The parameter estimation problem revisited

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based on
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Outline

- Parameter and state estimation problem.
- Bayesian formulation.
- Variational inverse problem.
- Ensemble methods.
- Examples.

Model equations

$$
\begin{aligned}
\frac{\partial \boldsymbol{\psi}}{\partial t} &= \boldsymbol{g}(\boldsymbol{\psi}, \boldsymbol{\alpha}), \\
\boldsymbol{\psi}|_{t_0} &= \boldsymbol{\Psi}_0, \\
\boldsymbol{\psi}|_{\partial \mathcal{D}} &= \boldsymbol{\psi}_b, \\
\boldsymbol{\alpha} &= \boldsymbol{\alpha}_0.
\end{aligned}
$$

$\Longrightarrow$ Well-posed problem with unique deterministic solution.

- $\boldsymbol{\psi}(\boldsymbol{x}, t)$ is model state vector.
- $\boldsymbol{\alpha}(\boldsymbol{x})$ is vector of model parameters.

Model equations and measurements

$$
\begin{aligned}
\frac{\partial \boldsymbol{\psi}}{\partial t} &= \boldsymbol{g}(\boldsymbol{\psi}, \boldsymbol{\alpha}), \\
\boldsymbol{\psi}|_{t_0} &= \boldsymbol{\Psi}_0, \\
\boldsymbol{\psi}|_{\partial \mathcal{D}} &= \boldsymbol{\psi}_b, \\
\boldsymbol{\alpha} &= \boldsymbol{\alpha}_0. \\
\boldsymbol{d} &= \mathcal{M}(\boldsymbol{\psi}, \boldsymbol{\alpha}).
\end{aligned}
$$

$\Longrightarrow$ Over-determined problem with no solution.

Example of direct measurement of $\psi(t)$:

$$\psi(t_i) = \mathcal{M}_i(\psi) = \int \psi(t)\delta(t - t_i)dt.$$

Allow for errors

Assume stochastic errors $\boldsymbol{q}(\boldsymbol{x},t)$, $\boldsymbol{a}(\boldsymbol{x})$, $\boldsymbol{b}(\boldsymbol{s},t)$, $\boldsymbol{\alpha}(\boldsymbol{x})$, and $\boldsymbol{\epsilon}$:

$$\begin{aligned}
\frac{\partial \boldsymbol{\psi}}{\partial t} &= \boldsymbol{g}(\boldsymbol{\psi},\boldsymbol{\alpha}) + \boldsymbol{q}, \\
\boldsymbol{\psi}|_{t_0} &= \boldsymbol{\Psi}_0 + \boldsymbol{a}, \\
\boldsymbol{\psi}|_{\partial\mathcal{D}} &= \boldsymbol{\psi}_b + \boldsymbol{b}, \\
\boldsymbol{\alpha} &= \boldsymbol{\alpha}_0 + \boldsymbol{\alpha}', \\
\boldsymbol{d} &= \mathcal{M}(\boldsymbol{\psi}^{\mathrm{t}},\boldsymbol{\alpha}^{\mathrm{t}}) + \boldsymbol{\epsilon}.
\end{aligned}$$

$\Longrightarrow$ Infinitively many solutions.

- Must specify statistics for error terms!
- Least squares problem.
- Find estimate for $\boldsymbol{\psi}$ and $\boldsymbol{\alpha}$ which “minimizes” errors.

State estimation

"Find an estimate of the state given a dynamical model and measurements."

- Standard data assimilation problem.
- Parameters fixed.
- Minimize errors in model and measurements.
- Solved by e.g. adjoint, representer or Kalman filter methods.

Parameter estimation

"Find an estimate of a set of parameters, resulting in a model solution which is close to the measurements."

- Standard parameter estimation problem.
- Minimization of a cost function.
- Solved using e.g. gradient methods.
- Solution is a single model realization.
- Model assumed perfect given the parameters.

A more general problem

"Find the pdf of the parameters and the model solution conditional on a set of measurements."

- Combined parameter and state estimation problem.
- Bayesian formulation.
- Optimal solution is the conditional pdf.
  - Different estimators for parameter and state.
  - Provides uncertainty estimates.

Part I

Bayesian formulation

Bayesian formulation

- Bayes theorem

$$f(\boldsymbol{\psi}, \boldsymbol{\alpha}|\boldsymbol{d}) \propto f(\boldsymbol{\psi}, \boldsymbol{\alpha}) f(\boldsymbol{d}|\boldsymbol{\psi}, \boldsymbol{\alpha}).$$

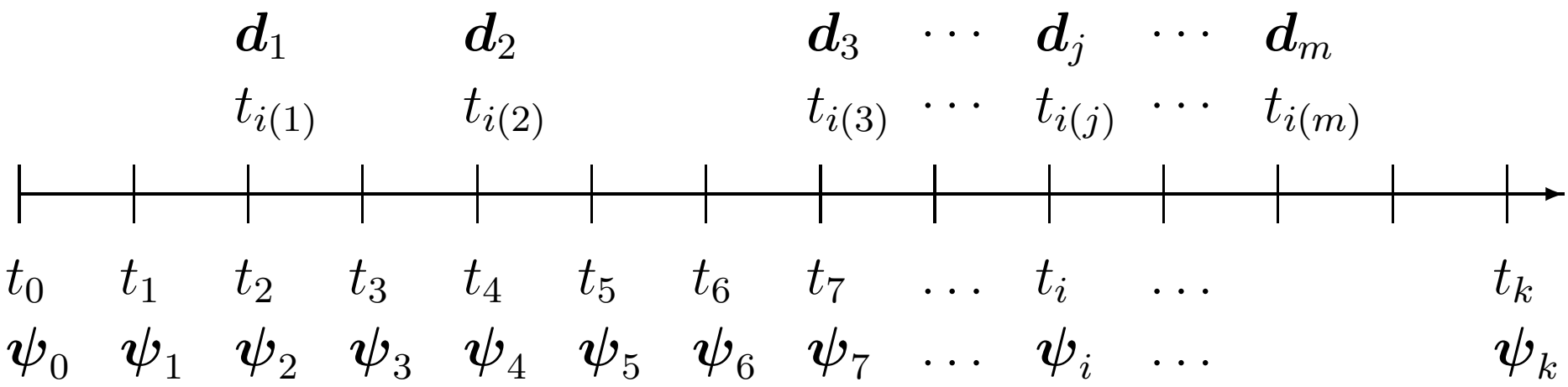
- The pdf for the model prediction is

$$f(\boldsymbol{\psi}, \boldsymbol{\alpha}, \boldsymbol{\psi}_0, \boldsymbol{\psi}_b) = f(\boldsymbol{\psi}|\boldsymbol{\alpha}, \boldsymbol{\psi}_0, \boldsymbol{\psi}_b) f(\boldsymbol{\psi}_0) f(\boldsymbol{\psi}_b) f(\boldsymbol{\alpha}).$$

- Bayes theorem then becomes

$$\boxed{f(\boldsymbol{\psi}, \boldsymbol{\alpha}, \boldsymbol{\psi}_0, \boldsymbol{\psi}_b|\boldsymbol{d}) \propto f(\boldsymbol{\psi}|\boldsymbol{\alpha}, \boldsymbol{\psi}_0, \boldsymbol{\psi}_b) f(\boldsymbol{\psi}_0) f(\boldsymbol{\psi}_b) f(\boldsymbol{\alpha}) f(\boldsymbol{d}|\boldsymbol{\psi}, \boldsymbol{\alpha}).}$$

Discretisation in time



- Time nodes t_i for $i = 0, \ldots, k$.
- Define $\boldsymbol{\psi}_i = \boldsymbol{\psi}(t_i)$.
- Then $\boldsymbol{\psi}$ is represented by $(\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_k)$
- Measurements $\boldsymbol{d}_j$ available at times, $t_{i(j)}$, $j = 1, \ldots, m$.

Assume

- Model is first order Markov process.

$$f(\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_k, \boldsymbol{\alpha}, \boldsymbol{\psi}_0, \boldsymbol{\psi}_b) \propto$$

$$f(\boldsymbol{\alpha}) f(\boldsymbol{\psi}_b) f(\boldsymbol{\psi}_0) \prod_{i=1}^{k} f(\boldsymbol{\psi}_i | \boldsymbol{\psi}_{i-1}, \boldsymbol{\alpha}, \boldsymbol{\psi}_b).$$

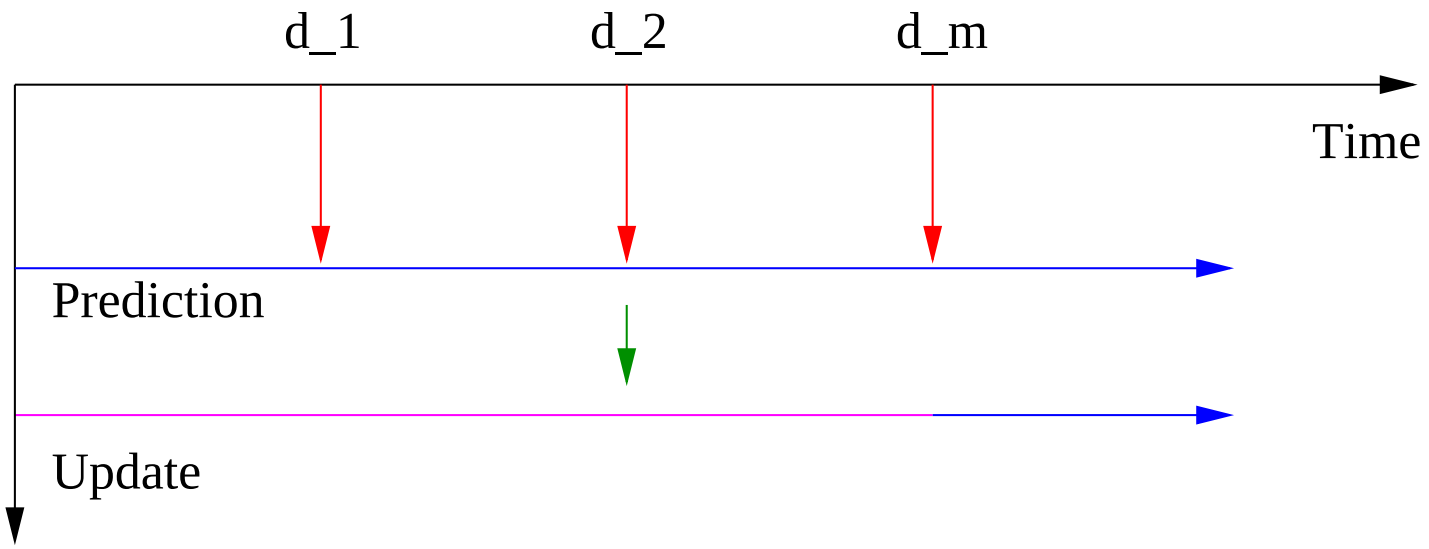
- Measurement errors are independent in time

$$f(\boldsymbol{d} | \boldsymbol{\psi}, \boldsymbol{\alpha}) = \prod_{j=1}^{m} f(\boldsymbol{d}_j | \boldsymbol{\psi}_{i(j)}, \boldsymbol{\alpha}).$$

Bayes for discrete state

- Bayes theorem then becomes

$$f(\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_k, \boldsymbol{\alpha}, \boldsymbol{\psi}_0, \boldsymbol{\psi}_b | \boldsymbol{d}) \propto f(\boldsymbol{\alpha}) f(\boldsymbol{\psi}_0) f(\boldsymbol{\psi}_b) \prod_{i=1}^{k} f(\boldsymbol{\psi}_i | \boldsymbol{\psi}_{i-1}, \boldsymbol{\alpha}) \prod_{j=1}^{m} f(\boldsymbol{d}_j | \boldsymbol{\psi}_{i(j)}, \boldsymbol{\alpha}),$$



Rewrite as:

$$f(\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_k, \boldsymbol{\alpha}, \boldsymbol{\psi}_0, \boldsymbol{\psi}_b | \boldsymbol{d}) \propto f(\boldsymbol{\alpha}) f(\boldsymbol{\psi}_0) f(\boldsymbol{\psi}_b)$$

$$\prod_{i=1}^{i(1)} f(\boldsymbol{\psi}_i | \boldsymbol{\psi}_{i-1}, \boldsymbol{\alpha}) f(\boldsymbol{d}_1 | \boldsymbol{\psi}_{i(1)}, \boldsymbol{\alpha})$$

$$\prod_{i=i(1)+1}^{i(2)} f(\boldsymbol{\psi}_i | \boldsymbol{\psi}_{i-1}, \boldsymbol{\alpha}) f(\boldsymbol{d}_2 | \boldsymbol{\psi}_{i(2)}, \boldsymbol{\alpha}) \cdots$$

$$\prod_{i=i(m-1)+1}^{i(m)} f(\boldsymbol{\psi}_i | \boldsymbol{\psi}_{i-1}, \boldsymbol{\alpha}) f(\boldsymbol{d}_m | \boldsymbol{\psi}_{i(m)}, \boldsymbol{\alpha})$$

$$\prod_{i=i(m)+1}^{k} f(\boldsymbol{\psi}_i | \boldsymbol{\psi}_{i-1}, \boldsymbol{\alpha})$$

Sequential processing of measurements

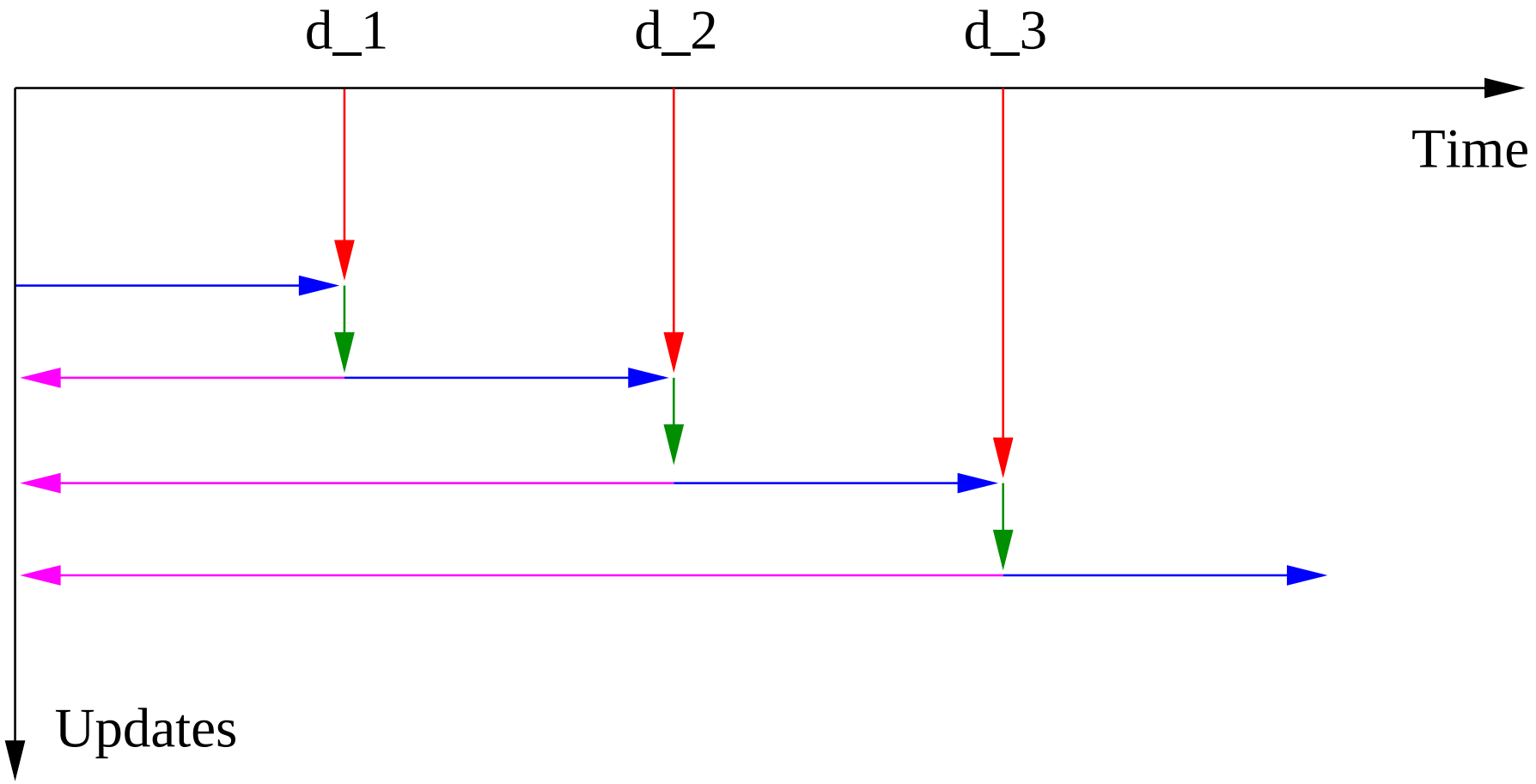
- First update

$$f(\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_{i(1)}, \boldsymbol{\alpha}, \boldsymbol{\psi}_0, \boldsymbol{\psi}_b | \boldsymbol{d}_1) \propto f(\boldsymbol{\alpha}) f(\boldsymbol{\psi}_0) f(\boldsymbol{\psi}_b) \prod_{i=1}^{i(1)} f(\boldsymbol{\psi}_i | \boldsymbol{\psi}_{i-1}, \boldsymbol{\alpha}) f(\boldsymbol{d}_1 | \boldsymbol{\psi}_{i(1)}, \boldsymbol{\alpha})$$

- Second update

$$f(\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_{i(2)}, \boldsymbol{\alpha}, \boldsymbol{\psi}_0, \boldsymbol{\psi}_b | \boldsymbol{d}_1, \boldsymbol{d}_2) \propto f(\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_{i(1)}, \boldsymbol{\alpha}, \boldsymbol{\psi}_0, \boldsymbol{\psi}_b | \boldsymbol{d}_1) \prod_{i=i(1)+1}^{i(2)} f(\boldsymbol{\psi}_i | \boldsymbol{\psi}_{i-1}, \boldsymbol{\alpha}) f(\boldsymbol{d}_2 | \boldsymbol{\psi}_{i(2)}, \boldsymbol{\alpha})$$

Sequential processing of measurements



Summary

- Independent measurements can be processed sequentially in time.
- Sequence of inverse problems.
- Solution of one sub-problem is prior for next.
- No approximations.

Part II

The generalized inverse

Generalized inverse formulation

$$f(\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_k, \boldsymbol{\alpha}, \boldsymbol{\psi}_0, \boldsymbol{\psi}_b | \boldsymbol{d}) \propto f(\boldsymbol{\alpha}) f(\boldsymbol{\psi}_0) f(\boldsymbol{\psi}_b)$$

$$\prod_{i=1}^{k} f(\boldsymbol{\psi}_i | \boldsymbol{\psi}_{i-1}, \boldsymbol{\alpha}) \prod_{j=1}^{m} f(\boldsymbol{d}_j | \boldsymbol{\psi}_{i(j)}, \boldsymbol{\alpha}),$$

Gaussian priors.

$\Downarrow$

Least squares variational inverse problem.

Gaussian priors

Prior for parameters:

- Prior estimate: $\boldsymbol{\alpha}_0(\boldsymbol{x})$.
- Error covariance: $\boldsymbol{C}_{\alpha\alpha}(\boldsymbol{x}_1, \boldsymbol{x}_2)$ with inverse $\boldsymbol{W}_{\alpha\alpha}(\boldsymbol{x}_1, \boldsymbol{x}_2)$

$$\int_{\mathcal{D}} \boldsymbol{C}_{\alpha\alpha}(\boldsymbol{x}_1, \boldsymbol{x}_3)\boldsymbol{W}_{\alpha\alpha}(\boldsymbol{x}_3, \boldsymbol{x}_2)d\boldsymbol{x}_3 = \boldsymbol{\delta}(\boldsymbol{x}_1 - \boldsymbol{x}_2).$$

- Prior pdf for $\boldsymbol{\alpha}$:

$$f(\boldsymbol{\alpha}) \propto \exp\left\{-\frac{1}{2}\iint_{\mathcal{D}} (\boldsymbol{\alpha}(\boldsymbol{x}_1) - \boldsymbol{\alpha}_0(\boldsymbol{x}_1))^{\mathrm{T}} \boldsymbol{W}_{\alpha\alpha}(\boldsymbol{x}_1, \boldsymbol{x}_2)(\cdots)d\boldsymbol{x}_1 d\boldsymbol{x}_2\right\}.$$

Conditional joint density

$$f(\boldsymbol{\psi}, \boldsymbol{\alpha}, \boldsymbol{\psi}_0, \boldsymbol{\psi}_b | \boldsymbol{d}) \propto \exp\left\{-\frac{1}{2}\mathcal{J}[\boldsymbol{\psi}, \boldsymbol{\alpha}]\right\},$$

$$\begin{aligned}
\mathcal{J}[\boldsymbol{\psi}, \boldsymbol{\alpha}] = & \left(\frac{\partial \boldsymbol{\psi}}{\partial t} - \boldsymbol{g}(\boldsymbol{\psi}, \boldsymbol{\alpha})\right)^{\mathrm{T}} \bullet \boldsymbol{W}_{qq} \bullet \left(\frac{\partial \boldsymbol{\psi}}{\partial t} - \boldsymbol{g}(\boldsymbol{\psi}, \boldsymbol{\alpha})\right) \\
& + (\boldsymbol{\psi}_0 - \boldsymbol{\Psi}_0)^{\mathrm{T}} \circ \boldsymbol{W}_{aa} \circ (\boldsymbol{\psi}_0 - \boldsymbol{\Psi}_0) \\
& + (\boldsymbol{\psi} - \boldsymbol{\psi}_b)^{\mathrm{T}} \star \boldsymbol{W}_{bb} \star (\boldsymbol{\psi} - \boldsymbol{\psi}_b) \\
& + (\boldsymbol{\alpha} - \boldsymbol{\alpha}_0)^{\mathrm{T}} \circ \boldsymbol{W}_{\alpha\alpha} \circ (\boldsymbol{\alpha} - \boldsymbol{\alpha}_0) \\
& + (\boldsymbol{d} - \mathcal{M}[\boldsymbol{\psi}])^{\mathrm{T}} \boldsymbol{W}_{\epsilon\epsilon} (\boldsymbol{d} - \mathcal{M}[\boldsymbol{\psi}]).
\end{aligned}$$

- Minimum of $\mathcal{J}$ is the MLH solution for $\boldsymbol{\psi}(\boldsymbol{x}, t)$ and $\boldsymbol{\alpha}(\boldsymbol{x})$.

Example with scalar model

Least squares penalty function

$$\begin{aligned}\mathcal{J}[\psi,\alpha] = &\left(\frac{\partial\psi}{\partial t} - g(\psi,\alpha)\right) \bullet W_{qq} \bullet \left(\frac{\partial\psi}{\partial t} - g(\psi,\alpha)\right)\\ &+ (\psi(t_0) - \Psi_0) W_{aa} (\psi(t_0) - \Psi_0)\\ &+ (\alpha - \alpha_0) W_{\alpha\alpha} (\alpha - \alpha_0)\\ &+ (\boldsymbol{d} - \mathcal{M}[\psi])^{\mathrm{T}} \boldsymbol{W}_{\epsilon\epsilon} (\boldsymbol{d} - \mathcal{M}[\psi])\end{aligned}$$

with

$$\bullet \equiv \int_{t_0}^{t_k} dt.$$

Euler-Lagrange equations

$$\frac{\partial \psi}{\partial t} = g(\psi, \alpha) + C_{qq} \bullet \lambda$$

$$\psi(t_0) = \Psi_0 + C_{aa}\lambda(t_0)$$

$$\frac{\partial \lambda}{\partial t} = -\left.\frac{\partial g}{\partial \psi}\right|_{\substack{\psi \\ \alpha}} \lambda - \mathcal{M}^{\mathrm{T}}[\delta]\boldsymbol{W}_{\epsilon\epsilon}(\boldsymbol{d} - \mathcal{M}[\psi])$$

$$\lambda(t_k) = 0$$

$$\alpha = \alpha_0 + C_{\alpha\alpha} \int_{t_0}^{t_k} \left.\frac{\partial g}{\partial \alpha}\right|_{\substack{\psi \\ \alpha}} \lambda \, dt$$

Euler-Lagrange equations

State estimation for each iterate α_{l+1}

$$\frac{\partial \psi}{\partial t} = g(\psi, \alpha) + C_{qq} \bullet \lambda$$

$$\psi(t_0) = \Psi_0 + C_{aa}\lambda(t_0)$$

$$\frac{\partial \lambda}{\partial t} = -\left.\frac{\partial g}{\partial \psi}\right|_{\substack{\psi \\ \alpha}} \lambda - \mathcal{M}^{\mathrm{T}}[\delta]\boldsymbol{W}_{\epsilon\epsilon}(\boldsymbol{d} - \mathcal{M}[\psi])$$

$$\lambda(t_k) = 0$$

Parameter estimation using iteration in α

$$\alpha_{l+1} = \alpha_l - \gamma \left(\alpha_l - \alpha_0 - C_{\alpha\alpha} \int_{t_0}^{t_k} \left.\frac{\partial g}{\partial \alpha}\right|_{\substack{\psi_l \\ \alpha_l}} \lambda_l \, dt \right)$$

Parameter estimation

State estimation with $C_{qq} = 0$ and $C_{aa} = 0$

$$\frac{\partial \psi}{\partial t} = g(\psi, \alpha)$$
$$\psi(t_0) = \Psi_0$$
$$\frac{\partial \lambda}{\partial t} = -\left.\frac{\partial g}{\partial \psi}\right|_{\substack{\psi \\ \alpha}} \lambda - \mathcal{M}^{\mathrm{T}}[\delta] \boldsymbol{W}_{\epsilon\epsilon}(\boldsymbol{d} - \mathcal{M}[\psi])$$
$$\lambda(t_k) = 0$$

$$\alpha_{l+1} = \alpha_l - \gamma \left(\alpha_l - \alpha_0 - C_{\alpha\alpha} \int_{t_0}^{t_k} \left.\frac{\partial g}{\partial \alpha}\right|_{\substack{\psi_l \\ \alpha_l}} \lambda_l \, dt \right)$$

- $\Rightarrow$ Adjoint method.

Reformulation

Define Lagrangian

$$\mathcal{L}[\psi, \alpha, \lambda, \mu] = \int_{t_0}^{t_k} \left(\frac{\partial \psi}{\partial t} - g(\psi, \alpha) \right) \lambda \, dt$$
$$+ (\psi(t_0) - \Psi_0)\mu$$
$$+ (\alpha - \alpha_0) W_{\alpha\alpha} (\alpha - \alpha_0)$$
$$+ (\boldsymbol{d} - \mathcal{M}[\psi])^{\mathrm{T}} \boldsymbol{W}_{\epsilon\epsilon} (\boldsymbol{d} - \mathcal{M}[\psi])$$

Variation with respect to:

- λ returns model.
- μ returns initial condition.
- α returns E-L equations for parameter estimation problem.

Summary

- The generalized inverse:
  - Combined parameter and state estimation.
  - MLH solution consistent with Gaussian priors.
- State estimation:
  - Solves only for model state (representer method).
- Parameter estimation:
  - Solves only for parameters (adjoint method).
- Issues:
  - Highly nonlinear problem!
  - Results in a single model realization!
  - Hard to compute uncertainty estimates!
  - Does not allow for sequential processing of measurements!

Part III

Ensemble methods

ES: Ensemble Smoother

EnKS: Ensemble Kalman Smoother

EnKF: Ensemble Kalman Filter

- Ensemble representation for pdfs.
- Ensemble predition for time evolution of pdfs.
- Assume Gaussian pdf for model prediction and use “variance minimizing” analysis schemes.

The error covariance matrix

Define ensemble covariances around the ensemble mean

$$\boldsymbol{C}_{\psi\psi} = \overline{\left(\boldsymbol{\psi} - \overline{\boldsymbol{\psi}}\right)\left(\boldsymbol{\psi} - \overline{\boldsymbol{\psi}}\right)^{\mathrm{T}}}$$

- The ensemble mean, $\overline{\boldsymbol{\psi}}$, is the best-guess.
- The error variance is defined by the ensemble spread.
- The smoothness of members defines the covariance.

$\Downarrow$

Representation by a finite ensemble of model states.

Ensemble representation

- Define ensemble matrix

$$\boldsymbol{A}(\boldsymbol{x}, t_i) = \begin{pmatrix} \boldsymbol{\psi}^1(\boldsymbol{x}, t_i) & \boldsymbol{\psi}^2(\boldsymbol{x}, t_i) & \dots & \boldsymbol{\psi}^N(\boldsymbol{x}, t_i) \\ \boldsymbol{\alpha}^1(\boldsymbol{x}, t_i) & \boldsymbol{\alpha}^2(\boldsymbol{x}, t_i) & \dots & \boldsymbol{\alpha}^N(\boldsymbol{x}, t_i) \end{pmatrix}.$$

- Parameters augmented to model state.
- The ensemble covariance becomes

$$\boldsymbol{C}^{\mathrm{e}}_{\psi\psi}(\boldsymbol{x}_1, \boldsymbol{x}_2, t_i) = \frac{\boldsymbol{A}'(\boldsymbol{x}_1, t_i)\boldsymbol{A}'^{\mathrm{T}}_i(\boldsymbol{x}_2, t_i)}{N-1}.$$

Dynamical evolution of error statistics

- Members evolve according to stochastic model dynamics

$$d\boldsymbol{\psi} = \boldsymbol{g}(\boldsymbol{\psi}, \boldsymbol{\alpha})dt + \boldsymbol{h}(\boldsymbol{\psi})dq$$
$$d\boldsymbol{\alpha} = 0.$$

- The pdf evolves according to Kolmogorov's equation

$$\frac{\partial f}{\partial t} + \sum_i \frac{\partial (g_i f)}{\partial \psi_i} = \frac{1}{2} \sum_{i,j} \frac{\partial^2 f \left(\boldsymbol{h}\boldsymbol{Q}\boldsymbol{h}^T\right)_{ij}}{\partial \psi_i \partial \psi_j}.$$

- Fundamental equation for evolution of error statistics.
- May be solved using Monte Carlo methods.

Variance minimizing analysis

Given

- First guess, $\boldsymbol{\psi}^{\mathrm{f}}$, and prediction error covariance, $\boldsymbol{C}^{\mathrm{f}}_{\psi\psi}$.
- Measurements, $\boldsymbol{d}$, and error covariance, $\boldsymbol{C}_{\epsilon\epsilon}$.

The variance minimizing analysis is minimum of

$$\mathcal{J}[\boldsymbol{\psi}^{\mathrm{a}}] = \left(\boldsymbol{\psi}^{\mathrm{a}} - \boldsymbol{\psi}^{\mathrm{f}}\right)^{\mathrm{T}} \bullet \boldsymbol{C}^{-1}_{\psi\psi} \bullet \left(\boldsymbol{\psi}^{\mathrm{a}} - \boldsymbol{\psi}^{\mathrm{f}}\right) + \left(\boldsymbol{d} - \mathcal{M}[\boldsymbol{\psi}^{\mathrm{a}}]\right)^{\mathrm{T}} \boldsymbol{C}^{-1}_{\epsilon\epsilon} \left(\boldsymbol{d} - \mathcal{M}[\boldsymbol{\psi}^{\mathrm{a}}]\right).$$

Analysis equations

Update of estimate

$$\boldsymbol{\psi}^{\mathrm{a}} = \boldsymbol{\psi}^{\mathrm{f}} + \mathcal{M}^{\mathrm{T}} \left[\boldsymbol{C}^{\mathrm{f}}_{\psi\psi} \right] \left(\mathcal{M}^{\mathrm{T}} \left[\mathcal{M} \left[\boldsymbol{C}^{\mathrm{f}}_{\psi\psi} \right] \right] + \boldsymbol{C}_{\epsilon\epsilon} \right)^{-1} \left(\boldsymbol{d} - \mathcal{M} \left[\boldsymbol{\psi}^{\mathrm{f}} \right] \right)$$

Error covariance for update

$$\boldsymbol{C}^{\mathrm{a}}_{\psi\psi} = \boldsymbol{C}^{\mathrm{f}}_{\psi\psi} - \mathcal{M}^{\mathrm{T}} \left[\boldsymbol{C}^{\mathrm{f}}_{\psi\psi} \right] \left(\mathcal{M}^{\mathrm{T}} \left[\mathcal{M} \left[\boldsymbol{C}^{\mathrm{f}}_{\psi\psi} \right] \right] + \boldsymbol{C}_{\epsilon\epsilon} \right)^{-1} \mathcal{M} \left[\boldsymbol{C}^{\mathrm{f}}_{\psi\psi} \right]$$

Ensemble analysis equations

- Define randomized measurements $\boldsymbol{D} = \boldsymbol{d} + \boldsymbol{E}$.
- Variance minimizing ensemble update becomes

$$
\begin{aligned}
\boldsymbol{A}^{\mathrm{a}} &= \boldsymbol{A} + \mathcal{M}^{\mathrm{T}}\left[\boldsymbol{C}^{\mathrm{e}}_{\psi\psi}\right] \\
&\quad \left(\mathcal{M}^{\mathrm{T}}\left[\mathcal{M}\left[\boldsymbol{C}^{\mathrm{e}}_{\psi\psi}\right]\right] + \boldsymbol{C}_{\epsilon\epsilon}\right)^{-1}\left(\boldsymbol{D} - \mathcal{M}\left[\boldsymbol{A}\right]\right) \\
&= \boldsymbol{A} + \boldsymbol{A}'\mathcal{M}^{\mathrm{T}}\left[\boldsymbol{A}'\right] \\
&\quad \left(\mathcal{M}\left[\boldsymbol{A}'\right]\mathcal{M}^{\mathrm{T}}\left[\boldsymbol{A}'\right] + \boldsymbol{E}\boldsymbol{E}^{\mathrm{T}}\right)^{-1}\left(\boldsymbol{D} - \mathcal{M}\left[\boldsymbol{A}\right]\right) \\
&\vdots \\
&= \boldsymbol{A}\boldsymbol{X}
\end{aligned}
$$

$\Rightarrow$ Updated ensemble with correct mean and covariance!

ES: The Ensemble Smoother

- Joint pdf for model prediction

$$f(\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_k, \boldsymbol{\alpha}, \boldsymbol{\psi}_0, \boldsymbol{\psi}_b) = f(\boldsymbol{\alpha}) f(\boldsymbol{\psi}_0) f(\boldsymbol{\psi}_b) \prod_{i=1}^{k} f(\boldsymbol{\psi}_i | \boldsymbol{\psi}_{i-1}, \boldsymbol{\alpha}).$$

- Ensemble representation for the prior pdfs.
- Ensemble integration gives the joint pdf.

Problem: how to compute the Bayesian update

$$f(\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_k, \boldsymbol{\alpha}, \boldsymbol{\psi}_0, \boldsymbol{\psi}_b | \boldsymbol{d}) =$$

$$f(\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_k, \boldsymbol{\alpha}, \boldsymbol{\psi}_0, \boldsymbol{\psi}_b) \prod_{j=1}^{m} f(\boldsymbol{d}_j | \boldsymbol{\psi}_{i(j)}, \boldsymbol{\alpha}),$$

ES: Ensemble representation

- Define ensemble matrix for joint state from t_0 to t_k as

$$\widetilde{\boldsymbol{A}}_k = \begin{pmatrix} \boldsymbol{A}(\boldsymbol{x}, t_0) \\ \vdots \\ \boldsymbol{A}(\boldsymbol{x}, t_k) \end{pmatrix}$$

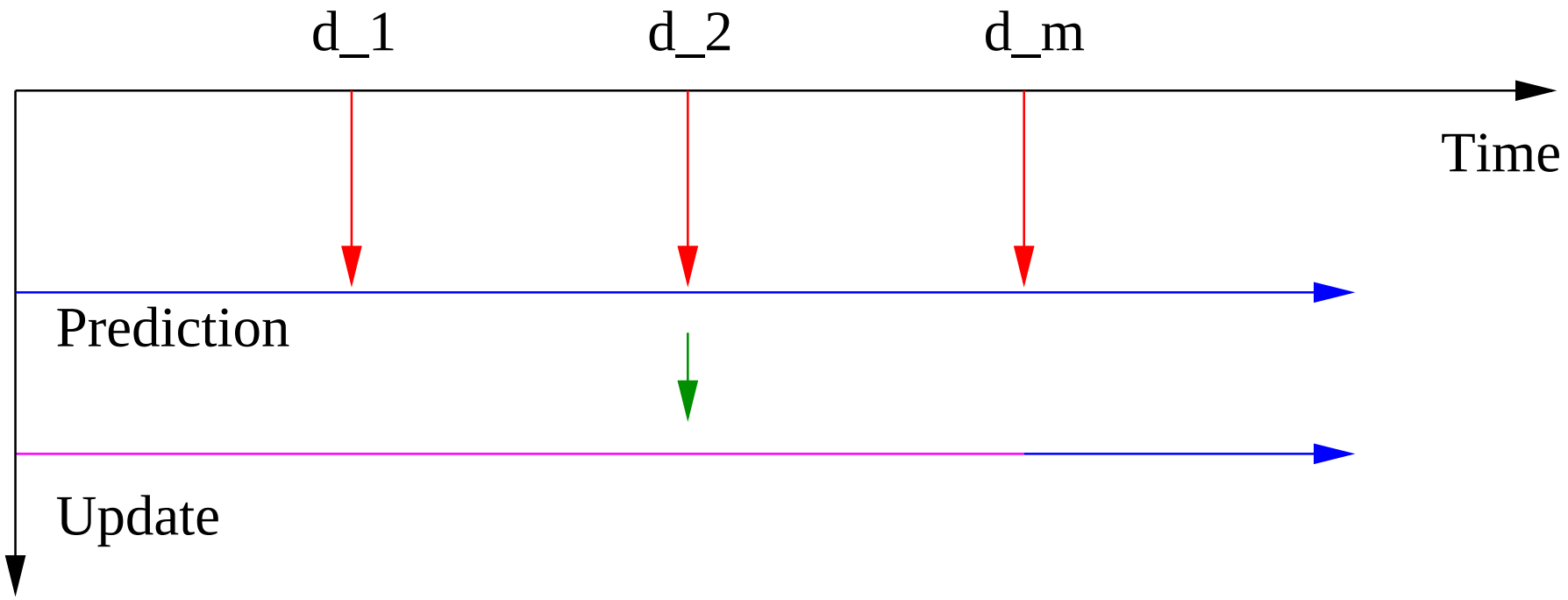
which defines the space–time ensemble covariance

$$\widetilde{\boldsymbol{C}}^{\mathrm{e}}_{\psi\psi}(\boldsymbol{x}_1, t_1, \boldsymbol{x}_2, t_2) = \frac{\widetilde{\boldsymbol{A}}'_k(\boldsymbol{x}_1, t_1)\widetilde{\boldsymbol{A}}'^{\mathrm{T}}_k(\boldsymbol{x}_2, t_2)}{N-1}$$

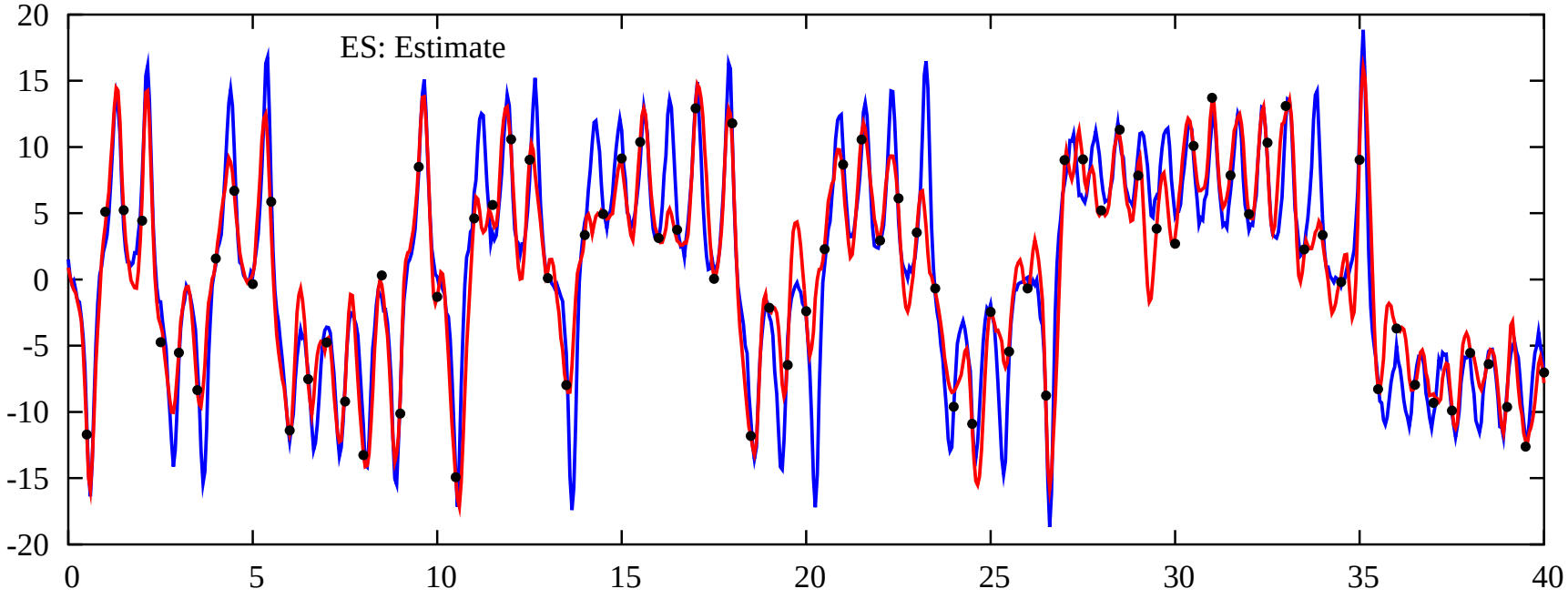
ES: Analysis scheme

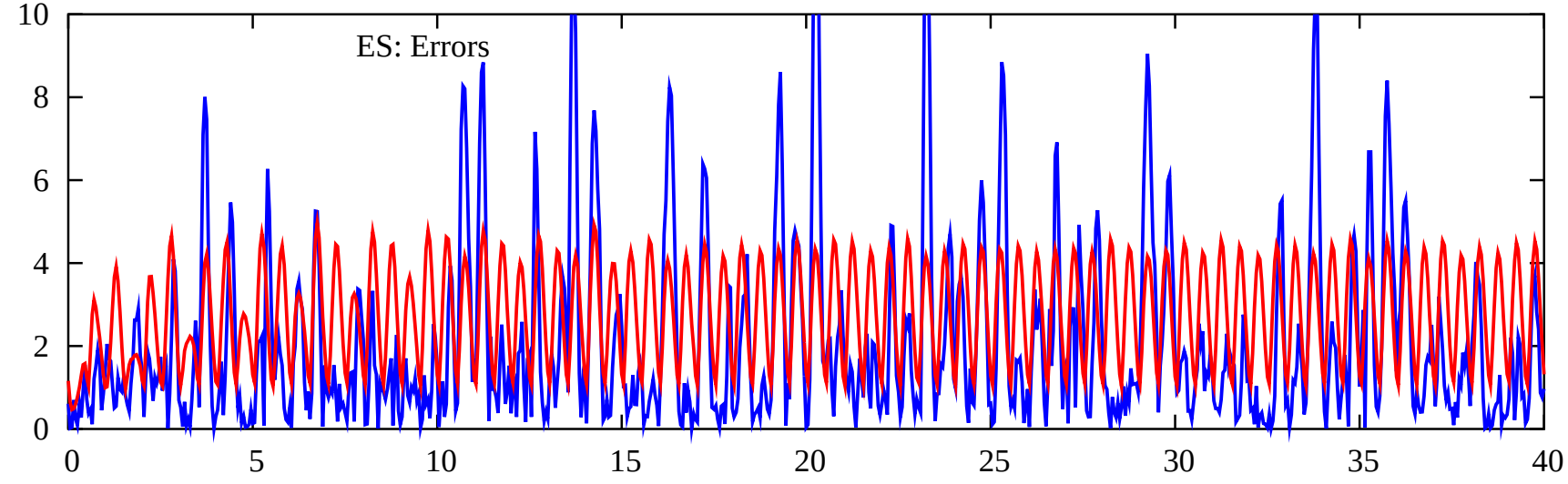
$$
\begin{aligned}
\widetilde{\boldsymbol{A}}_k^{\mathrm{a}} &= \widetilde{\boldsymbol{A}}_k + \mathcal{M}^{\mathrm{T}} \left[\widetilde{\boldsymbol{C}}_{\psi\psi}^{\mathrm{e}} \right] \\
&\quad \left(\mathcal{M}^{\mathrm{T}} \left[\mathcal{M} \left[\widetilde{\boldsymbol{C}}_{\psi\psi}^{\mathrm{e}} \right] \right] + \boldsymbol{C}_{\epsilon\epsilon} \right)^{-1} \left(\boldsymbol{D} - \mathcal{M} \left[\widetilde{\boldsymbol{A}}_k \right] \right) \\
&= \widetilde{\boldsymbol{A}}_k + \widetilde{\boldsymbol{A}}_k' \mathcal{M}^{\mathrm{T}} \left[\widetilde{\boldsymbol{A}}_k' \right] \\
&\quad \left(\mathcal{M} \left[\widetilde{\boldsymbol{A}}_k' \right] \mathcal{M}^{\mathrm{T}} \left[\widetilde{\boldsymbol{A}}_k' \right] + \boldsymbol{E}\boldsymbol{E}^{\mathrm{T}} \right)^{-1} \left(\boldsymbol{D} - \mathcal{M} \left[\widetilde{\boldsymbol{A}}_k \right] \right) \\
&\vdots \\
&= \widetilde{\boldsymbol{A}}_k \boldsymbol{X}
\end{aligned}
$$

ES solution procedure



ES: Example with Lorenz equations





ES: summary

Gauss–Markov interpolation in space and time.

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

EnKS: The ensemble Kalman smoother

- Starts from Bayes with sequential processing of data

E.g. first update:

$$f(\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_{i(1)}, \boldsymbol{\alpha}, \boldsymbol{\psi}_0, \boldsymbol{\psi}_b | \boldsymbol{d}_1) \propto$$

$$f(\boldsymbol{\alpha}) f(\boldsymbol{\psi}_0) f(\boldsymbol{\psi}_b) \prod_{i=1}^{i(1)} f(\boldsymbol{\psi}_i | \boldsymbol{\psi}_{i-1}, \boldsymbol{\alpha}) f(\boldsymbol{d}_1 | \boldsymbol{\psi}_{i(1)}, \boldsymbol{\alpha}),$$

Use ensemble representations

$$\widetilde{\boldsymbol{A}}_{i(1)} = \begin{pmatrix} \boldsymbol{A}(\boldsymbol{x}, t_0) \\ \vdots \\ \boldsymbol{A}(\boldsymbol{x}, t_{i(1)}) \end{pmatrix} \quad \text{and} \quad \boldsymbol{D}_1.$$

EnKS: Analysis equation

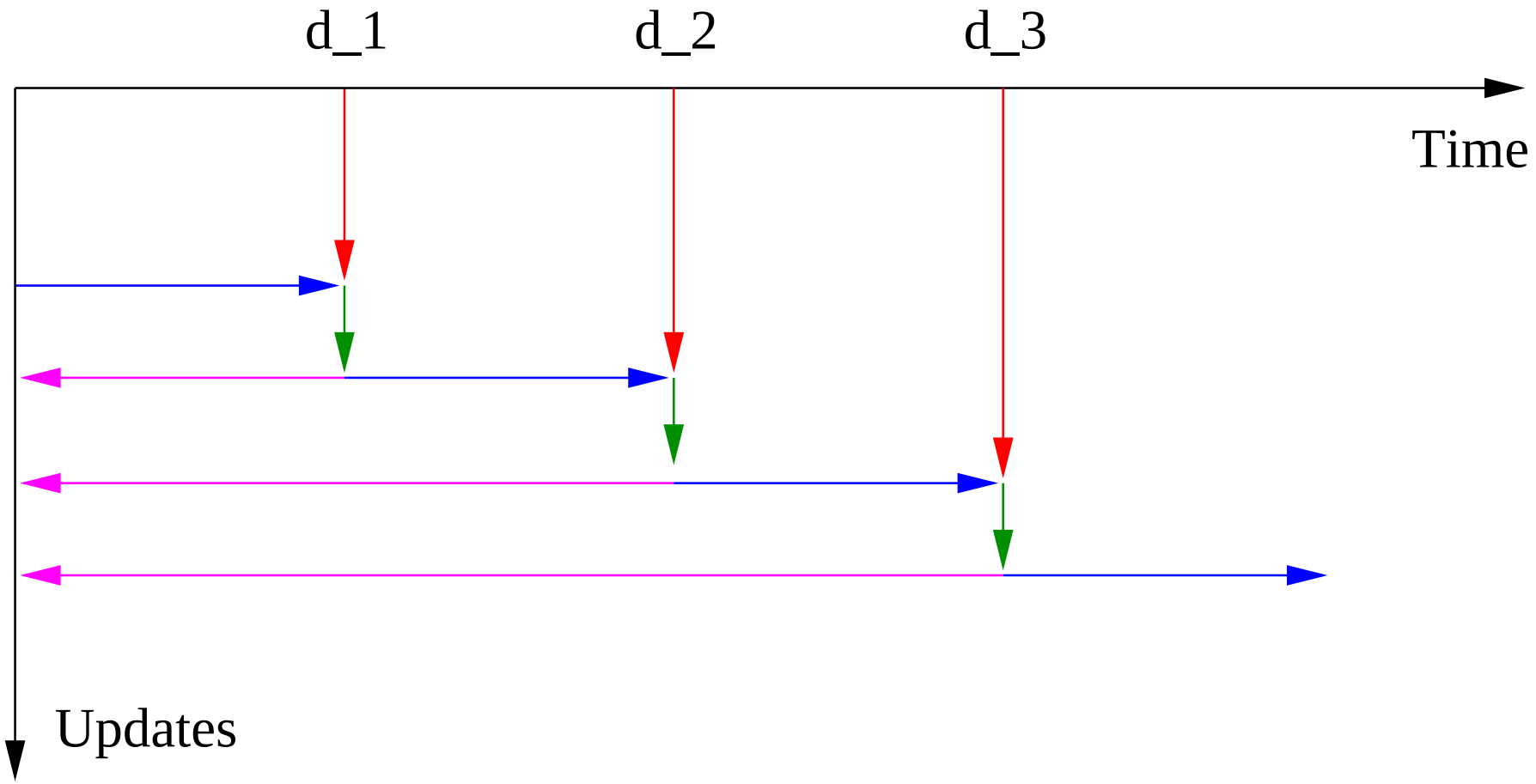
- The EnKS analysis equation for the first update is

$$\widetilde{\boldsymbol{A}}^{\mathrm{a}}_{i(1)} = \widetilde{\boldsymbol{A}}_{i(1)} + \widetilde{\boldsymbol{A}}'_{i(1)} \mathcal{M}_1^{\mathrm{T}} \left[\boldsymbol{A}'_{i(1)} \right]$$

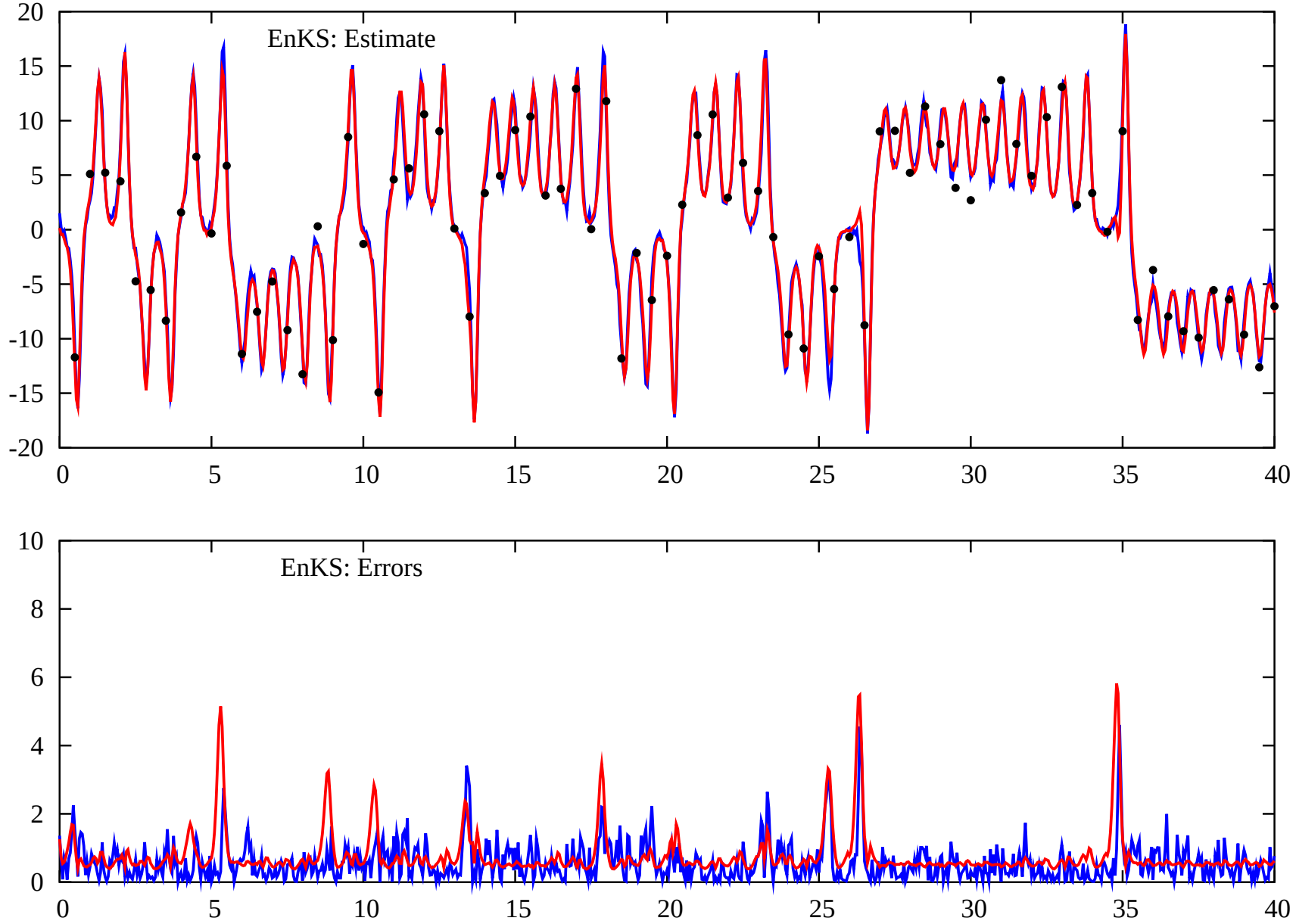
$$\left(\mathcal{M}_1 \left[\boldsymbol{A}'_{i(1)} \right] \mathcal{M}_1^{\mathrm{T}} \left[\boldsymbol{A}'_{i(1)} \right] + \boldsymbol{E}_1 \boldsymbol{E}_1^{\mathrm{T}} \right)^{-1} \left(\boldsymbol{D}_1 - \mathcal{M}_1 \left[\boldsymbol{A}_{i(1)} \right] \right)$$

$$= \widetilde{\boldsymbol{A}}_{i(1)} \boldsymbol{X}_1$$

EnKS solution procedure



EnKS solution



EnKS summary

- ES and EnKS gives 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.
- Accuracy of analysis is determined by:
  - the accuracy of $\boldsymbol{X}_j$,
  - the properties of the ensemble error space.

EnKF: Ensemble Kalman Filter

- Special case of EnKS.
- Only update state at data times

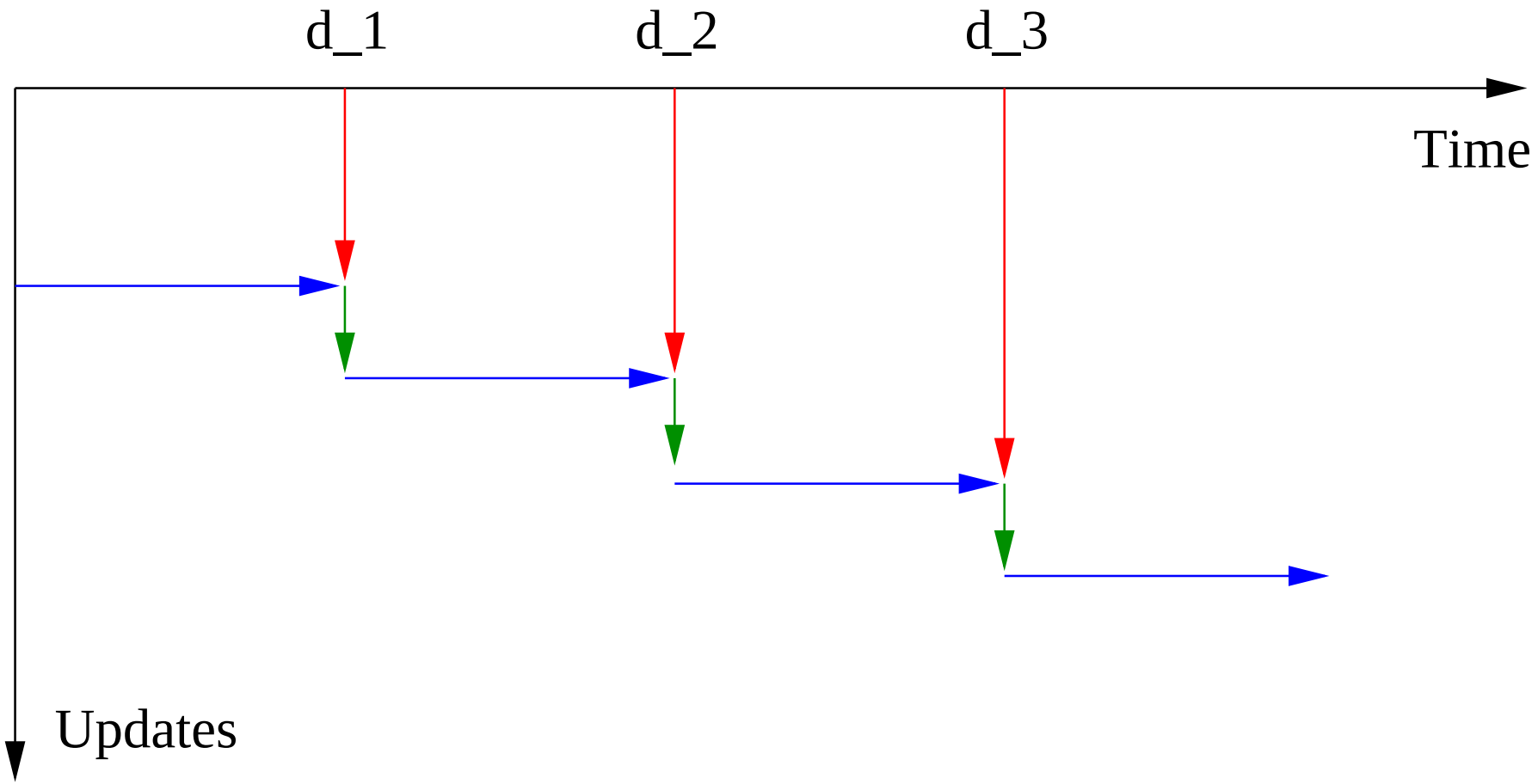
$$\boldsymbol{A}^{\mathrm{a}}_{i(1)} = \boldsymbol{A}_{i(1)} + \boldsymbol{A}'_{i(1)} \mathcal{M}_1^{\mathrm{T}} \left[\boldsymbol{A}'_{i(1)} \right]$$

$$\left(\mathcal{M}_1 \left[\boldsymbol{A}'_{i(1)} \right] \mathcal{M}_1^{\mathrm{T}} \left[\boldsymbol{A}'_{i(1)} \right] + \boldsymbol{E}_1 \boldsymbol{E}_1^{\mathrm{T}} \right)^{-1} \left(\boldsymbol{D}_1 - \mathcal{M}_1 \left[\boldsymbol{A}_{i(1)} \right] \right)$$

$$= \boldsymbol{A}_{i(1)} \boldsymbol{X}_1$$

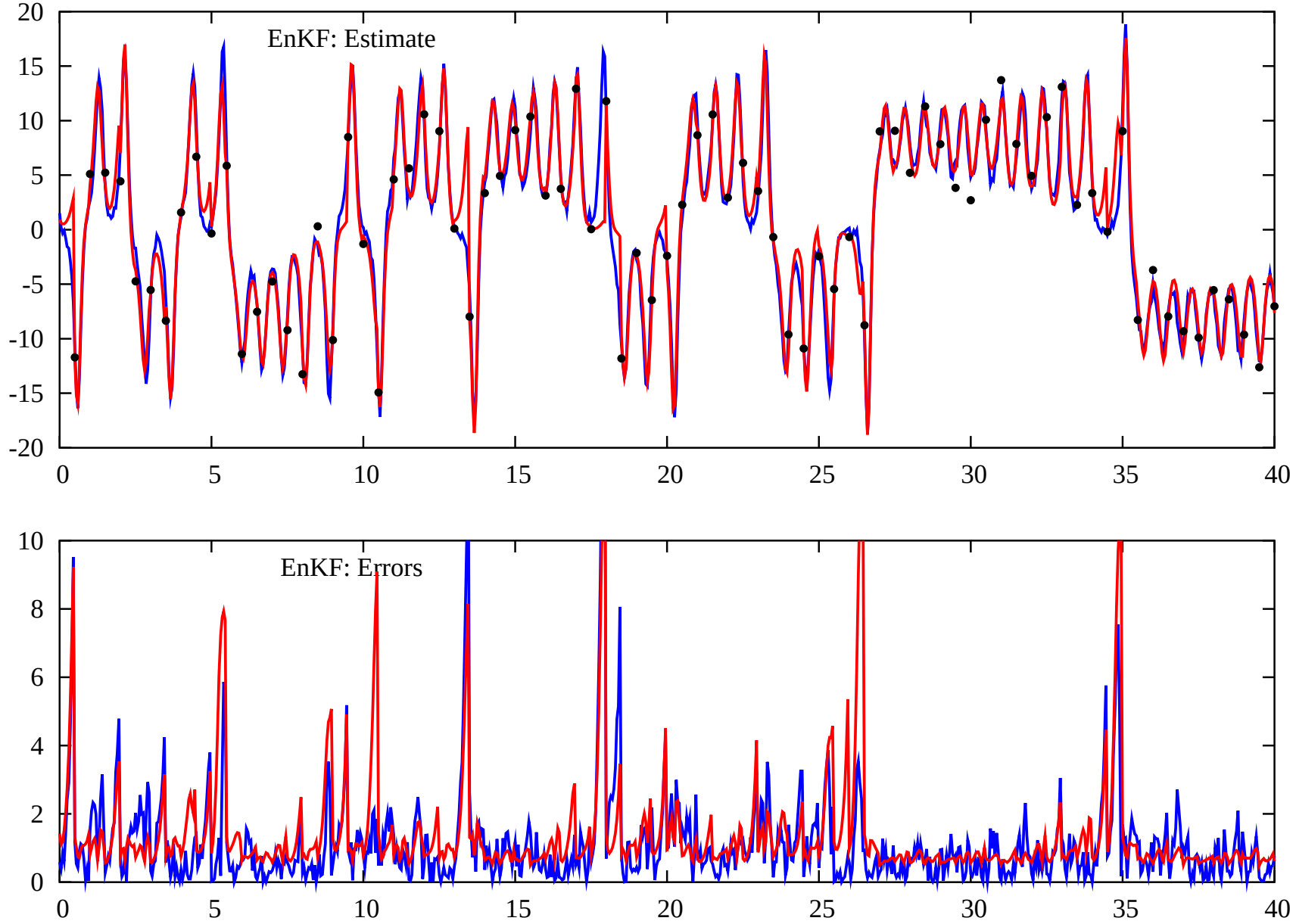
- EnKF forms a prior for the EnKS.

EnKF solution procedure



$$\boldsymbol{A}_{\mathrm{EnKS}}(\boldsymbol{x}, t_l) = \boldsymbol{A}_{\mathrm{EnKF}}(\boldsymbol{x}, t_l) \prod_{j'=j}^{m} \boldsymbol{X}_{j'}.$$

EnKF solution



EnKF summary

- A prediction from EnKF and EnKS will be identical.
- EnKF suitable for forecasting purposes.
- The EnKS solution can be computed using the EnKF solution as a prior.

Part IV

A simple example

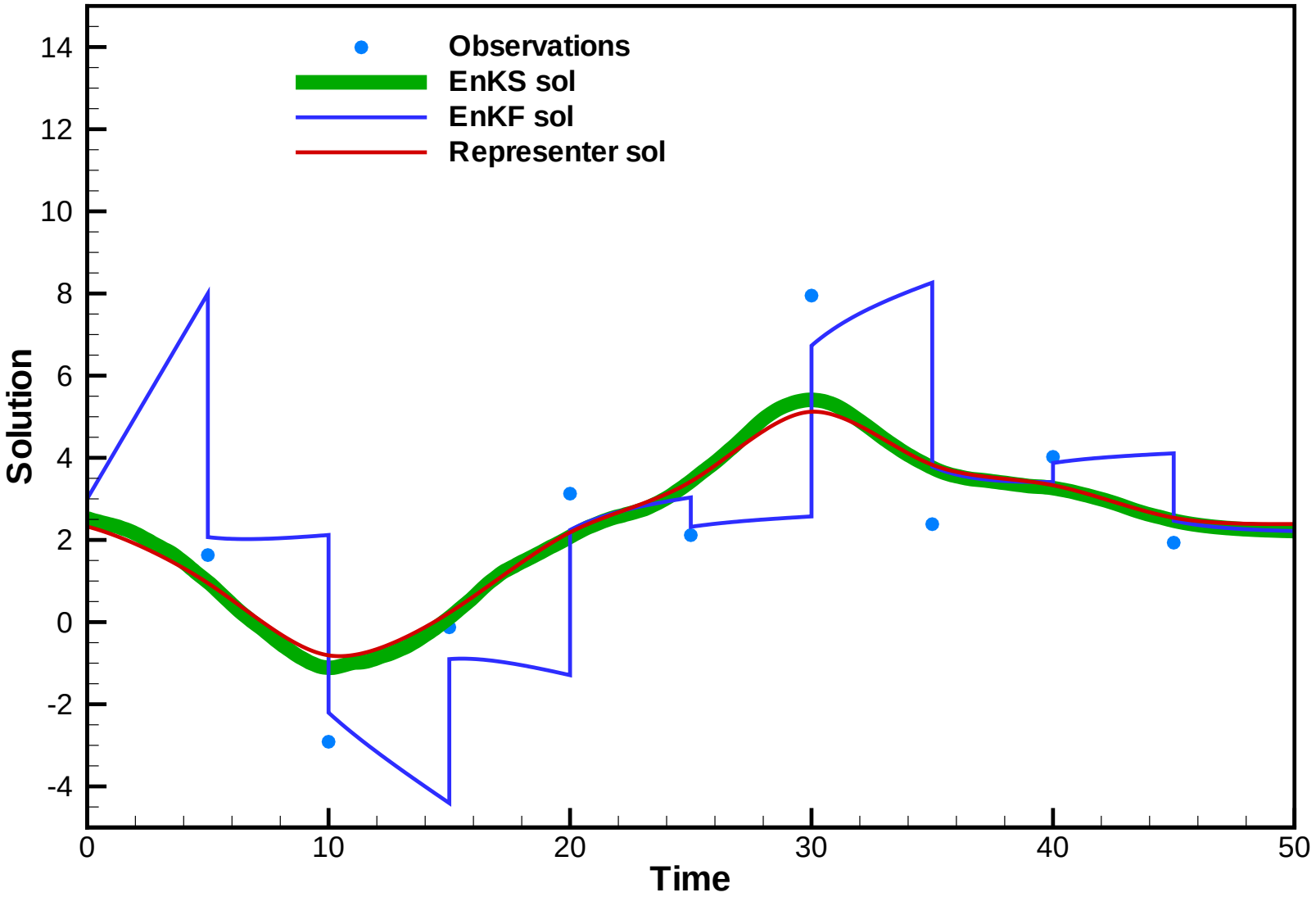
Example

- Scalar model

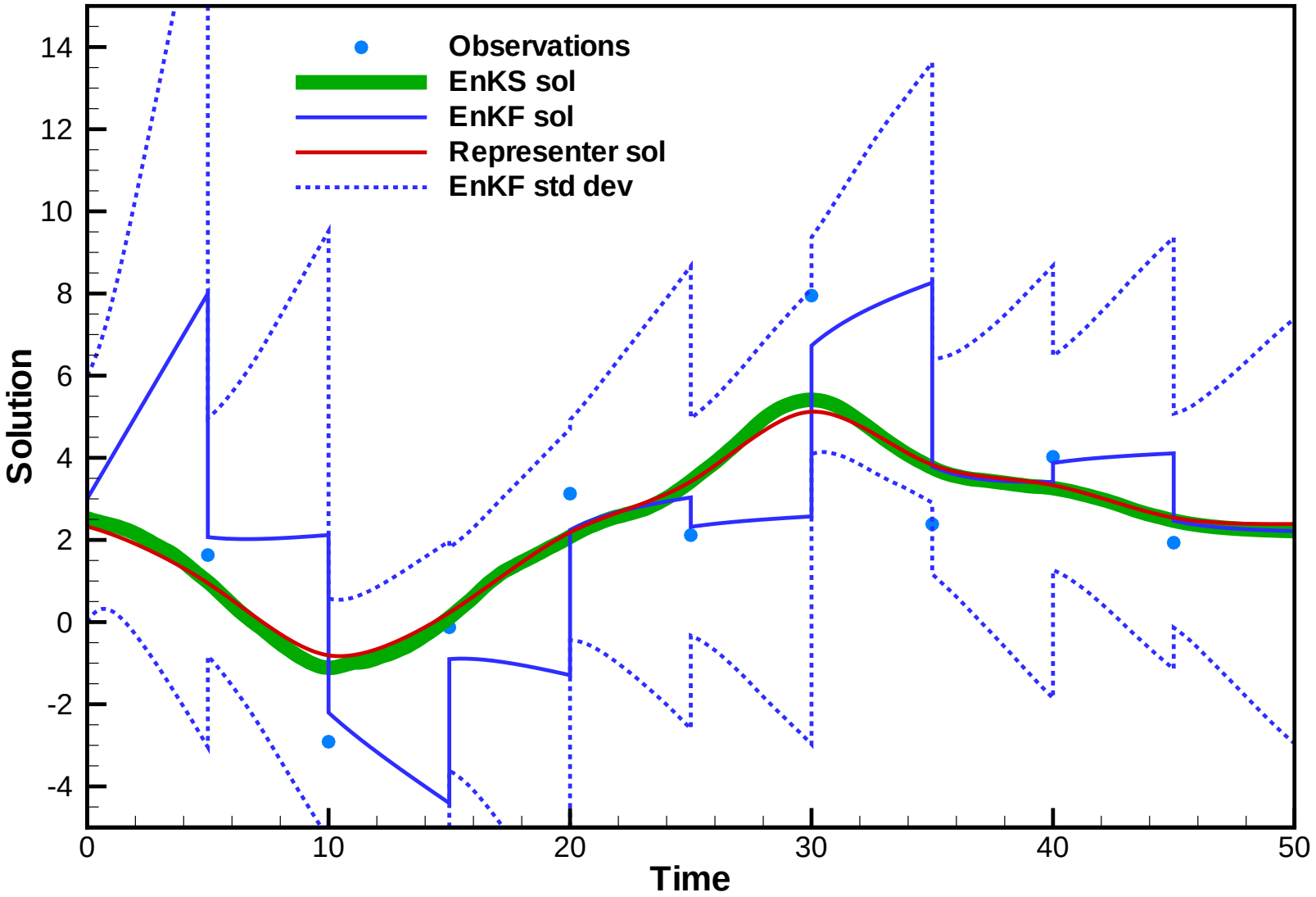
$$\frac{\partial \psi}{\partial t} = 1 - \alpha + q,$$
$$\psi(t=0) = 3 + a,$$
$$\alpha = 0 + \alpha',$$
$$\boldsymbol{d} = \mathcal{M}(\psi^t) + \boldsymbol{\epsilon}.$$

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

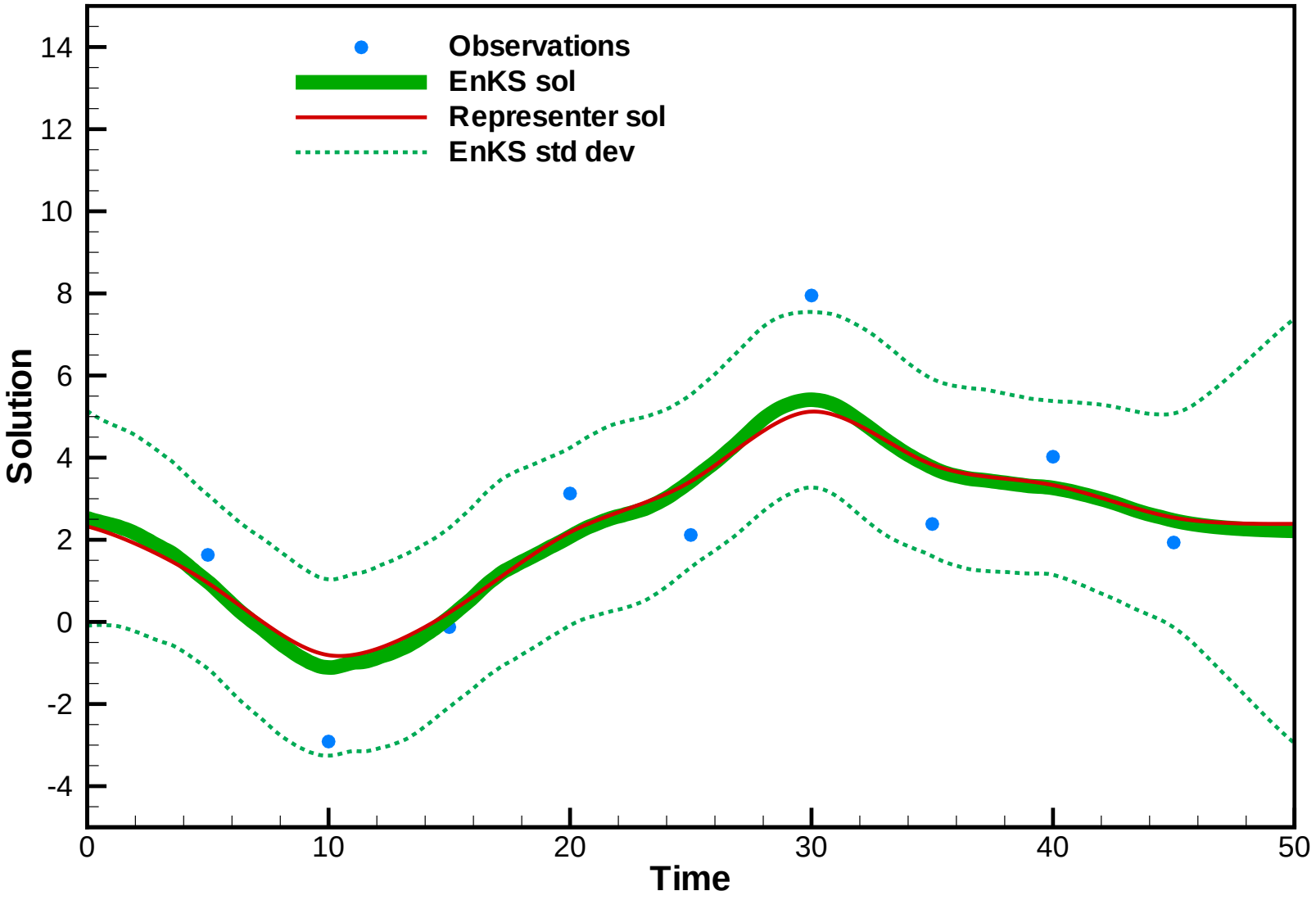
State and parameter estimation



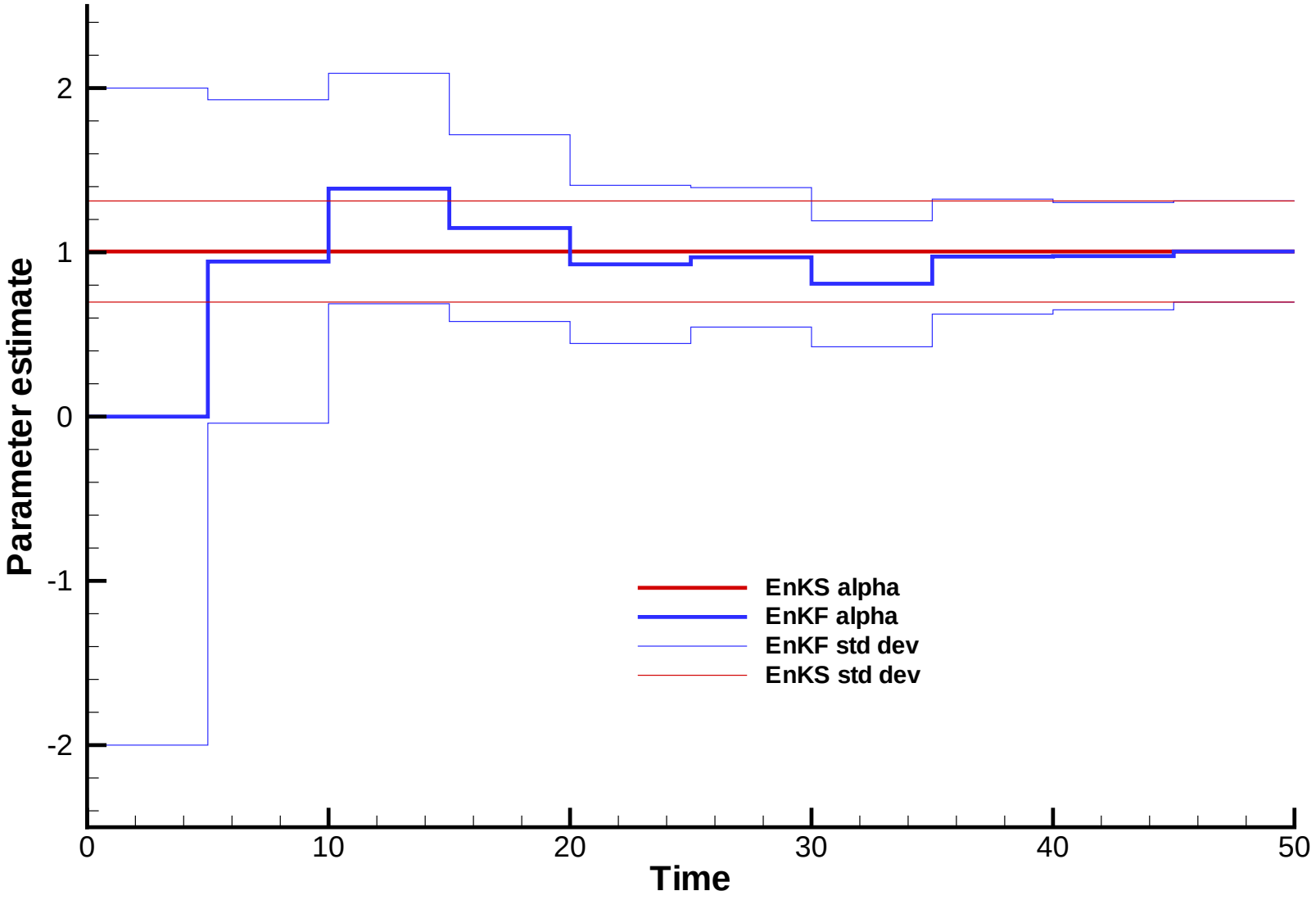
State and parameter estimation



State and parameter estimation



Estimate of parameter



Summary

www.nersc.no/∼geir/EnKF

- Joint state and parameter estimation problem!
- Bayesian formulation:
  - Variational methods (multiple minima; MLH).
    - Hard to compute error statistics!
    - Do not allow for sequential processing of measurements!
  - Ensemble methods (Gaussianity assumption; mean).
    - Provide estimate with error statistics.
    - Allow for sequential processing of measuremets.
      - Introduces Gaussianity!
      - Advantage with nonlinear dynamics.
- There is more to parameter estimation than just estimating the parameters!