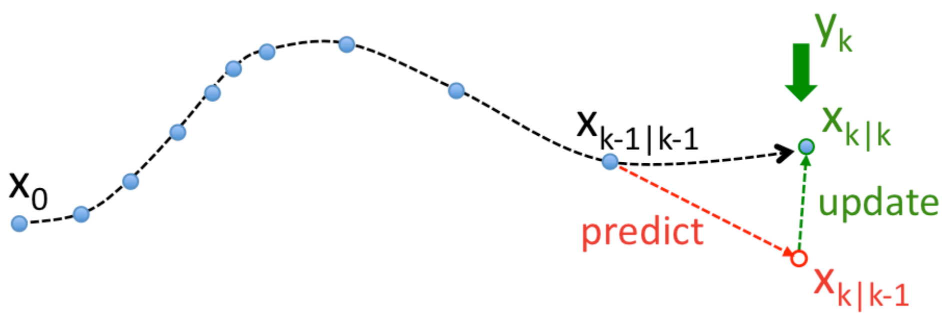
How do we solve it and what does the solution look like?

KF/PFs offer solutions to dynamical systems, nonlinear in general, using prediction and update as data becomes available. Tracking in time or space offers an ideal framework for studying KF/PF.



The Model

Consider the discrete, linear system,

$$\mathbf{x}_{k+1} = \mathbf{M}_k \mathbf{x}_k + \mathbf{w}_k, \quad k = 0, 1, 2, \ldots, \tag{1}$$

where

- $\mathbf{x}_k \in \mathbb{R}^n$ is the state vector at time t_k
- $\mathbf{M}_k \in \mathbb{R}^{n \times n}$ is the state transition matrix (mapping from time t_k to t_{k+1}) or model
- $\{\mathbf{w}_k \in \mathbb{R}^n; k = 0, 1, 2, \ldots\}$ is a white, Gaussian sequence, with $\mathbf{w}_k \sim N(\mathbf{0}, \mathbf{Q}_k)$, often referred to as model error
- $\mathbf{Q}_k \in \mathbb{R}^{n \times n}$ is a symmetric positive definite covariance matrix (known as the model error covariance matrix).

Some of the following slides are from: Sarah Dance, University of Reading

The Observations

We also have discrete, linear observations that satisfy

$$\mathbf{y}_k = \mathbf{H}_k \mathbf{x}_k + \mathbf{v}_k, \quad k = 1, 2, 3, \ldots, \tag{2}$$

where

- $\mathbf{y}_k \in \mathbb{R}^p$ is the vector of actual measurements or observations at time t_k
- $\mathbf{H}_k \in \mathbb{R}^{n \times p}$ is the observation operator. Note that this is not in general a square matrix.
- $\{\mathbf{v}_k \in \mathbb{R}^p; k = 1, 2, \ldots\}$ is a white, Gaussian sequence, with $\mathbf{v}_k \sim N(\mathbf{0}, \mathbf{R}_k)$, often referred to as observation error.
- $\mathbf{R}_k \in \mathbb{R}^{p \times p}$ is a symmetric positive definite covariance matrix (known as the observation error covariance matrix).

We assume that the initial state, $\mathbf{x}_0$ and the noise vectors at each step, $\{\mathbf{w}_k\}$, $\{\mathbf{v}_k\}$, are assumed mutually independent.

Summary of the Kalman filter

Prediction step

Mean update: $\widehat{\mathbf{x}}_{k+1|k} = \mathbf{M}_k \widehat{\mathbf{x}}_{k|k}$

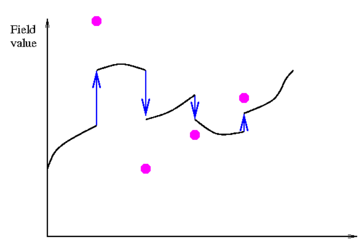
Covariance update: $\mathbf{P}_{k+1|k} = \mathbf{M}_k \mathbf{P}_{k|k} \mathbf{M}_k^T + \mathbf{Q}_k$.

Observation update step

Mean update: $\widehat{\mathbf{x}}_{k|k} = \widehat{\mathbf{x}}_{k|k-1} + \mathbf{K}_k(\mathbf{y}_k - \mathbf{H}_k \widehat{\mathbf{x}}_{k|k-1})$

Kalman gain: $\mathbf{K}_k = \mathbf{P}_{k|k-1} \mathbf{H}_k^T (\mathbf{H}_k \mathbf{P}_{k|k-1} \mathbf{H}^T + \mathbf{R}_k)^{-1}$

Covariance update: $\mathbf{P}_{k|k} = (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k) \mathbf{P}_{k|k-1}$.



CAGLARS HOMEWORK

Prediction step

We first derive the equation for one-step prediction of the mean using the state propagation model (1).

$$\begin{aligned}\widehat{\mathbf{x}}_{k+1|k} &= \mathbb{E}\left[\mathbf{x}_{k+1}|\mathbf{y}_1, \ldots \mathbf{y}_k\right], \\ &= \mathbb{E}\left[\mathbf{M}_k \overset{k+1|k}{}\mathbf{x}_k + \mathbf{w}_k\right], \\ &= \mathbf{M}_k \widehat{\mathbf{x}}_{k|k} \qquad (5)\end{aligned}$$

mesurement

$$\mathbf{x}_{k+1|k} = \mathbf{M}\mathbf{x}_{k|k} + \mathbf{B}\mathbf{w}$$

$$\widehat{\mathbf{x}}_{k+1|k} = E[\mathbf{x}_{k+1|k} \mid \mathbf{y}_1, \ldots, \mathbf{y}_k] = \mathbf{M}\hat{\mathbf{x}}_{k|k}$$

CAGLARS HOMEWORK

The one step prediction of the covariance is defined by,

$$\mathbf{P}_{k+1|k} = \mathbb{E}\left[(\mathbf{x}_{k+1} - \widehat{\mathbf{x}}_{k+1|k})(\mathbf{x}_{k+1} - \widehat{\mathbf{x}}_{k+1|k})^T|\mathbf{y}_1, \ldots \mathbf{y}_k\right]. \qquad (6)$$

Exercise: Using the state propagation model, (1), and one-step prediction of the mean, (5), show that

$$\mathbf{P}_{k+1|k} = \mathbf{M}_k \mathbf{P}_{k|k} \mathbf{M}_k^T + \mathbf{Q}_k. \qquad (7)$$

mesurement

$$\mathbf{x}_{k+1|k} = \mathbf{M}\mathbf{x}_{k|k} + \mathbf{B}\mathbf{w}$$

$$\mathbf{P}_{k+1|k} = E[(\mathbf{x}_{k+1|k} - \hat{\mathbf{x}}_{k+1|k})(\mathbf{x}_{k+1|k} - \hat{\mathbf{x}}_{k+1|k})^T \mid \mathbf{y}_1, \ldots, \mathbf{y}_k] = \mathbf{M}\mathbf{P}_{k|k}\mathbf{M}^T + \mathbf{B}\mathbf{Q}\mathbf{B}^T$$

Bayesian Framework

m : model parameter vector (unknown parameters to be estimated)
d : data vector relating to m via an equation h(.)
d = h(m) + noise

Classical parameter estimation framework: Unknown but deterministic m
Bayesian parameter estimation framework: Unknown and random variable m

Bayes' Formula

$$p(m,d) = p(m \mid d)p(d) = p(d \mid m)p(m)$$

POSTERIOR, LIKELIHOOD, PRIOR

$$\underbrace{p(\mathbf{m}|\mathbf{d})}_{\text{POSTERIOR}} = \frac{p(\mathbf{d}|\mathbf{m})p(\mathbf{m})}{p(\mathbf{d})} = \frac{\overbrace{p(\mathbf{d}|\mathbf{m})}^{\text{LIKELIHOOD}}\overbrace{p(\mathbf{m})}^{\text{PRIOR}}}{\underbrace{\int p(\mathbf{d}|\mathbf{m})p(\mathbf{m})d\mathbf{m}}_{\text{EVIDENCE}}}$$

EVIDENCE

Sequential updates

Bayes

$$p(\mathbf{m} \mid \mathbf{d}) \propto p(\mathbf{d} \mid \mathbf{m})p(\mathbf{m})$$

Consider **d** consisting of two independent data set

$$p(\mathbf{d}_1, \mathbf{d}_2) = p(\mathbf{d}_1)p(\mathbf{d}_2)$$

$$\begin{aligned} p(\mathbf{m} \mid \mathbf{d}) &= p(\mathbf{m} \mid \mathbf{d}_1, \mathbf{d}_2) \\ &= \frac{p(\mathbf{d}_2 \mid \mathbf{d}_1, \mathbf{m})p(\mathbf{m} \mid \mathbf{d}_1)}{p(\mathbf{d}_2 \mid \mathbf{d}_1)} \\ &= \frac{p(\mathbf{d}_2 \mid \mathbf{d}_1, \mathbf{m})}{p(\mathbf{d}_2)} \frac{p(\mathbf{d}_1 \mid \mathbf{m})p(\mathbf{m})}{p(\mathbf{d}_1)} \\ &\propto p(\mathbf{d}_2 \mid \mathbf{m})p(\mathbf{d}_1 \mid \mathbf{m})p(\mathbf{m}) \end{aligned}$$

Generalizing

$$p(\mathbf{m} \mid \mathbf{d}) \propto \prod_{i=1}^{N} p(\mathbf{d}_i \mid \mathbf{m})p(\mathbf{m})$$

Thus, in principle with no measurement equation,
you can update sequentially or just at once

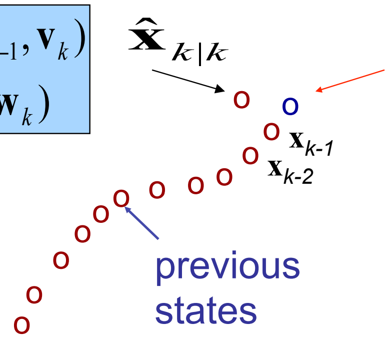
Inversion, Filtering and Smoothing

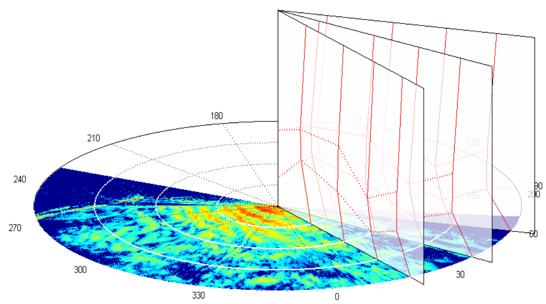
$p(\mathbf{x}_t \mid \mathbf{y}_t)$: Inversion, Only observations at time t

$p(\mathbf{x}_t \mid \mathbf{y}_{1:t})$: Filter, Observations from time $1:t$

$p(\mathbf{x}_t \mid \mathbf{y}_{1:T})$: Smoother, Observations from time $1:T$

$$\mathbf{x}_k = f_{k-1}(\mathbf{x}_{k-1}, \mathbf{v}_k)$$
$$\mathbf{y}_k = h_k(\mathbf{x}_k, \mathbf{w}_k)$$

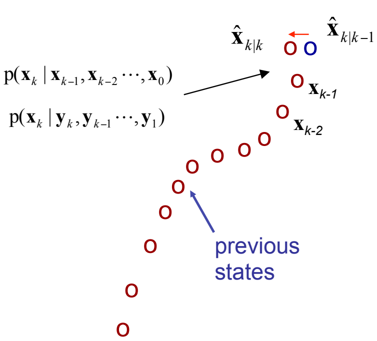




A Single Kalman Iteration

$$\mathbf{x}_k = \mathbf{F}_{k-1}\mathbf{x}_{k-1} + \mathbf{v}_k$$
$$\mathbf{y}_k = \mathbf{H}_k\mathbf{x}_k + \mathbf{w}_k$$

$$\mathbf{x}_{k|k} \sim \mathcal{N}(\hat{\mathbf{x}}_{k|k}, \mathbf{P}_{k|k})$$



PREDICT

1. Predict the mean $\hat{\mathbf{x}}_{k|k-1}$ using previous history.

   $\mathrm{p}(\mathbf{x}_k \mid \mathbf{x}_{k-1})$

   $$\hat{\mathbf{x}}_{k|k-1} = \mathrm{E}\{\mathbf{x}_k \mid \mathbf{x}_{k-1}\} = \int \mathbf{x}_k \, \mathrm{p}(\mathbf{x}_k \mid \mathbf{x}_{k-1}) d\mathbf{x}_k$$

2. Predict the covariance $\mathbf{P}_{k|k-1}$ using previous history.

UPDATE

3. Correct/update the mean using new data $\mathbf{y}_k$

   $\mathrm{p}(\mathbf{x}_k \mid \mathbf{Y}_k)$

   $$\hat{\mathbf{x}}_{k|k} = \mathrm{E}\{\mathbf{x}_k \mid \mathbf{Y}_k\} = \int \mathbf{x}_k \, \mathrm{p}(\mathbf{x}_k \mid \mathbf{Y}_k) d\mathbf{x}_k$$

4. Correct/update the covariance $\mathbf{P}_{k|k}$ using $\mathbf{y}_k$

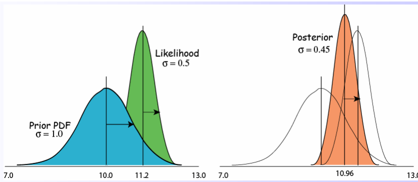
$$\cdots \Rightarrow \mathrm{p}(\mathbf{x}_{k-1} \mid \mathbf{Y}_{k-1}) \Rightarrow \mathrm{p}(\mathbf{x}_k \mid \mathbf{Y}_{k-1}) \Rightarrow \mathrm{p}(\mathbf{x}_k \mid \mathbf{Y}_k) \Rightarrow \cdots$$

PREDICTOR-CORRECTOR

DENSITY PROPAGATOR

Peter's slide from last week

Product of Gaussians=Gaussian:



One data point problem

For the general linear inverse problem we would have

Prior: $p(\boldsymbol{m}) \propto \exp\left\{-\frac{1}{2}(\boldsymbol{m}-\boldsymbol{m}_o)^T C_m^{-1}(\boldsymbol{m}-\boldsymbol{m}_o)\right\}$

Likelihood: $p(\boldsymbol{d}|\boldsymbol{m}) \propto \exp\left\{-\frac{1}{2}(\boldsymbol{d}-G\boldsymbol{m})^T C_d^{-1}(\boldsymbol{d}-G\boldsymbol{m})\right\}$

Posterior PDF

$$\propto \exp\left\{-\frac{1}{2}[(\boldsymbol{d}-G\boldsymbol{m})^T C_d^{-1}(\boldsymbol{d}-G\boldsymbol{m}) + (\boldsymbol{m}-\boldsymbol{m}_o)^T C_m^{-1}(\boldsymbol{m}-\boldsymbol{m}_o)]\right\}$$

$$\propto \exp\left\{-\frac{1}{2}\left[\mathbf{m}-\hat{\mathbf{m}}\right]^T \mathbf{S}^{-1}\left[\mathbf{m}-\hat{\mathbf{m}}\right]\right\}$$

$$\mathbf{S}^{-1} = \mathbf{G}^T\mathbf{C}_d^{-1}\mathbf{G} + \mathbf{C}_m^{-1}$$

$$\hat{\mathbf{m}} = \left(\mathbf{G}^T\mathbf{C}_d^{-1}\mathbf{G} + \mathbf{C}_m^{-1}\right)^{-1}\left(\mathbf{G}^T\mathbf{C}_d^{-1}\mathbf{d} + \mathbf{C}_m^{-1}\mathbf{m}_0\right)$$

$$= \mathbf{m}_0 + \left(\mathbf{G}^T\mathbf{C}_d^{-1}\mathbf{G} + \mathbf{C}_m^{-1}\right)^{-1}\mathbf{G}^T\mathbf{C}_d^{-1}\left(\mathbf{d} - \mathbf{G}\mathbf{m}_0\right)$$

DATA ASSIMILATION

Basic estimation theory

Observation: $T_0 = T + e_0$

First guess: $T_m = T + e_m$

$E\{e_0\} = 0$
$E\{e_m\} = 0$

$E\{e_0^2\} = s_0^2$
$E\{e_m^2\} = s_m^2$
$E\{e_0 e_m\} = 0$

Assume a linear best estimate: $T_n = a\,T_0 + b\,T_m$
with $T_n = T + e_n$.

Find a and b such that
1) $E\{e_n\} = 0$ 2) $E\{e_n^2\}$ minimal

1) Gives: $E\{e_n\} = E\{T_n\text{-}T\} = E\{aT_0+bT_m\text{-}T\} =$
$= E\{ae_0+be_m+ (a+b-1)\,T\} = (a+b-1)\,T = 0$

Hence $b=1-a$.

Basic estimation theory

2) $E\{e_n^2\}$ minimal gives:

$$E\{e_n^2\} = E\{(T_n - T)^2\} = E\{(aT_0 + bT_m - T)^2\} =$$
$$= E\{(ae_0+be_m)^2\} = a^2\,E\{e_0^2\} + b^2 E\{e_m^2\} =$$
$$= a^2\,s_0^2 + (1-a)^2\,s_m^2$$

This has to be minimal, so the derivative wrt a has to be zero:
$2\,a\,s_0^2 - 2(1-a)\,s_m^2 = 0$, so $(s_0^2 + s_m^2)a - s_m^2 = 0$, hence:

$$a = \frac{s_m^2}{s_0^2 + s_m^2} \quad \text{and} \quad b = 1-a = \frac{s_0^2}{s_0^2 + s_m^2}$$

$$s_n^2 = E\{e_n^2\} = \frac{s_m^4\,s_0^2 + s_0^4\,s_m^2}{(s_0^2 + s_m^2)^2} = \frac{s_0^2\,s_m^2}{s_0^2 + s_m^2}$$

Basic estimation theory

Solution: $T_n = \dfrac{s_m^2}{s_0^2 + s_m^2} T_0 + \dfrac{s_0^2}{s_0^2 + s_m^2} T_m$

and $\dfrac{1}{s_n^2} = \dfrac{1}{s_0^2} + \dfrac{1}{s_m^2}$

Note: s_n smaller than s_0 and s_m !

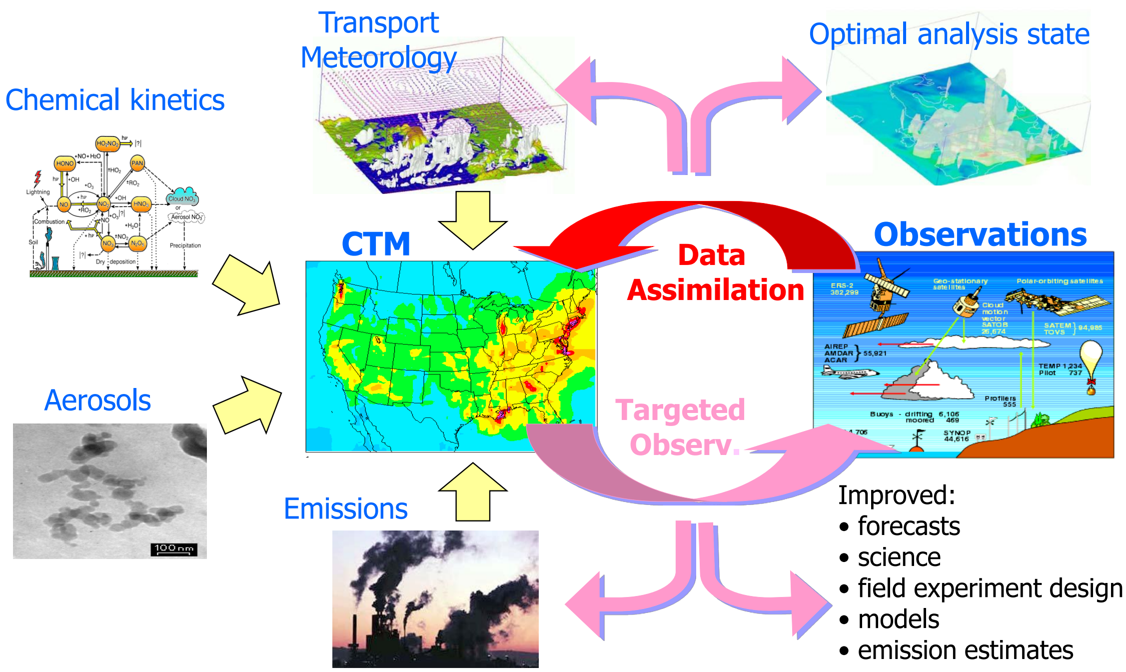
Best Linear Unbiased Estimate BLUE

Just least squares!!!

Tutorial Lecture: Data Assimilation

Adrian Sandu
Computational Science Laboratory
Virginia Polytechnic Institute
and State University

Data assimilation fuses information from (1) prior, (2) model, (3) observations to obtain consistent description of a physical system



Improved:

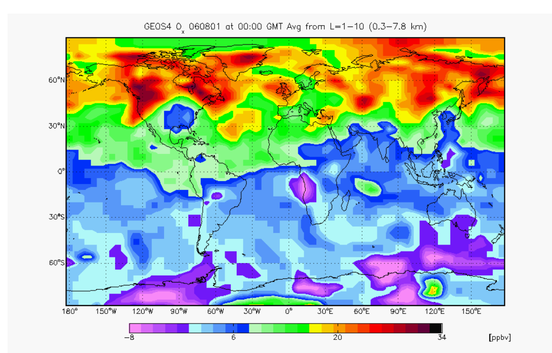
- forecasts
- science
- field experiment design
- models
- emission estimates

Source of information #1: **the prior** encapsulates our current knowledge about the state of the system

- Background (prior) pdf: $\mathcal{P}^{\rm b}(\mathbf{x})$
- Current best estimate: background state $\mathbf{x}^{\rm b}$.
- Typical assumption:

$$\varepsilon^{\rm b} = \mathbf{x}^{\rm b} - \mathcal{S}(\mathbf{x}^{\rm true}) \in \mathcal{N}\left(\mathbf{0}, \mathbf{B}\right) \, .$$

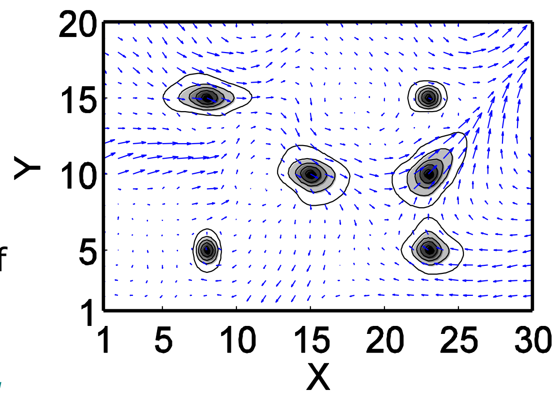
- With nonlinear models the normality assumption is difficult to justify, but is nevertheless used because of its convenience.



Correct models of background (prior) errors are very important for data assimilation

- Background error representation determines the spread of information, and impacts the assimilation results
- Needs: high rank, capture dynamic dependencies, efficient computations
- Traditionally estimated empirically (NMC, Hollingsworth-Lonnberg)

1. Tensor products of 1d correlations, decreasing with distance (Singh et al, 2010)
2. Multilateral AR model (Constantinescu et al 2007)
3. Hybrid methods in the context of 4D-Var (Cheng et al, 2009)



[Constantinescu and Sandu, 2007]

Source of information #2: **the model** encapsulates our knowledge about the physical laws that govern the evolution of the system

- The model evolves an initial state $\mathbf{x}_0 \in \mathbb{R}^n$ to future times

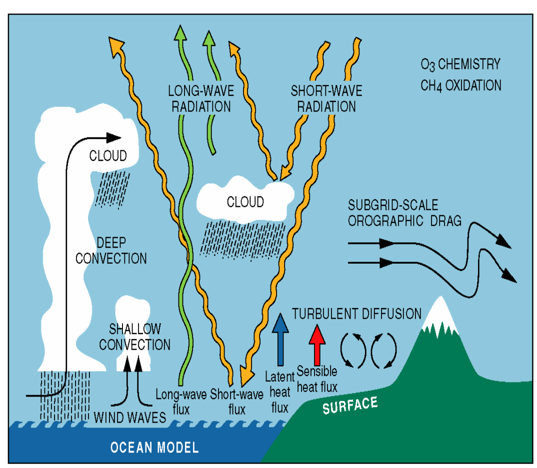
$$\mathbf{x}_i = \mathcal{M}_{t_0 \to t_i}\left(\mathbf{x}_0\right) \, .$$

- The model is imperfect

$$\mathcal{S}\left(\mathbf{x}_i^{\rm true}\right) = \mathcal{M}_{t_{i-1} \to t_i} \cdot \mathcal{S}\left(\mathbf{x}_{i-1}^{\rm true}\right) - \eta_i \, ,$$

where η_i is the model error in step i.

How large are the models of interest? Typically O(10^8) variables, and O(10) different physical processes



Picture: L. Isaksen (http://www.ecmwf.int)

Sep. 7, 2011. SAMSI UQ Methodology Workshop.

Source of information #3: **the observations** are sparse and noisy snapshots of reality

- Measurements $\mathbf{y}_i \in \mathbb{R}^m$ ($m \ll n$) taken at times $t_1, \dots, t_N$

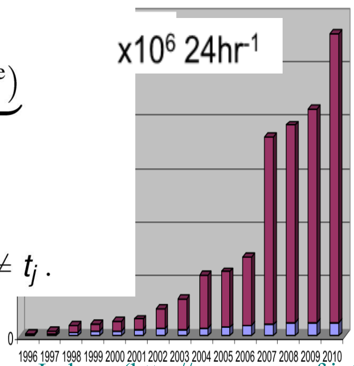
$$\mathbf{y}_i = \mathcal{H}^{\rm t}\left(\mathbf{x}_i^{\rm true}\right) - \varepsilon_i^{\rm instrument} = \mathcal{H}\left(\mathcal{S}(\mathbf{x}_i^{\rm true})\right) - \varepsilon_i^{\rm obs}, \quad i = 1, \cdots, N\,.$$

- Observation operators
  - $\mathcal{H}^{\rm t}$: physical space $\to$ observation space, while
  - $\mathcal{H}$: the model space $\to$ observation space.
- The *observation error*

$$\varepsilon_i^{\rm obs} = \underbrace{\varepsilon_i^{\rm instrument}}_{\text{instrument error}} + \underbrace{\mathcal{H}\left(\mathcal{S}(\mathbf{x}_i^{\rm true})\right) - \mathcal{H}^{\rm t}\left(\mathbf{x}_i^{\rm true}\right)}_{\text{representativeness error}}$$

- Typical assumptions:

$$\varepsilon_i^{\rm obs} \in \mathcal{N}\left(\mathbf{0}, \mathbf{R}_i\right)\ ; \quad \varepsilon_i^{\rm obs}\,,\ \varepsilon_j^{\rm obs} \quad \text{independent for} \quad t_i \neq t_j\,.$$

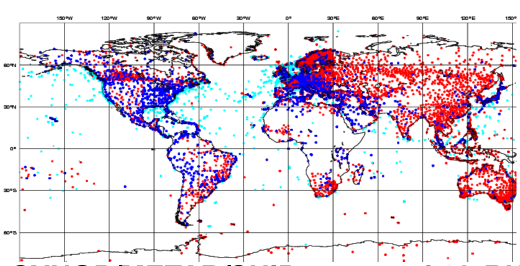


How many observations? ECMWF: O(10^7)

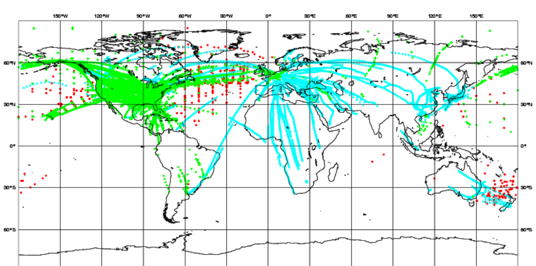
Lars Isaksen (http://www.ecmwf.int)

Some conventional and remote data sources used at ECMWF for numerical weather prediction

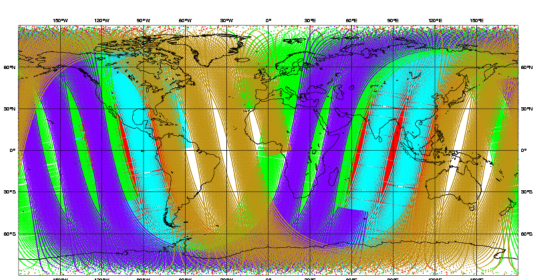
Lars Isaksen (http://www.ecmwf.int)



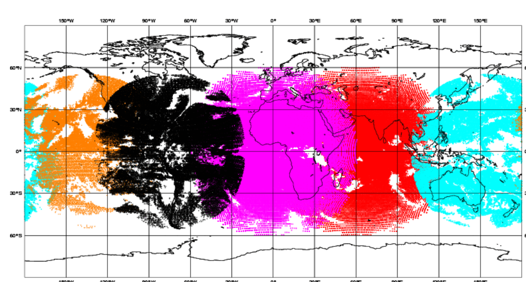
SYNOP/METAR/SHIP: pres., wind, RH



Aircraft: wind, temperature

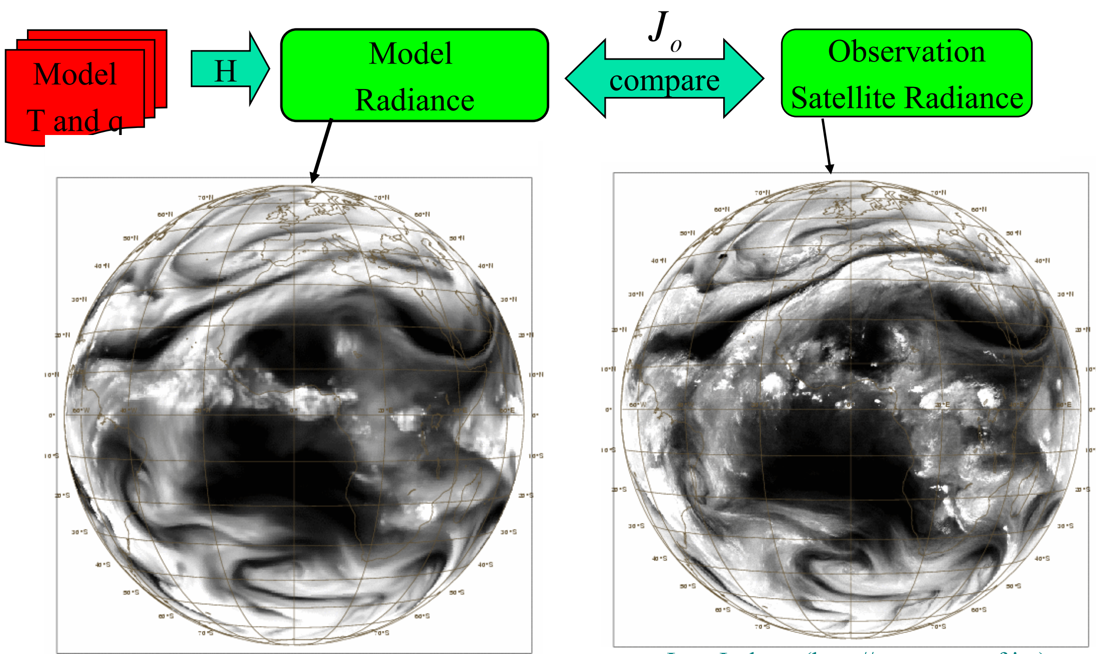


13 Sounders: NOAA AMSU-A/B, HIRS, AIRS, …



Geostationary, 4 IR and 5 winds

To allow model-data comparison, **observation operators** map the model state space to observation space



Lars Isaksen (http://www.ecmwf.int)

Result of DA: **the analysis**, which encapsulates our enhanced knowledge about the state of the system

- The analysis (posterior) probability density $\mathcal{P}^{\mathrm{a}}(\mathbf{x})$:

$$\text{Bayes:} \qquad \mathcal{P}^{\mathrm{a}}(\mathbf{x}) = \mathcal{P}(\mathbf{x}|\mathbf{y}) = \frac{\mathcal{P}(\mathbf{y}|\mathbf{x}) \cdot \mathcal{P}^{\mathrm{b}}(\mathbf{x})}{\mathcal{P}(\mathbf{y})}\,.$$

- Best posterior state estimate: the *analysis* $\mathbf{x}^{\mathrm{a}}$.
- Analysis estimation errors $\varepsilon^{\mathrm{a}} = \mathbf{x}^{\mathrm{a}} - \mathcal{S}(\mathbf{x}^{\mathrm{true}})$ characterized by *bias* $\beta^{\mathrm{a}} = \mathbb{E}^{\mathrm{a}}[\varepsilon^{\mathrm{a}}]$, *covariance* $\mathbf{A} = \mathrm{cov}(\varepsilon^{\mathrm{a}} - \beta^{\mathrm{a}}) \in \mathbb{R}^{n \times n}$.
- Kalman filter: analytical solution for $\mathcal{P}^{\mathrm{a}}(\mathbf{x})$ in Gaussian, linear case
- Methods of practical interest:
  - Suboptimal and Ensemble Kalman filters ($\sim$ min. var.)
  - Variational methods (MAP)

Result of DA: **the analysis**, which encapsulates our enhanced knowledge about the state of the system

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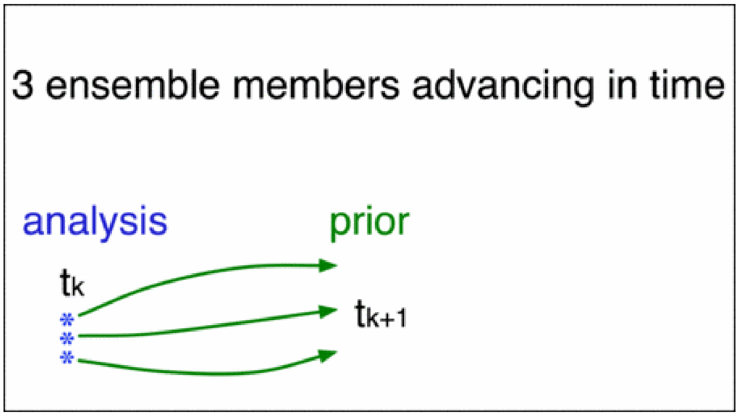
The ensemble Kalman filter (EnKF) is based on EKF, and uses a MC approach to propagate covariances



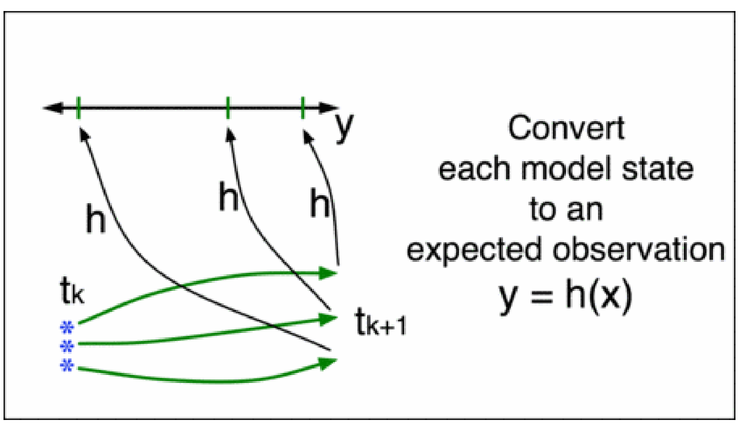
[Picture from J.L. Anderson]

$$\mathbf{x}_{k+1}^{b(i)} = M_{t_k \to t_{k+1}}\left(\mathbf{x}_k^{a(i)}\right) + \boldsymbol{\eta}_{k+1}^{(i)}$$

$$\mathbf{P}_k^b = \frac{1}{K}\sum_{i=1}^{K}\left(\mathbf{x}_k^{b(i)} - \overline{\mathbf{x}_k^b}\right)\left(\mathbf{x}_k^{b(i)} - \overline{\mathbf{x}_k^b}\right)^{\mathrm{T}}$$

Sequential approach to DA: Incorporates data in succession

The ensemble Kalman filter (EnKF) is based on EKF, and uses a MC approach to propagate covariances

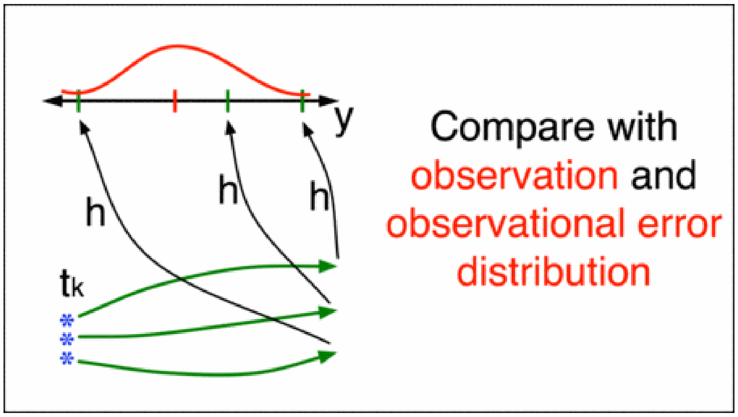


[Picture from J.L. Anderson]

$$\mathbf{P}_k^b\mathbf{H}^{\mathrm{T}} \approx \frac{1}{K}\sum_{i=1}^{K}\left(\mathbf{x}_k^{b(i)} - \overline{\mathbf{x}_k^b}\right)\left(H_k\left(\mathbf{x}_k^{b(i)}\right) - \overline{H_k\left(\mathbf{x}_k^b\right)}\right)^{\mathrm{T}}$$

$$\mathbf{H}_k\mathbf{P}_k^b\mathbf{H}_k^{\mathrm{T}} \approx \frac{1}{K}\sum_{i=1}^{K}\left(H_k\left(\mathbf{x}_k^{b(i)}\right) - \overline{H_k\left(\mathbf{x}_k^b\right)}\right)\left(H_k\left(\mathbf{x}_k^{b(i)}\right) - \overline{H_k\left(\mathbf{x}_k^b\right)}\right)^{\mathrm{T}}$$

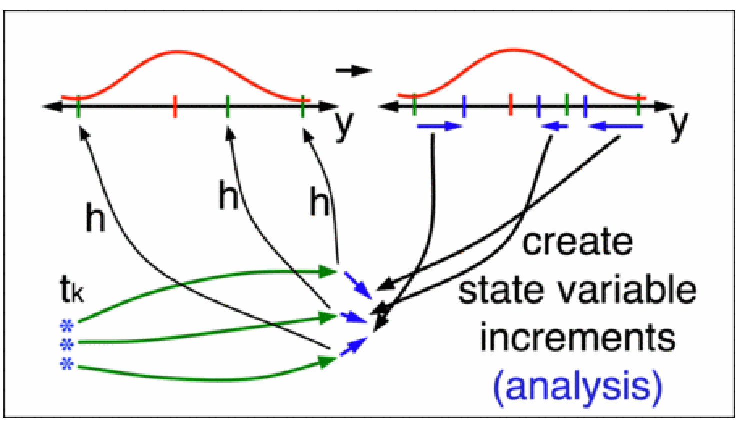
The ensemble Kalman filter (EnKF) is based on EKF, and uses a MC approach to propagate covariances



[Picture from J.L. Anderson]

$$\mathbf{x}_k^a = \mathbf{x}_k^b + \mathbf{K}_k\left(\mathbf{y}_k - \mathbf{H}_k\left(\mathbf{x}_k^b\right)\right)$$

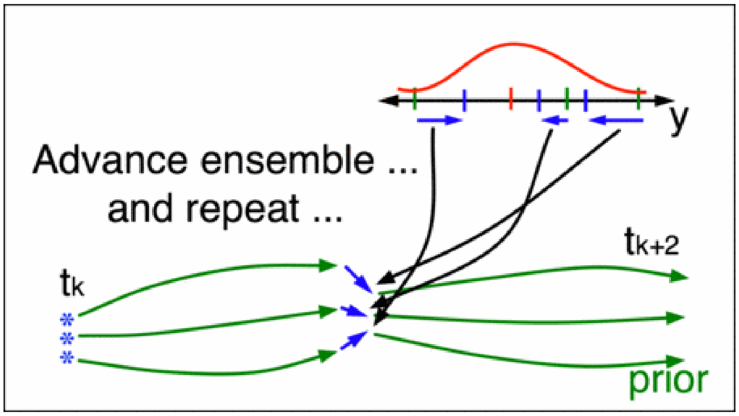
The ensemble Kalman filter (EnKF) is based on EKF, and uses a MC approach to propagate covariances



[Picture from J.L. Anderson]

$$\mathbf{x}_k^a = \mathbf{x}_k^b + \mathbf{K}_k\left(\mathbf{y}_k - \mathbf{H}_k\left(\mathbf{x}_k^b\right)\right)$$

The ensemble Kalman filter (EnKF) is based on EKF, and uses a MC approach to propagate covariances



[Picture from J.L. Anderson]