Assimilation Algorithms
Lecture 1: Basic Concepts

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A Covid story

Forehead	37.5°C
Armpit L	36.0°C

A Covid story

Forehead	37.5°C
Armpit L	36.0°C 36.3°C

A Covid story

Forehead	37.5°C
Armpit L	36.0°C
	36.3°C
Armpit R	36.2°C
	36.2°C

A Covid story

Forehead	37.5°C	A priori
Armpit L	36.0°C	Observation bias
	36.3°C	Observation error
Armpit R	36.2°C	Obs. operator error
	36.2°C	

Outline

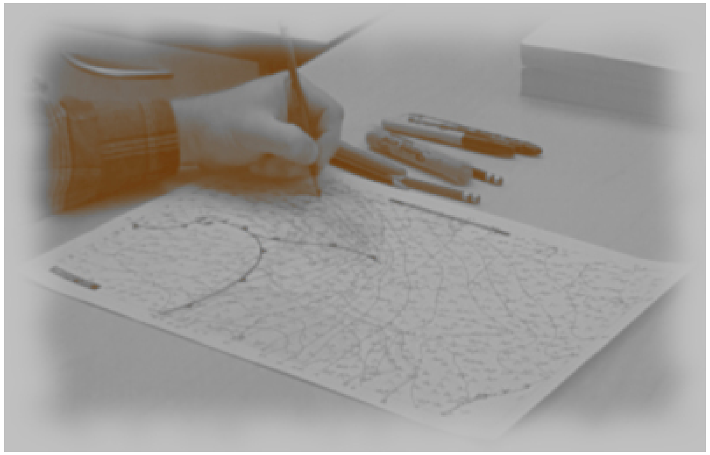
Outline

Interpreting the weather situation

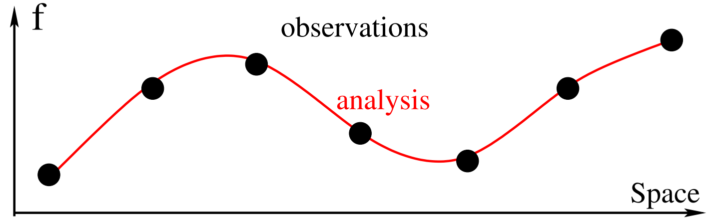
Definition

Analysis: The process of approximating the true state of a (geo-)physical system at a given time using the available knowledge.

- First hand analysis of synoptic observations in 1850 by LeVerrier and Fitzroy.



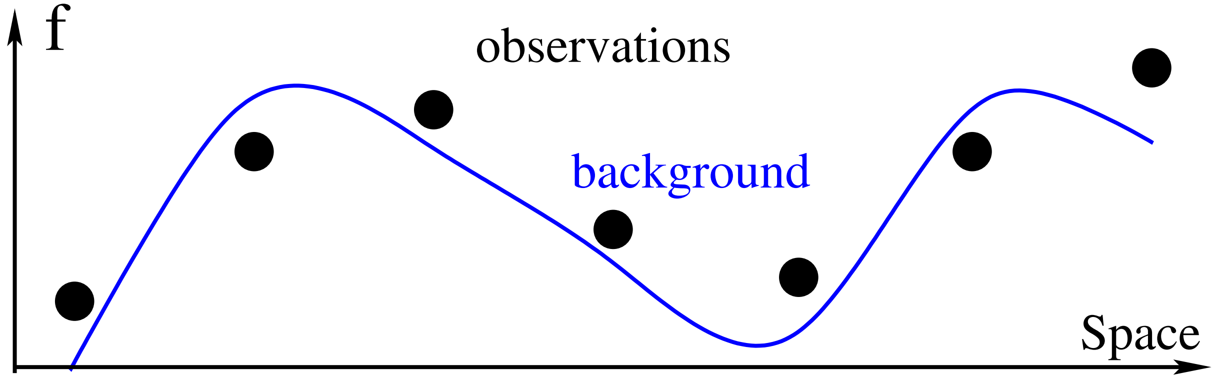
- Polynomial Interpolation in the 1950s by Panofsky with the developments of computers



The black dots denote the data points, while the red curve shows the polynomial interpolation.

Background

- An important step forward was made by Gilchrist and Cressman (1954), who introduced the idea of using a previous numerical forecast to provide a preliminary estimate of the analysis.



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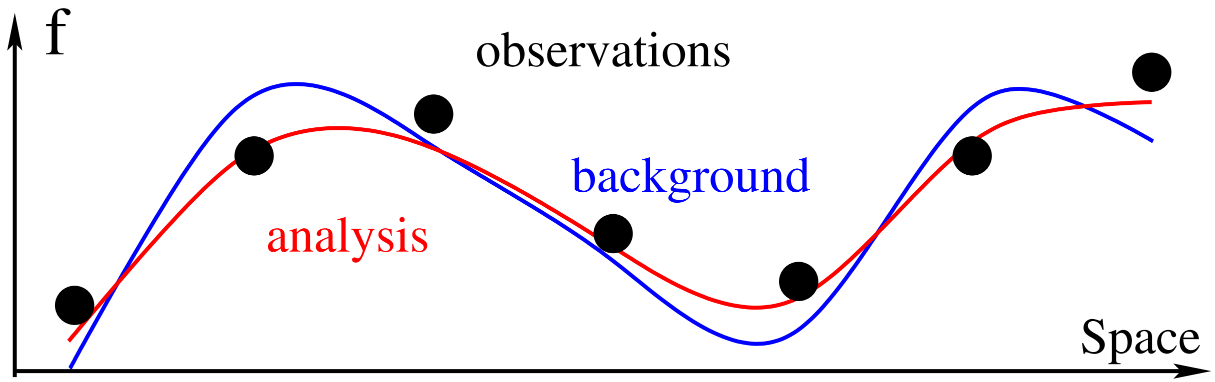

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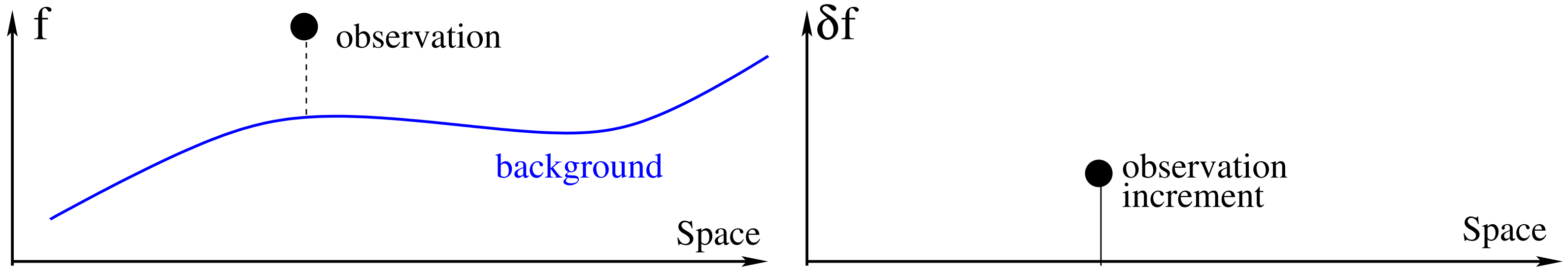
Optimal interpolation

- Bergthorsson and Döös (1955) took the idea of using a background field a step further by casting the analysis problem in terms of increments which were added to the background.



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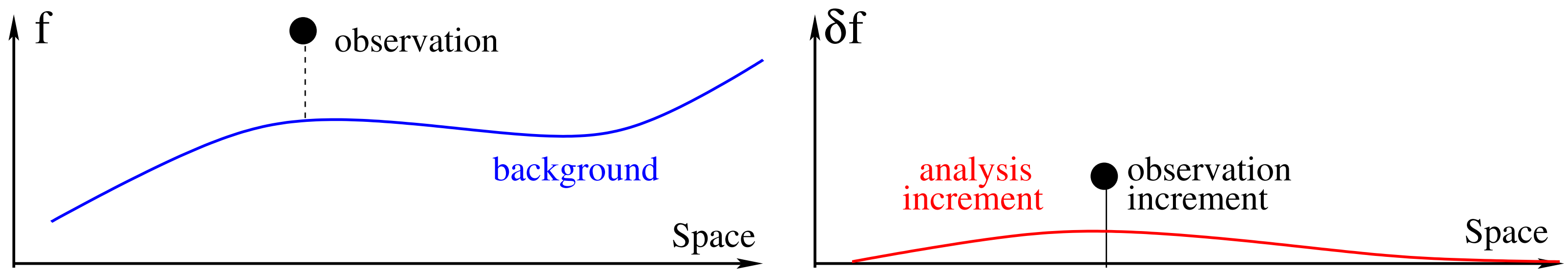

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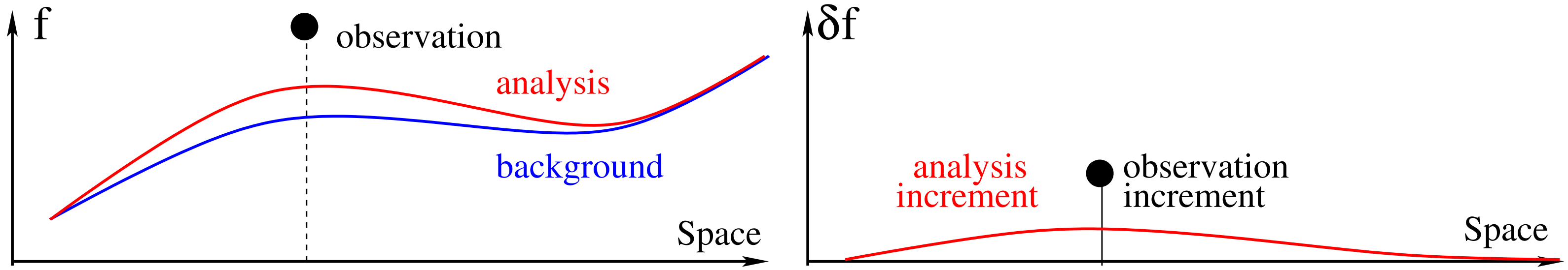

- The increments were weighted linear combinations of nearby observation increments (observation minus background), with the weights determined statistically.
- This idea of statistical combination of background and synoptic observations led ultimately to Optimal Interpolation.
- The use of statistics to merge model fields with observations is fundamental to all current methods of analysis.

Data Assimilation

- ✗ An important change of emphasis happened in the early 1970s with the introduction of primitive-equation models.
- ✗ Primitive equation models support inertia-gravity waves. This makes them much more fussy about their initial conditions than the filtered models that had been used hitherto.
- ✗ The analysis procedure became much more intimately linked with the model. The analysis had to produce an initial state that respected the model's dynamical balances.
- ✗ Unbalanced increments from the analysis procedure would be rejected as a result of geostrophic adjustment.
- ✗ Initialisation techniques (which suppress inertia-gravity waves) became important.

Data Assimilation

The idea that the analysis procedure must present observational information to the model in a way in which it can be absorbed (i.e. not rejected by geostrophic adjustment) led to the coining of the term data assimilation.

Wiktionary: Assimilate

1. To incorporate nutrients into the body, especially after digestion.
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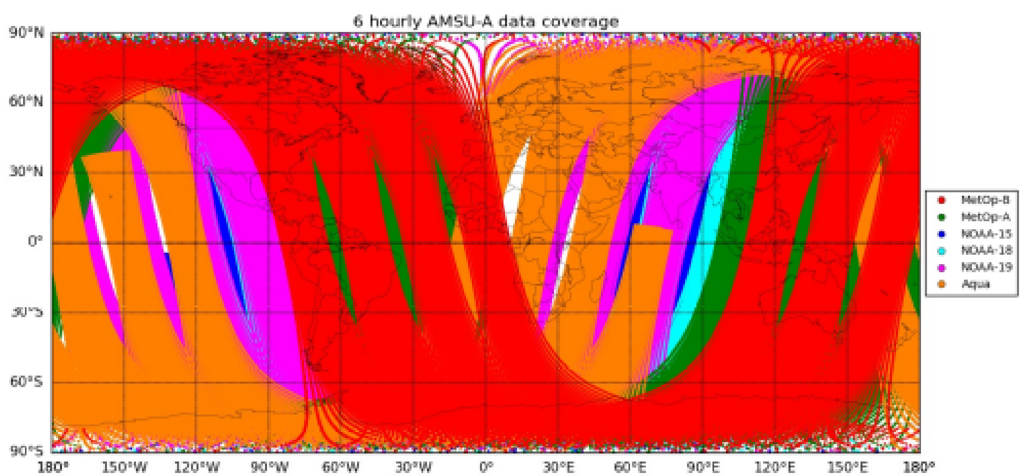
Our definition

✗ The process of objectively adapting the model state to observations in a statistically optimal way taking into account model and observation errors

Data Assimilation

- A final impetus towards the modern concept of data assimilation came from the increasing availability of asynoptic observations from satellite instruments.
- It was no longer sufficient to think of the analysis purely in terms of spatial interpolation of contemporaneous observations.
- The time dimension became important, and the model dynamics assumed the role of propagating observational information in time to allow a synoptic view of the state of the system to be generated from asynoptic data.



- Example of satellite data coverage in 6 hours (AMSU-A data).

Outline

Elementary Statistics

Problem

Suppose we want to estimate the body temperature of a person, given:

- A prior estimate: T_b.
- A thermometer: T_o.
- The true (unknown) body temperature T_t.

Errors

- The errors in T_b and T_o are:

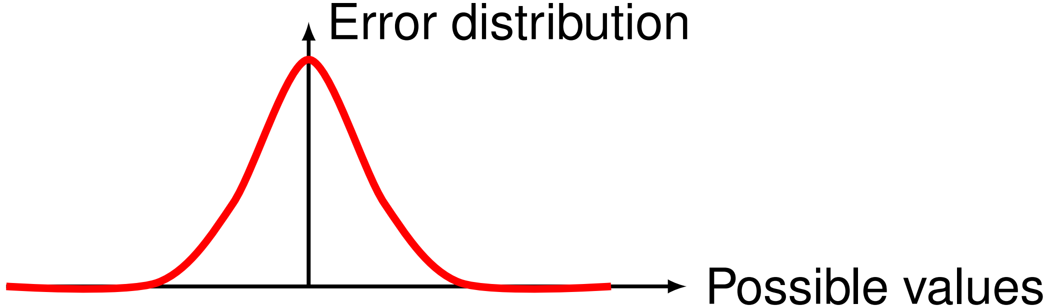
$$\begin{aligned} \varepsilon_b &= T_b - T_t \\ \varepsilon_o &= T_o - T_t \end{aligned}$$

- ε_b and ε_o are random variables (or stochastic variables)

Elementary Statistics

Hypotheses

- We will assume that the error statistics of T_b and T_o are known.



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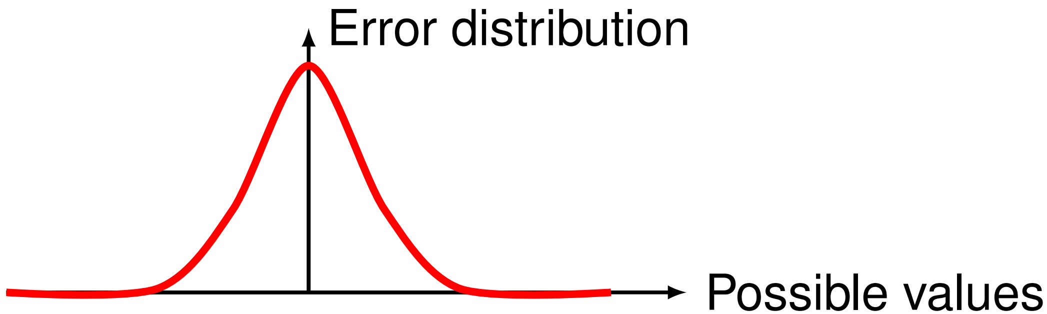

- We will assume that T_b and T_o have been adjusted (bias corrected) so that their mean errors are zero:

$$\overline{\varepsilon_b} = \overline{\varepsilon_o} = 0\,.$$

- There is usually no reason for ε_b and ε_o to be connected in any way:

$$\overline{\varepsilon_o \varepsilon_b} = 0\,.$$

- The quantity $\overline{\varepsilon_o \varepsilon_b}$ represents the covariance between the error of our prior estimate and the error of our thermometer measurement.

Elementary Statistics

- We estimate the body temperature as a linear combination of T_b and T_o:

$$T_a = \alpha T_o + \beta T_b + \gamma$$

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- Denote the error of our estimate as $\varepsilon_a = T_a - T_t$.
- We have:

$$T_a = T_t + \varepsilon_a = \alpha \left(T_t + \varepsilon_o \right) + \beta \left(T_t + \varepsilon_b \right) + \gamma$$

$$\text{or} \quad \varepsilon_a = (\alpha + \beta - 1)\, T_t + \alpha\, \varepsilon_o + \beta\, \varepsilon_b + \gamma$$

Elementary Statistics

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- We want the estimate to be unbiased: $\overline{\varepsilon_a} = 0$:

$$\overline{\varepsilon_a} = (\alpha + \beta - 1)\, T_t + \gamma = 0$$

- Since this holds for any T_t, we must have
  - ⇨ $\gamma = 0$ and $\alpha + \beta - 1 = 0$.
- Then

$$T_a = \alpha T_o + (1 - \alpha) T_b$$

Elementary Statistics

- The general Linear Unbiased Estimate is:

$$T_a = \alpha T_o + (1-\alpha) T_b$$

- Now consider the error of this estimate.
- Subtracting T_t from both sides of the equation gives

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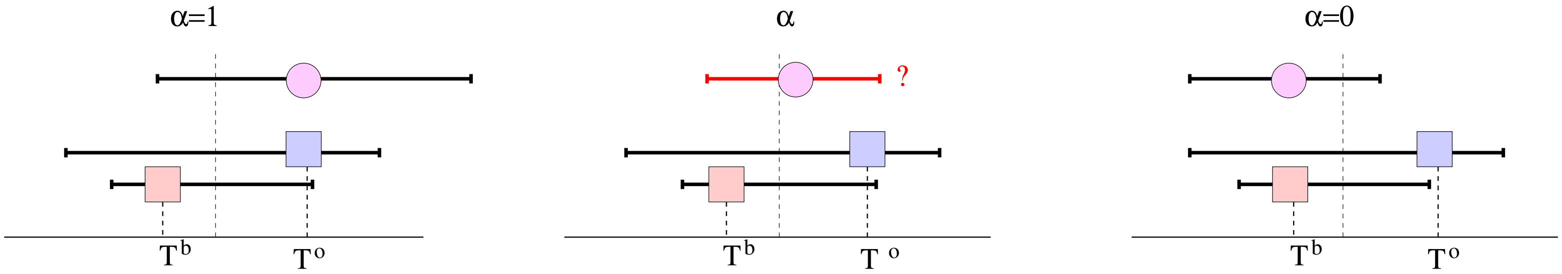

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$$\varepsilon_a = \alpha\, \varepsilon_o + (1-\alpha)\, \varepsilon_b$$

- The variance of the estimate is:

$$\overline{\varepsilon_a^2} = \alpha^2\, \overline{\varepsilon_o^2} + 2\alpha(1-\alpha)\, \overline{\varepsilon_o \varepsilon_b} + (1-\alpha)^2\, \overline{\varepsilon_b^2}$$

- With the previous hypothesis $\overline{\varepsilon_o \varepsilon_b} = 0$:

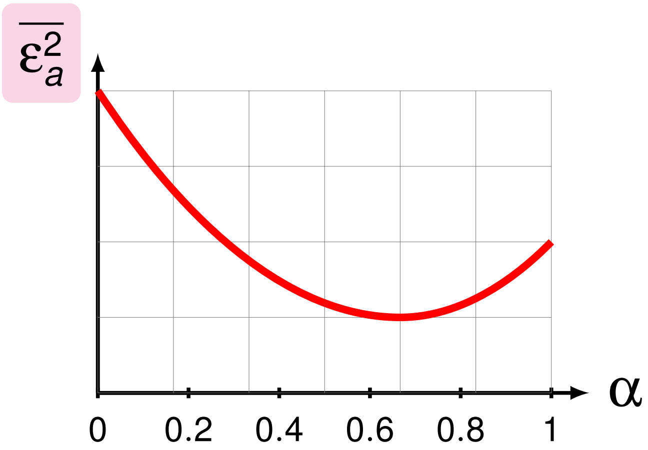
$$\overline{\varepsilon_a^2} = \alpha^2\, \overline{\varepsilon_o^2} + (1-\alpha)^2\, \overline{\varepsilon_b^2}$$

Elementary Statistics

$$\overline{\varepsilon_a^2} = \alpha^2 \, \overline{\varepsilon_o^2} + (1-\alpha)^2 \, \overline{\varepsilon_b^2}$$

We can easily derive some properties of our estimate:

- $\frac{d\overline{\varepsilon_a^2}}{d\alpha} = 2\alpha\overline{\varepsilon_o^2} - 2(1-\alpha)\overline{\varepsilon_b^2}$
- For $\alpha = 0$, $\overline{\varepsilon_a^2} = \overline{\varepsilon_b^2}$ and $\frac{d\overline{\varepsilon_a^2}}{d\alpha} = -2\overline{\varepsilon_b^2} < 0$
- For $\alpha = 1$, $\overline{\varepsilon_a^2} = \overline{\varepsilon_o^2}$ and $\frac{d\overline{\varepsilon_a^2}}{d\alpha} = 2\overline{\varepsilon_o^2} > 0$



From this we can deduce:

- For $0 \le \alpha \le 1$, $\overline{\varepsilon_a^2} \le \max(\overline{\varepsilon_b^2}, \overline{\varepsilon_o^2})$
- The minimum-variance estimate occurs for $\alpha \in (0, 1)$.
- The minimum-variance estimate satisfies $\overline{\varepsilon_a^2} < \min(\overline{\varepsilon_b^2}, \overline{\varepsilon_o^2})$, which means it is lower than the variance of each piece of information.

Elementary Statistics

The minimum-variance estimate occurs when

$$\frac{d\,\overline{\varepsilon_a^2}}{d\alpha} = 2\alpha\,\overline{\varepsilon_o^2} - 2(1-\alpha)\,\overline{\varepsilon_b^2} = 0$$

$$\Rightarrow \qquad \alpha = \frac{\overline{\varepsilon_b^2}}{\overline{\varepsilon_b^2} + \overline{\varepsilon_o^2}}.$$

It is not difficult to show that the error variance of this minimum-variance estimate is:

$$\frac{1}{\overline{\varepsilon_a^2}} = \frac{1}{\overline{\varepsilon_b^2}} + \frac{1}{\overline{\varepsilon_o^2}},$$

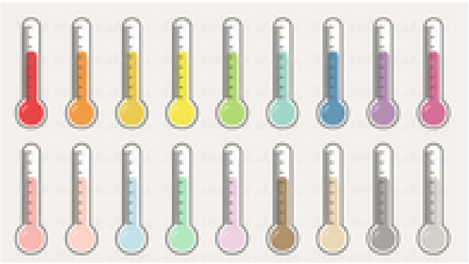
and the analysis is:

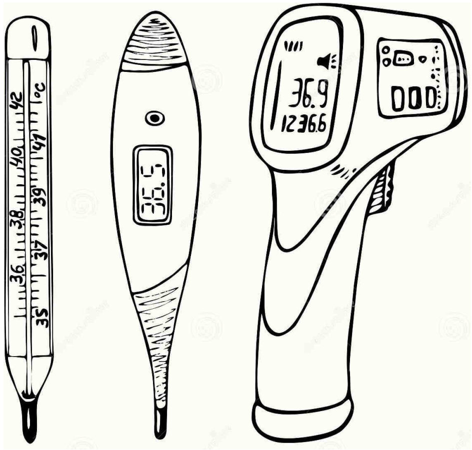
$$\frac{T_a}{\overline{\varepsilon_a^2}} = \frac{T_b}{\overline{\varepsilon_b^2}} + \frac{T_o}{\overline{\varepsilon_o^2}}.$$

Outline

A Covid story - Part 2

Forehead	37.5°C
Armpit L - T_1	36.0°C
	36.3°C
Armpit R - T_1	36.2°C
	36.2°C
Armpit L - T_2	36.1°C
	36.2°C
Armpit R - T_2	35.9°C
	36.0°C
Armpit L - T_3	···°C
	···°C
Armpit R - T_3	···°C
	···°C





Extension to Multiple Dimensions

- Now, let's turn our attention to the multi-dimensional case.
- Instead of a scalar prior estimate T_b, we now consider a vector $\mathbf{x}_b$.
- We can think of $\mathbf{x}_b$ as representing the entire state of a numerical model at some time.
- The elements of $\mathbf{x}_b$ might be grid-point values, spherical harmonic coefficients, etc., and some elements may represent temperatures, humidity, others wind components, etc.
- We refer to $\mathbf{x}_b$ as the background.
- Similarly, we generalise the observation to a vector $\mathbf{y}$.
- $\mathbf{y}$ can contain a disparate collection of observations at different locations, and of different variables.

Extension to Multiple Dimensions

- The major difference between the simple scalar example and the multi-dimensional case is that there is no longer a one-to-one correspondence between the elements of the observation vector and those of the background vector.

$\mathbf{x} \rightarrow$  $\leftarrow \mathbf{y}$

- It is no longer trivial to compare observations and background.
- When the background is a state of a numerical model at some time
  - Observations are not necessarily located at model gridpoints
  - The observed variables (e.g. radiances) may not correspond directly with any of the variables of the model.
  - To overcome this problem, we must assume that our model is a more-or-less complete representation of reality, so that we can always determine “model equivalents” of the observations.

Extension to Multiple Dimensions

- We formalise this by assuming the existence of an observation operator, $\mathcal{H}$.
- Given a model-space vector, $\mathbf{x}$, the vector $\mathcal{H}(\mathbf{x})$ can be compared directly with $\mathbf{y}$, and represents the "model equivalent" of $\mathbf{y}$.

$$\mathbf{x} \xrightarrow{\mathcal{H}(\cdot)} \mathcal{H}(\mathbf{x}) \rightarrow$$

$$\leftarrow \mathbf{y}$$

- For now, we will assume that $\mathcal{H}$ is perfect. I.e. it does not introduce any error, so that:

$$\mathcal{H}(\mathbf{x}_t) = \mathbf{y}_t$$

where $\mathbf{x}_t$ is the true state, and $\mathbf{y}_t$ contains the true values of the observed quantities.

Extension to Multiple Dimensions

- As we did in the scalar case, we will look for an analysis that is a linear combination of the available information:

$$\mathbf{x}_a = \mathbf{F}\mathbf{x}_b + \mathbf{K}\mathbf{y} + \mathbf{c}$$

  where **F** and **K** are matrices, and where **c** is a vector.
- If $\mathcal{H}$ is linear, we can proceed as in the scalar case and look for a linear unbiased estimate.
- In the more general case of nonlinear $\mathcal{H}$, we will require that error-free inputs ($\mathbf{x}_b = \mathbf{x}_t$ and $\mathbf{y} = \mathbf{y}_t$) produce an error-free analysis ($\mathbf{x}_a = \mathbf{x}_t$):

$$\mathbf{x}_t = \mathbf{F}\mathbf{x}_t + \mathbf{K}\mathcal{H}(\mathbf{x}_t) + \mathbf{c}$$

- Since this applies for any $\mathbf{x}_t$, we must have $\mathbf{c} = 0$ and

$$\mathbf{I} \equiv \mathbf{F} + \mathbf{K}\mathcal{H}(\cdot) \quad \text{or} \quad \mathbf{F} \equiv \mathbf{I} - \mathbf{K}\mathcal{H}(\cdot)$$

- Our analysis equation is thus:

$$\mathbf{x}_a = \mathbf{x}_b + \mathbf{K}(\mathbf{y} - \mathcal{H}(\mathbf{x}_b))$$

Extension to Multiple Dimensions

$$\mathbf{x}_a = \mathbf{x}_b + \mathbf{K}\left(\mathbf{y} - \mathcal{H}(\mathbf{x}_b)\right)$$

- Remember that in the scalar case, we had

$$\begin{aligned} T_a &= \alpha T_o + (1-\alpha) T_b \\ &= T_b + \alpha (T_o - T_b) \end{aligned}$$

- We see that the matrix **K** plays a role equivalent to that of the coefficient α.
- **K** is called the gain matrix.
- It determines the weight given to the innovation $\mathbf{y} - \mathcal{H}(\mathbf{x}_b)$
- It handles the transformation of information defined in “observation space” to the space of model variables.

Extension to Multiple Dimensions

- The next step in deriving the analysis equation is to describe the statistical properties of the analysis errors.
- We define

$$\begin{aligned} \varepsilon_a &= \mathbf{x}_a - \mathbf{x}_t \\ \varepsilon_b &= \mathbf{x}_b - \mathbf{x}_t \\ \varepsilon_o &= \mathbf{y} - \mathbf{y}_t \end{aligned}$$

- We will assume that the errors are small, so that

$$\mathcal{H}(\mathbf{x}_b) = \mathcal{H}(\mathbf{x}_t) + \mathbf{H}\,\varepsilon_b + O(\varepsilon_b^2)$$

where **H** is the Jacobian of $\mathcal{H}$ (if $\mathcal{H}$ is nonlinear).

Extension to Multiple Dimensions

- Substituting the expressions for the errors into our analysis equation, and using $\mathcal{H}(\mathbf{x}_t) = \mathbf{y}_t$, gives (to first order):

$$\varepsilon_a = \varepsilon_b + \mathbf{K}\left(\varepsilon_o - \mathbf{H}\varepsilon_b\right)$$

- As in the scalar example, we will assume that the mean errors have been removed, so that $\overline{\varepsilon_b} = \overline{\varepsilon_o} = 0$. We see that this implies that $\overline{\varepsilon_a} = 0$.
- In the scalar example, we derived the variance of the analysis error, and defined our optimal analysis to minimise this variance.
- In the multi-dimensional case, we must deal with covariances.

Covariance

- The covariance between two variables x_i and x_j is defined as

$$\mathrm{cov}(x_i, x_j) = \overline{(x_i - \overline{x_i})(x_j - \overline{x_j})}$$

- Given a vector $\mathbf{x} = (x_1, x_2, \cdots, x_N)^{\mathrm{T}}$, we can arrange the covariances into a covariance matrix, $\mathbf{C}$, such that $C_{ij} = \mathrm{cov}(x_i, x_j)$.
- Equivalently:

$$\mathbf{C} = \overline{(\mathbf{x} - \overline{\mathbf{x}})(\mathbf{x} - \overline{\mathbf{x}})^{\mathrm{T}}}$$

- Covariance matrices are symmetric and positive definite
  - symmetric: $\mathbf{C}^T = \mathbf{C}$
  - positive definite: $\mathbf{z}^T\mathbf{C}\,\mathbf{z}$ is positive for every non-zero vector $\mathbf{z}$

Extension to Multiple Dimensions

- The analysis error is:

$$
\begin{aligned}
\varepsilon_a &= \varepsilon_b + \mathbf{K}\left(\varepsilon_o - \mathbf{H}\varepsilon_b\right) \\
&= \left(\mathbf{I} - \mathbf{KH}\right)\varepsilon_b + \mathbf{K}\varepsilon_o
\end{aligned}
$$

Extension to Multiple Dimensions

- The analysis error is:

$$\begin{aligned} \varepsilon_a &= \varepsilon_b + \mathbf{K}\left(\varepsilon_o - \mathbf{H}\varepsilon_b\right) \\ &= (\mathbf{I} - \mathbf{KH})\varepsilon_b + \mathbf{K}\varepsilon_o \end{aligned}$$

- Forming the analysis error covariance matrix gives:

$$\begin{aligned} \overline{\varepsilon_a \varepsilon_a^{\mathrm{T}}} &= \overline{\left[(\mathbf{I} - \mathbf{KH})\varepsilon_b + \mathbf{K}\varepsilon_o\right]\left[(\mathbf{I} - \mathbf{KH})\varepsilon_b + \mathbf{K}\varepsilon_o\right]^{\mathrm{T}}} \\ &= (\mathbf{I} - \mathbf{KH})\overline{\varepsilon_b \varepsilon_b^{\mathrm{T}}}(\mathbf{I} - \mathbf{KH})^{\mathrm{T}} \\ &+ \mathbf{K}\overline{\varepsilon_o \varepsilon_o^{\mathrm{T}}}\mathbf{K}^{\mathrm{T}} \\ &+ \mathbf{K}\overline{\varepsilon_o \varepsilon_b^{\mathrm{T}}}(\mathbf{I} - \mathbf{KH})^{\mathrm{T}} + (\mathbf{I} - \mathbf{KH})\overline{\varepsilon_b \varepsilon_o^{\mathrm{T}}}\mathbf{K}^{\mathrm{T}} \end{aligned}$$

- Assuming that the background and observation errors are uncorrelated (i.e. $\overline{\varepsilon_o \varepsilon_b^{\mathrm{T}}} = \overline{\varepsilon_b \varepsilon_o^{\mathrm{T}}} = 0$), we find:

$$\overline{\varepsilon_a \varepsilon_a^{\mathrm{T}}} = (\mathbf{I} - \mathbf{KH})\overline{\varepsilon_b \varepsilon_b^{\mathrm{T}}}(\mathbf{I} - \mathbf{KH})^{\mathrm{T}} + \mathbf{K}\overline{\varepsilon_o \varepsilon_o^{\mathrm{T}}}\mathbf{K}^{\mathrm{T}}$$

Extension to Multiple Dimensions

$$\overline{\varepsilon_a \varepsilon_a^{\mathrm{T}}} = (\mathbf{I} - \mathbf{KH}) \, \overline{\varepsilon_b \varepsilon_b^{\mathrm{T}}} \, (\mathbf{I} - \mathbf{KH})^{\mathrm{T}} + \mathbf{K} \, \overline{\varepsilon_o \varepsilon_o^{\mathrm{T}}} \, \mathbf{K}^{\mathrm{T}}$$

- This expression is the equivalent of the expression we obtained for the error of the scalar analysis:

$$\begin{aligned} \overline{\varepsilon_a^2} &= (1-\alpha)^2 \, \overline{\varepsilon_b^2} + \alpha^2 \, \overline{\varepsilon_o^2} \\ &= (1-\alpha) \, \overline{\varepsilon_b^2} \, (1-\alpha) + \alpha \, \overline{\varepsilon_o^2} \, \alpha \end{aligned}$$

- Again, we see that **K** plays essentially the same role in the multi-dimensional analysis as α plays in the scalar case.
- In the scalar case, we chose α to minimise the variance of the analysis error.
- What do we mean by the minimum-variance analysis in the multi-dimensional case?

Extension to Multiple Dimensions

- Note that the diagonal elements of a covariance matrix are variances $C_{ii} = \mathrm{cov}(x_i, x_i) = \overline{(x_i - \overline{x_i})^2}$.
- Hence, we can define the minimum-variance analysis as the analysis that minimises the sum of the diagonal elements of the analysis error covariance matrix.
- The sum of the diagonal elements of a matrix is called the trace.
- In the scalar case, we found the minimum-variance analysis by setting $\frac{d\overline{\varepsilon_a^2}}{d\alpha}$ to zero.
- In the multidimensional case, we are going to set

$$\frac{\partial \mathrm{trace}(\overline{\varepsilon_a \varepsilon_a^{\mathrm{T}}})}{\partial \mathbf{K}} = \mathbf{0}$$

- Note: $\frac{\partial \mathrm{trace}(\overline{\varepsilon_a \varepsilon_a^{\mathrm{T}}})}{\partial \mathbf{K}}$ is the matrix whose ij^{th} element is $\frac{\partial \mathrm{trace}(\overline{\varepsilon_a \varepsilon_a^{\mathrm{T}}})}{\partial K_{ij}}$.

Extension to Multiple Dimensions

- We have: $\overline{\varepsilon_a \varepsilon_a^{\mathrm{T}}} = (\mathbf{I} - \mathbf{KH}) \overline{\varepsilon_b \varepsilon_b^{\mathrm{T}}} (\mathbf{I} - \mathbf{KH})^{\mathrm{T}} + \mathbf{K} \overline{\varepsilon_o \varepsilon_o^{\mathrm{T}}} \mathbf{K}^{\mathrm{T}}$.
- The following matrix identities come to our rescue:

$$\frac{\partial \mathrm{trace}(\mathbf{KAK}^{\mathrm{T}})}{\partial \mathbf{K}} = \mathbf{K}(\mathbf{A} + \mathbf{A}^{\mathrm{T}})$$

$$\frac{\partial \mathrm{trace}(\mathbf{KA})}{\partial \mathbf{K}} = \mathbf{A}^{\mathrm{T}}$$

$$\frac{\partial \mathrm{trace}(\mathbf{AK}^{\mathrm{T}})}{\partial \mathbf{K}} = \mathbf{A}$$

- Applying these to $\partial \mathrm{trace}(\overline{\varepsilon_a \varepsilon_a^{\mathrm{T}}}) / \partial \mathbf{K}$ gives:

$$\frac{\partial \mathrm{trace}(\overline{\varepsilon_a \varepsilon_a^{\mathrm{T}}})}{\partial \mathbf{K}} = 2\mathbf{K}\left[\mathbf{H} \overline{\varepsilon_b \varepsilon_b^{\mathrm{T}}} \mathbf{H}^{\mathrm{T}} + \overline{\varepsilon_o \varepsilon_o^{\mathrm{T}}}\right] - 2 \overline{\varepsilon_b \varepsilon_b^{\mathrm{T}}} \mathbf{H}^{\mathrm{T}} = \mathbf{0}$$

- Hence: $\mathbf{K} = \overline{\varepsilon_b \varepsilon_b^{\mathrm{T}}} \mathbf{H}^{\mathrm{T}} \left[\mathbf{H} \overline{\varepsilon_b \varepsilon_b^{\mathrm{T}}} \mathbf{H}^{\mathrm{T}} + \overline{\varepsilon_o \varepsilon_o^{\mathrm{T}}}\right]^{-1}$.

Extension to Multiple Dimensions

$$\mathbf{K} = \overline{\varepsilon_b \varepsilon_b^{\mathrm{T}}}\, \mathbf{H}^{\mathrm{T}} \left[\mathbf{H}\, \overline{\varepsilon_b \varepsilon_b^{\mathrm{T}}}\, \mathbf{H}^{\mathrm{T}} + \overline{\varepsilon_o \varepsilon_o^{\mathrm{T}}} \right]^{-1}$$

- This optimal gain matrix is called the Kalman Gain Matrix.
- Note the similarity with the optimal gain we derived for the scalar analysis:

$$\alpha = \overline{\varepsilon_b^2} \left[\overline{\varepsilon_b^2} + \overline{\varepsilon_o^2} \right]^{-1}$$

- The variance of analysis error for the optimal scalar problem was:

$$\frac{1}{\overline{\varepsilon_a^2}} = \frac{1}{\overline{\varepsilon_b^2}} + \frac{1}{\overline{\varepsilon_o^2}}$$

- The equivalent expression for the multi-dimensional case is:

$$\left[\overline{\varepsilon_a \varepsilon_a^{\mathrm{T}}} \right]^{-1} = \left[\overline{\varepsilon_b \varepsilon_b^{\mathrm{T}}} \right]^{-1} + \mathbf{H}^{\mathrm{T}} \left[\overline{\varepsilon_o \varepsilon_o^{\mathrm{T}}} \right]^{-1} \mathbf{H}$$

Notation

- The notation we have used for covariance matrices can get a bit cumbersome.
- The standard notation is:

$$\mathbf{P}^a \equiv \overline{\varepsilon_a \varepsilon_a^{\mathrm{T}}}$$

$$\mathbf{P}^b \equiv \overline{\varepsilon_b \varepsilon_b^{\mathrm{T}}}$$

$$\mathbf{R} \equiv \overline{\varepsilon_o \varepsilon_o^{\mathrm{T}}}$$

- In many analysis schemes, the true covariance matrix of background error, $\mathbf{P}^b$, is not known, or is too large to be used.
- In this case, we use an approximate background error covariance matrix. This approximate matrix is denoted by $\mathbf{B}$.

Alternative Expression for the Kalman Gain

Finally, we derive an alternative expression for the Kalman gain:

$$\mathbf{K} = \mathbf{P}^b\mathbf{H}^{\mathrm{T}}\left[\mathbf{H}\mathbf{P}^b\mathbf{H}^{\mathrm{T}} + \mathbf{R}\right]^{-1}$$

Multiplying both sides by $\left[\mathbf{P}^{b^{-1}} + \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\right]$ gives:

$$\begin{aligned}\left[\mathbf{P}^{b^{-1}} + \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\right]\mathbf{K} &= \left[\mathbf{H}^{\mathrm{T}} + \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\mathbf{P}^b\mathbf{H}^{\mathrm{T}}\right]\left[\mathbf{H}\mathbf{P}^b\mathbf{H}^{\mathrm{T}} + \mathbf{R}\right]^{-1} \\ &= \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\left[\mathbf{R} + \mathbf{H}\mathbf{P}^b\mathbf{H}^{\mathrm{T}}\right]\left[\mathbf{H}\mathbf{P}^b\mathbf{H}^{\mathrm{T}} + \mathbf{R}\right]^{-1} \\ &= \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\end{aligned}$$

Hence:

$$\mathbf{K} = \left[\mathbf{P}^{b^{-1}} + \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\right]^{-1}\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}$$

- ✘ Expression 1: need the inverse of a matrix of dimension size($\mathbf{R}$)
- ✘ Expression 2: need the inverse of a matrix of dimension size($\mathbf{P}^b$)
- ✘ Remember that $\mathbf{x}_a = \mathbf{x}_b + \mathbf{K}\left(\mathbf{y} - \mathcal{H}(\mathbf{x}_b)\right)$

Outline

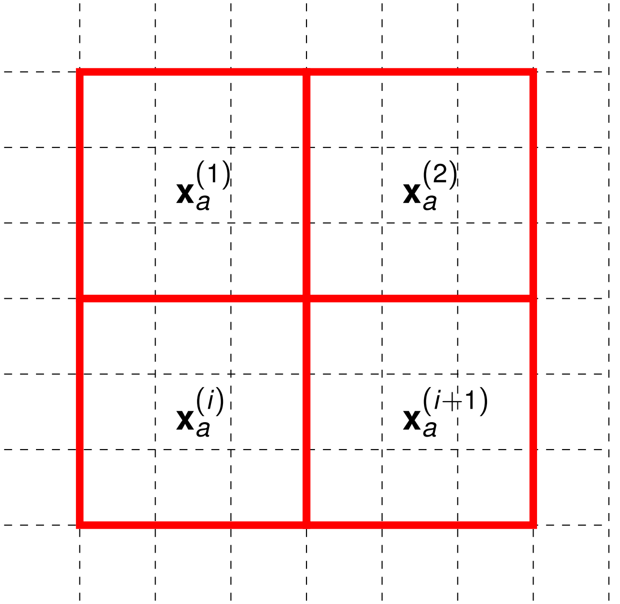
Optimal Interpolation

- Optimal Interpolation is a statistical data assimilation method based on the multi-dimensional analysis equations we have just derived.
- The Kalman gain $\mathbf{K}$ can not be computed because of the size of $\mathbf{P}^b$ and $\mathbf{R}$
- The basic idea is to split the global analysis into a number of boxes which can be analysed independently:

$$\mathbf{x}_a^{(i)} = \mathbf{x}_b^{(i)} + \mathbf{K}^{(i)} \left[\mathbf{y}^{(i)} - \mathcal{H}^{(i)}(\mathbf{x}_b) \right]$$

where

$$\mathbf{x}_a = \begin{pmatrix} \mathbf{x}_a^{(1)} \\ \mathbf{x}_a^{(2)} \\ \vdots \\ \mathbf{x}_a^{(M)} \end{pmatrix} \quad \mathbf{x}_b = \begin{pmatrix} \mathbf{x}_b^{(1)} \\ \mathbf{x}_b^{(2)} \\ \vdots \\ \mathbf{x}_b^{(M)} \end{pmatrix} \quad \mathbf{K} = \begin{pmatrix} \mathbf{K}^{(1)} \\ \mathbf{K}^{(2)} \\ \vdots \\ \mathbf{K}^{(M)} \end{pmatrix}$$

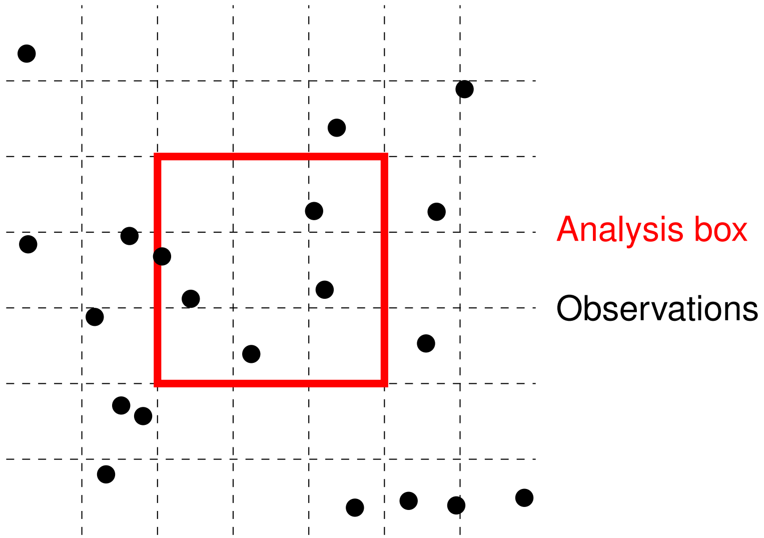


- The method was used operationally at ECMWF from 1979 until 1996, when it was replaced by 3D-Var.

Optimal Interpolation

$$\mathbf{x}_a^{(i)} = \mathbf{x}_b^{(i)} + \mathbf{K}^{(i)} \left(\mathbf{y}^{(i)} - \mathcal{H}^{(i)}(\mathbf{x}_b) \right)$$

- In principle, we should use *all* available observations to calculate the analysis for each box. However, this might be too expensive.
- To produce a computationally-feasible algorithm, Optimal Interpolation (OI) restricts the observations used for each box to those observations which lie in a surrounding selection area:



Optimal Interpolation

$$\mathbf{x}_a^{(i)} = \mathbf{x}_b^{(i)} + \mathbf{K}^{(i)} \left(\mathbf{y}^{(i)} - \mathcal{H}^{(i)}(\mathbf{x}_b) \right)$$

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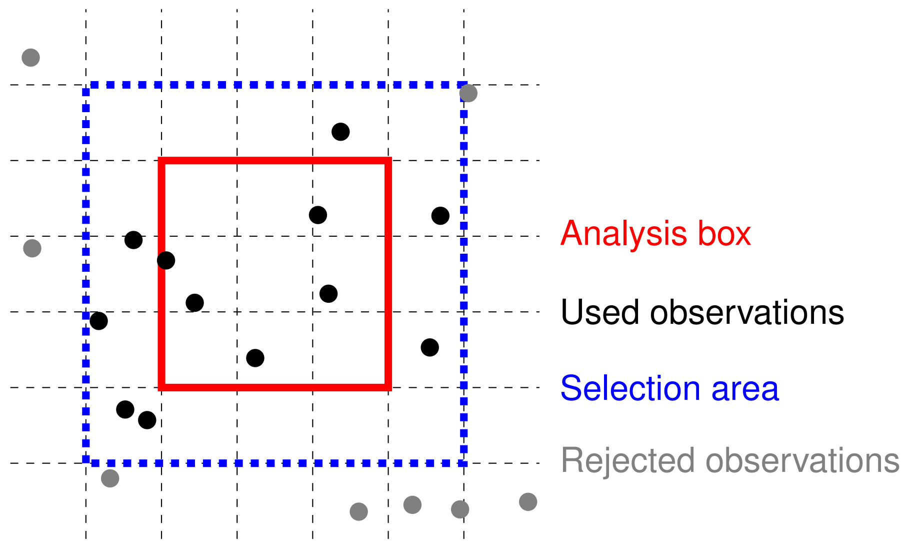

Optimal Interpolation

- The gain matrix used for each box is:

$$\mathbf{K}^{(i)} = \left(\mathbf{P}^b\mathbf{H}^{\mathrm{T}}\right)^{(i)} \left[\left(\mathbf{H}\mathbf{P}^b\mathbf{H}^{\mathrm{T}}\right)^{(i)} + \mathbf{R}^{(i)}\right]^{-1}$$

- Now, the dimension of the matrix $\left[\left(\mathbf{H}\mathbf{P}^b\mathbf{H}^{\mathrm{T}}\right)^{(i)} + \mathbf{R}^{(i)}\right]$ is equal to the number of observations in the selection box.
- Selecting observations reduces the size of this matrix, making it feasible to use direct solution methods to invert it.
- Note that to implement Optimal Interpolation, we have to specify $\left(\mathbf{P}^b\mathbf{H}^{\mathrm{T}}\right)^{(i)}$ and $\left(\mathbf{H}\mathbf{P}^b\mathbf{H}^{\mathrm{T}}\right)^{(i)}$. This effectively limits us to very simple observation operators, corresponding to simple interpolations.
- This, together with the artifacts introduced by observation selection, was one of the main reasons for abandoning Optimal Interpolation in favour of 3D-Var.

Outline

Summary

- We derived the linear analysis equation for a simple scalar example.
- We showed that a particular choice of the weight α given to the observation resulted in an optimal minimum-variance analysis.
- We repeated the derivation for the multi-dimensional case. This required the introduction of the observation operator.
- The derivation for the multi-dimensional case closely parallelled the scalar derivation.
- The expressions for the gain matrix and analysis error covariance matrix were recognisably similar to the corresponding scalar expressions.
- Finally, we considered the practical implementation of the analysis equation, in an Optimal Interpolation data assimilation scheme.