Presentation at Crash Course on Data Assimilation

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NORCE

Available from https://github.com/geirev/Presentations

The Variational Inverse Problem

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Simple scalar example

Given the model

$$\begin{aligned} \frac{dx}{dt} &= 1 \\ x(0) &= 0 \\ x(1) &= 2 \end{aligned}$$

- Overdetermined problem.
- No solution.

Allowing for errors

Relax model and conditions

$$\frac{dx}{dt} = 1 + q(t)$$
$$x(0) = 0 + a$$
$$x(1) = 2 + b$$

- Underdetermined problem.
- Infinitively many solutions.

Statistical assumption

Statistical null hypothesis, $\mathcal{H}_0$:

$$
\begin{aligned}
\overline{q(t)} &= 0, & \overline{q(t_1)q(t_2)} &= C_0\delta(t_1 - t_2), & \overline{q(t)a} &= 0,\\
\overline{a} &= 0, & \overline{a^2} &= C_0, & \overline{ab} &= 0,\\
\overline{b} &= 0, & \overline{b^2} &= C_0, & \overline{q(t)b} &= 0.
\end{aligned}
$$

Seeking a solution that:

- is close to the conditions, and
- almost satisfies the model,

by minimizing error terms.

Penalty function

- Define quadratic penalty function

$$\mathcal{J}[x] = W_0 \int_0^1 \left(\frac{dx}{dt} - 1\right)^2 dt + W_0 \big(x(0) - 0\big)^2 + W_0 \big(x(1) - 2\big)^2$$

with $W_0 = C_0^{-1}$.

- Then x is an extremum if

$$\delta\mathcal{J}[x] = \mathcal{J}[x + \delta x] - \mathcal{J}[x] = \mathcal{O}\big(\delta x^2\big)$$

when $\delta x \to 0$.

Variation of penalty function

We have

$$\mathcal{J}[x+\delta x] = W_0 \int_0^1 \left(\frac{dx}{dt} - 1 + \frac{d\delta x}{dt}\right)^2 dt$$
$$+ W_0\big(x(0) - 0 + \delta x(0)\big)^2 + W_0\big(x(1) - 2 + \delta x(1)\big)^2$$

and we must have

$$\int_0^1 \frac{d\delta x}{dt}\left(\frac{dx}{dt} - 1\right) dt + \delta x(0)\big(x(0) - 0\big) + \delta x(1)\big(x(1) - 2\big) = 0,$$

From integration by part we get

$$\delta x\left(\frac{dx}{dt} - 1\right)\Bigg|_0^1 - \int_0^1 \delta x \frac{d^2x}{dt^2} dt + \delta x(0)\big(x(0) - 0\big) + \delta x(1)\big(x(1) - 2\big) = 0.$$

Minimium of penalty function

This gives the following system of equations

$$\delta x(0)\left(-\frac{dx}{dt}+1+x\right)\bigg|_{t=0}=0,$$
$$\delta x(1)\left(\frac{dx}{dt}-1+x-2\right)\bigg|_{t=1}=0,$$
$$\int_0^1 \delta x\left(\frac{d^2x}{dt^2}\right)dt=0,$$

or since δx is arbitrary....

Euler-Lagrange equation

The Euler–Lagrange equation

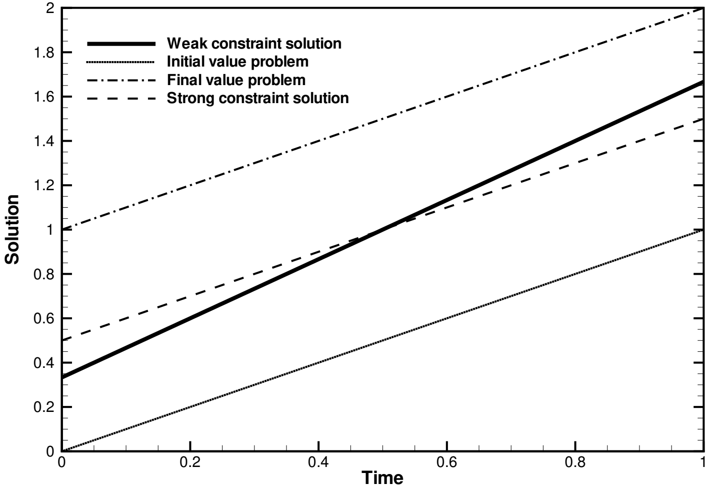
$$\frac{dx}{dt} - x = 1 \quad \text{for } t = 0,$$
$$\frac{dx}{dt} + x = 3 \quad \text{for } t = 1,$$
$$\frac{d^2x}{dt^2} = 0.$$

- Elliptic boundary value problem in time.
- It has a unique solution.

$$x = c_1 t + c_2,$$

with $c_1 = 4/3$ and $c_2 = 1/3$.

Results



Weak constraint solution
Initial value problem
Final value problem
Strong constraint solution
Solution
Time
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.2
0.4
0.6
0.8
1

Summary

- Model with conditions has a unique solution.
- Additional data makes problem over determined.
- Allowing for errors gives infinitely many solutions.
- Specify mean and covariance for error terms.
- Define variational inverse problem for least-squares solution.
- Weigths are the inverses of the error covariances.
- Least-squares solution is defined by Euler-Lagrange eqs.
- Boundary value problem in time.
- Weak-constraint solution: almost satisfies dynamics and data.
- Strong-constraint solution: satisfies dynamics, and close to data.

Bayes' and the data assimilation problem

Geir Evensen

Why Bayes Theorem?

- Provides a fundamental *framework* for data assimilation.
- All data-assimilation methods can be derived from Bayes'.

Properties of a probability denisty function

- The graph of the density function is continuous, since it is defined over a continuous range over a continuous variable.
- The total probability

$$P(x) = \int_{-\infty}^{\infty} f(x)dx = 1$$

- The probability of $x \in [a, b]$ is

$$P(x \in [a, b]) = \int_{a}^{b} f(x)dx$$

- And two special cases

$$P(x = c) = \int_{c}^{c} f(x)dx = 0 \qquad \text{and} \qquad \int_{-\infty}^{\infty} \delta(x)dx = 1$$

Also, we have

- The joint probability
$$f(x,y) = f(x)f(y|x) = f(y)f(x|y)$$
- Solving for $f(x|y)$ gives Bayes' theorem
$$f(x|y) = \frac{f(x)f(y|x)}{f(y)}$$
- Bayes states that "the probability of x given y, is equal to the probability of x, times the likelihood of y given x, divided by the probability of y."
- Here $f(y)$ is a normalization constant so that the integral of $f(x|y)$ becomes one.

Bayes' theorem

Given:

- A state variable $\boldsymbol{x}$ and its prior pdf: $f(\boldsymbol{x})$
- A vector of observations $\boldsymbol{d}$ and their likelihood: $f(\boldsymbol{d}|\boldsymbol{x})$
- Bayes' theorem defines the posterior pdf, $f(\boldsymbol{x}|\boldsymbol{d})$:

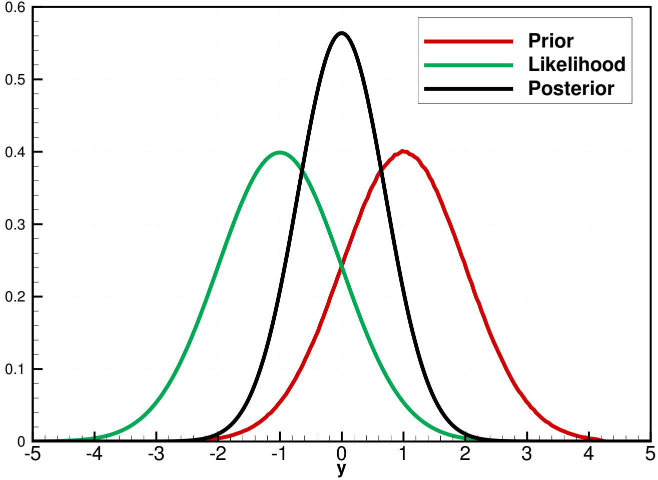
Bayes' theorem

$$f(\boldsymbol{x}|\boldsymbol{d}) = \frac{f(\boldsymbol{x})f(\boldsymbol{d}|\boldsymbol{x})}{f(\boldsymbol{d})}$$

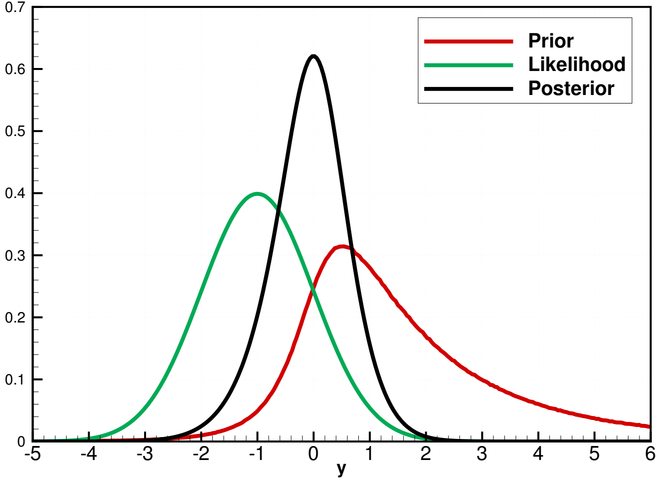
What is the likelihood function: $f(d|x)$

- The likelihood function $f(d|x)$ is the probability of the observed data d for various values of the unknown parameters x.
- The likelihood is used after data are available to describe a plausibility of a parameter value x.
- The likelihood does not have to integrate to one.

Example of using Bayes' theorem



Example of using Bayes' theorem



Revert to inverse problem again

With Gaussian errors

$$\frac{dx}{dt} = 1 + q(t) \qquad f(q(t)) \propto \exp\left\{-\frac{1}{2}\frac{q^2(t)}{C_{qq}}\right\}$$

$$x(0) = 0 + a \qquad f(a) \propto \exp\left\{-\frac{1}{2}\frac{a^2}{C_{aa}}\right\}$$

$$x(1) = 2 + b \qquad f(b) \propto \exp\left\{-\frac{1}{2}\frac{b^2}{C_{bb}}\right\}$$

$$f(a)f\left(\int_0^1 q(t)dt\right)f(b) = \exp\left(-\frac{1}{2}J[x]\right)$$

$$\mathcal{J}[x] = C_{qq}^{-1}\int_0^1 \left(\frac{dx}{dt} - 1\right)^2 dt + C_{aa}^{-1}\left(x(0) - 0\right)^2 + C_{bb}^{-1}\left(x(1) - 2\right)^2$$

Thus, Bayes' theorem leads to least-squares variational inverse problem for Gaussian error distributions.

Summary

- Bayes' theorem defines the "ultimate" data-assimilation problem.
- Impossible to solve in high dimensions.
- Gaussian approximation is key and leads to least-squares inverse problem.

Linear estimation theory and update equations

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Best Linear Unbiased Estimator

We have given a prediction x^{f} and a measurement d:

$$
\begin{aligned}
x^{\mathrm{f}} &= x^{\mathrm{t}} + p^{\mathrm{f}}, & \overline{p^{\mathrm{f}}} &= 0 & \overline{(p^{\mathrm{f}})^2} &= C^{\mathrm{f}}_{xx} & & \\
d &= x^{\mathrm{t}} + \epsilon, & \overline{\epsilon} &= 0 & \overline{(\epsilon)^2} &= C_{dd} & \overline{(\epsilon p^{\mathrm{f}})} &= 0
\end{aligned}
$$

What is the Best Linear Unbiased Estimator (BLUE) of x?

- x^{f} could be a Forecast or a First-guess solution.
- d is a measurement.

Original BLUE derivation from system control theory

Given

$$
\begin{aligned}
x^{\mathrm{f}} &= x^{\mathrm{t}} + p^{\mathrm{f}}, & \overline{p^{\mathrm{f}}} &= 0 & \overline{(p^{\mathrm{f}})^2} &= C_{xx}^{\mathrm{f}} \\
x^{\mathrm{a}} &= x^{\mathrm{t}} + p^{\mathrm{a}}, & \overline{p^{\mathrm{a}}} &= 0 & \overline{(p^{\mathrm{a}})^2} &= C_{xx}^{\mathrm{a}} \\
d &= x^{\mathrm{t}} + \epsilon, & \overline{\epsilon} &= 0 & \overline{(\epsilon)^2} &= C_{dd}
\end{aligned}
$$

A linear unbiased estimator is

$$
\begin{aligned}
x^{\mathrm{a}} &= (1-\alpha)x^{\mathrm{f}} + \alpha d \\
&= x^{\mathrm{f}} + \alpha(d - x^{\mathrm{f}})
\end{aligned}
$$

Inserting gives

$$
x^{\mathrm{a}} = x^{\mathrm{t}} + p^{\mathrm{a}} = x^{\mathrm{t}} + p^{\mathrm{f}} + \alpha(x^{\mathrm{t}} + \epsilon - x^{\mathrm{t}} - p^{\mathrm{f}})
$$

$$
p^{\mathrm{a}} = p^{\mathrm{f}} + \alpha(\epsilon - p^{\mathrm{f}})
$$

Derivation

$$
\begin{aligned}
\overline{(p^{\mathrm{a}})^2} = C^{\mathrm{a}}_{xx} &= \overline{(p^{\mathrm{f}} + \alpha(\epsilon - p^{\mathrm{f}}))^2} \\
&= \overline{(p^{\mathrm{f}})^2} + 2\alpha\overline{p^{\mathrm{f}}(\epsilon - p^{\mathrm{f}})} + \alpha^2\overline{\epsilon^2 - 2\epsilon p^{\mathrm{f}} + (p^{\mathrm{f}})^2} \\
&= C^{\mathrm{f}}_{xx} - 2\alpha C^{\mathrm{f}}_{xx} + \alpha^2(C_{dd} + C^{\mathrm{f}}_{xx}),
\end{aligned}
$$

Set derivative equal to zero

$$
\frac{\partial C^{\mathrm{a}}_{xx}}{\partial \alpha} = -2C^{\mathrm{f}}_{xx} + 2\alpha(C_{dd} + C^{\mathrm{f}}_{xx}) = 0.
$$

to get

$$
\alpha = \frac{C^{\mathrm{f}}_{xx}}{C^{\mathrm{f}}_{xx} + C_{dd}}
$$

Derivation

The optimal (BLUE) solution is

$$x^{\mathrm{a}} = x^{\mathrm{f}} + \frac{C^{\mathrm{f}}_{xx}}{C^{\mathrm{f}}_{xx} + C_{dd}}(d - x^{\mathrm{f}})$$

Error estimate when inserting for α

$$C^{\mathrm{a}}_{xx} = C^{\mathrm{f}}_{xx}\left(1 - \frac{C^{\mathrm{f}}_{xx}}{C^{\mathrm{f}}_{xx} + C_{dd}}\right)$$

Derivation from Bayes' Theorem

Assuming a Gaussian prior and likelihood

$$f(x) = \exp\left\{-\frac{1}{2}(x - x^{\mathrm{f}})C_{xx}^{-1}(x - x^{\mathrm{f}})\right\}$$
$$f(d|x) = \exp\left\{-\frac{1}{2}(d - x)C_{dd}^{-1}(d - x)\right\}$$

From Bayes

$$f(x|d) \propto f(x)f(d|x)$$

By taking the logarithm we get the cost function

$$\mathcal{J}(x) = (x - x^{\mathrm{f}})C_{xx}^{-1}(x - x^{\mathrm{f}}) + (d - x)C_{dd}^{-1}(d - x)$$

Derivation from Bayes' Theorem

Derivative of cost function set to zero

$$\begin{aligned}\frac{1}{2}\frac{\partial \mathcal{J}(x)}{\partial x} &= (x - x^{\mathrm{f}})C_{xx}^{-1} - (d - x)C_{dd}^{-1} \\ &= x(C_{xx}^{-1} + C_{dd}^{-1}) - x^{\mathrm{f}} C_{xx}^{-1} - dC_{dd}^{-1} = 0\end{aligned}$$

Solve for x

$$\begin{aligned}x &= x^{\mathrm{f}} \frac{C_{xx}^{-1}}{C_{xx}^{-1} + C_{dd}^{-1}} + d \frac{C_{dd}^{-1}}{C_{xx}^{-1} + C_{dd}^{-1}} && \times \frac{C_{dd} C_{xx}}{C_{dd} C_{xx}} \\ &= x^{\mathrm{f}} \frac{C_{dd}}{C_{dd} + C_{xx}} + d \frac{C_{xx}}{C_{dd} + C_{xx}} && + x^{\mathrm{f}} - \frac{C_{dd} + C_{xx}}{C_{dd} + C_{xx}} x^{\mathrm{f}} \\ &= x^{\mathrm{f}} + \frac{C_{xx}}{C_{xx} + C_{dd}}(d - x^{\mathrm{f}})\end{aligned}$$

Summary

- The BLUE is the optimal way of combining two linear estimates of a parameter.
- We can derive it from Bayes' formula when assuming Gaussian error statistics.

$$f(x|d) \propto f(x)f(d|x)$$

$$\mathcal{J}(x) = (x - x^{\mathrm{f}})C_{xx}^{-1}(x - x^{\mathrm{f}}) + (d - x)C_{dd}^{-1}(d - x)$$

$$x^{\mathrm{a}} = x^{\mathrm{f}} + \frac{C_{xx}}{C_{xx} + C_{dd}}(d - x^{\mathrm{f}})$$

$$C_{xx}^{\mathrm{a}} = C_{xx}^{\mathrm{f}}\left(1 - \frac{C_{xx}^{\mathrm{f}}}{C_{xx}^{\mathrm{f}} + C_{dd}}\right)$$

BLUE in vector form

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Vector state and data

Given a state vector $\boldsymbol{x} \in \Re^n$ and a data vector $\boldsymbol{d} \in \Re^m$.

$$\begin{aligned} \boldsymbol{x}^{\mathrm{f}} &= \boldsymbol{x}^{\mathrm{t}} + \boldsymbol{p} & \overline{\boldsymbol{p}} &= 0 & \overline{\boldsymbol{p}\boldsymbol{p}^{\mathrm{T}}} &= \boldsymbol{C}_{xx} & & \\ \boldsymbol{d} &= \boldsymbol{H}\boldsymbol{x}^{\mathrm{t}} + \boldsymbol{\epsilon} & \overline{\boldsymbol{\epsilon}} &= 0 & \overline{\boldsymbol{\epsilon}\boldsymbol{\epsilon}^{\mathrm{T}}} &= \boldsymbol{C}_{dd} & \overline{\boldsymbol{p}\boldsymbol{\epsilon}^{\mathrm{T}}} &= 0 \end{aligned}$$

where we define the measurement operator $\boldsymbol{H} \in \Re^{m \times n}$.

As an example consider the case with $m = 2$ and $n = 10$.

$$\begin{aligned} \boldsymbol{x}^{\mathrm{f}} &= [x_1, x_2, x_3, \ldots, x_{10}]^{\mathrm{T}} \\ \boldsymbol{d} &= [d_1, d_2]^{\mathrm{T}} \end{aligned}$$

with

$$\boldsymbol{H} = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}$$

implying that $d_1 = x_4^{\mathrm{t}} + \epsilon_1$ and $d_2 = x_7^{\mathrm{t}} + \epsilon_2$.

Start from Bayes' Theroem

Bayes for the state vector $\boldsymbol{x}$ given the measurement vector $\boldsymbol{d}$

$$f(\boldsymbol{x}|\boldsymbol{d}) \propto f(\boldsymbol{x})f(\boldsymbol{d}|\boldsymbol{x})$$

Assume Gaussian prior and measurement errors

$$f(\boldsymbol{x}|\boldsymbol{d}) \propto \exp -\frac{1}{2}\left\{(\boldsymbol{x}-\boldsymbol{x}^{\mathrm{f}})^{\mathrm{T}}\boldsymbol{C}_{xx}^{-1}(\boldsymbol{x}-\boldsymbol{x}^{\mathrm{f}}) + (\boldsymbol{d}-\boldsymbol{H}\boldsymbol{x})^{\mathrm{T}}\boldsymbol{C}_{dd}^{-1}(\boldsymbol{d}-\boldsymbol{H}\boldsymbol{x})\right\}$$

Maximizing $f(\boldsymbol{x}|\boldsymbol{d})$ identical to minimizing

$$\mathcal{J}(\boldsymbol{x}) = (\boldsymbol{x}-\boldsymbol{x}^{\mathrm{f}})^{\mathrm{T}}\boldsymbol{C}_{xx}^{-1}(\boldsymbol{x}-\boldsymbol{x}^{\mathrm{f}}) + (\boldsymbol{d}-\boldsymbol{H}\boldsymbol{x})^{\mathrm{T}}\boldsymbol{C}_{dd}^{-1}(\boldsymbol{d}-\boldsymbol{H}\boldsymbol{x})$$

Minimum is defined by zero-gradient of cost function

$$
\begin{aligned}
\frac{1}{2}\nabla\mathcal{J}(\boldsymbol{x}) &= \boldsymbol{C}_{xx}^{-1}(\boldsymbol{x}-\boldsymbol{x}^{\mathrm{f}}) - \boldsymbol{H}^{\mathrm{T}}\boldsymbol{C}_{dd}^{-1}(\boldsymbol{d}-\boldsymbol{H}\boldsymbol{x}) \\
&= \boldsymbol{C}_{xx}^{-1}\boldsymbol{x} - \boldsymbol{C}_{xx}^{-1}\boldsymbol{x}^{\mathrm{f}} - \boldsymbol{H}^{\mathrm{T}}\boldsymbol{C}_{dd}^{-1}\boldsymbol{d} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{C}_{dd}^{-1}\boldsymbol{H}\boldsymbol{x} = 0
\end{aligned}
$$

$$
\left(\boldsymbol{C}_{xx}^{-1} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{C}_{dd}^{-1}\boldsymbol{H}\right)\boldsymbol{x} = \boldsymbol{C}_{xx}^{-1}\boldsymbol{x}^{\mathrm{f}} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{C}_{dd}^{-1}\boldsymbol{d}
$$

$$
\boldsymbol{x} = \left(\boldsymbol{C}_{xx}^{-1} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{C}_{dd}^{-1}\boldsymbol{H}\right)^{-1}\left(\boldsymbol{C}_{xx}^{-1}\boldsymbol{x}^{\mathrm{f}} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{C}_{dd}^{-1}\boldsymbol{d}\right)
$$

Minimizing solution

State space formulation

$$\boldsymbol{x} = \left(\boldsymbol{C}_{xx}^{-1} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{C}_{dd}^{-1}\boldsymbol{H}\right)^{-1}\boldsymbol{C}_{xx}^{-1}\boldsymbol{x}^{\mathrm{f}} + \left(\boldsymbol{C}_{xx}^{-1} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{C}_{dd}^{-1}\boldsymbol{H}\right)^{-1}\boldsymbol{H}^{\mathrm{T}}\boldsymbol{C}_{dd}^{-1}\boldsymbol{d}$$

Using the following two lemmas (from the Woodbury matrix identity):

$$\boxed{\begin{aligned} \left(\boldsymbol{C}_{xx}^{-1} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{C}_{dd}^{-1}\boldsymbol{H}\right)^{-1}\boldsymbol{C}_{xx}^{-1} &= \boldsymbol{I} - \boldsymbol{C}_{xx}\boldsymbol{H}^{\mathrm{T}}(\boldsymbol{H}\boldsymbol{C}_{xx}\boldsymbol{H}^{\mathrm{T}} + \boldsymbol{C}_{dd})^{-1}\boldsymbol{H} \\ \left(\boldsymbol{C}_{xx}^{-1} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{C}_{dd}^{-1}\boldsymbol{H}\right)^{-1}\boldsymbol{H}^{\mathrm{T}}\boldsymbol{C}_{dd}^{-1} &= \boldsymbol{C}_{xx}\boldsymbol{H}^{\mathrm{T}}(\boldsymbol{H}\boldsymbol{C}_{xx}\boldsymbol{H}^{\mathrm{T}} + \boldsymbol{C}_{dd})^{-1} \end{aligned}}$$

we obtain the observation space formulation

$$\boldsymbol{x} = \boldsymbol{x}^{\mathrm{f}} + \boldsymbol{C}_{xx}\boldsymbol{H}^{\mathrm{T}}(\boldsymbol{H}\boldsymbol{C}_{xx}\boldsymbol{H}^{\mathrm{T}} + \boldsymbol{C}_{dd})^{-1}(\boldsymbol{d} - \boldsymbol{H}\boldsymbol{x}^{\mathrm{f}})$$

* What is the update error covariance

The error variance for the update is defined as

$$\boldsymbol{C}^{\mathrm{a}}_{xx} = \overline{(\boldsymbol{x}^{\mathrm{t}} - \boldsymbol{x}^{\mathrm{a}})(\boldsymbol{x}^{\mathrm{t}} - \boldsymbol{x}^{\mathrm{a}})^{\mathrm{T}}}$$

Let us define for simplicity

$$\begin{aligned}
\boldsymbol{C} &= \boldsymbol{H}\boldsymbol{C}^{\mathrm{f}}_{xx}\boldsymbol{H}^{\mathrm{T}} + \boldsymbol{C}_{dd} \\
\boldsymbol{R} &= \boldsymbol{H}\boldsymbol{C}^{\mathrm{f}}_{xx} \\
\boldsymbol{h} &= \boldsymbol{d} - \boldsymbol{H}\boldsymbol{x}^{\mathrm{f}} \\
&= \boldsymbol{H}\boldsymbol{x}^{\mathrm{t}} + \boldsymbol{\epsilon} - \boldsymbol{H}\boldsymbol{x}^{\mathrm{f}} = \boldsymbol{H}(\boldsymbol{x}^{\mathrm{t}} - \boldsymbol{x}^{\mathrm{f}}) + \boldsymbol{\epsilon}
\end{aligned}$$

And we can write

$$\boldsymbol{x}^{\mathrm{a}} = \boldsymbol{x}^{\mathrm{f}} + \boldsymbol{R}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{h}$$

* Update error covariance

$$
\begin{aligned}
C_{xx}^{\mathrm{a}} &= \overline{(x^{\mathrm{t}} - x^{\mathrm{a}})(x^{\mathrm{t}} - x^{\mathrm{a}})^{\mathrm{T}}} \\
&= \overline{(x^{\mathrm{t}} - x^{\mathrm{f}} - R^{\mathrm{T}}C^{-1}h)(x^{\mathrm{t}} - x^{\mathrm{f}} - R^{\mathrm{T}}C^{-1}h)^{\mathrm{T}}} \\
&= \overline{(x^{\mathrm{t}} - x^{\mathrm{f}})(x^{\mathrm{t}} - x^{\mathrm{f}})^{\mathrm{T}}} \qquad (\rightarrow C_{xx}^{\mathrm{f}}) \\
&- 2\overline{(x^{\mathrm{t}} - x^{\mathrm{f}})(R^{\mathrm{T}}C^{-1}h)^{\mathrm{T}}} \\
&+ \overline{(R^{\mathrm{T}}C^{-1}h)(R^{\mathrm{T}}C^{-1}h)^{\mathrm{T}}}
\end{aligned}
$$

* Second term

$$
\begin{aligned}
& -2\overline{(\boldsymbol{x}^{\mathrm{t}} - \boldsymbol{x}^{\mathrm{f}})(\boldsymbol{R}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{h})^{\mathrm{T}}} \\
&= -2\overline{(\boldsymbol{x}^{\mathrm{t}} - \boldsymbol{x}^{\mathrm{f}})\boldsymbol{h}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{R}} \\
&= -2\overline{(\boldsymbol{x}^{\mathrm{t}} - \boldsymbol{x}^{\mathrm{f}})(\boldsymbol{H}(\boldsymbol{x}^{\mathrm{t}} - \boldsymbol{x}^{\mathrm{f}}) + \boldsymbol{\epsilon})^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{R}} \\
&= -2\overline{(\boldsymbol{x}^{\mathrm{t}} - \boldsymbol{x}^{\mathrm{f}})(\boldsymbol{x}^{\mathrm{t}} - \boldsymbol{x}^{\mathrm{f}})^{\mathrm{T}}\boldsymbol{H}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{R}} \\
&= -2\boldsymbol{C}_{xx}^{\mathrm{f}}\boldsymbol{H}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{R} \\
&= -2\boldsymbol{R}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{R}
\end{aligned}
$$

* Third term

$$
\begin{aligned}
&\overline{(\boldsymbol{R}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{h})(\boldsymbol{R}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{h})^{\mathrm{T}}} \\
&= \overline{\boldsymbol{R}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{h}\boldsymbol{h}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{R}} \\
&= \overline{\boldsymbol{R}^{\mathrm{T}}\boldsymbol{C}^{-1}(\boldsymbol{H}(\boldsymbol{x}^{\mathrm{t}} - \boldsymbol{x}^{\mathrm{f}}) + \boldsymbol{\epsilon})(\boldsymbol{H}(\boldsymbol{x}^{\mathrm{t}} - \boldsymbol{x}^{\mathrm{f}}) + \boldsymbol{\epsilon})^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{R}} \\
&= \boldsymbol{R}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{C}\boldsymbol{C}^{-1}\boldsymbol{R} \\
&= \boldsymbol{R}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{R}
\end{aligned}
$$

* Update error covariance

$$\begin{aligned}
\boldsymbol{C}_{xx}^{\mathrm{a}} &= \boldsymbol{C}_{xx}^{\mathrm{f}} - 2\boldsymbol{R}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{R} + \boldsymbol{R}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{R} \\
&= \boldsymbol{C}_{xx}^{\mathrm{f}} - \boldsymbol{R}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{R} \\
&= \boldsymbol{C}_{xx}^{\mathrm{f}} - \boldsymbol{C}_{xx}^{\mathrm{f}}\boldsymbol{H}^{\mathrm{T}}\left(\boldsymbol{H}\boldsymbol{C}_{xx}^{\mathrm{f}}\boldsymbol{H}^{\mathrm{T}} + \boldsymbol{C}_{dd}\right)^{-1}\boldsymbol{H}\boldsymbol{C}_{xx}^{\mathrm{f}}
\end{aligned}$$

Minimizing solution in the Gaussian case

Kalman filter update equations

$$\boldsymbol{x}^{\mathrm{a}} = \boldsymbol{x}^{\mathrm{f}} + \boldsymbol{C}^{\mathrm{f}}_{xx}\boldsymbol{H}^{\mathrm{T}}\left(\boldsymbol{H}\boldsymbol{C}^{\mathrm{f}}_{xx}\boldsymbol{H}^{\mathrm{T}} + \boldsymbol{C}_{dd}\right)^{-1}\left(\boldsymbol{d} - \boldsymbol{H}\boldsymbol{x}^{\mathrm{f}}\right)$$

$$\boldsymbol{C}^{\mathrm{a}}_{xx} = \boldsymbol{C}^{\mathrm{f}}_{xx} - \boldsymbol{C}^{\mathrm{f}}_{xx}\boldsymbol{H}^{\mathrm{T}}\left(\boldsymbol{H}\boldsymbol{C}^{\mathrm{f}}_{xx}\boldsymbol{H}^{\mathrm{T}} + \boldsymbol{C}_{dd}\right)^{-1}\boldsymbol{H}\boldsymbol{C}^{\mathrm{f}}_{xx}.$$

Kalman gain matrix

The control theory community defines the Kalman Gain Matrix

$$\boldsymbol{K} = \boldsymbol{C}_{xx}^{\mathrm{f}} \boldsymbol{H}^{\mathrm{T}} \left(\boldsymbol{H} \boldsymbol{C}_{xx}^{\mathrm{f}} \boldsymbol{H}^{\mathrm{T}} + \boldsymbol{C}_{dd} \right)^{-1}$$

to obtain a simpler expression of the update:

$$\begin{aligned} \boldsymbol{x}^{\mathrm{a}} &= \boldsymbol{x}^{\mathrm{f}} + \boldsymbol{K}\left(\boldsymbol{d} - \boldsymbol{H}\boldsymbol{x}^{\mathrm{f}}\right) \\ \boldsymbol{C}_{xx}^{\mathrm{a}} &= \boldsymbol{C}_{xx}^{\mathrm{f}} - \boldsymbol{K}\boldsymbol{H}\boldsymbol{C}_{xx}^{\mathrm{f}} \end{aligned}$$

“Representer” formulation

$$\begin{aligned}\boldsymbol{x}^{\mathrm{a}} &= \boldsymbol{x}^{\mathrm{f}} + \boldsymbol{C}_{xx}^{\mathrm{f}}\boldsymbol{H}^{\mathrm{T}}\left(\boldsymbol{H}\boldsymbol{C}_{xx}^{\mathrm{f}}\boldsymbol{H}^{\mathrm{T}} + \boldsymbol{C}_{dd}\right)^{-1}\left(\boldsymbol{d} - \boldsymbol{H}\boldsymbol{x}^{\mathrm{f}}\right)\\ &= \boldsymbol{x}^{\mathrm{f}} + \boldsymbol{R}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{h}\end{aligned}$$

Define $\boldsymbol{b} = \boldsymbol{C}^{-1}\boldsymbol{h}$ as the solution of the linear system

$$\left(\boldsymbol{H}\boldsymbol{C}_{xx}^{\mathrm{f}}\boldsymbol{H}^{\mathrm{T}} + \boldsymbol{C}_{dd}\right)\boldsymbol{b} = \left(\boldsymbol{d} - \boldsymbol{H}\boldsymbol{x}^{\mathrm{f}}\right)$$

So we can write the update as

$$\begin{aligned}\boldsymbol{x}^{\mathrm{a}} &= \boldsymbol{x}^{\mathrm{f}} + \boldsymbol{R}^{\mathrm{T}}\boldsymbol{b}\\ \boldsymbol{C}_{xx}^{\mathrm{a}} &= \boldsymbol{C}_{xx}^{\mathrm{f}} - \boldsymbol{R}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{R}\end{aligned}$$

Note that the covariance update is independent of the actual measurement values.

Summary

- Introduced the concept of a measurement operator.
- Derived Kalman filter update equations in the vector case.
- We update both the state estimate and its error covariance.
- We defined the Kalman Gain.
- We heard about the Representer formulation.
- Original minimization problem is of dimension n.
- The KF update reduces the dimension to $m \ll n$.

Sequential and Smoother solutions from Bayes

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Starting from Bayes (again)

$$f(\boldsymbol{x}|\boldsymbol{d}) \propto f(\boldsymbol{x})f(\boldsymbol{d}|\boldsymbol{x})$$

- $f(\boldsymbol{x})$ is the density for the model state in space and time.
- $f(\boldsymbol{d}|\boldsymbol{x})$ is the measurement likelihood.

Assume that the model is 1st order Markov process

$$x_i = g(x_{i-1}) + q_i, \qquad\qquad q_i \leftarrow f(x_i|x_{i-1})$$

- Since the solution x_i only depends on x_{i-1} we can write

$$f(\boldsymbol{x}) = f(x_0, x_1, \ldots, x_k) = f(x_0) \prod_{i=1}^{k} f(x_i|x_{i-1}).$$

- Valid for most numerical prediction models.

Assume independent data in time

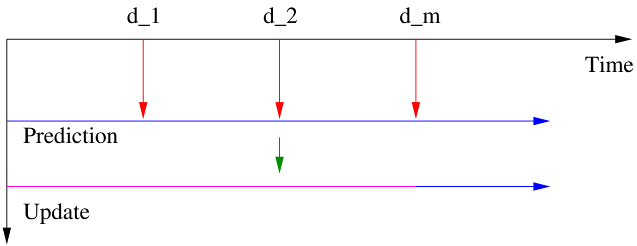
- When measurement errors are uncorrelated in time

$$f(\boldsymbol{d}|\boldsymbol{x}) = \prod_{j=1}^{m} f(d_j|x_j).$$

- Allows for recursive processing of measurements in time

Bayes' becomes

$$f(x_0, x_1, \ldots, x_k, |\boldsymbol{d}) \propto f(x_0) \prod_{i=1}^{k} f(x_i|x_{i-1}) \prod_{j=1}^{m} f(d_j|x_j)$$



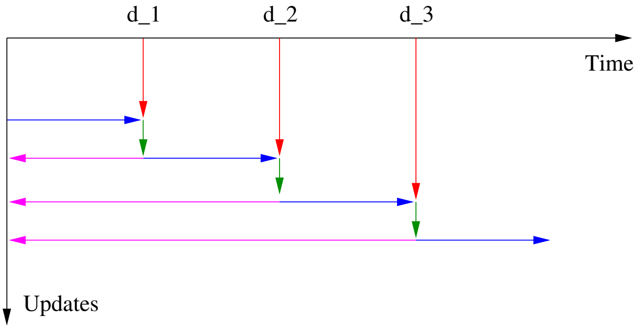
Rewrite as

$$
\begin{aligned}
f(\boldsymbol{x}|\boldsymbol{d}) \propto f(\boldsymbol{x})f(\boldsymbol{d}|\boldsymbol{x}) = \\
& f(x_0) \\
& f(x_1|x_0)f(d_1|x_1) \\
& f(x_2|x_1)f(d_2|x_2) \\
& \vdots \\
& f(x_k|x_{k-1})f(d_m|x_m) \\
& f(x_{k+1}|x_k)
\end{aligned}
$$

Recursive “smoother” updates

The recursive idea: "Today’s posterior is tomorrow’s prior"

$$f(x_0, x_1 | d_1) = f(x_0)\, f(x_1 | x_0)\, f(d_1 | x_1)$$
$$f(x_0, x_1, x_2 | d_1, d_2) = f(x_0, x_1 | d_1)\, f(x_2 | x_1)\, f(d_2 | x_2)$$

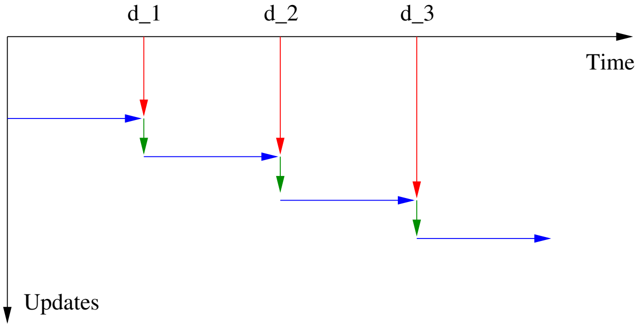


Recursive “filter” updates

Marginal pdfs

$$f(x_1|d_1) = \int_{x_0} f(x_0)f(x_1|x_0)dx_0\, f(d_1|x_1) \qquad = f(x_1)f(d_1|x_1)$$

$$f(x_2|d_1,d_2) = \int_{x_1} f(x_1|d_1)f(x_2|x_1)dx_1\, f(d_2|x_2) \qquad = f(x_2|d_1)f(d_2|x_2)$$



Summary

- Assume model is Marov process.
- Assume measurements are independent in time. (Not generally true.)
- We can process independent measurements sequentially in time.
- The solution of one sub-problem is prior for the next one.

Kalman Filter and Extended Kalman Filter

Geir Evensen

Kalman Filter

- Recursively updates model state and uncertainty.
- Variance minimizing update step.
- Estimate improves and uncertainty reduces at each update.

Error propagation

Derivation for linear scalar model

- Evolution of true state

$$x_k^{\mathrm{t}} = Gx_{k-1}^{\mathrm{t}} + q_{k-1}$$

- The model state evolves according to

$$x_k^{\mathrm{f}} = Gx_{k-1}^{\mathrm{a}}$$

- Difference is

$$x_k^{\mathrm{t}} - x_k^{\mathrm{f}} = G(x_{k-1}^{\mathrm{t}} - x_{k-1}^{\mathrm{a}}) + q_{k-1}$$

Predicting the errors

Square difference and take the expectation

$$\overline{(x_k^{\mathrm{t}} - x_k^{\mathrm{f}})^2} = G\overline{(x_{k-1}^{\mathrm{t}} - x_{k-1}^{\mathrm{a}})^2}G + \overline{q_{k-1}^2} + 2G\overline{(x_{k-1}^{\mathrm{t}} - x_{k-1}^{\mathrm{a}})q_{k-1}}$$

Error covariance evolution equation

$$C_{xx}^{\mathrm{f}}(t_k) = GC_{xx}^{\mathrm{a}}(t_{k-1})G + C_{qq}(t_{k-1}).$$

- Model errors uncorrelated with state error.

The full Kalman Filter (vector form)

Linear model prediction

$$\boldsymbol{x}_k^{\mathrm{f}} = \boldsymbol{G}\boldsymbol{x}_{k-1}^{\mathrm{a}}$$

Error covariance prediction

$$\boldsymbol{C}_{xx}^{\mathrm{f}}(t_k) = \boldsymbol{G}\boldsymbol{C}_{xx}^{\mathrm{a}}(t_{k-1})\boldsymbol{G}^{\mathrm{T}} + \boldsymbol{C}_{qq}(t_{k-1}).$$

Analysis update (skipped t_k index)

$$\boldsymbol{x}_k^{\mathrm{a}} = \boldsymbol{x}_k^{\mathrm{f}} + \boldsymbol{C}_{xx}^{\mathrm{f}}\boldsymbol{H}^{\mathrm{T}}\left(\boldsymbol{H}\boldsymbol{C}_{xx}^{\mathrm{f}}\boldsymbol{H}^{\mathrm{T}} + \boldsymbol{C}_{dd}\right)^{-1}\left(\boldsymbol{d}_k - \boldsymbol{H}\boldsymbol{x}_k^{\mathrm{f}}\right)$$

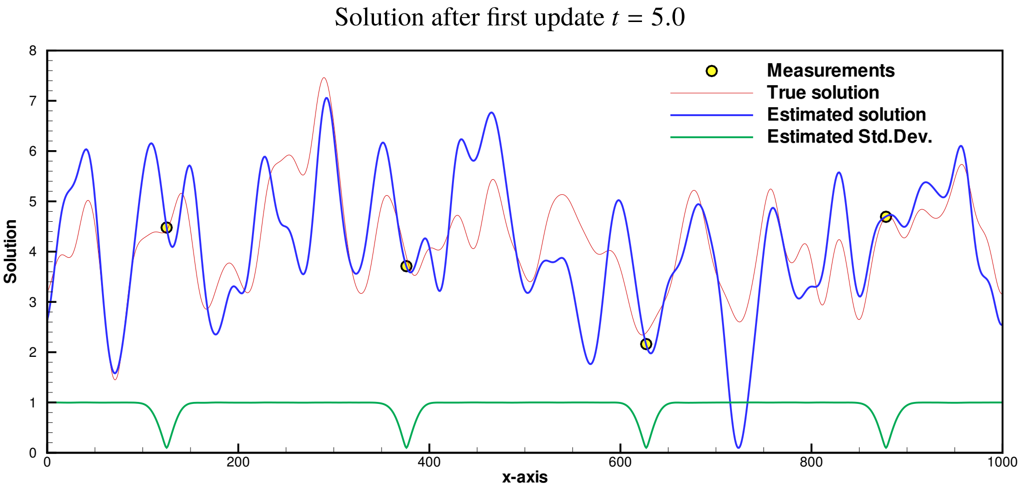
Error covariance update (for each t_k)

$$\boldsymbol{C}_{xx}^{\mathrm{a}} = \boldsymbol{C}_{xx}^{\mathrm{f}} - \boldsymbol{C}_{xx}^{\mathrm{f}}\boldsymbol{H}^{\mathrm{T}}\left(\boldsymbol{H}\boldsymbol{C}_{xx}^{\mathrm{f}}\boldsymbol{H}^{\mathrm{T}} + \boldsymbol{C}_{dd}\right)^{-1}\boldsymbol{H}\boldsymbol{C}_{xx}^{\mathrm{f}}.$$

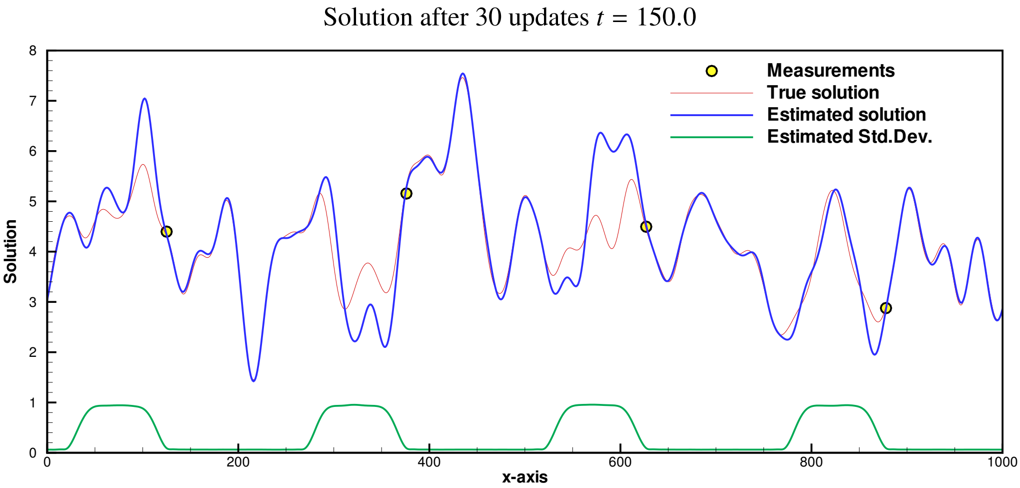
Kalman Filter Example

- Linear advection equation
- Periodic domain
- Random reference solution (truth).
- First guess is reference plus random perturbation.
- Initial variance is 1.0 m^2
- Four measurements every 5 time units.
- Measurement variance is 0.01 m^2.
- Cases without and including system noise of 0.0004 m^2.

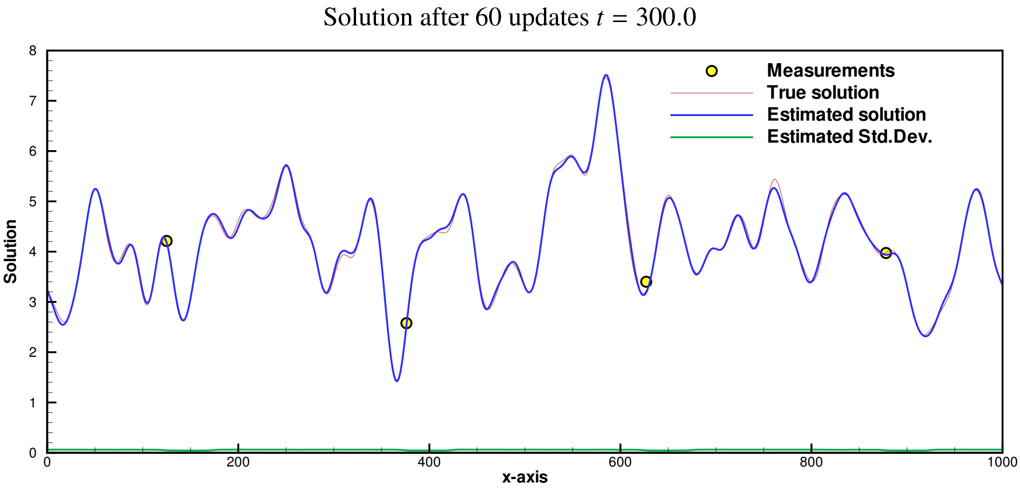
Kalman Filter example: Perfect model



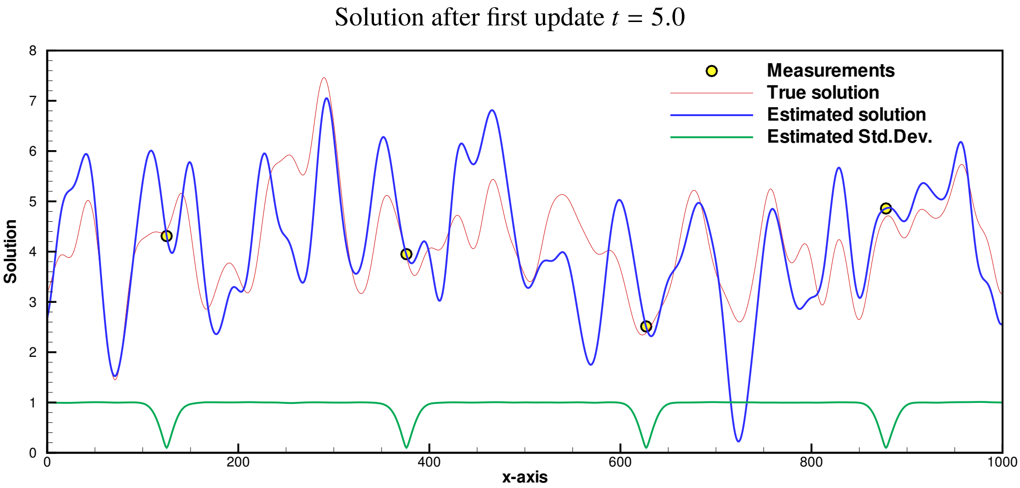
Kalman Filter example: Perfect model



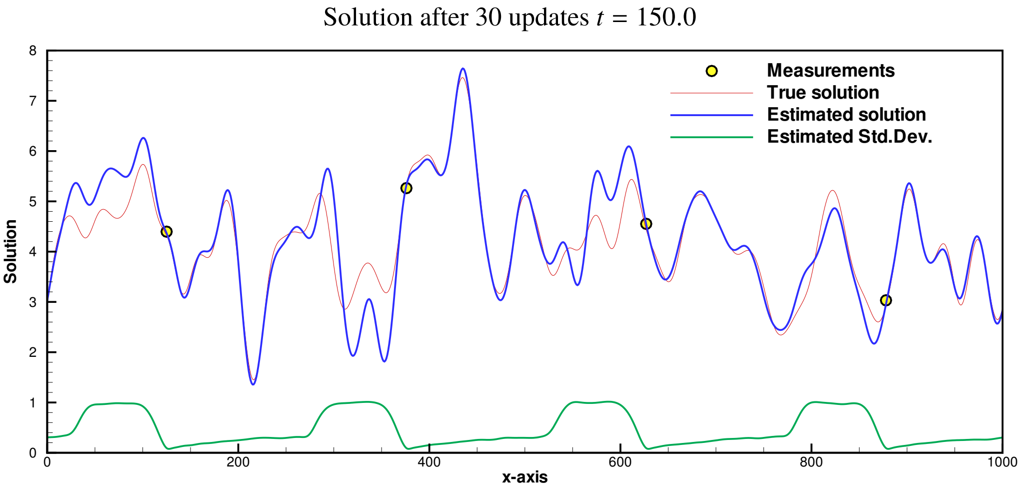
Kalman Filter example: Perfect model



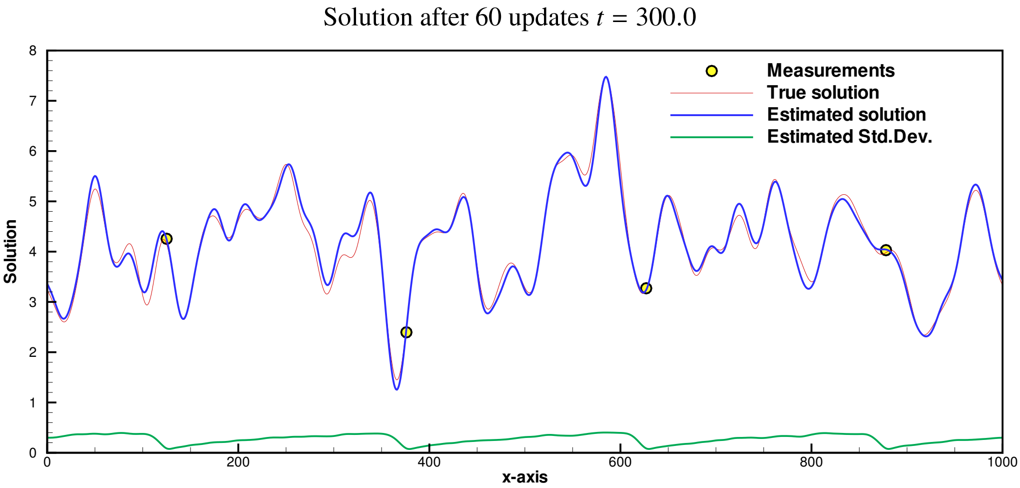
Kalman Filter example: with model error



Kalman Filter example: with model error



Kalman Filter example: with model error



Inverse problem revisited

What is the KF solution for the linear inverse problem?

$$\frac{dx}{dt} = 1$$
$$x(0) = 0$$
$$d = x(1) = 2$$

KF solution

Solve initial value problem

$$\frac{dx}{dt} = 1$$
$$x(0) = 0$$

$$\implies x^{\mathrm{f}}(t) = t$$

Predicted error variance

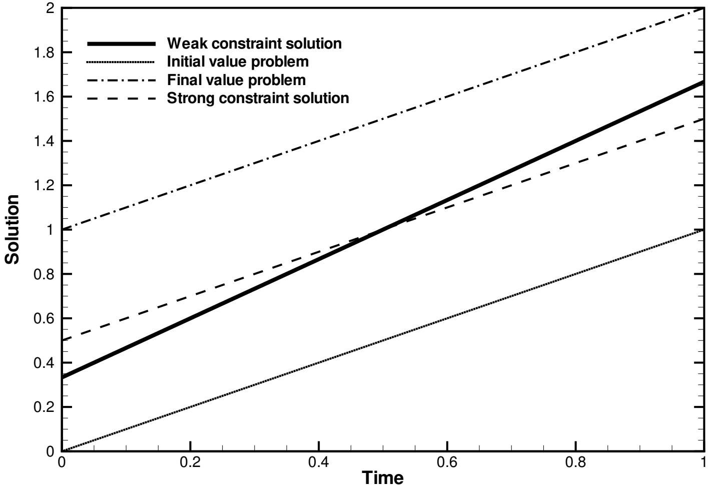
$$C^{\mathrm{f}}_{xx}(1) = C^{\mathrm{a}}_{xx}(0) + C_{qq} = 2C_0$$

Update at $t = 1$ is

$$x^{\mathrm{a}} = x^{\mathrm{f}} + \frac{C^{\mathrm{f}}_{xx}}{C_{dd} + C^{\mathrm{f}}_{xx}}(d - x^{\mathrm{f}}) = 1 + \frac{2C_0}{C_0 + 2C_0}(2 - 1) = 5/3$$

KF solution at final time equals the weak-constraint variational solution

Inverse problem revisited



Nonlinear dynamics

Derivation of Extended Kalman Filter (EKF)

$$
\begin{aligned}
\boldsymbol{x}_k^{\mathrm{t}} &= \boldsymbol{g}(\boldsymbol{x}_{k-1}^{\mathrm{t}}) + \boldsymbol{q}_{k-1}, \\
\boldsymbol{x}_k^{\mathrm{f}} &= \boldsymbol{g}(\boldsymbol{x}_{k-1}^{\mathrm{a}}), \\
\boldsymbol{x}_k^{\mathrm{t}} - \boldsymbol{x}_k^{\mathrm{f}} &= \boldsymbol{g}(\boldsymbol{x}_{k-1}^{\mathrm{t}}) - \boldsymbol{g}(\boldsymbol{x}_{k-1}^{\mathrm{a}}) + \boldsymbol{q}_{k-1}.
\end{aligned}
$$

Use Taylor expansion

$$
\boldsymbol{g}(\boldsymbol{x}_{k-1}^{\mathrm{t}}) = \boldsymbol{g}(\boldsymbol{x}_{k-1}^{\mathrm{a}}) + \boldsymbol{G}(\boldsymbol{x}_{k-1}^{\mathrm{a}})(\boldsymbol{x}_{k-1}^{\mathrm{t}} - \boldsymbol{x}_{k-1}^{\mathrm{a}}) + \frac{1}{2}\mathcal{H}(\boldsymbol{x}_{k-1}^{\mathrm{a}})(\boldsymbol{x}_{k-1}^{\mathrm{t}} - \boldsymbol{x}_{k-1}^{\mathrm{a}})^2 + \cdots .
$$

EKF: Derivation

Difference becomes

$$\boldsymbol{x}_k^{\mathrm{t}} - \boldsymbol{x}_k^{\mathrm{f}} = \boldsymbol{G}(\boldsymbol{x}_{k-1}^{\mathrm{a}})(\boldsymbol{x}_{k-1}^{\mathrm{t}} - \boldsymbol{x}_{k-1}^{\mathrm{a}}) + \frac{1}{2}\boldsymbol{\mathcal{H}}(\boldsymbol{x}_{k-1}^{\mathrm{a}})(\boldsymbol{x}_{k-1}^{\mathrm{t}} - \boldsymbol{x}_{k-1}^{\mathrm{a}})^2 + \cdots + \boldsymbol{q}_{k-1}.$$

By squaring and taking the expectation we get

$$\begin{aligned}
\boldsymbol{C}_{xx}^{\mathrm{f}}(t_k) &= \overline{(\boldsymbol{x}_k^{\mathrm{t}} - \boldsymbol{x}_k^{\mathrm{f}})(\boldsymbol{x}_k^{\mathrm{t}} - \boldsymbol{x}_k^{\mathrm{f}})^{\mathrm{T}}} \\
&= \boldsymbol{G}(\boldsymbol{x}_{k-1}^{\mathrm{a}})\overline{(\boldsymbol{x}_{k-1}^{\mathrm{t}} - \boldsymbol{x}_{k-1}^{\mathrm{a}})(\boldsymbol{x}_{k-1}^{\mathrm{t}} - \boldsymbol{x}_{k-1}^{\mathrm{a}})^{\mathrm{T}}}(\boldsymbol{G}(\boldsymbol{x}_{k-1}^{\mathrm{a}}))^{\mathrm{T}} + \cdots + \boldsymbol{C}_{qq}(t_{k-1}) \\
&= \boldsymbol{G}(\boldsymbol{x}_{k-1}^{\mathrm{a}})\boldsymbol{C}_{xx}^{\mathrm{a}}(t_{k-1})(\boldsymbol{G}(\boldsymbol{x}_{k-1}^{\mathrm{a}}))^{\mathrm{T}} + \cdots + \boldsymbol{C}_{qq}(t_{k-1}).
\end{aligned}$$

EKF: Error evolution

Close by discarding higher order moments to get

$$\begin{aligned} \boldsymbol{x}_k^{\mathrm{f}} &= \boldsymbol{g}(\boldsymbol{x}_{k-1}^{\mathrm{a}}), \\ \boldsymbol{C}_{xx}^{\mathrm{f}}(t_k) &\simeq \boldsymbol{G}_{k-1}\boldsymbol{C}_{xx}^{\mathrm{a}}(t_{k-1})\boldsymbol{G}_{k-1}^{\mathrm{T}} + \boldsymbol{C}_{qq}(t_{k-1}), \end{aligned}$$

together with standard analysis equations.

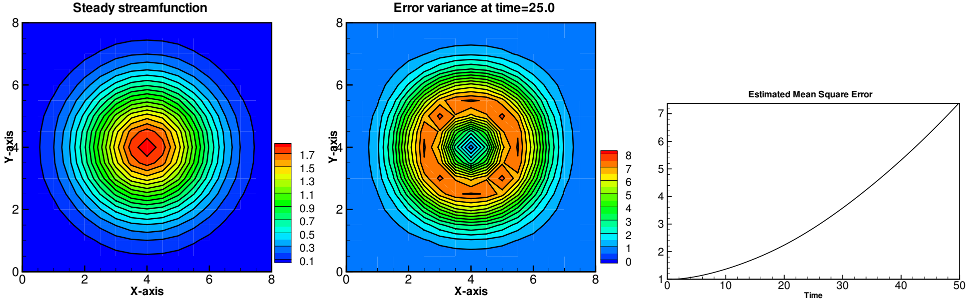
Example of Extended KF

Nonlinear quasi-geostrophic model

- Steady stream function solution.
- Curved and sheared flow.
- Supports instability.
- Initial variance is 1.0.

Example of Extended KF

Results (from Evensen 1992):



- Linear closure approximation not valid!
- Leads to linear instability and exponential error growth.

EKF: Summary

KF is optimal linear filter method!

- Storage of $\mathcal{O}(n^2)$ elements.
- Integration of $2n$ models.

EKF applies closure approximation in error covariance equation.

- Requires implementation of tangent linear model.
- Too simple closure may lead to linear instabilities.
- Does not work for strongly nonlinear models.

We need a better alternative!

Ensemble Kalman Filter

A Monte Carlo alternative to KF and EKF

Geir Evensen

NORCE

The error covariance matrix

Define ensemble covariances around the ensemble mean

$$
\begin{aligned}
\boldsymbol{C}^{\mathrm{f}}_{xx} &\simeq \overline{\boldsymbol{C}}^{\mathrm{f}}_{xx} = \overline{(\boldsymbol{x}^{\mathrm{f}} - \overline{\boldsymbol{x}^{\mathrm{f}}})(\boldsymbol{x}^{\mathrm{f}} - \overline{\boldsymbol{x}^{\mathrm{f}}})^{\mathrm{T}}} \\
\boldsymbol{C}^{\mathrm{a}}_{xx} &\simeq \overline{\boldsymbol{C}}^{\mathrm{a}}_{xx} = \overline{(\boldsymbol{x}^{\mathrm{a}} - \overline{\boldsymbol{x}^{\mathrm{a}}})(\boldsymbol{x}^{\mathrm{a}} - \overline{\boldsymbol{x}^{\mathrm{a}}})^{\mathrm{T}}}
\end{aligned}
$$

- The ensemble mean $\overline{\boldsymbol{x}}$ is the best-guess.
- The ensemble spread defines the error variance.
- The ensemble smoothness defines the error covariance.

Dynamical evolution of error statistics

- Ensemble of models (particles) defines probability $f(\boldsymbol{x})$.
- Ensemble members evolve according to the model dynamics.

$$d\boldsymbol{x} = \boldsymbol{g}(\boldsymbol{x})dt + d\boldsymbol{q}.$$

- Probability density evolve according to Kolmogorov's equation.

$$\frac{\partial f}{\partial t} + \sum_i \frac{\partial (g_i f)}{\partial x_i} = \frac{1}{2} \sum_{i,j} \boldsymbol{C}_{qq} \frac{\partial^2 f}{\partial x_i \partial x_j}.$$

- Fundamental equation for evolution of error statistics.
- Integrating a large ensemble of stochastic models is a MC method for solving Kolmogorov's equation

Analysis scheme (1)

Define the model-forcast error-covariance matrix

$$\boldsymbol{C}_{xx}^{\mathrm{f}} \simeq \overline{\boldsymbol{C}}_{xx}^{\mathrm{f}} = \overline{(\boldsymbol{x}^{\mathrm{f}} - \overline{\boldsymbol{x}^{\mathrm{f}}})(\boldsymbol{x}^{\mathrm{f}} - \overline{\boldsymbol{x}^{\mathrm{f}}})^{\mathrm{T}}}.$$

and the measurement error-covariance matrix

$$\boldsymbol{C}_{dd} \simeq \overline{\boldsymbol{C}}_{dd} = \overline{\boldsymbol{\epsilon}\boldsymbol{\epsilon}^{\mathrm{T}}}.$$

Create an ensemble of perturbed observations

$$\boldsymbol{d}_j = \boldsymbol{d} + \boldsymbol{\epsilon}_j,$$

where $\boldsymbol{d}$ is the vector of observed values and $\boldsymbol{\epsilon}_j$, is a vector of observation noise.

Analysis scheme (2)

Update each ensemble member according to

$$\boxed{\begin{aligned} \boldsymbol{x}_j^{\mathrm{a}} &= \boldsymbol{x}_j^{\mathrm{f}} + \overline{\boldsymbol{C}}_{xx}^{\mathrm{f}} \boldsymbol{H}^{\mathrm{T}} \left(\boldsymbol{H} \overline{\boldsymbol{C}}_{xx}^{\mathrm{f}} \boldsymbol{H}^{\mathrm{T}} + \overline{\boldsymbol{C}}_{dd} \right)^{-1} \left(\boldsymbol{d}_j - \boldsymbol{H} \boldsymbol{x}_j^{\mathrm{f}} \right) \\ &= \boldsymbol{x}_j^{\mathrm{f}} + \overline{\boldsymbol{K}} \left(\boldsymbol{d}_j - \boldsymbol{H} \boldsymbol{x}_j^{\mathrm{f}} \right) \end{aligned}}$$

Thus, the update of the mean becomes

$$\begin{aligned} \overline{\boldsymbol{x}^{\mathrm{a}}} &= \overline{\boldsymbol{x}^{\mathrm{f}}} + \overline{\boldsymbol{C}}_{xx}^{\mathrm{f}} \boldsymbol{H}^{\mathrm{T}} \left(\boldsymbol{H} \overline{\boldsymbol{C}}_{xx}^{\mathrm{f}} \boldsymbol{H}^{\mathrm{T}} + \overline{\boldsymbol{C}}_{dd} \right)^{-1} \left(\boldsymbol{d} - \boldsymbol{H} \overline{\boldsymbol{x}^{\mathrm{f}}} \right) \\ &= \overline{\boldsymbol{x}^{\mathrm{f}}} + \overline{\boldsymbol{K}} \left(\boldsymbol{d} - \boldsymbol{H} \overline{\boldsymbol{x}^{\mathrm{f}}} \right) \end{aligned}$$

Analysis scheme (3)

The error covariance update then becomes

$$
\begin{aligned}
\overline{C}^{\mathrm{a}}_{xx} &= \overline{\left(x^{\mathrm{a}} - \overline{x^{\mathrm{a}}}\right)\left(x^{\mathrm{a}} - \overline{x^{\mathrm{a}}}\right)^{\mathrm{T}}} \\
&= \overline{\left(\left(I - \overline{K}H\right)\left(x^{\mathrm{f}} - \overline{x^{\mathrm{f}}}\right) + \overline{K}\left(d - \overline{d}\right)\right)\left(\cdots\right)^{\mathrm{T}}} \\
&= \left(I - \overline{K}H\right)\overline{C}^{\mathrm{f}}_{xx}\left(I - H^{\mathrm{T}}\overline{K}^{\mathrm{T}}\right) + \overline{K}\,\overline{C}_{dd}\overline{K}^{\mathrm{T}} \\
&= \overline{C}^{\mathrm{f}}_{xx} - \overline{K}H\overline{C}^{\mathrm{f}}_{xx} - \overline{C}^{\mathrm{f}}_{xx}H^{\mathrm{T}}\overline{K}^{\mathrm{T}} + \overline{K}\left(H\overline{C}^{\mathrm{f}}_{xx}H^{\mathrm{T}} + \overline{C}_{dd}\right)\overline{K}^{\mathrm{T}} \\
&= \left(I - \overline{K}H\right)\overline{C}^{\mathrm{f}}_{xx} \\
&= \overline{C}^{\mathrm{f}}_{xx} - \overline{C}^{\mathrm{f}}_{xx}H^{\mathrm{T}}\left(H\overline{C}^{\mathrm{f}}_{xx}H^{\mathrm{T}} + \overline{C}_{dd}\right)^{-1}H\overline{C}^{\mathrm{f}}_{xx}
\end{aligned}
$$

Note that we need to perturb observations to have $\overline{C}_{dd} = \overline{(d - \overline{d})(d - \overline{d})^{\mathrm{T}}}$ (Burgers et al., 1998)

Ensemble Kalman Filter (EnKF)

- Represents error statistics using an ensemble of model states.
- Evolves error statistics by ensemble integrations.
- “Variance minimizing” analysis scheme operating on the ensemble.

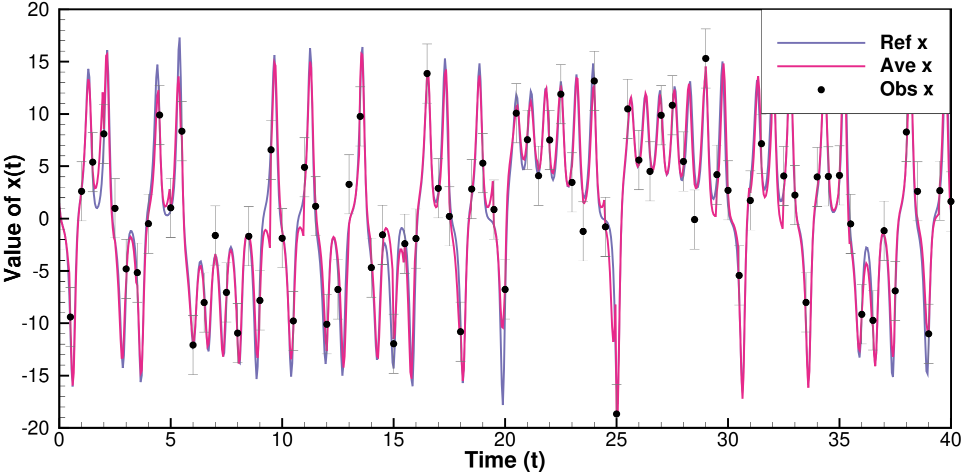
$$\Downarrow$$

- Monte Carlo, low rank, ensemble subspace method.
- Linear model: EnKF converges to the KF with large ensemble size.
- Fully nonlinear error evolution, contrary to EKF.
- Assumption of Gaussian statistics in analysis scheme.

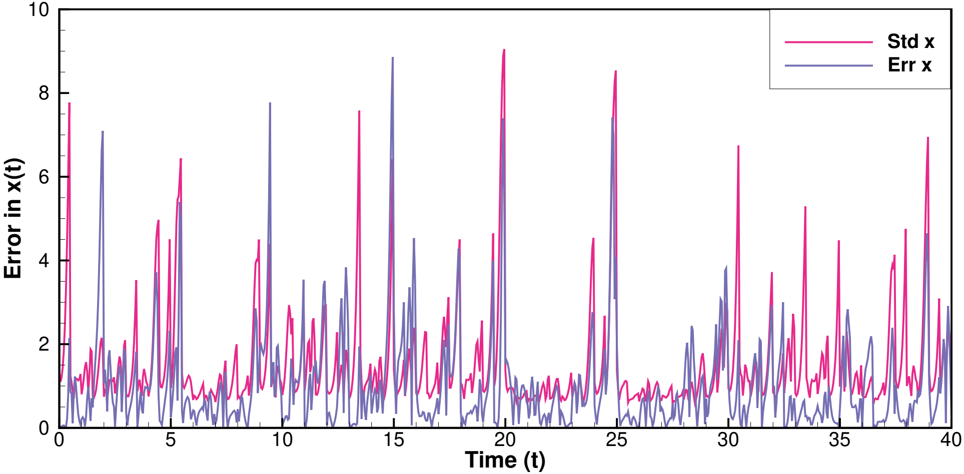
Example: Lorenz model

- Application with the chaotic Lorenz model.
- Illustrates properties with higly nonlinear dynamical models.
- From Evensen (1997), MWR.

EnKF solution



EnKF error variance



Analysis equation (1)

- Define the ensemble matrix
$$\boldsymbol{A} = (\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N) \in \Re^{n\times N}.$$
- The ensemble mean is (defining $\mathbf{1}_N \in \Re^{N\times N} \equiv 1/N$)
$$\overline{\boldsymbol{A}} = \boldsymbol{A}\mathbf{1}_N.$$
- The ensemble perturbations become
$$\boldsymbol{A}' = \boldsymbol{A} - \overline{\boldsymbol{A}} = \boldsymbol{A}(\boldsymbol{I} - \mathbf{1}_N).$$
- The ensemble covariance matrix $\overline{\boldsymbol{C}}_{xx} \in \Re^{n\times n}$ becomes
$$\overline{\boldsymbol{C}}_{xx} = \frac{\boldsymbol{A}'(\boldsymbol{A}')^{\mathrm{T}}}{N-1}.$$

Analysis equation (2)

- Given a vector of measurements $\boldsymbol{d} \in \Re^m$, define

$$\boldsymbol{d}_j = \boldsymbol{d} + \boldsymbol{\epsilon}_j, \qquad j = 1, \dots, N,$$

stored in

$$\boldsymbol{D} = (\boldsymbol{d}_1, \boldsymbol{d}_2, \dots, \boldsymbol{d}_N) \in \Re^{m \times N}.$$

- The ensemble perturbations are stored in

$$\boldsymbol{E} = (\boldsymbol{\epsilon}_1, \boldsymbol{\epsilon}_2, \dots, \boldsymbol{\epsilon}_N) \in \Re^{m \times N},$$

thus, the measurement error covariance matrix becomes

$$\overline{\boldsymbol{C}}_{dd} = \frac{\boldsymbol{E}\boldsymbol{E}^{\mathrm{T}}}{N-1}.$$

Analysis equation (3)

The analysis equation

$$\boldsymbol{A}^{\mathrm{a}} = \boldsymbol{A} + \overline{\boldsymbol{C}}_{xx}\boldsymbol{H}^{\mathrm{T}}\left(\boldsymbol{H}\overline{\boldsymbol{C}}_{xx}\boldsymbol{H}^{\mathrm{T}} + \overline{\boldsymbol{C}}_{dd}\right)^{-1}\left(\boldsymbol{D} - \boldsymbol{H}\boldsymbol{A}\right).$$

can now be written

$$\boldsymbol{A}^{\mathrm{a}} = \boldsymbol{A} + \boldsymbol{A}'(\boldsymbol{H}\boldsymbol{A}')^{\mathrm{T}}\left((\boldsymbol{H}\boldsymbol{A}')(\boldsymbol{H}\boldsymbol{A}')^{\mathrm{T}} + \boldsymbol{E}\boldsymbol{E}^{\mathrm{T}}\right)^{-1}\left(\boldsymbol{D} - \boldsymbol{H}\boldsymbol{A}\right).$$

The update is expressed entirely in terms of the ensemble

Define $\boldsymbol{S} = \boldsymbol{H}\boldsymbol{A}'$

$$\boldsymbol{A}^{\mathrm{a}} = \boldsymbol{A} + \boldsymbol{A}'\boldsymbol{S}^{\mathrm{T}}\left(\boldsymbol{S}\boldsymbol{S}^{\mathrm{T}} + \boldsymbol{E}\boldsymbol{E}^{\mathrm{T}}\right)^{-1}\left(\boldsymbol{D} - \boldsymbol{H}\boldsymbol{A}\right).$$

Analysis equation (4)

Define $\boldsymbol{C} = \boldsymbol{S}\boldsymbol{S}^{\mathrm{T}} + \boldsymbol{E}\boldsymbol{E}^{\mathrm{T}}$ and the innovations $\boldsymbol{D}' = \boldsymbol{D} - \boldsymbol{H}\boldsymbol{A}$.

$$
\begin{aligned}
\boldsymbol{A}^{\mathrm{a}} &= \boldsymbol{A} + \boldsymbol{A}'\boldsymbol{S}^{\mathrm{T}}\left(\boldsymbol{S}\boldsymbol{S}^{\mathrm{T}} + \boldsymbol{E}\boldsymbol{E}^{\mathrm{T}}\right)^{-1}\left(\boldsymbol{D} - \boldsymbol{H}\boldsymbol{A}\right). \\
&= \boldsymbol{A} + \boldsymbol{A}'\boldsymbol{S}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{D}' \\
&= \boldsymbol{A} + \boldsymbol{A}(\boldsymbol{I} - \mathbf{1}_N)\boldsymbol{S}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{D}' \\
&= \boldsymbol{A}\left(\boldsymbol{I} + \boldsymbol{S}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{D}'\right) \\
&= \boldsymbol{A}\boldsymbol{X}
\end{aligned}
$$

where we have used

- $\boldsymbol{A}' = \boldsymbol{A}(\boldsymbol{I} - \mathbf{1}_N)$.
- $\mathbf{1}_N\boldsymbol{S}^{\mathrm{T}} \equiv \mathbf{0}$.

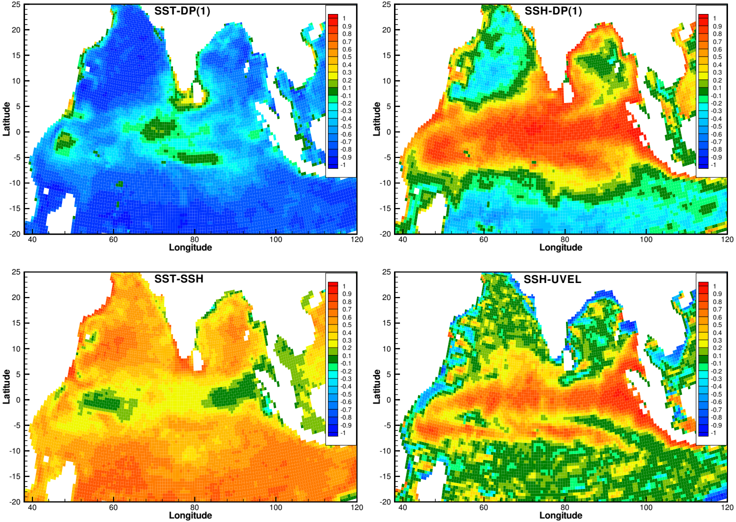
Remarks

- $\overline{\boldsymbol{C}}_{xx}$ is never computed.
- Even $\boldsymbol{H}\overline{\boldsymbol{C}}_{xx}\boldsymbol{H}^{\mathrm{T}} = \boldsymbol{S}\boldsymbol{S}^{\mathrm{T}}$ need not be computed.
- Analysis may be interpreted as:
    - combination of forecast ensemble members, or,
    - forecast plus combination of covariance functions.
- Accuracy of analysis is determined by:
    - the accuracy of $\boldsymbol{X}$,
    - the properties of the ensemble space.
- For a linear model, any choice of $\boldsymbol{X}$ will result in an analysis which is also a solution of the model.

Examples of ensemble statistics

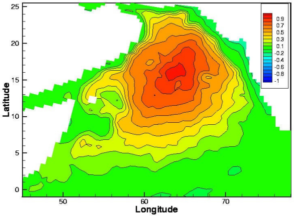
- Taken from Haugen et al. (2002), Ocean Dynamics.
- OGCM (MICOM) for the Indian Ocean.
- Assimilation of SST and SLA data.

Spatial correlations

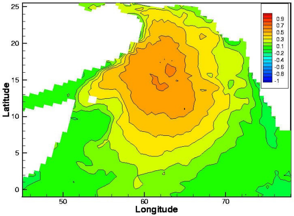


Correlation functions

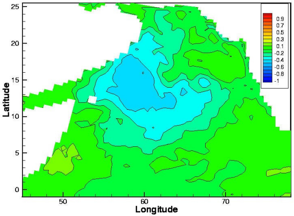
SSH–SSH



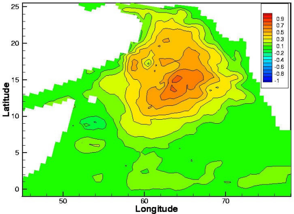
SSH–SST



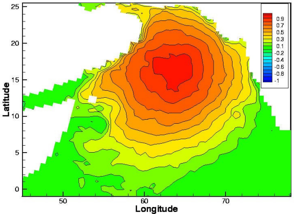
SSH–DP



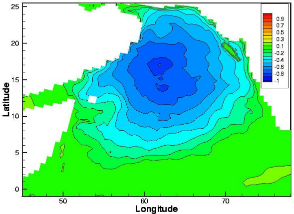
SST–SSH



SST–SST

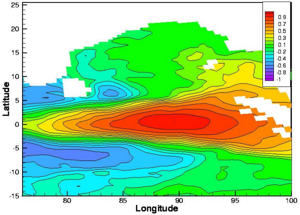


SST–DP

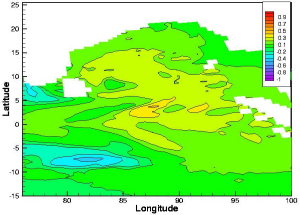


Correlation functions

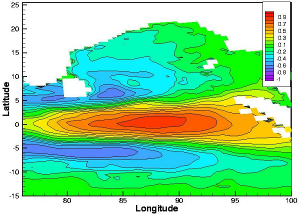
SSH–SSH



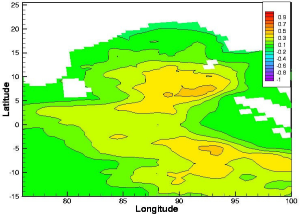
SSH–SST



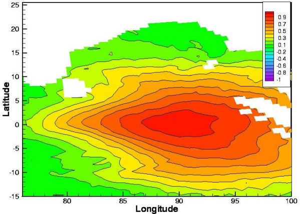
SSH–DP



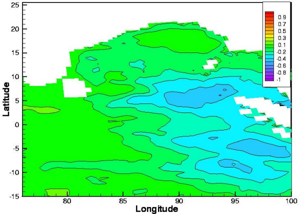
SST–SSH



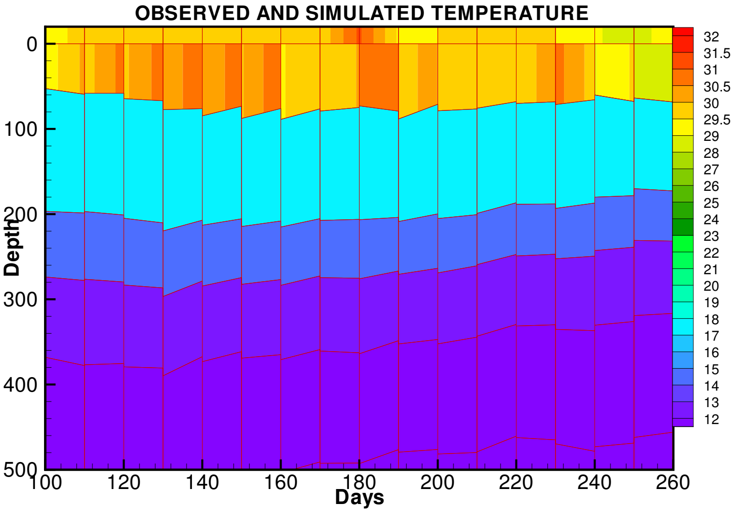
SST–SST



SST–DP



Time–Depth: Temperature



Computational aspects (1)

Analysis scheme

$$\boldsymbol{A}^{\mathrm{a}} = \boldsymbol{A}\boldsymbol{X} = \boldsymbol{A}\left(\boldsymbol{I} + \boldsymbol{S}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{D}'\right)$$

How to compute the inverse

$$\boldsymbol{C}^{-1} = \left(\boldsymbol{S}\boldsymbol{S}^{\mathrm{T}} + \boldsymbol{E}\boldsymbol{E}^{\mathrm{T}}\right)^{-1} \qquad\qquad (\approx \boldsymbol{Z}\boldsymbol{\Lambda}^{+}\boldsymbol{Z}^{\mathrm{T}})$$

- Low rank $(N-1)$.
- Dimension is number of measurents m.
- Direct inversion requires $\mathcal{O}(m^3)$ computations.

Subspace inversion

- Why invert m-dimensional matrix when solving for N coefficients?

$$
\begin{aligned}
\left(\boldsymbol{S}\boldsymbol{S}^{\mathrm{T}} + \boldsymbol{E}\boldsymbol{E}^{\mathrm{T}}\right)
&\approx \boldsymbol{S}\boldsymbol{S}^{\mathrm{T}} + (\boldsymbol{S}\boldsymbol{S}^{+})\boldsymbol{E}\boldsymbol{E}^{\mathrm{T}}(\boldsymbol{S}\boldsymbol{S}^{+})^{\mathrm{T}} \\
&= \boldsymbol{U}\boldsymbol{\Sigma}\left(\boldsymbol{I}_N + \boldsymbol{\Sigma}^{+}\boldsymbol{U}^{\mathrm{T}}\boldsymbol{E}\boldsymbol{E}^{\mathrm{T}}\boldsymbol{U}(\boldsymbol{\Sigma}^{+})^{\mathrm{T}}\right)\boldsymbol{\Sigma}^{\mathrm{T}}\boldsymbol{U}^{\mathrm{T}} \\
&= \boldsymbol{U}\boldsymbol{\Sigma}\left(\boldsymbol{I}_N + \boldsymbol{Z}\boldsymbol{\Lambda}\boldsymbol{Z}^{\mathrm{T}}\right)\boldsymbol{\Sigma}^{\mathrm{T}}\boldsymbol{U}^{\mathrm{T}} \\
&= \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{Z}\left(\boldsymbol{I}_N + \boldsymbol{\Lambda}\right)\boldsymbol{Z}^{\mathrm{T}}\boldsymbol{\Sigma}^{\mathrm{T}}\boldsymbol{U}^{\mathrm{T}}.
\end{aligned}
$$

$$
\left(\boldsymbol{S}\boldsymbol{S}^{\mathrm{T}} + \boldsymbol{E}\boldsymbol{E}^{\mathrm{T}}\right)^{-1} \approx \boldsymbol{U}(\boldsymbol{\Sigma}^{+})^{\mathrm{T}}\boldsymbol{Z}\left(\boldsymbol{I}_N + \boldsymbol{\Lambda}\right)^{-1}\left(\boldsymbol{U}(\boldsymbol{\Sigma}^{+})^{\mathrm{T}}\boldsymbol{Z}\right)^{\mathrm{T}}
$$

- Define singular value decomposition $\boldsymbol{S} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^{\mathrm{T}}$.
- Pseudo inverse $\boldsymbol{S}^{+} = \boldsymbol{V}\boldsymbol{\Sigma}^{+}\boldsymbol{U}^{\mathrm{T}}$.
- $(\boldsymbol{S}\boldsymbol{S}^{+})\boldsymbol{E}$ is orthogonal projection of $\boldsymbol{E}$ onto the $\boldsymbol{S}$ space.
- Cost is $\mathcal{O}(mN^2)$.

Square-Root Schemes

Mean updated using

$$\overline{\boldsymbol{x}^{\mathrm{a}}} = \overline{\boldsymbol{x}^{\mathrm{f}}} + \overline{\boldsymbol{C}}^{\mathrm{f}}_{xx}\boldsymbol{H}^{\mathrm{T}}\left(\boldsymbol{H}\overline{\boldsymbol{C}}^{\mathrm{f}}_{xx}\boldsymbol{H}^{\mathrm{T}} + \overline{\boldsymbol{C}}_{dd}\right)^{-1}\left(\boldsymbol{d} - \boldsymbol{H}\overline{\boldsymbol{x}^{\mathrm{f}}}\right).$$

Perturbations updated using factorization of posterior variance

$$\overline{\boldsymbol{C}}^{\mathrm{a}}_{xx} = \overline{\boldsymbol{C}}^{\mathrm{f}}_{xx} - \overline{\boldsymbol{C}}^{\mathrm{f}}_{xx}\boldsymbol{H}^{\mathrm{T}}\left(\boldsymbol{H}\overline{\boldsymbol{C}}^{\mathrm{f}}_{xx}\boldsymbol{H}^{\mathrm{T}} + \overline{\boldsymbol{C}}_{dd}\right)^{-1}\boldsymbol{H}\overline{\boldsymbol{C}}^{\mathrm{f}}_{xx}.$$

Ensemble notation and simple illustration

$$\boldsymbol{A}^{\mathrm{a}\prime}\boldsymbol{A}^{\mathrm{a}\prime\mathrm{T}} = \boldsymbol{A}^{\prime}\left(\boldsymbol{I} - \boldsymbol{S}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{S}\right)\boldsymbol{A}^{\prime\mathrm{T}}$$

Square-Root Schemes

Ensemble notation and simple illustration

$$
\begin{aligned}
\boldsymbol{A}^{\mathrm{a}\prime}\boldsymbol{A}^{\mathrm{a}\prime\mathrm{T}} &= \boldsymbol{A}'\left(\boldsymbol{I} - \boldsymbol{S}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{S}\right)\boldsymbol{A}'^{\mathrm{T}} \\
&= \boldsymbol{A}'\left(\boldsymbol{Z}\boldsymbol{\Lambda}\boldsymbol{Z}^{\mathrm{T}}\right)\boldsymbol{A}'^{\mathrm{T}} \\
&= \boldsymbol{A}'\boldsymbol{Z}\boldsymbol{\Lambda}^{\frac{1}{2}}\left(\boldsymbol{A}'\boldsymbol{Z}\boldsymbol{\Lambda}^{\frac{1}{2}}\right)^{\mathrm{T}} && \text{Non-symmetrical square root} \\
&= \boldsymbol{A}'\boldsymbol{Z}\boldsymbol{\Lambda}^{\frac{1}{2}}\boldsymbol{Z}\left(\boldsymbol{A}'\boldsymbol{Z}\boldsymbol{\Lambda}^{\frac{1}{2}}\boldsymbol{Z}\right)^{\mathrm{T}} && \text{Symmetrical square root}
\end{aligned}
$$

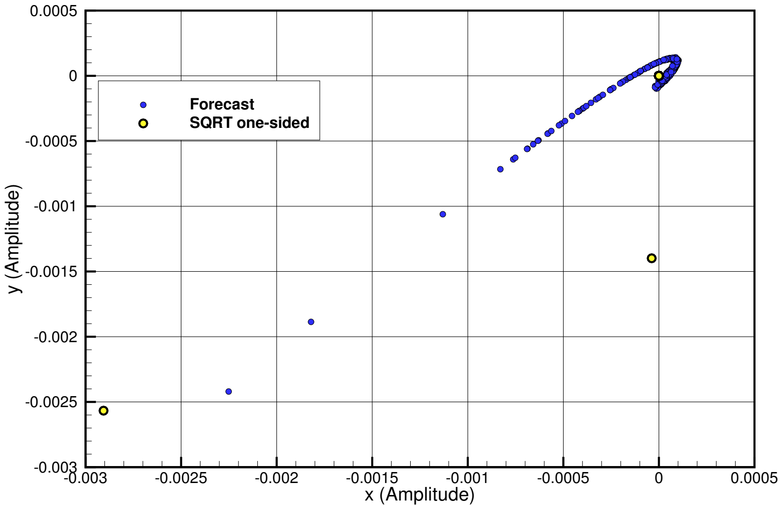
Update becomes

$$\boldsymbol{A}^{\mathrm{a}\prime} = \boldsymbol{A}'\boldsymbol{Z}\boldsymbol{\Lambda}^{\frac{1}{2}}\boldsymbol{Z}$$

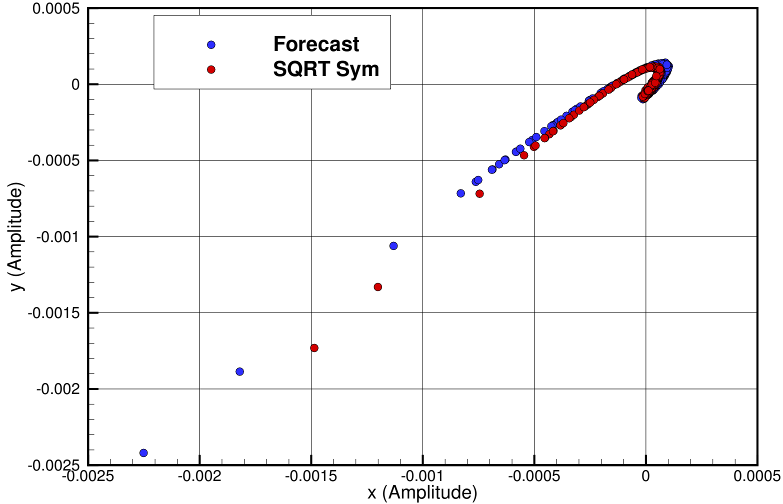
or when including mean preserving random rotation $\boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}} = \boldsymbol{I}$

$$\boldsymbol{A}^{\mathrm{a}\prime} = \boldsymbol{A}'\boldsymbol{Z}\boldsymbol{\Lambda}^{\frac{1}{2}}\boldsymbol{Z}\boldsymbol{\Phi}$$

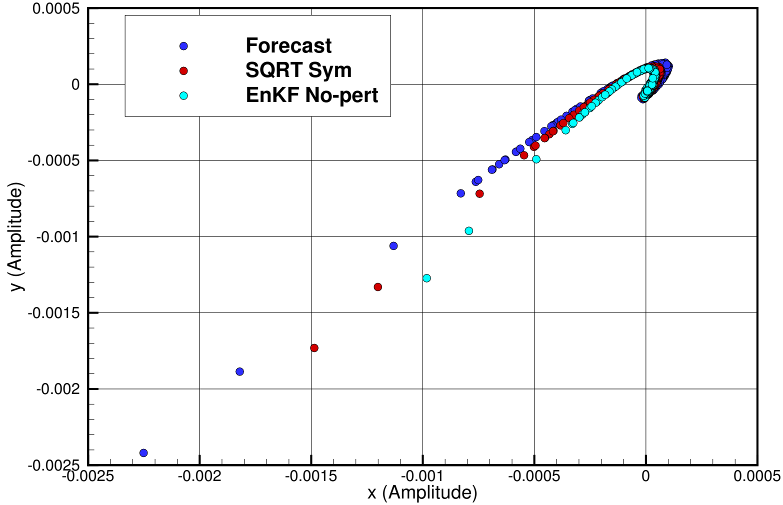
Square-root schemes: Non symmetrical



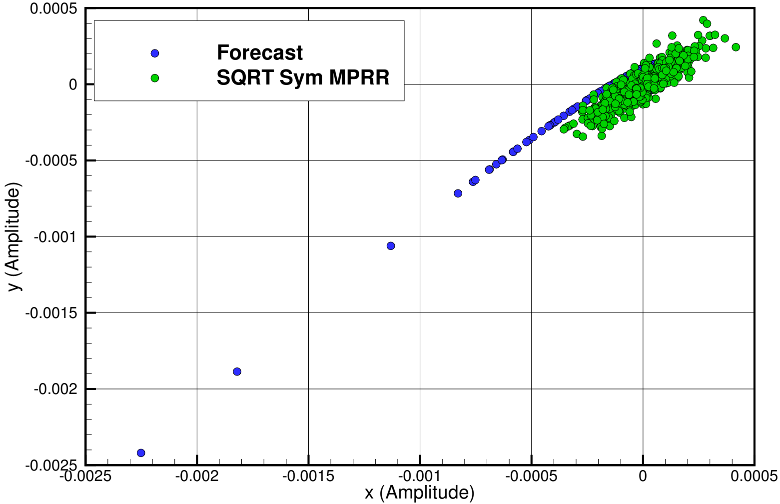
Square-root schemes: Symmetrical



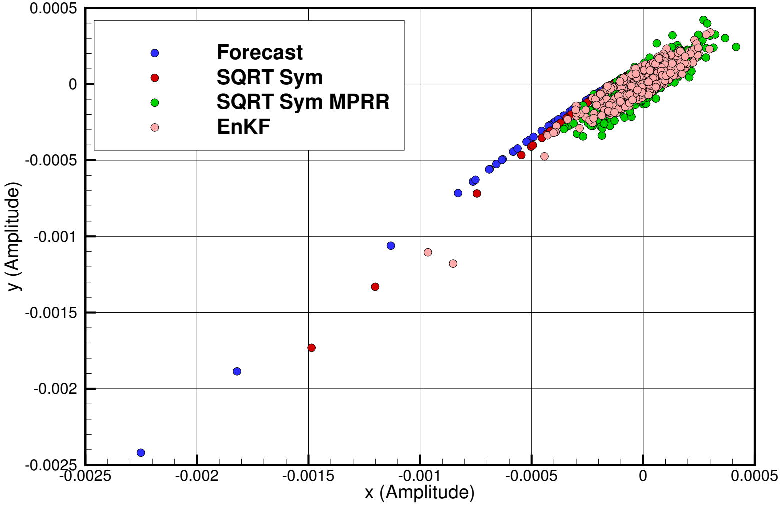
Square-root schemes vs no-pert EnKF



Square root schemes: Symmetrical with MPRR



Square root schemes vs EnKF



Summary

- The EnKF has worked well with highly nonlinear dynamics.
- The EnKF has worked well with high-dimensional models.
- There is no linearization in the evolution of error statistics.
- Major approximation is Gaussian assumption in update step.
- Another approximation is limited ensemble size.

More on ensemble methods

Geir Evensen

Ensemble methods

EnKF: Ensemble Kalman Filter

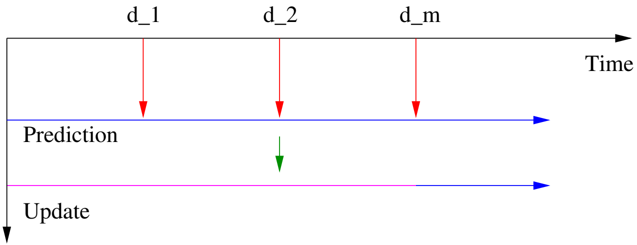
ES: Ensemble Smoother

EnKS: Ensemble Kalman Smoother

- Ensemble representation for pdfs.
- Ensemble prediction for time evolution of pdfs.
- Linear ensemble analysis scheme.

ES: The Ensemble Smoother

Smoother solution processing all data in one go.

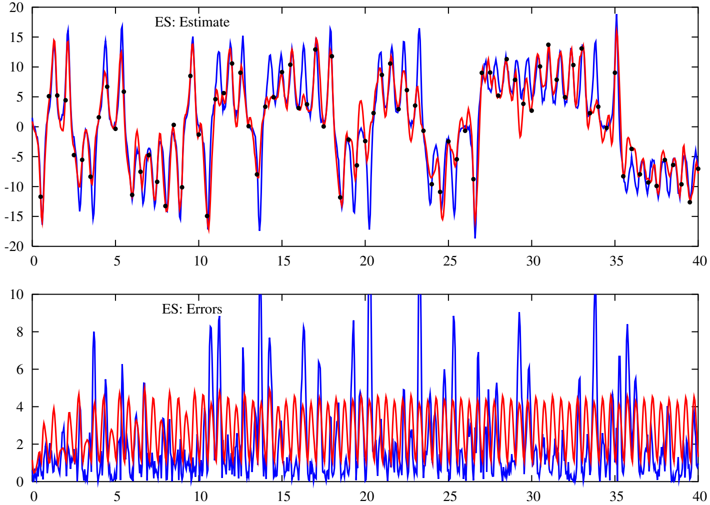


ES: summary

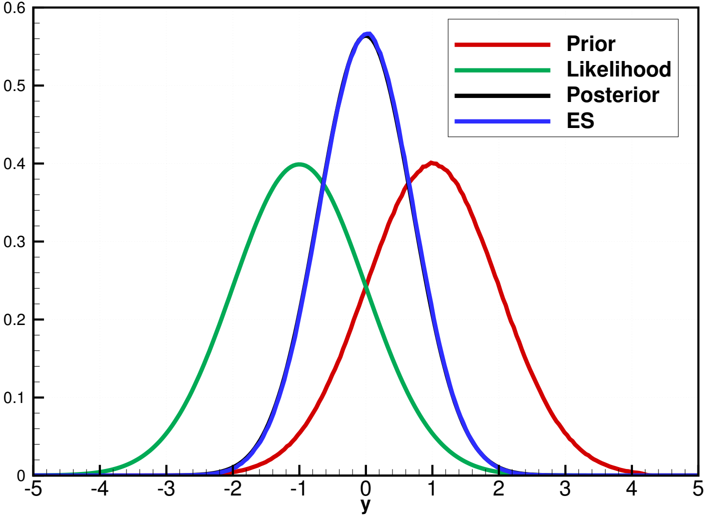
Gauss–Markov interpolation in space and time.

- Creates an ensemble for the model prediction.
- Assumes Gaussian pdf for model prediction.
- Computes variance minimizing ensemble analysis.
- Exact solution for linear problems.

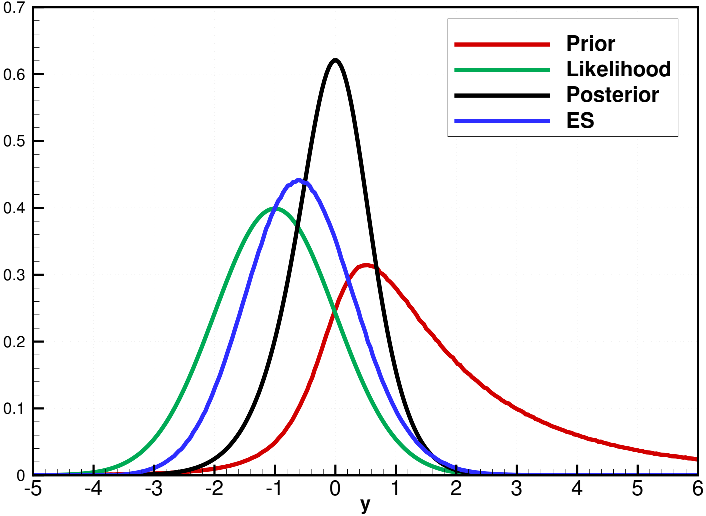
ES: Example with Lorenz equations



ES vs Bayes' (Gaussian prior)

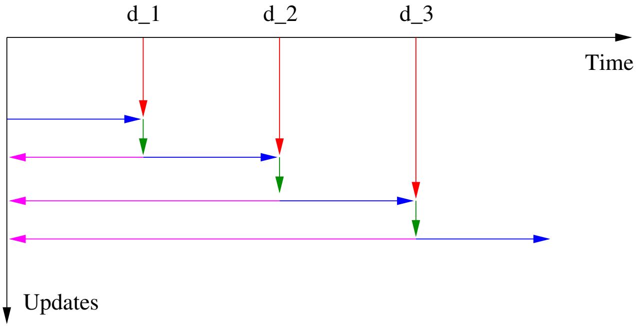


ES vs Bayes' (non-Gaussian prior)

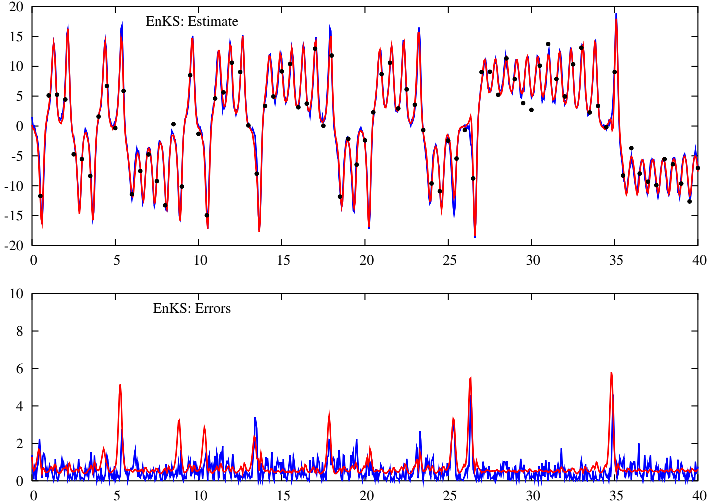


EnKS: The ensemble Kalman smoother

- Smoother solution with sequential processing of data



EnKS solution

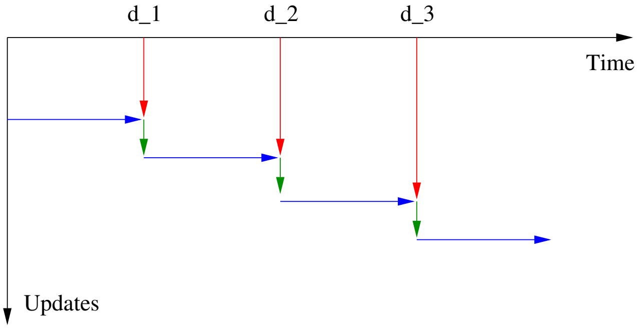


EnKS summary

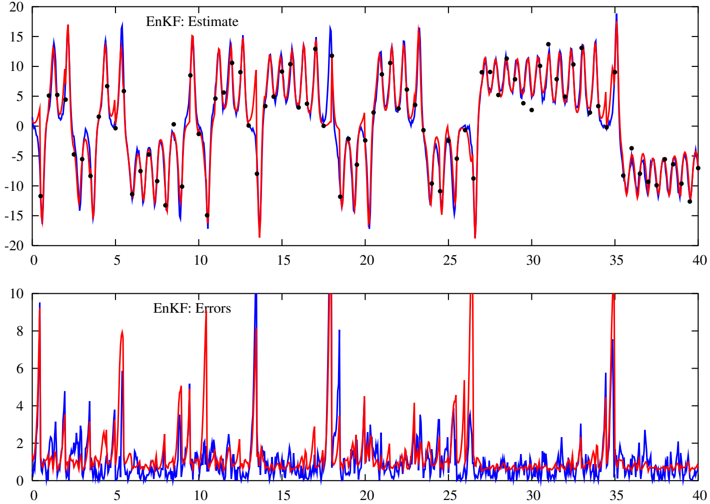
- ES and EnKS give identical results for linear models.
- EnKS is superior to the ES with nonlinear models.
  - Sequential processing of measurements introduces "Gaussianity".
  - Ensemble is kept close to the true state.

EnKF: Ensemble Kalman Filter

- Filtering solution



EnKF solution



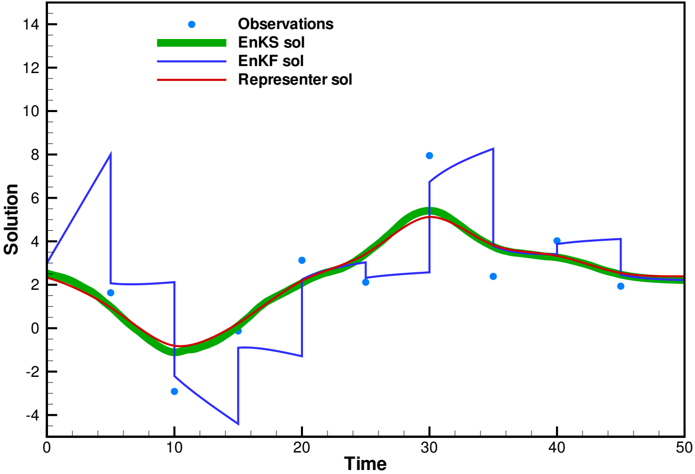
State and parameter estimation

- Scalar model for x with parameter α.

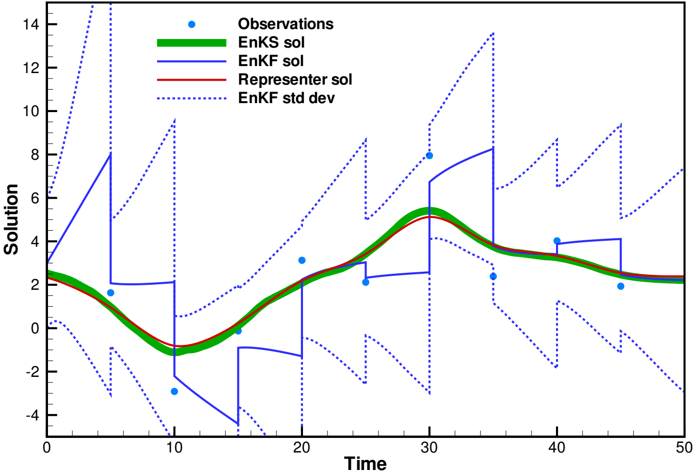
$$
\begin{aligned}
\frac{\partial x}{\partial t} &= 1 - \alpha + q, \\
x(t=0) &= 3 + a, \\
\alpha &= 0 + \alpha', \\
\mathcal{M}(x) &= \boldsymbol{d} + \boldsymbol{\epsilon}.
\end{aligned}
$$

- True parameter value is $\alpha = 1$.
- Truly linear model.
- Solved using EnKF, EnKS and Representer methods.
- Exponential time correlation for model errors.

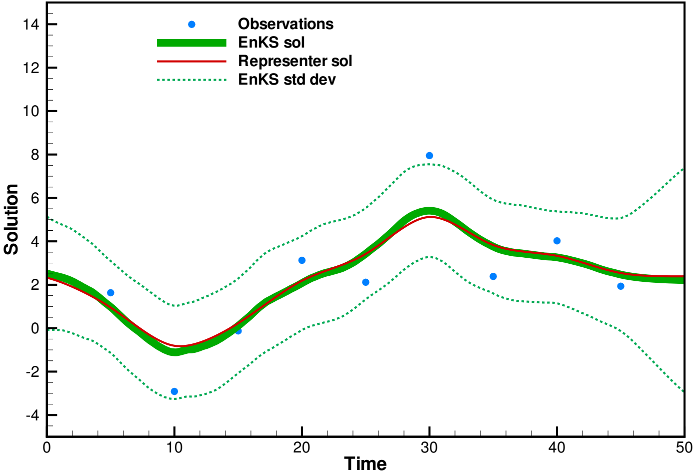
State and parameter estimation



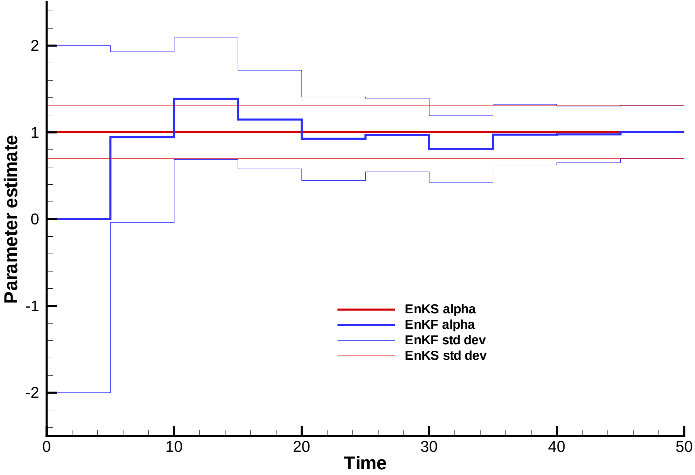
State and parameter estimation



State and parameter estimation



Estimate of parameter



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