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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.

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We now consider the complete NWP operational problem of finding an optimum analysis of a field of model variables $\mathbf{x}_a$, given

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$$[\textbf{Here } \dim(\mathbf{x}) = N_x N_y + 4 * N_x N_y N_z]$$

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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.

Helpful Hints

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- **Be aware whether vectors are row or column vectors.**

Forward Operator: General Remarks

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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

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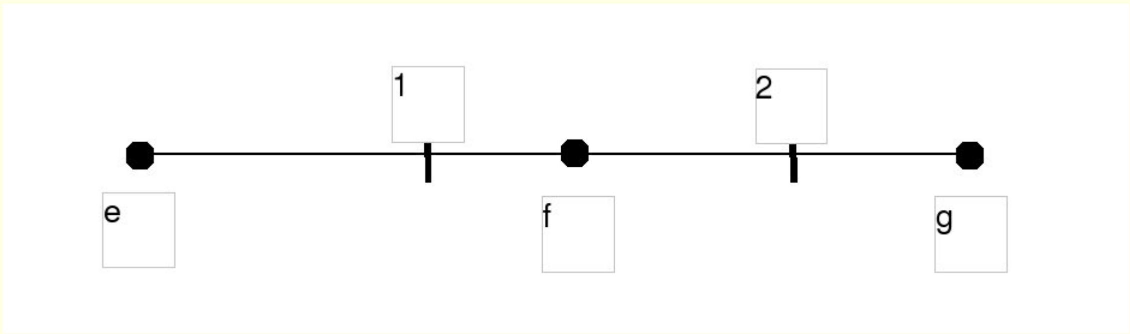

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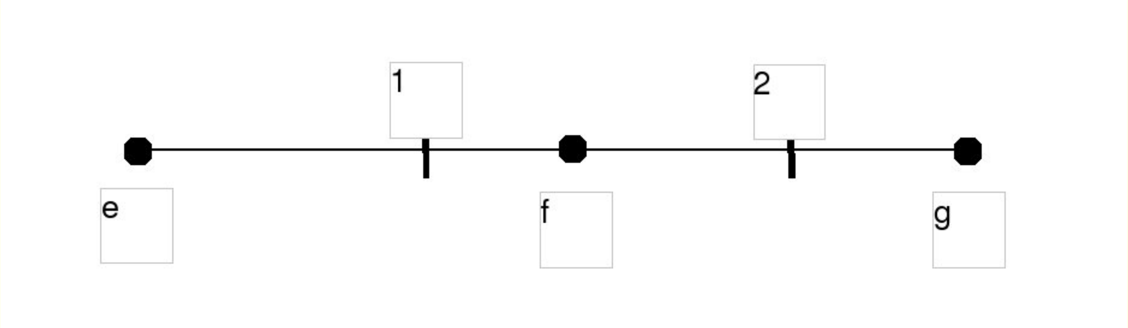

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Then

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

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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.

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The observational error variance R is the sum of the instrument error variance $\mathbf{R}_{\mathrm{instr}}$ and the representativity error variance $\mathbf{R}_{\mathrm{repr}}$, assuming that these errors are not correlated:

$$\mathbf{R} = \mathbf{R}_{\mathrm{instr}} + \mathbf{R}_{\mathrm{repr}}$$

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

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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 $\overline{e_i e_j}/\sigma_i \sigma_j = \mathbf{corr}(e_i, e_j) = \rho_{ij}$**, 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

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

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$$\mathbf{P} = \mathbf{D}^{\mathbf{1/2}}\mathbf{C}\mathbf{D}^{\mathbf{1/2}}$$

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

Some General Rules

The transpose of a matrix product is the product of the transposes, but in reverse order:

$$[\mathbf{AB}]^T = \mathbf{B}^T \mathbf{A}^T$$

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Exercise: Prove these statements.

Note: The transpose $\mathbf{A}^T$ 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 x:**

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

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Therefore,

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

Conclusion of the foregoing.

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We derive the <u>best linear unbiased estimation</u> of x in terms of y, i.e., the optimal value of the weight matrix 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** $E(\varepsilon^T \varepsilon)$**.**

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To derive W we write the regression equation matrix components explicitly:

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$$\sum_{i=1}^{n} \varepsilon_i^2(t) = \sum_{i=1}^{n} \left[\sum_{k=1}^{p} w_{ik} y_k(t) - x_i(t) \right]^2 \quad = \varepsilon^T \varepsilon$$

The derivative of this with respect to the weight matrix components is

$$\begin{aligned}\frac{\partial}{\partial w_{ij}}\sum_{i=1}^{n}\varepsilon_i^2(t) &= 2\left[\sum_{k=1}^{p} w_{ik}y_k(t) - x_i(t)\right]\left[y_j(t)\right] \\ &= 2\left[\sum_{k=1}^{p} w_{ik}y_k(t)y_j(t) - x_i(t)y_j(t)\right]\end{aligned}$$

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Setting this to zero, and taking the long-time average, we get a system of equations for w_{ik}:

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This is a linear system of equations for the weights w_{ik}.

The derivative of this with respect to the weight matrix components is

$$\frac{\partial}{\partial w_{ij}} \sum_{i=1}^{n} \varepsilon_i^2(t) = 2 \left[\sum_{k=1}^{p} w_{ik} y_k(t) - x_i(t) \right] \left[y_j(t) \right]$$
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We will re-cast the system in matrix form:

$$\mathbf{W} \overline{\mathbf{y}\mathbf{y}^T} = \overline{\mathbf{x}\mathbf{y}^T}$$

In matrix form, the derivative of the error variance is

$$\frac{\partial}{\partial \mathbf{W}}(\varepsilon^T \varepsilon) = \frac{\partial}{\partial \mathbf{W}}\left[(\mathbf{y}^T \mathbf{W}^T - \mathbf{x}^T)(\mathbf{W}\mathbf{y} - \mathbf{x})\right]$$

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Expanding, and taking the derivative, we get

$$\frac{\partial}{\partial \mathbf{W}}\varepsilon^T \varepsilon = 2\left\{\left[\mathbf{W}\mathbf{y}(t)\mathbf{y}^T(t)\right] - \left[\mathbf{x}(t)\mathbf{y}^T(t)\right]\right\}$$

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If we take a long time mean, and choose W to minimize the mean squared error, we get the normal equation

$$\mathbf{W}E\left(\mathbf{y}\mathbf{y}^T\right) - E\left(\mathbf{x}\mathbf{y}^T\right) = 0$$

or

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

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This gives the best linear unbiased estimation

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

Formal Derivation of BLUE

The analysis error covariance can be written

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Statistical Assumptions

We define the background error and the analysis error as vectors of length n:

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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:

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

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

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

Note that H is a nonlinear vector function while H is a matrix.

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So, the innovation vector $\mathbf{d} = \mathbf{y}_0 - H(\mathbf{x}_b)$ **can be written**

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

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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Its transpose or adjoint $\mathbf{H}^T$ transforms vectors in observation space to vectors in analysis space.

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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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We may expand it as

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

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

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

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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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 H is the linear tangent perturbation of H.

The Optimal Weight Matrix

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

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

Analysis Error Covariance Matrix

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

End of §5.4.1