Introduction to Data Assimilation

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How do we combines 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 $k = 1, \ldots, K$.
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- e_k^m, e_k^o and e^b are independent.

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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.**

Outline

Best linear unbiased estimate (BLUE)

The Kalman filter

3D Var

4D Var

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

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

respectively.

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Let us make the Ansatz that

$$x^a = Lx^b + Ky, \quad \text{where} \quad L \in \mathbb{R}^{n\times n} \quad \text{and} \quad K \in \mathbb{R}^{n\times p}.$$

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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 $\mathbb{E}[\left\|x^a - x^t\right\|^2]$.

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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which implies that

$$e^a = Le^b + Ke^o + (L + KH - \mathrm{Id})x^t.$$

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

$$L = \mathrm{Id} - KH,$$

The analysis covariance

From the choice of $L = \mathrm{Id} - KH$,

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$$e^a = e^b + K(e^o - He^b) = Le^b + Ke^o$$

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The covariance matrix is therefore

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

Minimal error

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

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

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

$$\begin{aligned}\delta(\mathrm{tr}(P^a)) &= \lim_{\varepsilon\to 0} \frac{1}{\varepsilon}(\mathrm{tr}(P^a_{K+\varepsilon\delta K}) - \mathrm{tr}(P^a_K)) \\ &= 2\,\mathrm{tr}\left((-LBH^\top + KR)(\delta K)^\top\right)\end{aligned}$$

and so

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

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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

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

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

Example

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 σ_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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- Observation is

$$y \stackrel{\text{def.}}{=} v_o = Hx + \varepsilon, \quad \text{where} \quad H = (0, 1), \quad \varepsilon \sim \mathcal{N}(0, \sigma_o^2).$$

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- The background is $x^b = \binom{0}{v_b}$ with covariance matrix $B = \sigma_b^2 \mathrm{Id}_2$.

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The posterior error is

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Denoting σ_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 σ_o^2 as time progresses.

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

The Kalman filter

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

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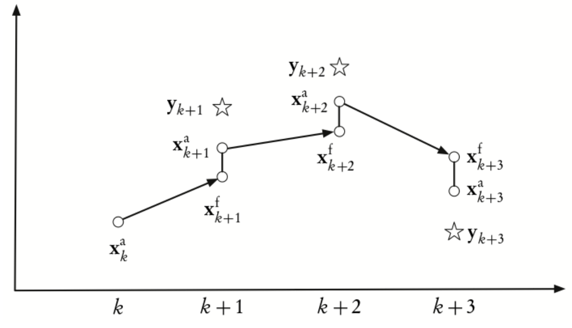
It alternates between

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



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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

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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,

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

Example

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 σ_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 $x_{k+1} = x_k + \xi_k$ whre $\xi_k \sim \mathcal{N}(0, \sigma_m^2 \mathrm{Id}_2)$.
- 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 $M_k = \mathrm{Id}_2$ and $Q_k = \sigma_m^2 \mathrm{Id}_2$.
- We have $x_0^f = (u, v)$ and $P_0^f = \sigma_b^2 \mathrm{Id}_2$.

Example

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Assume that $P_k^a = \mathrm{diag}(\lambda_{1,k}, \lambda_{2,k})$ and $P_k^f = \mathrm{diag}(\nu_{1,k}, \nu_{2,k})$ are diagonal matrices (we will check this afterwards).

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

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

The error covariance is $P_k^a = (\mathrm{Id} - K_k^* H_k) P_k^f$.

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

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

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

Kalman filter forecast step

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

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

Forecast step

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- The model does not change our estimate

$$\begin{pmatrix} u_{k+1}^f \\ v_{k+1}^f \end{pmatrix} = \begin{pmatrix} u_k^a \\ v_k^a \end{pmatrix}.$$

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- The forecast covariance error diagonal entries are

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

Example

To summarise:

$$u^f_{k+1} = u^f_k \quad \text{and} \quad v^f_{k+1} = \frac{\sigma_o^2}{\sigma_o^2 + \nu_{2,k}} v^f_k + \frac{\nu_{2,k}}{\sigma_o^2 + \nu_{2,k}} y_k$$

and

$$\nu_{1,k+1} = \nu_{1,k} + \sigma_m^2 = k\sigma_m^2 + \sigma_b^2 \quad \text{and} \quad \frac{1}{\nu_{2,k+1} - \sigma_m^2} = \frac{1}{\sigma_o^2} + \frac{1}{\nu_{2,k}}$$

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This leads to a fixed point equation $\nu_*^2 - \sigma_m^2\nu_* - \sigma_o^2\sigma_m^2 = 0$ 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 the the observation and the uncertainty due to the uncontrolled drift of the boat.

The extended Kalman filter

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 $k = 1, \ldots, K$, 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 $k = 1, \ldots, K$ where $e_k^m \sim \mathcal{N}(0, Q_k)$.

Assume independence between the background, observation and model.

What to do if H_k and M_k are nonlinear operators?

The extended Kalman filter

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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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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.

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

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

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

$$\begin{aligned} e_{k+1}^f = x_{k+1}^f - x_{k+1}^t &= M_{k+1}(x_k^a) - x_{k+1} \\ &= M_{k+1}(x_k^a - x_k^t + x_k^t) - x_{k+1} \\ &= M_{k+1}(x_k^a - x_k^t + x_k^t) - M_{k+1}(x_k) - e_{k+1}^m \\ &\approx \mathbb{M}_{k+1}(x_k^t) e_k^a - e_{k+1}^m. \end{aligned}$$

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

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

The extended Kalman filter

For **the analysis step**, we compute

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

The analysis error is

$$\begin{aligned} e_k^a = x_k^a - x_k^t = x_k^f - x_k^t + K_k(y_k - H_k[x_k^t] + H_k[x_k^t] - H_k[x_k^f - x_k^t + x_k^t]) \\ \approx e_k^f + K_k(e_k^o - \mathbb{H}_k[x_k^t]e_k^f) = (\mathrm{Id} - K_k\mathbb{H}_k[x_k^t])e_k^f + K_k e_k^o \end{aligned}$$

So, set

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

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

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

and the analysis covariance is now

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

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 $t_k = 1, 2, \ldots,$

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

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

   with

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

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

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

2. Given x_k^a, compute the forecast

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

   and covariance

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

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

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.

The stochastic ensemble Kalman filter (Geir Evensen, 1994) aims to alleviate the above 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: The analysis step

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 $i = 1, \ldots, m$, let

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

3. The analysis covariance is

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

How would this compare with BLUE analysis? Suppose now that H is linear, then the ensemble anomalies $e_i^a \stackrel{\text{def.}}{=} x_i^a - \bar{x}^a$ satisfy

$$e_i^a = e_i^f + K^*(0 - He_i^f) = (\mathrm{Id} - K^*H)e_i^f$$

which leads to

$$P^a = \frac{1}{m-1}\sum_{i=1}^{m}(x_i^a - \bar{x}^a)(x_i^a - \bar{x}^a)^\top = (\mathrm{Id} - K^*H)P^f(\mathrm{Id} - K^*H)^\top.$$

So there is a $K^*RK^\top$ 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 $R_u = \frac{1}{m-1} \sum_{i=1}^{m} u_i u_i^\top \quad \xrightarrow{m\to\infty} \quad R$
3. compute the Kalman gain matrix as $K^* = P^f H^\top (HP^f H^\top + R)^{-1}$.

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

$$e_i^a = e_i^f + K^*(e_i^o - He_i^f) = (\mathrm{Id} - K^* H)e_i^f + K^* e_i^o.$$

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

$$\mathbb{E}[P^a] = \mathbb{E}[(E^a)(E^a)^\top] = (\mathrm{Id} - K^* H)\mathbb{E}[P^f](\mathrm{Id} - K^* H) + R = (\mathrm{Id} - K^* H)\mathbb{E}[P^f]$$

We let

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

and

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

The stochastic ensemble Kalman filter: The forecast step

We let

$$x_i^f = M(x_i^a), \qquad i = 1, \ldots, m$$

and

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

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.

The stochastic ensemble Kalman filter: no linearisation

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

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

$$\bar{y}^f \stackrel{\text{def.}}{=} \frac{1}{m}\sum_{i=1}^{m} H(x_i^f)$$

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

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

The stochastic ensemble Kalman filter

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

For $k = 1, 2, \ldots$

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 $i = 1, \ldots, m$, $x_{i,k}^a = x_{i,k}^f + K_k(y_{i,k} - H_k(x_{i,k}^f))$,
- $\bar{x}_k^a = \frac{1}{m}\sum_i x_{i,k}^a$ and $P_k^a = \frac{1}{m-1}\sum_{i=1}^m (x_{i,k}^a - \bar{x}^a)(x_{i,k}^a - \bar{x}_k^a)^\top$.

Forecast step:

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

Outline

Given a positive definite matrix Σ, 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.

3D Var

We choose x^a to minimise the cost function

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

Note that

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

Equivalence to BLUE

The following lemma shows that the 3D Var solution is precisely the BLUE estimate.

Lemma 3.1

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,

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

Note that $\mathrm{Hess}(J) = B^{-1} + H^\top R^{-1} H$, so $P^a = \mathrm{Hess}(J)^{-1}$ and the analysis precision is proportional to the curvature of J – the narrower the minimum, the better the analysis. In the following lemma, we present an alternative argument for this fact.

Lemma 3.2

Let $P^a = (x^a - x^t)(x^a - x^t)^\top$. Then $P^a = \mathrm{Hess}(J)^{-1}$.

Proof.

From $\nabla J(x^a) = 0$, we have

$$
\begin{aligned}
& 0 = B^{-1}(x^a - x^b) - H^\top R^{-1}(y - Hx^a) \\
\Longrightarrow\ & 0 = B^{-1}(x^a - x^t + x^t - x^b) - H^\top R^{-1}(y - Hx^t + Hx^t - Hx^a) \\
\Longrightarrow\ & v_1 \overset{\text{def.}}{=} (B^{-1} + H^\top R^{-1} H)(x^a - x^t) = B^{-1}(x^b - x^t) + H^\top R^{-1}(y - Hx^t) \overset{\text{def.}}{=} v_2.
\end{aligned}
$$

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

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

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

Dual formulation

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

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

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

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

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

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

The dual problem is therefore

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

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 $p \ll n$).

Advantages of 3D Var

Computational One advantage of this variational interpretation is that BLUE requires the storage and inversion of a large matrix, whereas, since 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.

The nonlinear case Another advantage of 3D Var is in the handling of the case were H is nonlinear. There is no need to explicitly linearise. For

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

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.

4D Var

In 4D Var is a sequential extension of 3D Var (the 4 refers to the time dimension). The cost function still depends on the initial state x_0, but also includes the model.

We assume

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

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

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

The 4d var estimate is the minimiser of the cost

$$J(x_0) = \frac{1}{2}\left\|x_0 - x^b\right\|_{B^{-1}}^2 + \frac{1}{2}\sum_{k=0}^{K}\|H_k(x_k) - y_k\|_{R_k^{-1}}^2 \qquad \text{subject to } x_k = M_k(x_{k-1})$$

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

Outline

Best linear unbiased estimate (BLUE)

The Kalman filter

3D Var

4D Var

4D Var

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

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

we have

$$J(x_0) = \frac{1}{2} \left\| x_0 - x^b \right\|_{B^{-1}}^2 + \frac{1}{2} \sum_{k=0}^{K} \| d_k \|_{R_i^{-1}}^2$$

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The gradient is

$$\nabla_{x_0} J = B^{-1}(x_0 - x^b) - \sum_{k=0}^{K} (M_1^\top M_2^\top \dots M_k^\top) H_k^\top \Delta_k$$

$$= B^{-1}(x_0 - x^b) - \left(H_0^\top \Delta_0 + M_1^\top \left(H_1^\top \Delta_1 + M_2^\top \left(H_2^\top \Delta_2 + \dots + M_K^\top \left(H_K^\top \Delta_K \right) \right) \right) \right)$$

4D Var: Computation of the gradient

We can therefore compute the gradient as follows

1. First compute x_k recursively using the resolvent matrix M_k and initial state x_0.
2. Compute $\Delta_k = R_k^{-1}(y_k - H_k x_k)$.
3. Define $\tilde{x}_k \in \mathbb{R}^n$ (the adjoint state variable). Initialise with $\tilde{x}_K = H_K^\top \Delta_K$. Then, given $\tilde{x}_{k+1}$, $\tilde{x}_k = H_k^\top \Delta_k + M_{k+1}^\top \tilde{x}_{k+1}$.
4. $\nabla_{x_0} J = B^{-1}(x_0 - x^b) - \tilde{x}_0$.

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 $P^a = \mathrm{Hess}(J)^{-1}$.

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

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

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 filters

In the case of no model errors and when M_k and H_k are both linear, M_k are invertible, one can show that the output x_K of 4D-Var is precisely the output of the Kalman filter. Note however that there is no equivalence between the intermediate outputs x_k for $k < K$.

Equivalence to the Kalman filter

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 $j = 0, \ldots, K$.

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

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We have

$$x_0 \in \operatorname{argmin} J(x) = \frac{1}{2}\left\|x - x^b\right\|^2_{B^{-1}} + \frac{1}{2}\sum_{k=0}^{K}\|H_k(M_{k,0}x) - y_k\|^2_{R_k^{-1}}$$

if and only if $M_{j,0}x_0 = x_j$ where writing $x_j^b = M_{j,0}x^b$ and $B_j^{-1} \stackrel{\text{def.}}{=} M_{0,j}^\top B_0^{-1} M_{0,j}$

$$x_j \in \operatorname{argmin}_x \tilde{J}_j(x) \stackrel{\text{def.}}{=} \frac{1}{2}\left\|x - x_j^b\right\|^2_{B_j^{-1}} + \frac{1}{2}\sum_{k=0}^{K}\|H_k(M_{k,j}x) - y_k\|^2_{R_k^{-1}}$$

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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

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

2. Transferability of optimality

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

Lemma 4.1

Consider the following:

- *Let x_0 be the minimiser of* $J(x) = \frac{1}{2}\left\|x - x^b\right\|^2_{B^{-1}} + \frac{1}{2}\sum_{k=0}^{K}\left\|H_k(M_{k,0}x) - y_k\right\|^2_{R_k^{-1}}$.
- *Let $m < K$ and x^a be the minimiser of* $J_m(x) = \frac{1}{2}\left\|x - x^b\right\|^2_{B^{-1}} + \frac{1}{2}\sum_{k=0}^{m}\left\|H_k(M_{k,0}x) - y_k\right\|^2_{R_k^{-1}}$. *Then, by defining $P^a \overset{\text{def.}}{=} \mathcal{H}_{x^a}^{-1}$ where $\mathcal{H}_{x^a}$ is the Hessian of J_m at x^a, let*

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

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

2. Transferability of optimality

Proof.

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

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,

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

Therefore,

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

as required. $\square$

Weak constrained 4D Var

When the model is inexact $x^t_{k+1} = M_{k+1} x^t_k + e^m_k$ and consider the cost

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

This is called weak constrained 4D Var. However, this requires optimisation over $x_0, \ldots, x_j$ and is therefore much more computationally expensive.

Summary

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.