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Later, we show that **3D-Var** is equivalent to the OI method, although the **method for solving** it is quite different.

Optimal interpolation (OI)

We now consider the complete NWP operational problem of finding an optimum analysis of a field of model variables x_a , given

- A **background field** x_b available at grid points in two or three dimensions
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$$[\text{Here } \dim(\mathbf{x}) = N_x N_y + 4 * N_x N_y N_z]$$

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Examples of these measurements are **radar** reflectivities and Doppler shifts, satellite **radiances**, and global positioning system (GPS) atmospheric **refractivities**.

Just as for a scalar variable, the analysis is cast as the background *plus* weighted innovation:

$$\mathbf{x}_a = \mathbf{x}_b + \mathbf{W}[\mathbf{y}_o - H(\mathbf{x}_b)] = \mathbf{x}_b + \mathbf{W}\mathbf{d}$$

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The **weights** are given by a matrix of dimension $(n \times p)$.

They are determined from **statistical interpolation**.

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- For every matrix expression, **check the orders** of the components to ensure that the expression is meaningful.
- Be aware whether vectors are **row** or **column** vectors.

Forward Operator: General Remarks

In general, **we do not directly observe** the grid-point variables that we want to analyze.

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Thus, we have to perform horizontal and vertical **interpolations**.

We also have remote sensing instruments (like satellites and radars) that measure quantities like radiances, reflectivities, refractivities, and Doppler shifts, rather than the variables themselves.

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The **direct assimilation** of radiances, using the forward observational model H to convert the first guess into **first guess TOVS radiances** has resulted in **major improvements** in forecast skill.

Simple Low-order Example

As an illustration, let us consider the simple case of **three grid points** e , f , g , and **two observations**, 1 and 2.

Simple Low-order Example

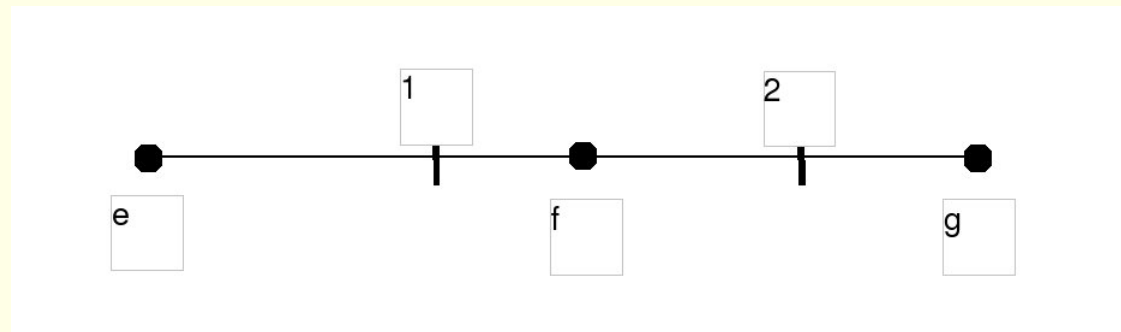
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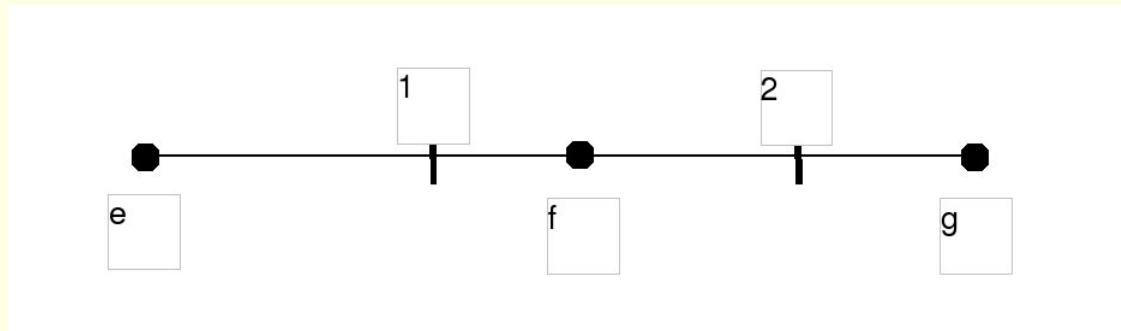


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Then

$$\mathbf{x}^a = (x_e^a, x_f^a, x_g^a)^T = \begin{pmatrix} x_e^a \\ x_f^a \\ x_g^a \end{pmatrix} \quad \text{and} \quad \mathbf{x}^b = (x_e^b, x_f^b, x_g^b)^T = \begin{pmatrix} x_e^b \\ x_f^b \\ x_g^b \end{pmatrix}$$

The Observational Operator H

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Note: The operator H is a **nonlinear vector function**. It maps from the n -dimensional analysis space to the p -dimensional observation space.

Observation Error Variances

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The observational error variance R is the sum of the instrument error variance R_{instr} and the representativity error variance R_{repr} , assuming that these errors are **not correlated**:

$$R = R_{\text{instr}} + R_{\text{repr}}$$

Error Covariance Matrix

The **error covariance matrix** is obtained by multiplying the vector error

$$\varepsilon = \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{bmatrix}$$

by its transpose

$$\varepsilon^T = [e_1 \ e_2 \ \dots \ e_n]$$

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We **average over many cases**, to obtain the expected value:

$$\mathbf{P} = \overline{\varepsilon \varepsilon^T} = \begin{bmatrix} \overline{e_1 e_1} & \overline{e_1 e_2} & \cdots & \overline{e_1 e_n} \\ \overline{e_2 e_1} & \overline{e_2 e_2} & \cdots & \overline{e_2 e_n} \\ \vdots & \vdots & & \vdots \\ \overline{e_n e_1} & \overline{e_n e_2} & \cdots & \overline{e_n e_n} \end{bmatrix}$$

The overbar represents the expected value ($E(\)$).

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If we normalize the covariance matrix, dividing each component by the product of the standard deviations $\overline{e_i e_j} / \sigma_i \sigma_j = \text{corr}(e_i, e_j) = \rho_{ij}$, we obtain a **correlation matrix**

$$\mathbf{C} = \begin{bmatrix} 1 & \rho_{12} & \cdots & \rho_{1n} \\ \rho_{12} & 1 & \cdots & \rho_{2n} \\ \vdots & \vdots & & \vdots \\ \rho_{1n} & \rho_{12} & \cdots & 1 \end{bmatrix}$$

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Warning: Do not confuse $\varepsilon \varepsilon^T$ and $\varepsilon^T \varepsilon$. Write expressions for both. Experiment with the 2×2 case.

If

$$\mathbf{D} = \begin{bmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \sigma_n^2 \end{bmatrix}$$

is the diagonal matrix of the variances, then we can write

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Exercise: Verify the last expression explicitly for a low-order (say, $n = 3$) matrix.

Some General Rules

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Exercise: Prove these statements.

Note: The transpose A^T exists for any matrix. However, the (two-sided) inverse only exists for non-singular square matrices.

The general form of a **quadratic function** is

$$F(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T \mathbf{A}\mathbf{x} + \mathbf{d}^T \mathbf{x} + c,$$

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To find the **gradient** of this scalar function $\nabla_{\mathbf{x}}F = \partial F / \partial \mathbf{x}$ (a column vector), we use the following properties of the gradient with respect to \mathbf{x} :

$$\nabla(\mathbf{d}^T \mathbf{x}) = \nabla(\mathbf{x}^T \mathbf{d}) = \mathbf{d} \quad \text{i.e.} \quad \frac{\partial}{\partial x_i}(d_1 x_1 + \dots d_n x_n) = d_i$$

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Therefore,

$$\nabla F(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{d} \qquad \nabla^2 F(\mathbf{x}) = \mathbf{A} \qquad \text{and} \qquad \delta F = (\nabla F)^T \delta \mathbf{x}$$

Conclusion of the foregoing.

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We derive the best linear unbiased estimation of \mathbf{x} in terms of \mathbf{y} , i.e., the optimal value of the weight matrix \mathbf{W} in the multiple linear regression

$$\mathbf{x}_a(t) = \mathbf{W}\mathbf{y}(t)$$

This approximates the true relationship

$$\mathbf{x}(t) = \mathbf{W}\mathbf{y}(t) - \varepsilon(t)$$

where $\varepsilon(t) = \mathbf{x}_a(t) - \mathbf{x}(t)$ is the linear regression (“analysis”) error, and \mathbf{W} is an $n \times p$ matrix that minimizes the mean squared error $E(\varepsilon^T \varepsilon)$.

Formal Derivation of BLUE

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Setting this to zero and taking time means give the normal equations:

$$\mathbf{W} = E \left(\mathbf{x} \mathbf{y}^T \right) \left[E \left(\mathbf{y} \mathbf{y}^T \right) \right]^{-1}$$

Statistical Assumptions

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We don't know the **truth**, \mathbf{x}_t , thus we don't know the errors of the available background and observations ...

... but we can make a number of assumptions about their statistical properties.

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The p observations available at irregularly spaced points $\mathbf{y}_o(\mathbf{r}_k)$ have observational errors

$$\varepsilon_{ok} = \mathbf{y}_o(\mathbf{r}_k) - \mathbf{y}_t(\mathbf{r}_k) = \mathbf{y}_o - H(\mathbf{x}_t)$$

We don't know the **truth**, \mathbf{x}_t , thus we don't know the errors of the available background and observations ...

... but we can make a number of assumptions about their statistical properties.

The background and observations are assumed to be **unbiased**:

$$\left. \begin{aligned} E\{\varepsilon_b\} &= E\{\mathbf{x}_b\} - E\{\mathbf{x}_t\} = 0 \\ E\{\varepsilon_o\} &= E\{\mathbf{y}_o\} - E\{\mathbf{y}_t\} = 0 \end{aligned} \right\}$$

We define the **error covariance matrices** for the analysis, background and observations respectively:

$$\left. \begin{aligned} \mathbf{P}_a &= \mathbf{A} = E\{\varepsilon_a \varepsilon_a^T\} && (n \times n) \\ \mathbf{P}_b &= \mathbf{B} = E\{\varepsilon_b \varepsilon_b^T\} && (n \times n) \\ \mathbf{P}_o &= \mathbf{R} = E\{\varepsilon_o \varepsilon_o^T\} && (p \times p) \end{aligned} \right\}$$

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Here \mathbf{H} is a $p \times n$ matrix, called the linear observation operator with elements

$$\mathbf{H}_{ij} = \frac{\partial H_i}{\partial x_j} \quad (p \times n)$$

Note that H is a nonlinear vector function while \mathbf{H} is a matrix.

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$$\begin{aligned}\mathbf{d} &= \mathbf{y}_o - H(\mathbf{x}_b) = \mathbf{y}_o - H(\mathbf{x}_t + (\mathbf{x}_b - \mathbf{x}_t)) \\ &= \mathbf{y}_o - H(\mathbf{x}_t) - \mathbf{H}(\mathbf{x}_b - \mathbf{x}_t) = \varepsilon_o - \mathbf{H}\varepsilon_b\end{aligned}$$

Here we use

$$H(\mathbf{x} + \varepsilon) = H(\mathbf{x}) + \left(\frac{\partial H}{\partial \mathbf{x}} \right)_{\mathbf{x}} \varepsilon = H(\mathbf{x}) + \mathbf{H}\varepsilon$$

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So, the optimal weight matrix \mathbf{W} that minimizes $\varepsilon_a^T \varepsilon_a$ is

$$\mathbf{W} = E\{(\mathbf{x} - \mathbf{x}_b)[\mathbf{y}_o - H(\mathbf{x}_b)]^T\} \left[E\{[\mathbf{y}_o - H(\mathbf{x}_b)][\mathbf{y}_o - H(\mathbf{x}_b)]^T\}\right]^{-1}$$

Clarification

- The BLUE problem we are solving is

$$(\mathbf{x} - \mathbf{x}^b) = \mathbf{W}(\mathbf{y}^o - H(\mathbf{x}^b))$$

- Therefore the optimal weight matrix is

$$\mathbf{W} = E\left[(\mathbf{x} - \mathbf{x}^b)(\mathbf{y}^o - H(\mathbf{x}^b))^T\right]E\left[(\mathbf{y}^o - H(\mathbf{x}^b))(\mathbf{y}^o - H(\mathbf{x}^b))^T\right]^{-1}$$

This can be written as

$$\mathbf{W} = E[(-\varepsilon_b)(\varepsilon_o - \mathbf{H}\varepsilon_b)^T] \{E[(\varepsilon_o - \mathbf{H}\varepsilon_b)(\varepsilon_o - \mathbf{H}\varepsilon_b)^T]\}^{-1}$$

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$$\mathbf{W} = [E(\varepsilon_b \varepsilon_b^T) \mathbf{H}] [E(\varepsilon_o \varepsilon_o^T) + \mathbf{H} E(\varepsilon_b \varepsilon_b^T) \mathbf{H}^T]^{-1}$$

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Substituting the definitions of background error covariance \mathbf{B} and observational error covariance \mathbf{R} into this, we obtain the optimal weight matrix:

$$\mathbf{W} = \mathbf{B} \mathbf{H}^T (\mathbf{R} + \mathbf{H} \mathbf{B} \mathbf{H}^T)^{-1}$$

Repeat:

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Using the relationship

$$\varepsilon_a = \varepsilon_b + \mathbf{W}[\varepsilon_0 - \mathbf{H}(\varepsilon_b)]$$

we can derive the analysis error covariance $E\{\varepsilon_a \varepsilon_a^T\}$.

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Substituting

$$\mathbf{W} = \mathbf{B}\mathbf{H}^T(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^T)^{-1}$$

we obtain

$$\mathbf{P}_a = (\mathbf{I} - \mathbf{W}\mathbf{H})\mathbf{B}$$

The Full Set of OI Equations

For convenience, we collect the full set of basic equations of OI, and then examine their meaning in detail.

They are formally similar to the equations for the scalar least squares *‘two temperatures problem’*.

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The interpretation of these equations is very similar to the scalar case discussed earlier.

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The first guess of the observations is obtained by applying the observation operator H to the background vector.

Note that from $H(\mathbf{x} + \delta\mathbf{x}) = H(\mathbf{x}) + \mathbf{H}\delta\mathbf{x}$, we get

$$H(\mathbf{x}_b) = H(\mathbf{x}_t) + \mathbf{H}(\mathbf{x}_b - \mathbf{x}_t) = H(\mathbf{x}_t) + \mathbf{H}\varepsilon_b,$$

where the matrix \mathbf{H} is the linear tangent perturbation of H .

The Optimal Weight Matrix

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Check the result if $\mathbf{R} = 0$.

Analysis Error Covariance Matrix

$$\mathbf{P}_a = (\mathbf{I} - \mathbf{WH})\mathbf{B}$$

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The error covariance of the analysis is given by the error covariance of the background, reduced by a matrix equal to the identity matrix minus the optimal weight matrix.

Note that \mathbf{I} is the $n \times n$ identity matrix.

End of §5.4.1