

Ensemble Methods in Atmospheric Data Assimilation

Harald Anlauf

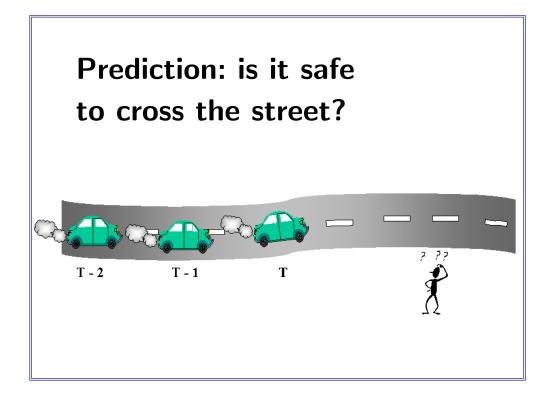
Research and Development, Data Assimilation Section Deutscher Wetterdienst, Offenbach, Germany

DESY Monte Carlo Workshop, DESY, Hamburg 19.-21. February 2013

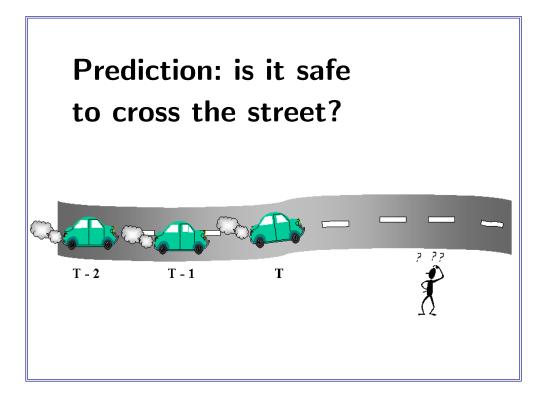




Data assimilation in everyday life



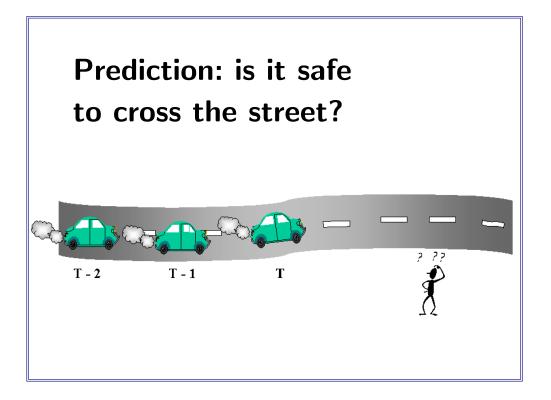
Data assimilation in everyday life



Used information:

- Observations
- Knowledge about cars, roads
- ► Experience (⇒ statistics)

Data assimilation in everyday life



Used information:

- Observations
- Knowledge about cars, roads
- ► Experience (⇒ statistics)

• Forecast error due to:

- Observation error
- Model error (icy road)
- Current conditions not represented by statistics

Operational NWP Models at DWD

GME

Global model, hydrostatic

Triangular grid, mesh size: 20 km

 $(1474562\times60 \text{ grid points})$

Forecast times:

174h from 00Z, 12Z;

48h from 06Z, 18Z

COSMO-EU

Non-hydrostatic

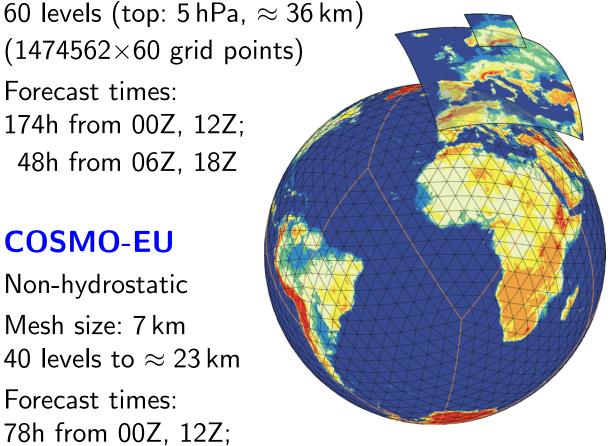
Mesh size: 7 km

40 levels to $\approx 23 \, \mathrm{km}$

Forecast times:

78h from 00Z, 12Z;

48h from 06Z, 18Z



COSMO-DE

Non-hydrostatic, "convection permitting"

Mesh size: 2.8 km

50 levels to $\approx 22 \text{ km}$

Forecast times:

21h from 00Z, 03Z, . . . , 21Z

COSMO-DE-EPS

Ensemble prediction system 20 ensemble members (in 2013: 40 members)

Forecast times:

21h from 00Z, 03Z, . . . , 21Z

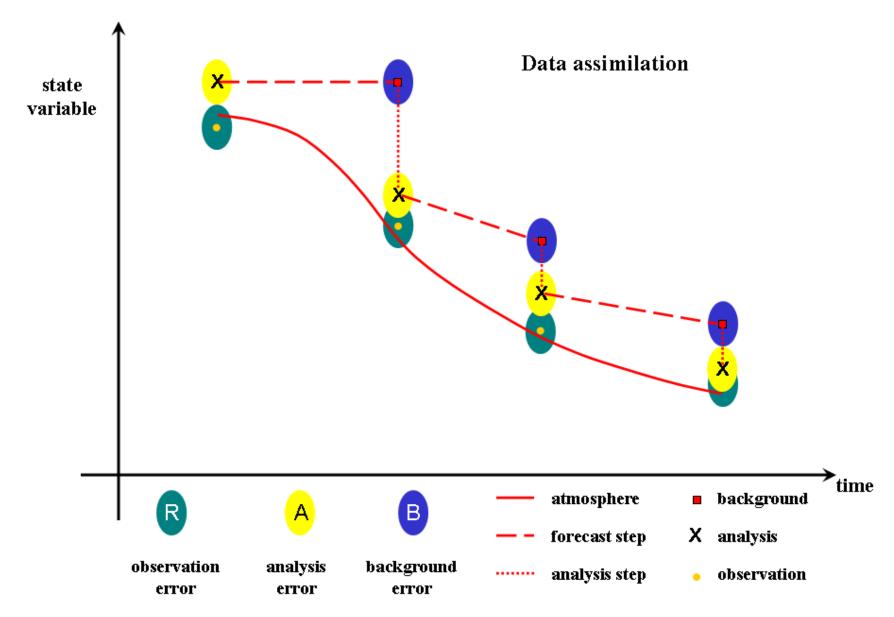
The Global Observing System

- In-Situ Observations
 - Surface observations (land, ship, buoys)
 - Radiosondes
 - Aircraft reports
- Remote Sensing Observations
 - Satellite based
 - ★ geostationary
 - **★** polar orbiting
 - ★ LEOs (low-earth orbit), partly research satellites
 - RADAR
 - LIDAR
 - GNSS (GPS) ground observations
- Network very inhomogeneous, some areas not well observed!



4) Q (2)

Intermittent (Cycled) Data Assimilation



Outline

- Introduction
 - What is Data Assimilation?
 - Data Assimilation for Dynamical Systems
 - Kalman Filter
 - Variational methods and Bayes method
- 2 Ensemble Methods
 - Ensemble Kalman Filters
 - Local Ensemble Transform Kalman-Filter
 - Particle Filter
 - Implicit Particle Filter
 - Equivalent-Weights Particle Filter
- Concluding Remarks

Data Assimilation for Dynamical Systems

• Dynamical system: State space \mathcal{X} , model operator (flow):

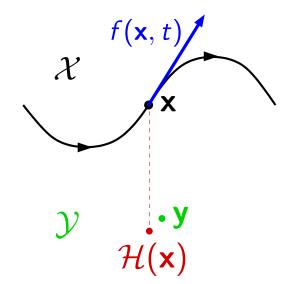
$$\mathcal{M}: \mathbb{R} imes \mathcal{X} o \mathcal{X}$$

so that for all $x \in \mathcal{X}$, $s, t \in \mathbb{R}$:

$$\mathcal{M}(0,x) = x$$
, $\mathcal{M}(s,\mathcal{M}(t,x)) = \mathcal{M}(t+s,x)$



- Observation operator $\mathcal{H}: \mathcal{X} \ni x \to y \in \mathcal{Y}$
- Given observations y_1, \ldots, y_n , determine x(t)!



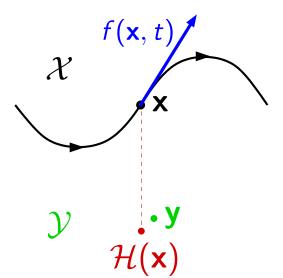
Data Assimilation for Dynamical Systems

• Dynamical system: State space \mathcal{X} , model operator (flow):

$$\mathcal{M}: \mathbb{R} imes \mathcal{X} o \mathcal{X}$$

so that for all $x \in \mathcal{X}$, $s, t \in \mathbb{R}$:

$$\mathcal{M}(0,x) = x$$
, $\mathcal{M}(s,\mathcal{M}(t,x)) = \mathcal{M}(t+s,x)$



- ullet Observation space: ${\cal Y}$
- Observation operator $\mathcal{H}: \mathcal{X} \ni x \to y \in \mathcal{Y}$
- Given observations y_1, \ldots, y_n , determine x(t)!
 - Under-determined (ill-posed) inverse problem: number of observations much smaller than degrees of freedom (related problem: tomography)
 - Observations and models have errors
 - Model variables may not be directly observed,
 observation operator (in general) not injective, not invertible
 - ▶ Data assimilation: combine observations with prior information

Linear Systems: Kalman Filter (I)

- Linear model, linear observation operator: $\mathcal{H}(x) = \mathbf{H}x$
 - ▶ Forecast error covariance $(x^f$: forecast, x_t : true state)

$$\mathbf{P}^{f} = \mathsf{E} \left\{ (x^{f} - x_{t})(x^{f} - x_{t})^{\mathsf{T}} \right\}$$

▶ Observation error covariance $(y_t$: true observation)

$$\mathbf{R} = \mathsf{E}\left\{ (y - y_t)(y - y_t)^\mathsf{T} \right\}$$

Analysis: weighted linear combination of forecast and observations

$$x^a = x^f + \mathbf{K}(y - \mathbf{H}x^f)$$

Optimal "Kalman gain"

$$\mathbf{K} = \mathbf{P}^f \mathbf{H}^\mathsf{T} \left(\mathbf{H} \mathbf{P}^f \mathbf{H}^\mathsf{T} + \mathbf{R} \right)^{-1}$$

minimizes analysis error:

$$\mathbf{P}^{a} = (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{P}^{f} = \left((\mathbf{P}^{f})^{-1} + \mathbf{H}^{\mathsf{T}}\mathbf{R}^{-1}\mathbf{H}\right)^{-1}$$

Kalman Filter (II)

• Forecast step $(\mathbf{M}_i = \mathbf{M}(t_i \rightarrow t_{i+1}))$:

$$x^f(t_{i+1}) = \mathbf{M}_i x^a(t_i)$$

 $\mathbf{P}^f(t_{i+1}) = \mathbf{M}_i \mathbf{P}^a(t_i) \mathbf{M}_i^\mathsf{T} + \mathbf{Q}(t_i)$

Q: model error (system noise) covariance

 Kalman filter gives optimal (minimal variance) solution for linear models, linear observations, and Gaussian observation errors

Kalman Filter (II)

• Forecast step $(\mathbf{M}_i = \mathbf{M}(t_i \rightarrow t_{i+1}))$:

$$x^f(t_{i+1}) = \mathbf{M}_i x^a(t_i)$$

 $\mathbf{P}^f(t_{i+1}) = \mathbf{M}_i \mathbf{P}^a(t_i) \mathbf{M}_i^\mathsf{T} + \mathbf{Q}(t_i)$

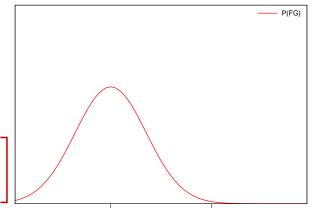
Q: model error (system noise) covariance

- Kalman filter gives optimal (minimal variance) solution for linear models, linear observations, and Gaussian observation errors
- Kalman filter computationally expensive:
 - lacktriangle Solve large linear systems for many observations $\left(\mathcal{O}(10^5\dots 10^6)\right)$
 - ▶ Memory requirement: \mathbf{P}^f has N^2 elements (N: grid points \times d.o.f.)
 - ▶ Computation of \mathbf{P}^a , forecast of \mathbf{P}^f : $\sim N^3$ operations
 - ⇒ some approximations will be needed anyway
- Generalization to more realistic, non-linear models required
 - Observation impact in Kalman filter depends only on specified errors, not on model state ("actual weather situation")!

Variational Method and Bayes Method

- Maximum-likelihood method
 - Likelihood for forecast

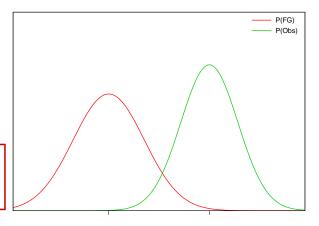
$$L_{\mathbf{P}^f}(x|x^f) \sim \exp\left[-\frac{1}{2}(x^f-x)^{\mathsf{T}}\mathbf{P}^{f-1}(x^f-x)\right]$$



Variational Method and Bayes Method

- Maximum-likelihood method
 - Likelihood for forecast

$$L_{\mathbf{P}^f}(x|x^f) \sim \exp\left[-\frac{1}{2}(x^f-x)^{\mathsf{T}}\mathbf{P}^{f-1}(x^f-x)\right]$$



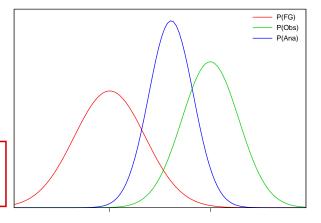
Likelihood for new observations

$$L_{\mathbf{R}}(x|y) \sim \exp\left[-\frac{1}{2}(y - \mathcal{H}(x))^{\mathsf{T}}\mathbf{R}^{-1}(y - \mathcal{H}(x))\right]$$

Variational Method and Bayes Method

- Maximum-likelihood method
 - Likelihood for forecast

$$L_{\mathbf{P}^f}(x|x^f) \sim \exp\left[-\frac{1}{2}(x^f-x)^{\mathsf{T}}\mathbf{P}^{f-1}(x^f-x)\right]$$



Likelihood for new observations

$$L_{\mathsf{R}}(x|y) \sim \exp\left[-\frac{1}{2}(y-\mathcal{H}(x))^{\mathsf{T}}\mathsf{R}^{-1}(y-\mathcal{H}(x))\right]$$

► Forecast and observations are independent ⇒ Likelihood function

$$L(x|x^f, y) = L_{\mathbf{P}^f}(x|x^f) L_{\mathbf{R}}(x|y)$$

▶ Bayesian interpretation: maximize a-posteriori probability for given observations y and prior p(x):

$$p(x|y) = \frac{p(y|x)p(x)}{p(y)}$$

Variational method (3D-Var)

• Cost function $(J \equiv -2 \ln p + \text{const.})$:

$$J(x) = (x^f - x)^\mathsf{T} \left(\mathbf{P}^f \right)^{-1} (x^f - x) + (y - \mathcal{H}(x))^\mathsf{T} \mathbf{R}^{-1} (y - \mathcal{H}(x))$$

- Minimization: conjugate-gradient (CG), quasi-Newton methods
 - control variable: x
 - \blacktriangleright dual formulation (control variable y): "Physical Space Analysis System"

Variational method (3D-Var)

• Cost function $(J \equiv -2 \ln p + \text{const.})$:

$$J(x) = (x^f - x)^\mathsf{T} \left(\mathbf{P}^f \right)^{-1} (x^f - x) + (y - \mathcal{H}(x))^\mathsf{T} \mathbf{R}^{-1} (y - \mathcal{H}(x))$$

- Minimization: conjugate-gradient (CG), quasi-Newton methods
 - control variable: x
 - \triangleright dual formulation (control variable y): "Physical Space Analysis System"
- Gradient of *J*:

$$\frac{1}{2}\nabla_{x}J(x) = \left(\mathbf{P}^{f}\right)^{-1}(x - x^{f}) + \mathbf{H}^{\mathsf{T}}\mathbf{R}^{-1}(\mathcal{H}(x) - y)$$

with **H** from linearization of $\mathcal{H}(x)$

• J quadratic near minimum \Rightarrow Hessian:

$$\frac{1}{2} \nabla_{\mathsf{X}} \nabla_{\mathsf{X}} J(\mathsf{X}^{\mathsf{a}}) = \left(\mathsf{P}^{\mathsf{f}} \right)^{-1} + \mathsf{H}^{\mathsf{T}} \mathsf{R}^{-1} \mathsf{H} = \left(\mathsf{P}^{\mathsf{a}} \right)^{-1}$$

• Solution x is best fit in model state space at $t = t_0$

General variational method (4D-Var)

• Cost function for model trajectory $x(t) = \mathcal{M}(t, x(0))$

$$J(x) = (x^{f}(0) - x(0))^{T} \mathbf{P}^{f^{-1}}(x^{f}(0) - x(0)) + \sum_{i} (y^{(i)} - \mathcal{H}(x(t_{i})))^{T} \mathbf{R}^{-1}(y^{(i)} - \mathcal{H}(x(t_{i}))) + (terms for model error) + ...$$

General variational method (4D-Var)

• Cost function for model trajectory $x(t) = \mathcal{M}(t, x(0))$

$$J(x) = (x^{f}(0) - x(0))^{T} \mathbf{P}^{f^{-1}}(x^{f}(0) - x(0)) + \sum_{i} (y^{(i)} - \mathcal{H}(x(t_{i})))^{T} \mathbf{R}^{-1}(y^{(i)} - \mathcal{H}(x(t_{i}))) + (terms for model error) + ...$$

Remarks

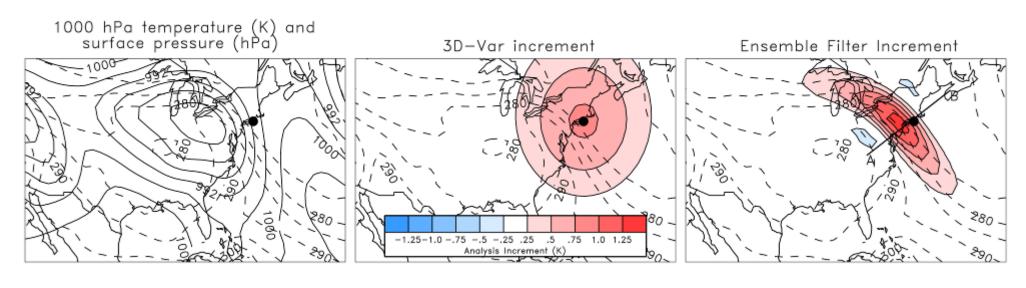
- \odot 4D-Var solution: x(0), model trajectory with best fit to observations within time window
- \odot Implicit evolution of \mathbf{P}^f matrix (but only in time window)
- © For linear model mathematically equivalent to Kalman filter/smoother
- © Huge development efforts necessary (tangent linear and adjoint model)
- Large computational ressources required, but poor scaling on modern HPC architectures
- \bigcirc Long-window 4D-Var \longleftrightarrow strong nonlinearities at small scales

Ensemble Methods in Data Assimilation

• Why Ensemble Data Assimilation?

Motivation: Impact of observations (determined by \mathbf{R} and by \mathbf{P}^{t}) should depend on actual weather situation (e.g. near fronts)

 \implies explicit or implicit evolution of \mathbf{P}^f essential!



Ensemble Methods in Data Assimilation

Whitaker (2005)

Ensemble Kalman Filters

- Represent mean forecast, forecast uncertainty by ensemble (size: N) of (equal-weight) model states x_i^f drawn from appropriate p.d.f.
- Gaussian distribution characterized by first two moments:

Departures:
$$x'_i^f = x_i^f - \bar{x}^f$$
 (\bar{x}^f : Ensemble mean)

Ensemble covariance: $\mathbf{P}^f = \frac{1}{N-1} \sum_{i=1}^N x'_i^f (x'_i^f)^T$

Generalized analysis equations

Analysis mean:
$$\bar{x}^a = \bar{x}^f + \mathbf{K}(\bar{y} - \mathbf{H}\bar{x}^f)$$

Analysis departures: $x'^a = x'^f + \tilde{\mathbf{K}}(y' - \mathbf{H}x'^f)$

Choose K, \tilde{K} such that P^a represents true analysis error covariance

Implement model error Q as random forcing of forecast model

"The" Ensemble Kalman Filter (EnKF)

- Stochastic EnKF (Evensen, 1994; Burgers et al., 1998)
- $\tilde{\mathbf{K}} = \mathbf{K} = \mathbf{P}^f \mathbf{H}^\mathsf{T} (\mathbf{H} \mathbf{P}^f \mathbf{H}^\mathsf{T})^{-1} \iff \mathsf{E} \{ y'(y')^T \} = \mathbf{R}$ Observations must be randomly perturbed using true error covariance!

"The" Ensemble Kalman Filter (EnKF)

- Stochastic EnKF (Evensen, 1994; Burgers et al., 1998)
- $\tilde{\mathbf{K}} = \mathbf{K} = \mathbf{P}^f \mathbf{H}^\mathsf{T} (\mathbf{H} \mathbf{P}^f \mathbf{H}^\mathsf{T})^{-1} \iff \mathsf{E} \{ y'(y')^\mathsf{T} \} = \mathbf{R}$ Observations must be randomly perturbed using true error covariance!
- rank(\mathbf{P}^f)=N-1: analysis increments projected onto low-dimensional subspace of state space, leading to underestimation of analysis error and risk of filter collapse
 - Use cross-validation approach by splitting the ensemble
 - Artificially increase forecast error ("covariance inflation")

"The" Ensemble Kalman Filter (EnKF)

- Stochastic EnKF (Evensen, 1994; Burgers et al., 1998)
- $\tilde{\mathbf{K}} = \mathbf{K} = \mathbf{P}^f \mathbf{H}^\mathsf{T} (\mathbf{H} \mathbf{P}^f \mathbf{H}^\mathsf{T})^{-1} \iff \mathsf{E} \{ y'(y')^\mathsf{T} \} = \mathbf{R}$ Observations must be randomly perturbed using true error covariance!
- rank(\mathbf{P}^f)=N-1: analysis increments projected onto low-dimensional subspace of state space, leading to underestimation of analysis error and risk of filter collapse
 - Use cross-validation approach by splitting the ensemble
 - Artificially increase forecast error ("covariance inflation")
- ${f P}^f$ has spurious long-range correlations $(\sim N^{-1})$
 - Suppressing the influence of distant observations requires
 "localization":
 Schur product of P^f with suitably chosen correlation function or local analysis method (c.f. LETKF below)
 - ightharpoonup Localization effectively increases the rank of \mathbf{P}^f (and \mathbf{K})
 - Localization is computationally expensive, disturbs model balance
- ullet EnKF operationally used by Canadian Meteorological Service since 2005, now using 192 ensemble members (4 sub-ensembles imes 48)

Deterministic Ensemble Kalman Filters

- Large family of Deterministic EnKF w/o need of perturbation of observations: Ensemble Square-Root-Filters (EnSRF) (see Whitaker and Hamill, 2002)
 - Ensemble Adjustment Kalman Filter (EAKF)
 - Ensemble Transform Kalman Filter (ETKF)

 - Different localization concepts, differing computational efficiency

Deterministic Ensemble Kalman Filters

- Large family of Deterministic EnKF w/o need of perturbation of observations: Ensemble Square-Root-Filters (EnSRF) (see Whitaker and Hamill, 2002)
 - Ensemble Adjustment Kalman Filter (EAKF)
 - Ensemble Transform Kalman Filter (ETKF)

 - Different localization concepts, differing computational efficiency
- Atmospheric dynamics locally low-dimensional (Patil et al., 2001)
 - λ_i : Eigenvalues of covariance matrices of (fast-growing) "bred-vectors" in a limited domain (1100 km imes 1100 km)
 - "Bred-vector"-dimension:

$$\psi(\lambda_1,\ldots,\lambda_k) = \frac{(\sum_i \sqrt{\lambda_i})^2}{\sum_i \lambda_i} \ll k$$

 For local covariances, about 40–100 ensemble members needed from storm to global scales (Kalnay et al.)

LETKF: Local Ensemble Transform Kalman-Filter

- LETKF (Ott et al., 2004; Hunt et al., 2004, 2007):
 - Forecast perturbations: $\mathbf{X}^f = [x_1 \bar{x} | \dots | x_N \bar{x}]$ Obs. in ensemble space: $\mathbf{Y} = [y_1 - \bar{y} | \dots | y_N - \bar{y}]$, $y_i \equiv \mathcal{H}(x_i)$
 - ▶ Local analysis in ensemble space, at each grid point:

$$ilde{\mathbf{P}}^f = (\mathcal{N}-1)^{-1}\mathbf{I} \;, \quad ilde{\mathbf{P}}^a = \left[(\mathcal{N}-1)\mathbf{I} + \mathbf{Y}^\mathsf{T}\mathbf{R}^{-1}\mathbf{Y}
ight]^{-1}$$

using all observations in the local region.

LETKF: Local Ensemble Transform Kalman-Filter

- LETKF (Ott et al., 2004; Hunt et al., 2004, 2007):
 - Forecast perturbations: $\mathbf{X}^f = [x_1 \bar{x} | \dots | x_N \bar{x}]$ Obs. in ensemble space: $\mathbf{Y} = [y_1 - \bar{y} | \dots | y_N - \bar{y}]$, $y_i \equiv \mathcal{H}(x_i)$
 - ▶ Local analysis in ensemble space, at each grid point:

$$ilde{\mathbf{P}}^f = (\mathcal{N}-1)^{-1}\mathbf{I} \;, \quad ilde{\mathbf{P}}^a = \left[(\mathcal{N}-1)\mathbf{I} + \mathbf{Y}^\mathsf{T}\mathbf{R}^{-1}\mathbf{Y}
ight]^{-1}$$

using all observations in the local region.

- Analysis mean: $\bar{x}^a = \bar{x}^f + \mathbf{X}^f \bar{w}$, $\bar{w} = \tilde{\mathbf{P}}^a \mathbf{Y} \mathbf{R}^{-1} (y \bar{y})$ Analysis ensemble: $\mathbf{X}^a = \mathbf{X}^f \mathbf{W} + \bar{x}^a$, $\mathbf{W} = \left[(N - 1) \tilde{\mathbf{P}}^a \right]^{1/2}$
- ► Localization: apply to (inverse) observation error!
- ▶ Computationally very efficient, well parallelizable: symmetric square-roots of $N \times N$ matrices at each grid-point
- ▶ No minimization ⇒ no adjoint of observation operators needed

LETKF: Local Ensemble Transform Kalman-Filter

- LETKF (Ott et al., 2004; Hunt et al., 2004, 2007):
 - Forecast perturbations: $\mathbf{X}^f = [x_1 \bar{x} | \dots | x_N \bar{x}]$ Obs. in ensemble space: $\mathbf{Y} = [y_1 - \bar{y} | \dots | y_N - \bar{y}]$, $y_i \equiv \mathcal{H}(x_i)$
 - ▶ Local analysis in ensemble space, at each grid point:

$$ilde{\mathbf{P}}^f = (\mathcal{N}-1)^{-1}\mathbf{I} \;, \quad ilde{\mathbf{P}}^a = \left[(\mathcal{N}-1)\mathbf{I} + \mathbf{Y}^\mathsf{T}\mathbf{R}^{-1}\mathbf{Y}
ight]^{-1}$$

using all observations in the local region.

- Analysis mean: $\bar{\mathbf{x}}^a = \bar{\mathbf{x}}^f + \mathbf{X}^f \bar{\mathbf{w}}$, $\bar{\mathbf{w}} = \tilde{\mathbf{P}}^a \mathbf{Y} \mathbf{R}^{-1} (y \bar{y})$ Analysis ensemble: $\mathbf{X}^a = \mathbf{X}^f \mathbf{W} + \bar{\mathbf{x}}^a$, $\mathbf{W} = \left[(N - 1) \tilde{\mathbf{P}}^a \right]^{1/2}$
- ► Localization: apply to (inverse) observation error!
- ▶ Computationally very efficient, well parallelizable: symmetric square-roots of $N \times N$ matrices at each grid-point
- ▶ No minimization ⇒ no adjoint of observation operators needed
- DWD: KENDA (experimental LETKF for COSMO-DE-EPS)
- Hybrid global 3D-Var/LETKF, with high-resolution deterministic analysis: e.g. GFS at NCEP (operational); GME at DWD (experim.)

Nonlinear filtering & Particle Filter

Nonlinear filtering & Particle Filter

Bayes theorem

$$p(x|y) = \frac{p(y|x)p(x)}{\int p(y|x)p(x)dx}$$

Nonlinear filtering & Particle Filter

Bayes theorem

$$p(x|y) = \frac{p(y|x)p(x)}{\int p(y|x)p(x)dx}$$

Ensemble representation of probability density ("particles")

$$p(x) = \sum_{i=1}^{N} \frac{1}{N} \delta(x - x_i)$$

Posterior density

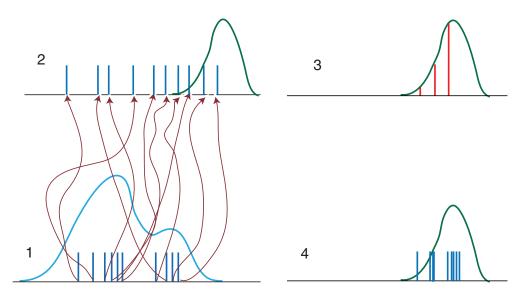
$$p(x|y) = \sum_{i=1}^{N} w_i \, \delta(x - x_i) \qquad \text{with weights} \quad w_i = \frac{p(y|x_i)}{\sum_i p(y|x_i)}$$

For Gaussian distributed observations

$$w_i \propto \exp\left[-\frac{1}{2}(y - \mathcal{H}(x_i))^\mathsf{T}\mathbf{R}^{-1}(y - \mathcal{H}(x_i))\right]$$

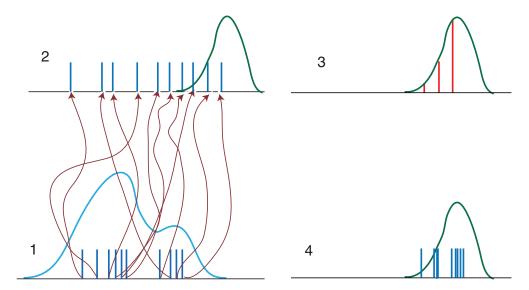
Standard Particle Filter

- Sequential Importance Resampling Filter (van Leeuwen, 2003)
 - (1) Generate Ensemble as sample of the probability density, run the model
 - (2) Assign weights accordings to probability density given the observations
 - (3) Reject particles with small weights and
 - (4) replace by particles according to posteriory density (resampling)



Standard Particle Filter

- Sequential Importance Resampling Filter (van Leeuwen, 2003)
 - (1) Generate Ensemble as sample of the probability density, run the model
 - (2) Assign weights accordings to probability density given the observations
 - (3) Reject particles with small weights and
 - (4) replace by particles according to posteriory density (resampling)



- Standard PF inefficient: many particles lost for many observations!
- Required ensemble size $\sim \exp$ (number of observations)!
- For particle filters to be useful, we need importance sampling!

Bayes Theorem and proposal transition density (I)

• Stochastic model equation (β : model error, e.g. with $\beta \sim N(0, \mathbf{Q})$)

$$x^n = f(x^{n-1}) + \beta^{n-1}$$

Transition density

$$p(x^n|x^{n-1}) = N(f(x^{n-1}), \mathbf{Q})$$

• Use transition density to derive marginal prior p.d.f. at time n

$$p(x^n) = \int p(x^n | x^{n-1}) p(x^{n-1}) dx^{n-1}$$

 \bullet Rewrite Bayes theorem using (arbitrary) proposal transition density q

$$p(x^{n}|y^{n}) = \frac{p(y^{n}|x^{n})p(x^{n})}{p(y^{n})}$$

$$= \frac{p(y^{n}|x^{n})}{p(y^{n})} \int p(x^{n}|x^{n-1})p(x^{n-1}) dx^{n-1}$$

$$= \frac{p(y^{n}|x^{n})}{p(y^{n})} \int \frac{p(x^{n}|x^{n-1})}{q(x^{n}|x^{n-1},y^{n})} q(x^{n}|x^{n-1},y^{n})p(x^{n-1}) dx^{n-1}$$

Proposal transition density (II)

• Starting with equal-weight particles at n-1, we have:

$$p(x^n|y^n) = \frac{p(y^n|x^n)}{p(y^n)} \frac{1}{N} \sum_{i=1}^{N} \frac{p(x^n|x_i^{n-1})}{q(x^n|x_i^{n-1}, y^n)} q(x^n|x_i^{n-1}, y^n)$$

• For each particle at n-1 draw from proposal transition density q

$$p(x^{n}|y^{n}) = \frac{1}{N} \sum_{i=1}^{N} \frac{p(y^{n}|x_{i}^{n})}{p(y^{n})} \frac{p(x_{i}^{n}|x_{i}^{n-1})}{q(x_{i}^{n}|x_{i}^{n-1}, y^{n})} \delta(x^{n} - x_{i}^{n})$$

Weights

$$w_{i} = \underbrace{\frac{p(y^{n}|x_{i}^{n})}{p(y^{n})}}_{\text{Likelihood weight}} \times \underbrace{\frac{p(x_{i}^{n}|x_{i}^{n-1})}{q(x_{i}^{n}|x_{i}^{n-1},y^{n})}}_{\text{Proposal weight}}$$

The proposal transition density is essentially arbitrary!
 Can we use it to draw the particles closer to the observations?

Implicit particle filter (I)

• For weakly non-linear observation operators $(\mathcal{H}(x_i) \approx \mathbf{H}x_i)$

$$w_i \cdot q \propto \exp \left[-\frac{1}{2} (y - \mathbf{H} x_i)^{\mathsf{T}} \mathbf{R}^{-1} (y - \mathbf{H} x_i) - \frac{1}{2} (x_i^n - f(x_i^{n-1}))^{\mathsf{T}} \mathbf{Q}^{-1} (x_i^n - f(x_i^{n-1})) \right]$$

This is a quadratic function in $(x_i^n - \mu_i)$ with Hessian H.

• The minimum μ_i can be determined by e.g. variational methods. Choose proposal density as:

$$q(x_i^n|x_i^{n-1},y^n) = N(\mu_i,H^{-1})$$

Resulting weights:

$$w_i \propto \exp\left[-rac{1}{2}\left(y^n - \mathbf{H}f(x_i^{n-1})
ight)^{\mathsf{T}}\left(\mathbf{H}\mathbf{Q}\mathbf{H}^{\mathsf{T}} + \mathbf{R}
ight)^{-1}\left(y^n - \mathbf{H}f(x_i^{n-1})
ight)
ight]$$

Implicit particle filter (II)

- Implicit particle filter: run special 4D-Var for each particle to obtain μ_i
- Determine (approximate) Hessian H
- Generate proposal particles from

$$q(x_i^n|x_i^{n-1},y^n) = N(\mu_i,H^{-1})$$

- Calculate weights
 (Note: no explicit expression for weights for non-linear models).
- Resample
- See Atkins et al., 2013, and references for a review and the connection between variational methods and implicit particle methods.

Equivalent-Weights Particle Filter

- Van Leeuwen, 2010:
 - Assume that model needs several time steps between observations
 - Use simple proposal at each time step, e.g. corresponding to nudging:

$$q(x^{n}|x^{n-1},y^{n}) = N(f(x^{n-1}) + S(y^{n} - \mathcal{H}(x^{n-1})), \mathbf{Q})$$

• Use different proposal at final time step to achieve similar weights. Determine maximum achievable weight (w_i^{max}) during last time step(s) and choose target weight w^{target} . Then set:

$$q(x^n|x^{n-1},y^n) = \begin{cases} q_1(x^n|x^{n-1},y^n) & \text{for } w_i^{\text{max}} > w^{\text{target}} \\ q_2(x^n|x^{n-1},y^n) & \text{for } w_i^{\text{max}} < w^{\text{target}} \end{cases}$$

For particles that cannot reach the target weight, one uses:

$$q_2(x^n|x^{n-1},y^n) = N(f(x^{n-1}),\mathbf{Q})$$

Choose "special move" (different forcing) for high-weight particles

Calculate weights, resample "lost" particles

Comments on Particle Filters

- Particle Filters do not need state covariances
- No assumptions on linearity, Gaussianity, . . . , needed
- Perfectly scalable (number of particles, dimensionality of problem)
- Proposal transition density may solve the degeneracy problem connected with many observations, apparently highly flexible
- In practice, particle filters have only been shown yet to work with toy models (Lorenz '63, Lorenz '96, barotropic vorticity equation, . . .), no experience with general circulation models:
 - Arbitrary forcing terms may destroy model balances
 - How to resample efficiently?
 - Some kind of localization similar to Ensemble Kalman Filters may be beneficial, but it is not clear how to do this (cannot linearly combine particles!)
- Many interesting ideas are being investigated . . .

Concluding Remarks

- Ensemble methods have been established as a valuable method in data assimilation to estimate the analysis uncertainties
 - Several competitive methods which are also efficient on modern massively parallel computer architectures (EnKF, LETKF, hybrid Var/EnKF methods, . . .)
 - Ensemble DA already operationally used at some meteorological centers, more centers to follow
 - ightharpoonup Key challenges have shifted: from poorly known \mathbf{P}^f in deterministic DA to poorly understood model error (\mathbf{Q}) in ensemble DA
 - ---- many ideas, but mostly ad-hoc solutions and lots of tuning

Concluding Remarks

- Ensemble methods have been established as a valuable method in data assimilation to estimate the analysis uncertainties
 - Several competitive methods which are also efficient on modern massively parallel computer architectures (EnKF, LETKF, hybrid Var/EnKF methods, . . .)
 - Ensemble DA already operationally used at some meteorological centers, more centers to follow
 - ► Key challenges have shifted: from poorly known \mathbf{P}^f in deterministic DA to poorly understood model error (\mathbf{Q}) in ensemble DA \longrightarrow many ideas, but mostly ad-hoc solutions and lots of tuning
- While Ensemble Kalman Filters work well on the synoptic scale,
 DA for the convective scale is still a subject of current research
 - Ensemble methods are essential to capture the flow dependence of uncertainties
 - Strong non-linearities in models and observation operators pose challenges to all methods
 - Particle filters are a promising candidate, but efficient importance sampling is a challenge to prevent ensemble collapse, still a lot to learn!

Selected References

Ensemble Kalman Filter (EnKF)

- G. Burgers et al., 1998. On the analysis scheme of the Ensemble Kalman Filter, Monthly Weather Rev., 126, 1719–1724.
- Evensen, G., 1994. Sequential data assimilation with a nonlinear quasi-geostrophic model using Monte Carlo methods to forecast error statistics, J. Geophys. Res., 99(C5), 10,143–10,162.
- P. L. Houtekamer, et al., 2005. Atmospheric data assimilation with an ensemble Kalman filter: results with real observations, Mon. Wea. Rev. 133, 604–620.

Ensemble Square Root Filters, Ensemble Transform Kalman Filters

- ▶ Hunt et al., 2004. Four-dimensional ensemble Kalman filtering, Tellus, 56A, 273–277.
- Ott et al., 2004. A local ensemble Kalman filter for atmospheric data assimilation, Tellus, 56A, 415–428.
- Patil et al., 2001. Local Low Dimensionality of Atmospheric Dynamics, Phys. Rev. Lett., 86, 5878-5881
- Whitaker, J.S. and Hamill, T.H., 2002. Ensemble Data Assimilation without perturbed observations, Mon. Wea. Rev. 130, 1913–1924.

Particle Filter

- Van Leeuwen, P.J., 2010. Nonlinear data assimilation in geosciences: an extremely efficient particle filter, Q. J. R. Meteorol. Soc. 136: 1991–1999. DOI:10.1002/qj.699
- Snyder et al., 2008. Obstacles to high-dimensional particle filtering, Mon. Wea. Rev. 136, 4629–4640.
- Atkins et al., 2013. Implicit particle methods and their connection with variational data assimilation, Mon. Wea. Rev., in print.



Localization

ullet Let ${f P}$ be symmetric positive semi-definite, and ${f C}$ (the localization) be a correlation function. The Schur product

$$\widetilde{\mathbf{P}} \equiv \mathbf{P} \odot \mathbf{C}$$

defines the localized version of P

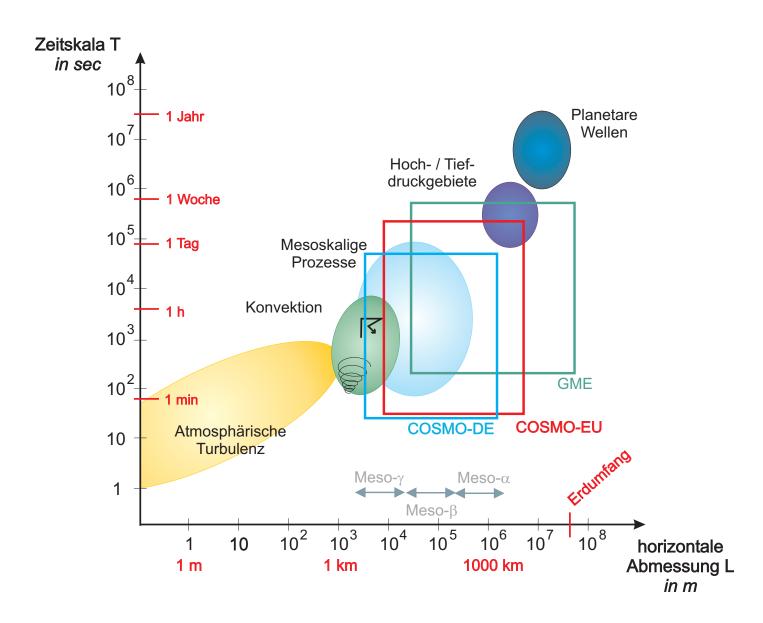
$$(\mathbf{P}\odot\mathbf{C})(x,y)\equiv P(x,y)C(x,y)$$

which is also positive semi-definite.

(See Gaspari & Cohn, 1999, for a treatment of localization on the sphere.)

• In practice, localization of \mathbf{P}^f is too expensive. Many authors apply localization to $(\mathbf{H}\mathbf{P}^f\mathbf{H}^T)$ and $(\mathbf{P}^f\mathbf{H}^T)$, which leads to small but systematic errors.

Length- and time-scales in the atmosphere



Global Observing System

Observation usage of DWD's global data assimilation on 2011-02-01

Observation type	variable	Total	used	monitored
TEMP	T, rh , u , v	57 258	5.4 %	199 973
PILOT	u, v	4 200	0.4 %	15 122
SYNOP	p_s, u, v	112 647	10.7%	114 558
DRIBU	p_s, u, v	6 353	0.6 %	6 643
Aircraft	T, u, v	225 947	21.4%	250 578
AMV geo	u, v	86 620	8.2 %	99 844
AMV polar	u, v	25 332	2.4 %	25 384
SCATT	u_{10}, v_{10}	188 774	17.9%	224 412
AMSU-A	T_b	287 950	27.3 %	18 838 147
GPSRO	bending angle	60 659	5.7 %	65 052
All data		1 055 740	100.0 %	19839713
Polar satellites		562 715	53.3 %	19 152 995