}_{n+1}^{(j)} \quad \text{and} \quad \hat{C}_{m+1} = \frac{1}{J-1} \sum_{j=1}^{J} (\hat{z}_{n+1}^{(j)} - \hat{m}_{n+1}) \otimes (\hat{z}_{n+1}^{(j)} - \hat{m}_{n+1})$$

3: Kalman update formulas

$$\begin{split} m_{n+1} &= \hat{m}_{n+1} + K_{n+1}(y_{n+1} - H\hat{m}_{n+1}) \qquad C_{n+1} = \hat{C}_{n+1} - K_{n+1}H\hat{C}_{n+1} \\ \text{with } K_{n+1} &= \hat{C}_{n+1}H^{\top}(H\hat{C}_{n+1}H^{\top} + \Gamma)^{-1}. \\ \text{4: Define } (z_{n+1}^{(j)})_{j=1}^{J} \text{ by a linear transformation } D \text{ with } z_{n+1}^{(j)} = \sum_{i=1}^{J} \hat{z}_{n+1}^{(i)} d_{ij} \\ \text{ such that } \end{split}$$

$$\frac{1}{J}\sum_{j=1}^{J} z_{n+1}^{(j)} = m_{n+1} \quad \text{and} \quad \frac{1}{J-1}\sum_{j=1}^{J} (z_{n+1}^{(j)} - m_{n+1}) \otimes (z_{n+1}^{(j)} - m_{n+1}) = C_{n+1} \,.$$

5: $n \leftarrow n+1$, go to 2.

Ensemble Kalman Filter

EnKF with perturbed observations

$$z_{n+1}^{(j)} = \sum_{i=1}^{J} \hat{z}_{n+1}^{(i)} d_{ij}$$

with observations $y_{n+1}^{(j)} = y_{n+1} + \eta_{n+1}^{(j)}, \ \eta_{n+1}^{(j)} \sim N(0,\Gamma)$ and $d_{ij} = \delta_{ij} - \frac{1}{J-1} (\hat{z}_{n+1}^{(j)} - \hat{m}_{n+1})^\top H^\top (H\hat{C}_{n+1}H^\top + \Gamma)^{-1} (Hz_{n+1}^{(j)} - y_{n+1}^{(j)}).$

Ensemble square root filter (ESFR)

$$z_{n+1}^{(j)} = \sum_{i=1}^{J} \hat{z}_{n+1}^{(i)} d_{ij}$$

with $d_{ij} = w_i - \frac{1}{J} + s_{ij}$, where $\hat{C}_{n+1} = \frac{1}{J-1} P_{n+1} P_{n+1}^{\top}$, $S = (s_{ij})_{i,j} = (I + \frac{1}{J-1} (HP_{n+1})^{\top} \Gamma^{-1} HP_{n+1})^{-\frac{1}{2}}$ and $w = \frac{1}{J} 1 - \frac{1}{J-1} S^2 P_{n+1}^{\top} H^{\top} \Gamma^{-1} (H\hat{m}_{n+1} - y_{n+1}).$

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Ensemble Kalman Filter

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with observations $y_{n+1}^{(j)} = y_{n+1} + \eta_{n+1}^{(j)}, \ \eta_{n+1}^{(j)} \sim N(0,\Gamma)$ and $d_{ij} = \delta_{ij} - \frac{1}{J-1} (\hat{z}_{n+1}^{(j)} - \hat{m}_{n+1})^\top H^\top (H\hat{C}_{n+1}H^\top + \Gamma)^{-1} (Hz_{n+1}^{(j)} - y_{n+1}^{(j)}).$

Ensemble square root filter (ESFR)

$$z_{n+1}^{(j)} = \sum_{i=1}^{J} \hat{z}_{n+1}^{(i)} d_{ij}$$

with $d_{ij} = w_i - \frac{1}{J} + s_{ij}$, where $\hat{C}_{n+1} = \frac{1}{J-1} P_{n+1} P_{n+1}^{\top}$, $S = (s_{ij})_{i,j} = (I + \frac{1}{J-1} (HP_{n+1})^{\top} \Gamma^{-1} HP_{n+1})^{-\frac{1}{2}}$ and $w = \frac{1}{J} 1 - \frac{1}{J-1} S^2 P_{n+1}^{\top} H^{\top} \Gamma^{-1} (H\hat{m}_{n+1} - y_{n+1}).$

- The ensemble parameter estimate lies in the linear span of the initial ensemble [23].
- In the linear case, the EnKF estimate converges in the limit J → ∞ to the solution of the regularised least-squares problem [24, 31]. In the nonlinear setting, convergence to the mean-field Kalman filter is proven in [30].
- Ernst et al. [21] showed that the EnKF is not consistent with the Bayesian perspective in the nonlinear setting, but can be interpreted as a point estimator of the unknown parameters.
- Kelly et al. [28, 29, 42, 41] presented an analysis of the long-time behavior and ergodicity of the ensemble Kalman filter with arbitrary ensemble size establishing time uniform bounds to control the filter divergence and ensuring in addition the existence of an invariant measure.
- Long term stability and accuracy is established for ensemble Kalman-Bucy filters applied to continuous-time filtering problems [20, 44].
- Higher order updates by polynomial chaos expansion can be found in [34].
Connection to inverse problems

Find the unknown data $u \in X$ from noisy observations

 $y = \mathcal{G}(u) + \eta$

Bridging Sequence

Introduction of an artificial discrete time dynamical system which maps the prior μ_0 into the posterior μ . The effective variance is amplified by N = 1/h at each step, compensating for the redundant, repeated use of the data.

Analysis of Ensemble Kalman Inversion

Assumption: The forward operator is linear , i.e. $\mathcal{G} = A \in \mathcal{L}(X, \mathbb{R}^{n_y})$. EnKF with perturbed observations

$$du^{(j)} = C(u)A^*\Gamma^{-1}A(u^{\dagger} + \eta - u^{(j)}) dt + C(u)A^*\Gamma^{-\frac{1}{2}} dW^{(j)}$$

where $W^{(1)}, \ldots, W^{(J)}$ are pairwise cylindrical Wiener processes and y denotes the noisy observational data.

(a) Global Existence of Solutions (b) Ensemble Collapse

(c) Convergence of Residuals

Strongly convergent discretization scheme

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(a) Global Existence of Solutions(b) Ensemble Collapse

(c) Convergence of Residuals

Strongly convergent discretization scheme .

Continuous Time Limit (Linear Case)

Assumption: Linear response operator $\mathcal{G}(u) = Au$ with $A \in \mathcal{L}(X, Y)$

$$u_{n+1}^{(j)} = u_n^{(j)} + hC(u_n)A^*\Gamma^{-1}(y_{n+1}^{(j)} - Au_{n+1}^{(j)})$$

with $C(u_n) = \frac{1}{J} \sum_{j=1}^J (u_n^{(j)} - \overline{u}_n) \otimes (u_n^{(j)} - \overline{u}_n)$ and $\overline{u}_n = \frac{1}{J} \sum_{j=1}^J u_n^{(j)}$.

Limiting SDE

$$du^{(j)} = C(u)A^*\Gamma^{-1}A(u^{\dagger} + \eta - u^{(j)}) dt + C(u)A^*\Gamma^{-\frac{1}{2}} dW^{(j)},$$

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Noise-free Case

Limiting ODE

$$du^{(j)} = C(u)A^*\Gamma^{-1}A(u^{\dagger} + \eta - u^{(j)}) dt + C(u)A^*\Gamma^{-\frac{1}{2}} dW^{(j)},$$

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Noise-free Case

Limiting ODE

$$du^{(j)} = C(u)A^*\Gamma^{-1}A(u^{\dagger} - u^{(j)}) dt,$$

or equivalently,

$$\frac{\mathrm{d}}{\mathrm{d}t}u^{(j)} = -C(u)D_u\Phi(u^{(j)};y)$$

with potential $\Phi(u; y) = \frac{1}{2} \|\Gamma^{-\frac{1}{2}}(y - Au)\|^2$.

(a) Global Existence of Solutions

(b) Ensemble Collapse

(c) Convergence of Residuals

(a) Global Existence of Solutions

Assume that y is the image of a truth $u^{\dagger} \in \mathcal{X}$ under A. Let $u^{(j)}(0) \in \mathcal{X}$ for $j = 1, \ldots, J$ and define \mathcal{X}_0 to be the linear span of the $\{u^{(j)}(0)\}_{j=1}^J$.

Then, the limiting ODE has a unique solution $u^{(j)}(\cdot) \in C([0,\infty); \mathcal{X}_0)$ for $j = 1, \ldots, J$.

(a) Global Existence of Solutions

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Then, the limiting ODE has a unique solution $u^{(j)}(\cdot) \in C([0,\infty); \mathcal{X}_0)$ for $j = 1, \ldots, J$.

Sketch of Proof

Quantities

$$\begin{split} e^{(j)} &= u^{(j)} - \overline{u} , \qquad \qquad r^{(j)} = u^{(j)} - u^{\dagger} , \\ E_{lj} &= \langle Ae^{(l)}, Ae^{(j)} \rangle_{\Gamma} , \qquad R_{lj} = \langle Ar^{(l)}, Ar^{(j)} \rangle_{\Gamma} , \qquad F_{lj} = \langle Ar^{(l)}, Ae^{(j)} \rangle_{\Gamma} , \end{split}$$

(a) Global Existence of Solutions

Assume that y is the image of a truth $u^{\dagger} \in \mathcal{X}$ under A. Let $u^{(j)}(0) \in \mathcal{X}$ for $j = 1, \ldots, J$ and define \mathcal{X}_0 to be the linear span of the $\{u^{(j)}(0)\}_{j=1}^J$.

Then, the limiting ODE has a unique solution $u^{(j)}(\cdot) \in C([0,\infty); \mathcal{X}_0)$ for $j = 1, \ldots, J$.

Sketch of Proof

$$\frac{\mathrm{d}}{\mathrm{d}t}e^{(j)} = -\frac{1}{J}\sum_{k=1}^{J}E_{jk}e^{(k)}, \quad \frac{\mathrm{d}}{\mathrm{d}t}r^{(j)} = -\frac{1}{J}\sum_{k=1}^{J}F_{jk}r^{(k)}, \qquad j = 1, \dots, J$$
$$\frac{\mathrm{d}}{\mathrm{d}t}E = -\frac{2}{J}E^{2}, \qquad \qquad \frac{\mathrm{d}}{\mathrm{d}t}R = -\frac{2}{J}FF^{\top}, \qquad \frac{\mathrm{d}}{\mathrm{d}t}F = -\frac{2}{J}FE$$

Global existence of E, R and F \Rightarrow global existence of r and e

(b) Ensemble Collapse

Assume that y is the image of a truth $u^{\dagger} \in \mathcal{X}$ under A. Let $u^{(j)}(0) \in \mathcal{X}$ for $j = 1, \ldots, J$.

Then, the matrix valued quantity E(t) converges to 0 for $t\to\infty$ and, indeed $\|E(t)\|=\mathcal{O}(Jt^{-1}).$

(b) Ensemble Collapse

Assume that y is the image of a truth $u^{\dagger} \in \mathcal{X}$ under A. Let $u^{(j)}(0) \in \mathcal{X}$ for $j = 1, \ldots, J$.

Then, the matrix valued quantity E(t) converges to 0 for $t \to \infty$ and, indeed $||E(t)|| = O(Jt^{-1})$.

The rate of convergence of E and F is algebraic with a constant growing with larger ensemble size J.

(c) Convergence of Residuals

Assume that y is the image of a truth $u^{\dagger} \in \mathcal{X}$ under A and the forward operator A is one-to-one. Let Y^{\parallel} denote the linear span of the $\{Ae^{(j)}(0)\}_{j=1}^{J}$ and let Y^{\perp} denote the orthogonal complement of Y^{\parallel} in \mathcal{Y} with respect to the inner product $\langle \cdot, \cdot \rangle_{\Gamma}$ and assume that the initial ensemble members are chosen so that Y^{\parallel} has the maximal dimension $\min\{J-1,\dim(\mathcal{Y})\}.$

Then $Ar^{(j)}(t)$ may be decomposed uniquely as

$$Ar_{\parallel}^{(j)}(t) + Ar_{\perp}^{(j)}(t) \quad \text{with } Ar_{\parallel}^{(j)} \in Y^{\parallel} \text{ and } Ar_{\perp}^{(j)} \in Y^{\perp}.$$

Furthermore $Ar_{\parallel}^{(j)}(t) \to 0$ as $t \to \infty$ and $Ar_{\perp}^{(j)}(t) = Ar_{\perp}^{(j)}(0) = Ar_{\perp}^{(1)}$.

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 $\text{Furthermore } Ar^{(j)}_{\parallel}(t) \to 0 \text{ as } t \to \infty \text{ and } Ar^{(j)}_{\perp}(t) = Ar^{(j)}_{\perp}(0) = Ar^{(1)}_{\perp}.$

Adaptive choice of the initial ensemble to ensure convergence of the residuals.

Long-time Behaviour (Linear Case) Idea of Proof

Subspace property

$$Ae^{(j)}(t) = \sum_{k=1}^{J} \ell_{jk}(t) Ae^{(k)}(0)$$

where the matrix $L = \{\ell_{jk}\}$ is invertible.

Decomposition of the residual

$$Ar^{(j)}(t) = \sum_{k=1}^{J} \alpha_k Ae^{(k)}(t) + Ar_{\perp}^{(1)}$$

Convergence of the residuals

Boundedness of the coefficient vector

$$|\alpha(t)|^2 \le \frac{\lambda_0^{(J)}}{\lambda_0^{\min}} |\alpha(0)|^2$$

gives convergence of the residuals.

(a) Global Existence of Solutions(b) Ensemble Collapse(c) Convergence of Residuals

- No Gaussian prior assumption.
- Convergence result opens up the perspective to use the EnKF as a linear solver in case of a boundedly invertible forward operator.
- In the finite dimensional setting, the results can be used to characterise the parameter space informed by the data.

Continuous Time Limit

EnKF with perturbed observations

$$du^{(j)} = C(u)A^*\Gamma^{-1}A(u^{\dagger} + \eta - u^{(j)}) dt + C(u)A^*\Gamma^{-\frac{1}{2}} dW^{(j)},$$

where $W^{(1)}, \ldots, W^{(J)}$ are pairwise independent cylindrical Wiener processes and y denotes the noisy observational data.

Continuous Time Limit

EnKF with perturbed observations

$$du^{(j)} = C(u)A^*\Gamma^{-1}A(u^{\dagger} - u^{(j)}) dt,$$

or equivalently,

$$\frac{\mathrm{d}}{\mathrm{d}t}u^{(j)} = -C(u)D_u\Phi(u^{(j)};y)$$

with potential $\Phi(u; y) = \frac{1}{2} \|\Gamma^{-\frac{1}{2}}(y - Au)\|^2$.

CIS and Stuart A M 2017 Analysis of the ensemble Kalman filter for inverse problems SINUM.

CIS and Stuart A M 2017 Convergence analysis of ensemble Kalman inversion: the linear, noisy case Applicable Analysis.

Continuous time limit of the EnKF

 $du^{(j)} = C(u)A^*\Gamma^{-1}A(u^{\dagger} + \eta - u^{(j)}) dt + C(u)A^*\Gamma^{-\frac{1}{2}} dW^{(j)},$

(a) Global Existence of Solutions

(b) Ensemble Collapse

(c) Convergence of Residuals

Let S be the linear span of $\{u_0^{(j)}\}_{j=1}^J$, then $u_t^{(j)} \in S$ for all $(t,j) \in [0,\infty) \times \{1,\ldots,J\}$ almost surely.

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Transformation to SDE in finite dimensional space

- Assume that the initial ensemble $(u_0^{(j)})_{j\in\{1,\ldots,J\}}$ is linearly independent almost surely.
- Transformation of the original SDE to

$$du_t^{(j)} = C(u_t) A^* \Gamma^{-1}(y - Au_t^{(j)}) dt + C(u_t) A^* \Gamma^{-1/2} dW_t^{(j)}.$$

with linear operator $A : \mathbb{R}^J \to \mathbb{R}^K$.

(a) Global Existence of Solutions [Blömker, CIS, Wacker, Weissmann 18] Let $u_0 = (u_0^{(j)})_{j \in \{1,...,J\}}$ be \mathcal{F}_0 -measurable maps $u_0^{(j)} : \Omega \to X$ which are linearly independent almost surely.

Then for all $T \ge 0$ there exists a unique strong solution $(u_t)_{t \in [0,T]}$ (up to \mathbb{P} -indistinguishability) of the set of coupled SDEs

$$du_t^{(j)} = C(u_t)A^*\Gamma^{-1}(y - Au_t^{(j)}) dt + C(u_t)A^*\Gamma^{-1/2} dW_t^{(j)}.$$
 (1)

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$$du_t^{(j)} = C(u_t) A^* \Gamma^{-1}(y - Au_t^{(j)}) dt + C(u_t) A^* \Gamma^{-1/2} dW_t^{(j)}.$$
 (1)

Sketch of Proof

- Local weak monotonicity
- Local weak coercivity
- Existence of a stochastic Lyapunov function $V \in C^2(X; \mathcal{R}_+)$ such that for some c > 0

$$\begin{split} LV(x) &:= V_x(x)F(x) + \frac{1}{2}\operatorname{trace}(G^T(x)V_{xx}(x)G(x)) \leq cV(x),\\ \inf_{|x|>R} V(x) \to \infty \text{ as } R \to \infty \,. \end{split}$$

Quantities of Interest

$$e^{(j)} = u^{(j)} - \overline{u}, \quad \mathfrak{e}^{(j)} := \Gamma^{-\frac{1}{2}} A e^{(j)}$$

(b) Ensemble Collapse [Blömker, CIS, Wacker, Weissmann 18]

Let $u_0 = (u_0^{(j)})_{j \in \{1,...,J\}}$ be \mathcal{F}_0 -measurable maps with $C_0 = \mathbb{E}[\frac{1}{J} \sum_{j=1}^J |\mathfrak{e}_0^{(j)}|^2] < \infty$.

Then, the ensemble collapse is quantified by

$$\mathbb{E}[\frac{1}{J}\sum_{j=1}^{J}|\mathfrak{e}_{t}^{(j)}|^{2}] \leq \frac{1}{\frac{J+1}{J^{2}}t + \frac{1}{C_{0}}}$$

Quantities of Interest

$$e^{(j)} = u^{(j)} - \overline{u}, \quad \mathfrak{e}^{(j)} := \Gamma^{-\frac{1}{2}} A e^{(j)}$$

(b) Ensemble Collapse (Parameter Space) [Blömker, CIS, Wacker, Weissmann 18]

Let $u_0 = (u_0^{(j)})_{j \in \{1,...,J\}}$ be \mathcal{F}_0 -measurable maps with $C_0 = \mathbb{E}[\frac{1}{J} \sum_{j=1}^J |\mathfrak{e}_0^{(j)}|^2] < \infty$. Further assume that the linear operator A is one-to-one.

Then, the ensemble collapse is quantified by

$$\mathbb{E}\left[\frac{1}{J}\sum_{j=1}^{J}|e_{t}^{(j)}|^{2}\right] \leq \frac{1}{\sigma_{\min}}\frac{1}{\frac{J+1}{J^{2}}t + \frac{1}{C_{0}}},$$

where σ_{\min} is the smallest eigenvalue of $A^*\Gamma^{-1}A$.

Quantities of Interest

$$e^{(j)} = u^{(j)} - \overline{u}, \quad \mathfrak{e}^{(j)} := \Gamma^{-\frac{1}{2}} A e^{(j)}$$

(c) Almost Sure Ensemble Collapse [Blömker, CIS, Wacker, Weissmann 18] Let $u_0 = (u_0^{(j)})_{j \in \{1,...,J\}}$ be \mathcal{F}_0 -measurable maps and $\gamma : \mathcal{R}_+ \to \mathcal{R}_+$ a positive, monotonically increasing and differentiable function such that $\int_0^\infty \frac{\gamma'(s)^2}{\gamma(s)} ds < \infty$. Then the trivial solution of

$$\mathrm{d}\mathfrak{e}_t^{(j)} = -C(\mathfrak{e}_t)\mathfrak{e}_t^{(j)}\mathrm{d}t + C(\mathfrak{e}_t)\mathrm{d}(W_t^{(j)} - \overline{W}_t)$$

is almost surely asymptotically stable with rate function $\rho(t) = (\gamma(t))^{-\frac{1}{2}}$. In particular, $(\mathfrak{e}_t^{(j)})_{j=1,\dots,J}$ converges to zero almost surely as $t \to \infty$.

Quantities of Interest

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(c) Almost Sure Ensemble Collapse [Blömker, CIS, Wacker, Weissmann 18] Let $u_0 = (u_0^{(j)})_{j \in \{1,...,J\}}$ be \mathcal{F}_0 -measurable maps and $\gamma : \mathcal{R}_+ \to \mathcal{R}_+$ a positive, monotonically increasing and differentiable function such that $\int_0^\infty \frac{\gamma'(s)^2}{\gamma(s)} ds < \infty$. Then the trivial solution of

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is almost surely asymptotically stable with rate function $\rho(t) = (\gamma(t))^{-\frac{1}{2}}$. In particular, $(\mathfrak{e}_t^{(j)})_{j=1,\dots,J}$ converges to zero almost surely as $t \to \infty$.

Under the assumption that \boldsymbol{A} is one-to-one, the result holds true in the parameter space too.

C. Schillings (U Mannheim)

Quantities of Interest

$$r^{(j)} = u^{(j)} - u^{\dagger}, \quad \mathfrak{r}^{(j)} := \Gamma^{-\frac{1}{2}} A r^{(j)}$$

(c) Convergence of the Residuals [Blömker, CIS, Wacker, Weissmann 18] Let y be the image of a truth $u^{\dagger} \in \mathcal{X}$ under A and $u_0 = (u_0^{(j)})_{j \in \{1,...,J\}}$ be \mathcal{F}_0 -measurable maps $u_0^{(j)} : \Omega \to \mathcal{X}$ such that $\mathbb{E}[\frac{1}{J} \sum_{j=1}^{J} |\mathfrak{r}_0^{(j)}|^2] < \infty$.

Then

$$\mathbb{E}\left[\frac{1}{J}\sum_{j=1}^{J}|\mathfrak{r}_{t}^{(j)}|^{2}\right]^{\frac{1}{2}}$$

is monotonically decreasing.

Quantities of Interest

$$r^{(j)} = u^{(j)} - u^{\dagger}, \quad \mathfrak{r}^{(j)} := \Gamma^{-\frac{1}{2}} A r^{(j)}$$

(c) Convergence of the Residuals with Variance Inflation [Blömker, CIS, Wacker, Weissmann 18]

Assume that y is the image of a truth $u^{\dagger} \in \mathcal{X}$ under A and let $\mathfrak{r}_0 = (\mathfrak{r}_0^{(j)})_{j \in \{1,...,J\}}$ be \mathcal{F}_0 -measurable maps such that $\mathbb{E}[\frac{1}{J}\sum_{j=1}^J |\mathfrak{r}_0^{(j)}|^2] < \infty$, $B \in \mathcal{L}(\mathcal{R}^K, \mathcal{R}^K)$ a positive definite operator and $(\mathfrak{r}_t^{(j)})_{t \ge 0, j=1,...,J}$ the solution of

$$\mathrm{d}\mathfrak{r}_t^{(j)} = -(C(\mathfrak{r}_t) + \frac{1}{t^\alpha + R}B)\mathfrak{r}_t^{(j)}\,\mathrm{d}t + C(\mathfrak{r}_t)\,\mathrm{d}W_t^{(j)}, \quad \alpha \in (0,1), R > 0.$$

Then it holds true that

$$\lim_{t \to \infty} \mathbb{E}\left[\frac{1}{J} \sum_{j=1}^{J} |\mathfrak{r}_t^{(j)}|^2\right] = 0.$$

Quantities of Interest

$$r^{(j)} = u^{(j)} - u^{\dagger}, \quad \mathfrak{r}^{(j)} := \Gamma^{-\frac{1}{2}} A r^{(j)}$$

(c) Convergence of the Residuals with Variance Inflation [Blömker, CIS, Wacker, Weissmann 18]

Assume that y is the image of a truth $u^{\dagger} \in \mathcal{X}$ under A and let $\mathfrak{r}_0 = (\mathfrak{r}_0^{(j)})_{j \in \{1,...,J\}}$ be \mathcal{F}_0 -measurable maps, $B \in \mathcal{L}(\mathcal{R}^K, \mathcal{R}^K)$ a positive definite operator and $(\mathfrak{r}_t^{(j)})_{t \geq 0, j=1,...,J}$ the solution of

$$\mathrm{d}\mathfrak{r}_t^{(j)} = -(C(\mathfrak{r}_t) + \frac{1}{t^\alpha + R}B)\mathfrak{r}_t^{(j)}\,\mathrm{d}t + C(\mathfrak{r}_t)\,\mathrm{d}W_t^{(j)}, \quad \alpha \in (0,1), R > 0$$

Then the solution is almost surely asymptotically stable with rate function $\rho(t) = t^{-\frac{\beta}{2}}$ for all $\beta \in (0, 1 - \alpha)$. In particular, $(\mathfrak{r}_t^{(j)})_{j=1,\dots,J}$ converges to zero almost surely as $t \to \infty$.

Variance Inflation in the Parameter Space

Let $y \in AS$ with $AS = \operatorname{span}\{Au_0^{(1)}, \dots, Au^{(J)}\}.$

$$du_t^{(j)} = (C(u_t) + \frac{1}{t^{\alpha} + R}B)A^*\Gamma^{-1}(y - Au_t^{(j)}) dt + C(u_t)A^*\Gamma^{-\frac{1}{2}} dW_t^{(j)} \quad (VI)$$

 $j=1,\ldots,J,$ for B positive definite, R>0 and $\alpha\in(0,1)$

Variance Inflation in the Parameter Space Let $y \in AS$ with $AS = \text{span}\{Au_0^{(1)}, \dots, Au^{(J)}\}$.

$$du_t^{(j)} = (C(u_t) + \frac{1}{t^{\alpha} + R}B)A^*\Gamma^{-1}(y - Au_t^{(j)}) dt + C(u_t)A^*\Gamma^{-\frac{1}{2}} dW_t^{(j)}$$
(VI)

 $j = 1, \ldots, J$, for B positive definite, R > 0 and $\alpha \in (0, 1)$

Let $y \in AS$ and assume that y is the image of a truth $u^{\dagger} \in \mathcal{X}$ under A and let $(u_t^{(j)})_{t \geq 0, j=1,...,J}$ be the solution of (VI). Then,

• $\lim_{t\to\infty} \mathbb{E}\left[\frac{1}{J}\sum_{j=1}^{J} |\mathfrak{e}_t^{(j)}|^2\right] = 0.$

•
$$\lim_{t \to \infty} \mathbb{E}\left[\frac{1}{J} \sum_{j=1}^{J} |\mathbf{r}_t^{(j)}|^2\right] = 0.$$

• $(\mathfrak{r}_t^{(j)})_{t\geq 0}$ converges almost surely to zero with rate function $\rho(t) = t^{-\frac{\beta}{2}}$ for all $\beta \in (0, 1 - \alpha)$.

(a) Global Existence of Solutions(b) Ensemble Collapse(c) Convergence of Residuals

- No Gaussian prior assumption (in the case of the EnKF with perturbed observations).
- The discretization via the ensemble particles and properties of the forward operator allow to transfer the results to the parameter space informed by the data.

Numerical Experiments (Linear Case)

1-dimensional elliptic equation

$$-\frac{\mathrm{d}^2 p}{\mathrm{d} x^2} + p = u \quad \text{in } D := (0,\pi) \,, \ p = 0 \quad \text{in } \partial D \;,$$

where

$$\begin{split} A &= \mathcal{O} \circ L^{-1} \text{ with } L = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + id \text{ and } D(L) = H^2(D) \cap H^1_0(D) \\ \mathcal{O} : X \mapsto \mathbb{R}^K \text{, equispaced observation points in } D \text{ with spacing } \tau_N^{\mathcal{O}} = 2^{-N_K} \text{ at } \\ x_k &= \frac{k}{2^{N_K}}, \ k = 1, \dots, 2^{N_K} - 1, \ o_k(\cdot) = \delta(\cdot - x_k) \text{ with } K = 2^{N_K} - 1. \end{split}$$

Numerical Experiments (Linear Case)

1-dimensional elliptic equation

$$-\frac{\mathrm{d}^2 p}{\mathrm{d} x^2} + p = u \quad \text{in } D := (0,\pi) \,, \ p = 0 \quad \text{in } \partial D \,.$$

The goal of computation is to recover the unknown data u^\dagger from observations

$$y = \mathcal{O}L^{-1}u^{\dagger} = Au^{\dagger} .$$

Numerical Experiments (Linear Case)

1-dimensional elliptic equation

$$-\frac{\mathrm{d}^2 p}{\mathrm{d} x^2} + p = u \quad \text{in } D := (0,\pi) \,, \ p = 0 \quad \text{in } \partial D \,.$$

The goal of computation is to recover the unknown data u^{\dagger} from observations

$$y = \mathcal{O}L^{-1}u^{\dagger} = Au^{\dagger} .$$

Computational Setting

- Noise-free case, $\Gamma = I$.
- $u \sim \mathcal{N}(0, C)$ with $C = \beta (A id)^{-1}$ and with $\beta = 10$.
- Finite element method using continuous, piecewise linear ansatz functions on a uniform mesh with meshwidth h = 2⁻⁸ (the spatial discretisation leads to a discretisation of u, i.e. u ∈ ℝ^{2⁸-1}).

• The space $\mathcal{A} = \operatorname{span}\{u_0^{(j)}\}_{j=1}^J$ is chosen based on the KL expansion of $C = \beta (A - id)^{-1}$.
Numerical Experiments (Linear Case)



Numerical Experiments (Linear Case)



Numerical Experiments (Ensemble Collapse)



Numerical Experiments (Ensemble Collapse)



Numerical Experiments (Convergence of the Residuals)



Numerical Experiments (Convergence of the Residuals)



Extensions

• Variance inflation, Localization

G. EVENSEN 2006 Data Assimilation: The Ensemble Kalman Filter Springer

E. KALNAY 2003 Atmospheric Modeling, Data Assimilation and Predictability Cambridge

Multilevel strategies

A. CHERNOV, H. HOEL, K. LAW, F. NOBILE AND R. TEMPONE 2016 Multilevel ensemble Kalman filtering for spatially extended models

Regularization

N. CHADA, A. STUART, X. TONG 2019 Tikhonov regularization within Ensemble Kalman Inversion

- Subsampling strategies M. HANU, J. LATZ, CLS 2021(in preparation)
- Ensemble tranform filters
- Hybrid Methods ...

Summary

- Basic concepts of smoothing, filtering.
- (Ensemble) Kalman filter.
- Particle filter.

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