

# Introduction to Data Assimilation

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This is a special case of inverse problems and approximates the true states of some physical system at a given time by combining time observations with some dynamic model in an optimal way.

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*How do we combine all this information?*

## Typical data assimilation framework

The aim is to estimate a sequence of true states  $x_k^t \in \mathbb{R}^n$  for  $k = 1, \dots, K$ .  
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**Goal:** combine the above to obtain an estimate  $x^a$ . We call this the **analysis**.

We will discuss two approaches to DA:

1. Statistical interpolation techniques, these include **BLUE** and **Kalman filters**.
2. Variational techniques, these include **3D-Var** and **4D-Var**.

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Assume that the background error  $e^b \stackrel{\text{def.}}{=} x^b - x^t$  and the observation error  $e^o$  are uncorrelated with symmetric covariance matrices

$$B \stackrel{\text{def.}}{=} \mathbb{E}[e^b(e^b)^\top] \quad \text{and} \quad R \stackrel{\text{def.}}{=} \mathbb{E}[e^o(e^o)^\top]$$

respectively.

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How do we choose  $L$  and  $K$  such that  $x^a$  is “statistically optimal”?

1. an unbiased estimate:  $\mathbb{E}[x^a - x^t] = 0$
2. to minimise  $\mathbb{E}[\|x^a - x^t\|^2]$ .

**Unbiased analysis for  $x^a = Lx^b + Ky$  :**

Using  $y = Hx^t + e^o$ :

$$x^a - x^t = L(x^b - x^t + x^t) + K(Hx^t + e^o) - x^t$$

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So, to ensure that our analysis state is unbiased, a **sufficient** (although not necessary) condition is

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and recalling that  $y = Hx^t + e^o$ , we have

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The covariance matrix is therefore

$$\begin{aligned} P^a &= \mathbb{E}[e^a(e^a)^\top] = LBL^\top + KRK^\top \\ &= (\text{Id} - KH)B(\text{Id} - KH)^\top + KRK^\top. \end{aligned}$$

We just deduced that  $P^a = (\text{Id} - KH)B(\text{Id} - KH)^\top + KRK^\top$ .

We want to choose  $K$  to minimise  $\mathbb{E}[\|x^a - x^t\|^2] = \text{tr}(P^a)$ .

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Look at the variation of  $\text{tr}(P^a)$  with respect to  $K$ :

$$\begin{aligned}\delta(\text{tr}(P^a)) &= \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} (\text{tr}(P_{K+\varepsilon\delta K}^a) - \text{tr}(P_K^a)) \\ &= 2 \text{tr} \left( (-LBH^\top + KR)(\delta K)^\top \right)\end{aligned}$$

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$$-(\text{Id} - KH)BH^\top + KR = 0 \iff K = BH^\top(R + HBH^\top)^{-1}.$$

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To summarise:

### BLUE

Let  $K = BH^\top(R + HBH^\top)^{-1}$ .

- $x^a = x^b + K(y - Hx^b)$  is called the BLUE estimator with covariance

$$P^a = (\text{Id} - KH)B + \left( -(\text{Id} - KH)BH^\top + KR \right) K^\top = (\text{Id} - KH)B.$$

- We call  $K$  the gain matrix and  $y - Hx^b$  the innovation.

### Scenario

Suppose you are shipwrecked at sea, a few km from shore.

- Before boarding a small lifeboat, you measure your coordinates  $(u, v) = (0, v_b)$  with high accuracy. The first axis is parallel to shore, the second axis is perpendicular to shore.
- After 1 hour, you want to estimate your new coordinates. So, you guess your distance to shore:  $v_o$  with variance  $\sigma_o^2$ .
- Assume that the probability that the boat remains at  $(u_b, v_b)$  follows  $\mathcal{N}(0, \sigma_b^2)$ .

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- The background is  $x^b = \begin{pmatrix} 0 \\ v_b \end{pmatrix}$  with covariance matrix  $B = \sigma_b^2 \text{Id}_2$ .





## Example

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Denoting  $\sigma_a^2$  as the error on the  $v$  coordinate, we have

$$\frac{1}{\sigma_a^2} = \frac{1}{\sigma_b^2} + \frac{1}{\sigma_o^2}$$

This will be dominated by  $\sigma_o^2$  as time progresses.

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NB: we are assuming that the model and observation are linear.

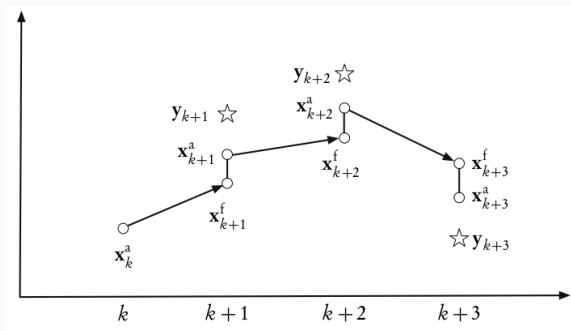
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# The Kalman filter

The Kalman filter is a **sequential statistical interpolation method**.

It alternates between

1. **Analysis**. Interpolates the observations and the background at time  $t_k$ .
2. **Forecast**. Advances to the next time point using the model.



## The Kalman filter

We initialise with a state  $x_0^f = x^b$  and covariance matrix  $P_0^f = \mathbb{E}[e^b(e^b)^\top]$ .

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1. Compute the **analysis estimate**: Just as for BLUE, let

$$x_k^a = x_k^f + K_k(y_k - H_k x_k^f)$$

with

$$K_k^* = P_k^f H_k^\top (H_k P_k^f H_k^\top + R_k)^{-1}$$

which is called the Kalman gain matrix. Moreover, the error covariance is

$$P_k^a = (\text{Id} - K_k^* H_k) P_k^f$$

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$$K_k^* = P_k^f H_k^\top (H_k P_k^f H_k^\top + R_k)^{-1}$$

which is called the Kalman gain matrix. Moreover, the error covariance is

$$P_k^a = (\text{Id} - K_k^* H_k) P_k^f$$

2. Given  $x_k^a$ , compute the **forecast**

$$x_{k+1}^f \stackrel{\text{def.}}{=} M_{k+1} x_k^a.$$

Thanks to the linearity of  $M_{k+1}$ , this is unbiased. Moreover,

$$e_{k+1}^f = M_{k+1} e_k^a + e_{k+1}^m \quad \text{and} \quad P_{k+1}^f = M_{k+1} P_k^a M_{k+1}^\top + Q_{k+1}$$



### Scenario

Suppose you are shipwrecked at sea, a few km from shore. You want to estimate your new coordinates on an **hourly basis**.

- Before boarding a small lifeboat, you measure your coordinates  $(u, v) = (0, v_b)$  with high accuracy. The first axis is parallel to shore, the second axis is perpendicular to shore.
- at hour  $k$ , you guess your distance to shore:  $y_k$  with variance  $\sigma_o^2$ .
- Denote the true coordinates at time  $k$  by  $x_k = (u_k, v_k)$ . Between time  $k$  and  $k + 1$ , assume the boat has drifted with  $x_{k+1} = x_k + \xi_k$  where  $\xi_k \sim \mathcal{N}(0, \sigma_m^2 \text{Id}_2)$ .
- Assume that the probability that the boat remains at  $(u_b, v_b)$  follows  $\mathcal{N}(0, \sigma_b^2)$ .

## Example

- The state vectors are of the form  $x_k = (u_k, v_k)^\top$ .
- As before,  $H_k = (0, 1)$  and  $R_k = \sigma_o^2$ .
- We have  $M_k = \text{Id}_2$  and  $Q_k = \sigma_m^2 \text{Id}_2$ .
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Assume that  $P_k^a = \text{diag}(\lambda_{1,k}, \lambda_{2,k})$  and  $P_k^f = \text{diag}(\rho_{1,k}, \rho_{2,k})$  are diagonal matrices (we will check this afterwards).

## Example: Analysis step

### Kalman filter analysis step

Given  $x_k^f$  and  $P_k^f$ , set  $x_k^a = x_k^f + K_k(y_k - H_k x_k^f)$  where

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$$\begin{pmatrix} u_k^a \\ v_k^a \end{pmatrix} = \begin{pmatrix} u_k^f \\ v_k^f \end{pmatrix} + K_k^* \left( y_k - (0, 1) \begin{pmatrix} u_k^f \\ v_k^f \end{pmatrix} \right) = \begin{pmatrix} u_k^f \\ v_k^f + \frac{\rho_{2,k}}{\sigma_o^2 + \rho_{2,k}} (y_k - v_k^f) \end{pmatrix}$$

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The covariance  $P_k^a = (\text{Id} - K_k^* H_k) P_k^f$  has diagonal entries

$$\lambda_{1,k} = \rho_{1,k} \quad \text{and} \quad \frac{1}{\lambda_{2,k}} = \frac{1}{\sigma_o^2} + \frac{1}{\rho_{2,k}}$$

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### Kalman filter forecast step

Given  $x_k^a$  and  $P_k^a$ , the forecast and associated covariance matrix are

$$x_{k+1}^f \stackrel{\text{def.}}{=} M_{k+1} x_k^a \quad \text{and} \quad P_{k+1}^f = M_{k+1} P_k^a M_{k+1}^\top + Q_{k+1}.$$



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- The forecast covariance error diagonal entries are

$$\rho_{1,k+1} = \lambda_{1,k} + \sigma_m^2 \quad \text{and} \quad \rho_{2,k+1} = \lambda_{2,k} + \sigma_m^2$$

## Example: summary

To summarise:

$$u_{k+1}^f = u_k^f \quad \text{and} \quad v_{k+1}^f = \frac{\sigma_o^2}{\sigma_o^2 + \rho_{2,k}} v_k^f + \frac{\rho_{2,k}}{\sigma_o^2 + \rho_{2,k}} y_k$$

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This leads to a fixed point equation  $\rho_*^2 - \sigma_m^2\rho_* - \sigma_o^2\sigma_m^2 = 0$  with solution

$$\nu_*^2 = \frac{\sigma_m^2}{2} \left( 1 + \sqrt{1 + 4 \frac{\sigma_o^2}{\sigma_m^2}} \right)$$

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Compromise between the uncertainty due to the observation and the uncertainty due to the uncontrolled drift of the boat.

Best linear unbiased estimate (BLUE)

The Kalman filter

**The extended Kalman filter**

The stochastic ensemble Kalman filter

3D Var

4D Var



## Setup

We want to estimate a sequence of true state  $(x_k^t)_{k=1}^K \subset \mathbb{R}^n$  given

- an initial background state  $x^b = x_0^t + e^b \in \mathbb{R}^n$  where  $e^b \in \mathcal{N}(0, B)$ .
- observations  $y_k = H_k[x_k^t] + e_k^o \in \mathbb{R}^p$  for  $k = 1, \dots, K$ , where  $e_k^o \sim \mathcal{N}(0, R_k)$ .
- a model  $x_k^t = M_k[x_{k-1}^t] + e_k^m$  for  $k = 1, \dots, K$  where  $e_k^m \sim \mathcal{N}(0, Q_k)$ .

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Assume independence between the background, observation and model.

What to do if  $H_k$  and  $M_k$  are **nonlinear operators**?

Linearise in the computation of the covariance matrices  $P_k^a$ ,  $P_k^f$  and the Kalman gain matrix  $K_k$ .

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The tangent linear (Jacobian) of  $M_k$  and  $H_k$  at  $x$  are defined to be the  $n \times n$  matrices

$$(\mathbb{M}_k(x))_{ij} \stackrel{\text{def.}}{=} \frac{\partial (M_k)_i}{\partial x_j}(x) \quad \text{and} \quad (\mathbb{H}_k(x))_{ij} \stackrel{\text{def.}}{=} \frac{\partial (H_k)_i}{\partial x_j}(x)$$

## The extended Kalman filter: the forecast step

The forecast step is simply  $x_{k+1}^f = M_{k+1}(x_k^a)$ .

To compute the forecast covariance, we look at the linearisation of the error:

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Computation of  $P_{k+1}^f$  is replaced by

$$P_{k+1}^f = \mathbb{M}_{k+1}(x_k^t) P_k^a \mathbb{M}_{k+1}(x_k^t)^\top + Q_{k+1}$$

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So, set

$$P_k^a = (\text{Id} - K_k\mathbb{H}_k[x_k^t])P_k^f(\text{Id} - K_k\mathbb{H}_k[x_k^t])^\top + K_k R_k K_k^\top$$



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The Kalman gain matrix which minimises  $\mathbb{E}[\text{tr}(P_k^a)]$  is therefore

$$K_k = P_k^f\mathbb{H}_k^\top(R_k + \mathbb{H}_kP_k^f\mathbb{H}_k^\top)^{-1}$$

and the analysis covariance is now  $P_k^a = (\text{Id} - K_k\mathbb{H}_k[x_k^t])P_k^f$

# The extended Kalman filter

We initialise with a state  $x_0^f = x^b$  and covariance matrix  $P_0^f = \mathbb{E}[e^b(e^b)^\top]$ .

For  $t_k = 1, 2, \dots$ ,

1. Compute the **analysis** estimate: let  $\mathbb{H}_k \stackrel{\text{def.}}{=} \mathbb{H}_k[x_k^f]$ .

$$x_k^a = x_k^f + K_k(y_k - H_k[x_k^f])$$

with Kalman gain matrix.

$$K_k = P_k^f \mathbb{H}_k^\top (\mathbb{H}_k P_k^f \mathbb{H}_k^\top + R_k)^{-1}$$

The error covariance is

$$P_k^a = (\text{Id} - K_k^* \mathbb{H}_k) P_k^f$$

2. Given  $x_k^a$ , compute the **forecast**

$$x_{k+1}^f \stackrel{\text{def.}}{=} M_{k+1}[x_k^a].$$

and covariance

$$P_{k+1}^f = \mathbb{M}_{k+1} P_k^a \mathbb{M}_{k+1}^\top + Q_{k+1}$$

where  $\mathbb{M}_{k+1} \stackrel{\text{def.}}{=} \mathbb{M}_{k+1}[x_k^a]$ .

## Disadvantages of the Kalman filter

1. The storage of the covariance matrices  $P_k^f$ . This requires  $n(n+1)/2$  scalars to be stored. Much more expensive than storing only the state vectors.
2. We require  $2n$  computations with the model  $M_k$  for the computation of  $P_k^f$  since we apply  $M_k$  and  $M_k^\top$  on the left and right hand sides.
3. In the extended Kalman filter for nonlinear models, this is an approximation, and the approximation may diverge if the timestep between consecutive updates is too large.

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## The stochastic ensemble Kalman filter

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The stochastic ensemble Kalman filter (Geir Evensen, 1994) aims to alleviate these issue problems.

**Idea:** instead of propagating the covariance matrices  $P_k^f$ ,

- maintain a collection of state vectors (particles) whose variability represent the uncertainty of the system's state.
- the particles are propagated by the model without any linearisation.

# The stochastic ensemble Kalman filter: naive formulation

Suppose we now have **an ensemble of  $m$  particles** from the previous forecast step  $\{x_i^f\}_{i=1}^m \subset \mathbb{R}^n$ . At each time, we have observation  $y$ .

1. Compute the empirical mean and covariance:

$$\bar{x}^f \stackrel{\text{def.}}{=} \frac{1}{m} \sum_{i=1}^m x_i^f \quad \text{and} \quad P^f = \frac{1}{m-1} \sum_{i=1}^m (x_i^f - \bar{x}^f)(x_i^f - \bar{x}^f)^\top.$$

2. For each  $i = 1, \dots, m$ , let

$$x_i^a = x_i^f + K(y_i - H(x_i^f)), \quad \text{where} \quad y_i = y.$$

3. The analysis covariance is

$$P^a = \frac{1}{m-1} \sum_{i=1}^m (x_i^a - \bar{x}^a)(x_i^a - \bar{x}^a)^\top$$



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Suppose now that  $H$  is linear, from

$$\begin{cases} x_i^a = x_i^f + K(y - H(x_k^f)) \\ \bar{x}^a \stackrel{\text{def.}}{=} \frac{1}{m} \sum_i x_i^a = \bar{x}^f + K(y - H(\bar{x}^f)) \end{cases}$$

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we have the ensemble anomalies  $e_i^a \stackrel{\text{def.}}{=} x_i^a - \bar{x}^a$  satisfy

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which leads to

$$P^a = \frac{1}{m-1} \sum_{i=1}^m (e_i^a)(e_i^a)^\top = (\text{Id} - KH)P^f(\text{Id} - KH)^\top.$$

There is a  $KRK^\top$  term missing if we wanted to emulate the BLUE analysis.

### Fix:

1. Perturb  $y_i = y + u_i$  where  $u_i \sim \mathcal{N}(0, R)$ .
2. Define  $R_u = \frac{1}{m-1} \sum_{i=1}^m u_i u_i^\top \xrightarrow{m \rightarrow \infty} R$
3. compute the Kalman gain matrix as  $K = P^f H^\top (H P^f H^\top + R_u)^{-1}$ .

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Let  $e_i^o \stackrel{\text{def.}}{=} u_i - \bar{u}$  and  $\bar{u} = \frac{1}{m} \sum_{i=1}^m u_i$ . We then have

$$e_i^a = e_i^f + K(e_i^o - H e_i^f) = (\text{Id} - KH)e_i^f + K e_i^o.$$

Then, letting  $E^a$  be the matrix with columns  $\frac{e_i^a}{\sqrt{m-1}}$  and  $E^o$  be the matrix with columns  $\frac{e_i^o}{\sqrt{m-1}}$ , we have

$$P^a = (E^a)(E^a)^\top = (\text{Id} - KH)P^f(\text{Id} - KH)^\top + KR_u K^\top = (\text{Id} - KH)P^f$$

## The forecast step

We let

$$x_i^f = M(x_i^a), \quad i = 1, \dots, m$$

and

$$\bar{x}^f \stackrel{\text{def.}}{=} \frac{1}{m} \sum_{i=1}^m x_i^f \quad \text{and} \quad P^f = \frac{1}{m-1} \sum_{i=1}^m (x_i^f - \bar{x}^f)(x_i^f - \bar{x}^f)^\top.$$

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NB: Previously,  $P_{k+1}^f = \mathbb{M}_{k+1} P_k^a \mathbb{M}_{k+1}^\top + Q_{k+1}$ , so we avoid having to apply  $\mathbb{M}_{k+1}$  and there is also no need to explicitly compute  $P_k^a$ .



For the extended Kalman filter, we would have computed using the tangent linear  $\mathbb{H}$  in the computation of  $K$ :  $K = P^f \mathbb{H}^\top (\mathbb{H} P^f \mathbb{H}^\top + R)^{-1}$ .

## No need for linearisation

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For the ensemble Kalman filter, this is done without linearisation of  $H$ :  
Consider the matrix products  $P^f \mathbb{H}^\top$  and  $\mathbb{H} P^f \mathbb{H}^\top$ :

$$\bar{y}^f \stackrel{\text{def.}}{=} \frac{1}{m} \sum_{i=1}^m H(x_i^f)$$
$$P^f \mathbb{H}^\top = \sum_{i=1}^m \frac{(x_i^f - \bar{x}^f)(\mathbb{H}(x_i^f - \bar{x}^f))^\top}{m-1} \approx \sum_{i=1}^m \frac{(x_i^f - \bar{x}^f)(H(x_i^f) - \bar{y}^f))^\top}{m-1}$$

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# The stochastic ensemble Kalman filter

Initialise  $\{x_{i,0}^f\}_{i=1}^m$  and initial error covariance matrix  $P_0^f$ .

For  $k = 1, 2, \dots$

Let  $y_{i,k} = y_k + u_i$  where  $u_i \sim \mathcal{N}(0, R)$ .

Analysis step:

- $\bar{x}_k^f \stackrel{\text{def.}}{=} \frac{1}{m} \sum_{i=1}^m x_{i,k}^f$ ,  $\bar{u} = \frac{1}{m} \sum_{i=1}^m u_i$ ,  $\bar{y}_k^f \stackrel{\text{def.}}{=} \frac{1}{m} \sum_{i=1}^m H_k[x_{i,k}^f]$ .
- $[E_k^f]_i = \frac{1}{\sqrt{m-1}}(x_{i,k}^f - \bar{x}_k^f)_{i=1}^m$  and  $[Y_k^f]_i = \frac{H_k[x_{i,k}^f] - u_i - \bar{y}_k^f + \bar{u}}{\sqrt{m-1}}$ .
- $K_k = X_k^f(Y_k^f)(Y_k^f(Y_k^f)^\top)^{-1}$ .
- For  $i = 1, \dots, m$ ,  $x_{i,k}^a = x_{i,k}^f + K_k(y_{i,k} - H_k(x_{i,k}^f))$ ,
- $\bar{x}_k^a = \frac{1}{m} \sum_i x_{i,k}^a$  and  $P_k^a = \frac{1}{m-1} \sum_{i=1}^m (x_{i,k}^a - \bar{x}_k^a)(x_{i,k}^a - \bar{x}_k^a)^\top$ .

Forecast step:

- For  $i = 1, \dots, m$ ,  $x_{i,k}^f = M(x_{i,k}^a)$
- $P_k^f = \frac{1}{m-1} \sum_{i=1}^m (x_{i,k}^f - \bar{x}_k^f)(x_{i,k}^f - \bar{x}_k^f)^\top$ .

Best linear unbiased estimate (BLUE)

The Kalman filter

The extended Kalman filter

The stochastic ensemble Kalman filter

**3D Var**

4D Var

Given a positive definite matrix  $\Sigma$ , let  $\|v\|_{\Sigma} \stackrel{\text{def.}}{=} \langle \Sigma v, v \rangle$ .

### Setup

We want to estimate the true state  $x^t \in \mathbb{R}^n$  given

- a background state  $x^b \in \mathbb{R}^n$ .
- observation  $y = H[x^t] + e^o \in \mathbb{R}^p$ , where  $H \in \mathbb{R}^{p \times n}$  is a matrix, typically,  $p \ll n$ .

Let  $e^b \stackrel{\text{def.}}{=} x^b - x^t$  and  $e^o = x^b - x^t$  be the background and observation errors.

They are assumed to be uncorrelated with symmetric covariance matrices  $B \stackrel{\text{def.}}{=} \mathbb{E}[e^b(e^b)^{\top}]$  and  $R \stackrel{\text{def.}}{=} \mathbb{E}[e^o(e^o)^{\top}]$  respectively.

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### 3D Var

We choose  $x^a$  to minimise the cost function

$$J(x) = \frac{1}{2} \|x - x^b\|_{B^{-1}}^2 + \frac{1}{2} \|Hx - y\|_{R^{-1}}^2 \quad (3\text{dVar})$$

**Notation:** For positive definite  $A \in \mathbb{R}^{n \times n}$  and  $v \in \mathbb{R}^n$ ,  $\|v\|_A^2 \stackrel{\text{def.}}{=} \langle Av, v \rangle$ .

Recall the Bayesian viewpoint of variational problems...



## Recall the Bayesian viewpoint of variational problems...

- Our data model is  $y = Hx^t + e^o$  where  $e^o \sim \mathcal{N}(0, R)$ . So,  
 $P(y|x) = \exp\left(-\frac{1}{2} \|Hx - y\|_{R^{-1}}^2\right)$ .
- Since we assume that  $x^t = x^b + e^b$  where  $e^b \sim \mathcal{N}(0, B)$ , our a-priori probability density is  $P(x) = \exp\left(-\frac{1}{2} \|x - x^b\|_{B^{-1}}^2\right)$ .

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By Baye's rule,  $P(x|y)P(y) = P(y|x)P(x)$ . we have

$$P(x|y) = \exp\left(-\frac{1}{2} \|Hx - y\|_{R^{-1}}^2 - \frac{1}{2} \|x - x^b\|_{B^{-1}}^2\right)$$

So the maximum a-posterior estimate is

$$x \in \operatorname{argmin} J(x) = \frac{1}{2} \|x - x^b\|_{B^{-1}}^2 + \frac{1}{2} \|Hx - y\|_{R^{-1}}^2.$$

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In fact, the minimiser coincides with the BLUE estimate!

## 3D Var is equivalent to BLUE

### Lemma 1 (3D Var is equivalent to BLUE)

*The minimiser  $x^a$  to (3dVar) is*

$$x^a = x^b + K(y - Hx^b)$$

*where  $K = (B^{-1} + H^{\top} R^{-1} H)^{-1} H^{\top} R^{-1}$ . Moreover,*

$$K = BH^{\top} (R + HBH^{\top})^{-1} = (B^{-1} + H^{\top} R^{-1} H)^{-1} H^{\top} R^{-1}.$$

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### Proof.

Note that

$$\nabla J(x) = B^{-1}(x - x^b) - H^T R^{-1}(y - Hx).$$

So, the minimiser  $x^a$  to (3dVar) satisfies  $\nabla J(x^a) = 0$  which yields the first statement.

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The second statement follows from the Sherman-Morrison-Woodbury formula:

$$(B^{-1} + H^T R^{-1} H)^{-1} = B - BH^T (R + HBH^T)^{-1} HB$$



Recall

$$J(x) = \frac{1}{2} \|x - x^b\|_{B^{-1}}^2 + \frac{1}{2} \|Hx - y\|_{R^{-1}}^2$$

Its gradient is

$$\nabla J(x) = B^{-1}(x - x^b) + H^* R^{-1}(Hx - y)$$

and its Hessian is

$$\text{Hess}(J) = B^{-1} + H^* R^{-1} H$$

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### Error estimate

We have  $\text{Hess}(J)^{-1} = \mathbb{E}[(x^a - x^t)(x^a - x^t)]$ .

So, the narrower the minimum, the better the analysis.



### Lemma 2

Let  $P^a = \mathbb{E}[(x^a - x^t)(x^a - x^t)^\top]$ . Then  $P^a = \text{Hess}(J)^{-1}$ .

### Proof.

From  $\nabla J(x^a) = 0$ , we have  $B^{-1}(x^a - x^b) - H^\top R^{-1}(y - Hx^a) = 0$



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$$\implies 0 = B^{-1}(x^a - x^t + x^t - x^b) - H^\top R^{-1}(y - Hx^t + Hx^t - Hx^a)$$



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Considering  $\mathbb{E}[v_i^\top v_j]$  for  $i = 1, 2$  and since  $x^b$  and  $y$  are uncorrelated, we have

$$\text{Hess}(J)P_a\text{Hess}(J) = B^{-1} + H^\top R^{-1}H = \text{Hess}(J)$$

which yields  $P_a = \text{Hess}(J)^{-1}$ . □

Note that  $J$  is convex and we can write  $\min_{x \in \mathbb{R}^n} J(x)$  as

$$\min_{x, z \in \mathbb{R}^n} \frac{1}{2} \|x - x^b\|_{B^{-1}}^2 + \frac{1}{2} \|z\|_{R^{-1}}^2 \quad \text{s.t.} \quad Hx - y = z$$

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The Lagrange function is a function over  $\lambda \in \mathbb{R}^p$

$$H(\lambda) = \min_{x, z} \frac{1}{2} \|x - x^b\|_{B^{-1}}^2 + \frac{1}{2} \|z\|_{R^{-1}}^2 + \langle \lambda, z - Hx + y \rangle$$

## Dual formulation

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The optimum is achieved at  $x = x^b + BH^\top \lambda$  and  $z = -R\lambda$ , so

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The dual problem is therefore

$$\sup_{\lambda \in \mathbb{R}^p} -\frac{1}{2} \langle (HBH^\top + R)\lambda, \lambda \rangle - \langle \lambda, y - Hx^b \rangle$$

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The dual formulation is called the **Physical Statistical space Assimilation System (PSAS)** and has the advantage of operating over the measurement space  $\mathbb{R}^p$  as opposed to  $\mathbb{R}^n$  (recall that often  $p \ll n$ ).



## Computational:

- BLUE requires the storage and inversion of a large matrix
- 3D var is simply the minimisation of a function  $J$ , we only need to compute the product of  $B^{-1}$  and  $R^{-1}$  against vectors several times – this is computationally less demanding.

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**The nonlinear case:** There is no need to explicitly linearise. For

$$J(x) = \frac{1}{2} \|x - x^b\|_{B^{-1}}^2 + \frac{1}{2} \|y - H[x]\|_{R^{-1}}^2$$

the gradient is

$$\nabla J(x) = B^{-1}(x - x^b) - \mathbb{H}^\top R^{-1}(y - H[x])$$

where  $\mathbb{H}$  is the so called *tangent linear* of  $H$  at  $x$ .

Best linear unbiased estimate (BLUE)

The Kalman filter

The extended Kalman filter

The stochastic ensemble Kalman filter

3D Var

4D Var

In 4D Var is a sequential extension of 3D Var ('4' refers to the time dimension).

### Setup

We assume

- a given background  $x^b = x^t + e^b$  with  $e^b \in \mathcal{N}(0, B)$
- observations for  $k = 1, \dots, K$ ,

$$y_k = H_k[x_k^t] + e_k^o, \quad e_k^o \sim \mathcal{N}(0, R_k).$$

- the true states  $x_k^t$  follow some model  $x_k^t = M_k[x_{k-1}^t]$  for  $k = 1, \dots, K$ .

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### 4D Var

The 4d var estimate is the minimiser of the cost

$$J(x_0) = \frac{1}{2} \|x_0 - x^b\|_{B^{-1}}^2 + \frac{1}{2} \sum_{k=0}^K \|H_k(x_k) - y_k\|_{R_k^{-1}}^2 \quad \text{s.t. } x_k = M_k(x_{k-1})$$

This is called **strong constraint 4D Var**: the model is assumed to be exact.

## 4D Var: unconstrained

We first assume that  $M_k$  and  $H_k$  are both linear.

We can write  $x_{k+1} = M_{k+1}M_k \dots M_1 x_0$ , so writing

$$d_k = y_k - H_k M_k M_{k-1} \dots M_2 M_1 x_0 \quad \text{and} \quad \Delta_k = R_k^{-1} d_k$$

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## 4D Var: Computation of the gradient

We can therefore compute the gradient

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**Remark:** In practice,  $M_k$  is computed using a numerical code of thousands of lines. It is common to resort to **auto-differentiation** to compute  $M_k^\top$ , given the code of  $M_k$ .

**Error estimate** Just as for 3D Var, one can show that  $P^a = \text{Hess}(J)^{-1}$ .

## 4D Var: error estimate and the nonlinear case

**Error estimate** Just as for 3D Var, one can show that  $P^a = \text{Hess}(J)^{-1}$ .

**The nonlinear case** Let  $\mathbb{M}$  and  $\mathbb{H}$  be the tangent linear of  $M$  and  $H$  with respect to  $x$ . Let  $d_k = y_k - H_k M_k(M_{k-1}(\dots(M_2(M_1 x_0))))$  and  $\Delta_k$  be as before. By Leibnitz's rule,

$$\nabla_{x_0} J = - \sum_{k=0}^K \left( \mathbb{M}_1^\top(x_0) \mathbb{M}_2^\top(x_1) \dots \mathbb{M}_k^\top(x_{k-1}) \right) \mathbb{H}_k^\top(x_k) \Delta_k.$$

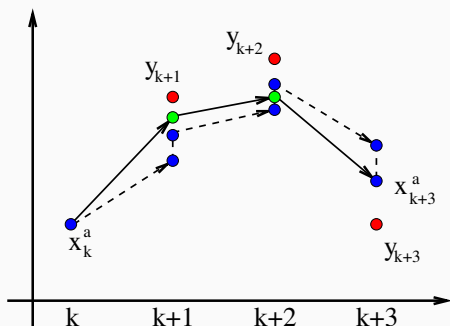
Note only do we need to know the adjoint, but also the differential (tangent linear) of  $M_k$  and  $H_k$ . This can again be done using automatic differentiation.



## Equivalence to Kalman filter

In the case of no model errors and when  $M_k$  and  $H_k$  are both linear, and  $M_k$  are invertible,

- one can show that the output  $x_K$  of 4D-Var is precisely the output of the Kalman filter.
- however, there is no equivalence between the intermediate outputs  $x_k$  for  $k < K$ .



## Property 1: Minimisation over any $x_j$ is equivalent

The evolution model is assumed to be perfect. So we can minimise over any  $x_j$  for  $j = 0, \dots, K$ .

Write for  $k \geq \ell$ ,  $M_{k,\ell} \stackrel{\text{def.}}{=} M_k M_{k-1} \dots M_{\ell+1}$  and for  $k < \ell$ ,  $M_{k,\ell} = M_{\ell,k}^{-1}$ .

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Let  $P_j^a = \mathbb{E}[(x_j^a - x_j^t)(x_j^a - x_j^t)^\top]$  and  $\mathcal{H}_j$  be the Hessian of  $J_j$  at its optimum  $x_j^a$

$$(P_j^a)^{-1} = \mathcal{H}_j = B_j^{-1} + \sum_{k=0}^K M_{k,j}^\top H_k^\top R_k^{-1} H_k M_{k,j} = M_{\ell,j}^\top (P_\ell^a)^{-1} M_{\ell,j}.$$

KF is causal in that error at  $k$  depends on observations before the analysis, but this is not the case for 4D Var.

## Property 2: Transferability of optimality

Minimising over  $[0, K]$  is equivalent to minimising over  $[0, m]$  and  $[m, K]$ :

### Lemma 3

Consider the following:

- Let  $x_0$  be the minimiser of

$$J(x) = \frac{1}{2} \|x - x^b\|_{B^{-1}}^2 + \frac{1}{2} \sum_{k=0}^K \|H_k(M_{k,0}x) - y_k\|_{R_k^{-1}}^2.$$

- Let  $m < K$  and  $x^a$  be the minimiser of

$$J_m(x) = \frac{1}{2} \|x - x^b\|_{B^{-1}}^2 + \frac{1}{2} \sum_{k=0}^m \|H_k(M_{k,0}x) - y_k\|_{R_k^{-1}}^2. \text{ Then, by defining } P^a \stackrel{\text{def.}}{=} \mathcal{H}_{x^a}^{-1} \text{ where } \mathcal{H}_{x^a} \text{ is the Hessian of } J_m \text{ at } x^a, \text{ let}$$

$$\hat{x}_0 \in \operatorname{argmin}_x \frac{1}{2} \|x - x^a\|_{\mathcal{H}_{x^a}^{-1}}^2 + \frac{1}{2} \sum_{k=m+1}^K \|H_k(M_{k,0}x) - y_k\|_{R_k^{-1}}^2.$$

Then,  $\hat{x}_0 = x_0$ .

## Property 2: Transferability of optimality

### Proof.

Define  $J_{K,m} \stackrel{\text{def.}}{=} \frac{1}{2} \sum_{k=m+1}^K \|H_k(M_{k,0}x) - y_k\|_{R_k}^2$ .

NB:  $J(x) = J_m(x) + J_{K,m}(x)$ .

Since  $J_m$  is a quadratic function, it coincides with its 2nd order Taylor expansion around  $x^a$ :

$$J_m(x) = J_m(x^a) + \nabla J_m(x^a)(x - x^a) + \frac{1}{2}(x - x^a)^\top \mathcal{H}_{x^a}(x - x^a).$$

By optimality of  $x^a$ ,  $\nabla J_m(x^a) = 0$ . Therefore,

$$J(x) = J_m(x^a) + \frac{1}{2} \|x - x^a\|_{\mathcal{H}_{x^a}}^2 + J_{K,m}(x).$$

Therefore,

$$\operatorname{argmin}_x J(x) = \operatorname{argmin}_x \frac{1}{2} \|x - x^a\|_{\mathcal{H}_{x^a}}^2 + J_{K,m}(x)$$

as required. □

When the model is inexact  $x_{k+1}^t = M_{k+1}x_k^t + e_k^m$  and consider the cost

$$J(x_0, \dots, x_K) = \frac{1}{2} \left\| x - x^b \right\|_{B^{-1}}^2 + \sum_{i=0}^j \left\| H_i x_i - y_i \right\|_{R_i^{-1}} + \left\| M_i x_{i-1} - x_i \right\|_{Q_i^{-1}}^2 .$$

This is called **weak constrained 4D Var**.

However, this requires optimisation over  $x_0, \dots, x_j$  and is therefore much more computationally expensive.



## Back to the equivalence between KF and 4D Var...

Let  $m = 0$  in the previous lemma, then

1.  $x^a \in \operatorname{argmin}_x J_0(x) = \frac{1}{2} \|x - x^b\|_{B^{-1}}^2 + \frac{1}{2} \|H_0(x) - y_0\|_{R_0^{-1}}^2.$

2. Let

$$\hat{x}_0 \in \operatorname{argmin}_x J_{1,K}(x) = \frac{1}{2} \|x - x^a\|_{\mathcal{H}_{x^a}}^2 + \frac{1}{2} \sum_{k=1}^K \|H_k(M_{k,0}x) - y_k\|_{R_k^{-1}}^2.$$

We know that  $\hat{x}_0$  coincides with the 4D Var output.

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By writing  $M_{1,0}^{-1}z = x$  and  $P^f = M_{1,0}\mathcal{H}_{x^a}^{-1}M_{1,0}^\top$  this is equivalent to solving

$$\operatorname{argmin}_z \frac{1}{2} \|z - M_{1,0}x^a\|_{(P^f)^{-1}}^2 + \frac{1}{2} \|H_k(z) - y_1\|_{R_1^{-1}}^2 .$$

which is equivalent to one forecast step followed by one analysis step in KF.

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**Repeating this shows that the outputs of 4D Var and KF coincide.**

Data assimilation is a set of statistical tools to improve knowledge of present or future system states by combining experimental data and theoretical knowledge of the system.

- BLUE is a statistical interpolation technique for combining observation with an a-priori guess. The BLUE estimate can be written as the solution to a variational problem, 3d Var.
- The Kalman filter is a sequential statistical interpolation technique. It alternates between performing a analysis step (BLUE), and a forecast step (propagating states using a known model).
- 4D Var is a sequential version of 3D Var, and can be seen to be equivalent to the Kalman filter in the case of linear observation and model operators.
- Extensions of the Kalman filter: extended Kalman filter, ensemble Kalman filter.