Introduction to Variational Data Assimilation

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Plan of talk

- Non-Variational Sequential DA Methods
- Sasaki
- 3D VAR
- Adjoints
- 4D VAR
- Incremental Var
- Background Error Covariance models

NON-VARIATIONAL SEQUENTIAL DATA ASSIMILATION METHODS 15

CHAPTER OUTLINE

15.3.1 BERGTHÓRSSON AND DÖÖS [142]

An interesting feature of Bergthórsson and Döös's [142] paper is the description of how numerical weather prediction began to be undertaken in the 1950s. Here are the first two paragraphs of the 1955 paper:

> The first attempts at numerical weather forecasting on a routine basis have been characterized by a combination of tedious manual work on one hand and electronic computations with extremely high speed on the other. The weather observations are plotted on maps, examined and analyzed. From this manual analysis values are interpolated at a great number of grid points and punched on a paper copied. Finally the electronic computer can start the forecasting procedure. The manual part of these operations consumes time that is out of proportion to the time required for the machine computation. This, however, is not the only disadvantage.
>
> The manual analyst cannot be expected to use systematic and quantitative methods in his interpolations and extrapolations. His work is rather a complicated curve-fitting by the eye based on a number of more or less well established rules. The analysis will, in other words, be subjective and depending on the skill of the meteorologist. It is furthermore very difficult to avoid wiggles and irregularities of small scale which are neither desirable nor justified by observations. These may frequently amplify in the forecast computation and thus reduce the value of the final forecast. Errors in the reading and punching of values in grid points are also highly probable.

The starting point for the derivation of what would become successive correction in [2] in [142] was to use the observations of the wind and height fields at the 500 mb height as the "informations," along with the 12- or 24-hour barotropic forecast valid for the same time as the analysis, and the normal height of the 500 mb level for the particular month when the analysis is made.

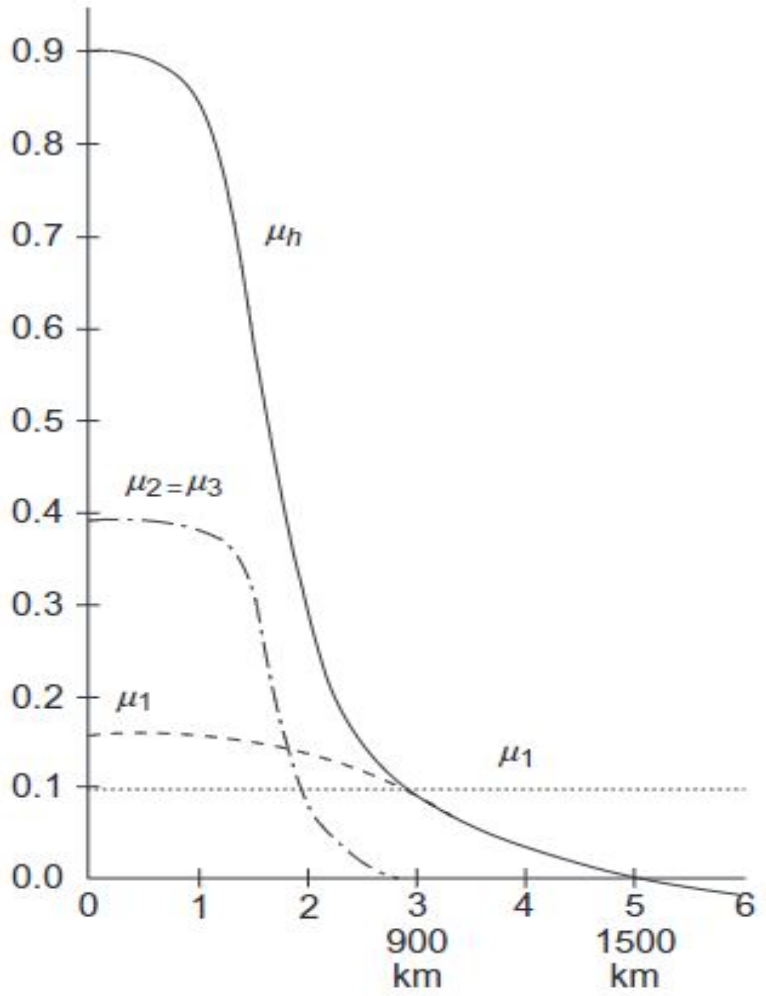

FIG. 15.1

Copy of figure 3 from [142] from the first version of objective analysis.

15.4.1 UNIVARIATE LINEAR LEAST SQUARES

The best way to introduce least squares, and weighted least squares, is through a toy problem. A classic example, which is used in many classes/lectures on least squares, is to consider the case where you are recording a temperature of a situation, either in a room, or at a specific location. You start with a prior estimate of the temperature, referred to here as T_b, and that you have an observation of that temperature, denoted T_o. There will also exist a true temperature that we do not know but is denoted T_t. We can define the *errors* in the background and the observation as

$$\varepsilon_b = T_b - T_t,$$
$$\varepsilon_o = T_o - T_t.$$

We now assume that the errors above are *unbiased*; this then implies that $\overline{\varepsilon_b} = \overline{\varepsilon_o} = 0$, where the bar refers to the mean of the errors.

The next step is to form an *analysis*, which is a linear combination of the background and the observed value of the temperature. The analysis temperature is denoted by T_a and is defined as

$$T_a = \alpha_1 T_o + \alpha_2 T_b + \alpha_3, \tag{15.29}$$

where α_3 is a constant. We now define the *analysis error* as $\varepsilon_a = T_a - T_t$, where we require this error to be unbiased, which implies that $\overline{\varepsilon_a} = 0$. If we now express the analysis state in terms of the true state and the background and observation errors, then we have

$$T_a = T_t + \varepsilon_a = \alpha_1 (T_t + \varepsilon_b) + \alpha_2 (T_t + \varepsilon_o) + \alpha_3. \tag{15.30}$$

If we now take the expectation of (15.30), which is also referred to as taking the mean, we see that using the fact that the mean of the background and observation errors have been assumed to be zero, then we obtain an expression for the mean analysis error, $\overline{\varepsilon_a}$, as

$$\overline{\varepsilon_a} = (\alpha_1 + \alpha_2 - 1)\, T_t + \alpha_3 = 0. \tag{15.31}$$

Since (15.31) must hold for all true temperature values, including the case where $T_t = 0$, then $\alpha_3 = 0$. This implies that $\alpha_1 + \alpha_2 = 1$, which implies that $\alpha_2 = 1 - \alpha_1$. We shall now drop the subscripts on α as there is only one remaining. Therefore the **general linear unbiased estimate** for this problem is

$$T_a = \alpha T_o + (1 - \alpha)\, T_b. \tag{15.32}$$

The next step is to determine what the value of α is. To achieve this we consider the error of the estimate in (15.32). If we now subtract the true state from both sides of the equation in (15.32), and recall the definitions for the various errors, we have

$$\varepsilon_a = \alpha \varepsilon_o + (1 - \alpha)\, \varepsilon_b, \tag{15.33}$$

If we now form the variance of (15.33), which we shall denote by σ_i^2 for $i = a, b, o$, then we have

$$\sigma_a^2 = \alpha^2 \sigma_o^2 + 2\alpha (1 - \alpha) \sigma_o \sigma_b + (1 - \alpha)^2 \sigma_b^2, \tag{15.34}$$

where we have used the property

$$VAR[aX_1 + bX_2] = a^2 VAR[X_1] + b^2 VAR[X_2] + 2abCOV[X_1 X_2].$$

We now assume that there is no covariance between the background error and the observation error, which then leaves

$$\sigma_a^2 = \alpha^2 \sigma_o^2 + (1 - \alpha) \sigma_b^2. \tag{15.35}$$

We now wish to consider three properties of the estimate in (15.35). If we take the first derivative of (15.35) with respect to α, then we obtain

$$\frac{d\sigma_a^2}{d\alpha} = 2\alpha \sigma_o^2 - 2(1 - \alpha) \sigma_b^2. \tag{15.36}$$

If we consider the case when $\alpha = 0$, then we have that $\sigma_a^2 = \sigma_b^2$ and from (15.36) that $\frac{d\sigma_a^2}{d\alpha} = -2\sigma_b^2 < 0$. If we now consider the case when $\alpha = 1$, then we now have that $\sigma_a^2 = \sigma_o^2$, and again from (15.36) that $\frac{d\sigma_a^2}{d\alpha} = 2\sigma_o^2 > 0$.

Given this information about $\alpha = 0$ and $\alpha = 1$, we can deduce that for $0 \leq \alpha \leq 1$, analysis variance is less than or equal to the maximum of the background or observation variance, that is to say, $\sigma_a^2 \leq \max\left(\sigma_b^2, \sigma_0^2\right)$. We also have that the minimum variance estimate occurs for a value of α that lies between 0 and 1 but not including them, that is to say, for $\alpha \in (0, 1)$. Finally, we have that the minimum variance estimate satisfies

$$\sigma_a^2 < \min\left(\sigma_b^2, \sigma_o^2\right).$$

Therefore, the minimum variance estimate occurs when the derivative in (15.36) is equal to zero,

$$\frac{d\sigma_a^2}{d\alpha} = 2\alpha\sigma_o^2 - 2(1-\alpha)\sigma_b^2 = 0, \quad \Rightarrow \quad \alpha = \frac{\sigma_b^2}{\sigma_o^2 + \sigma_b^2}. \tag{15.37}$$

Thus, the error variance of this now **minimum variance** estimate is

$$\sigma_a^2 = \left(\frac{1}{\sigma_b^2} + \frac{1}{\sigma_o^2}\right)^{-1}. \tag{15.38}$$

Therefore, the estimate with value of α derived in (15.37) is referred to as the **best linear unbiased estimate**, or **BLUE**.

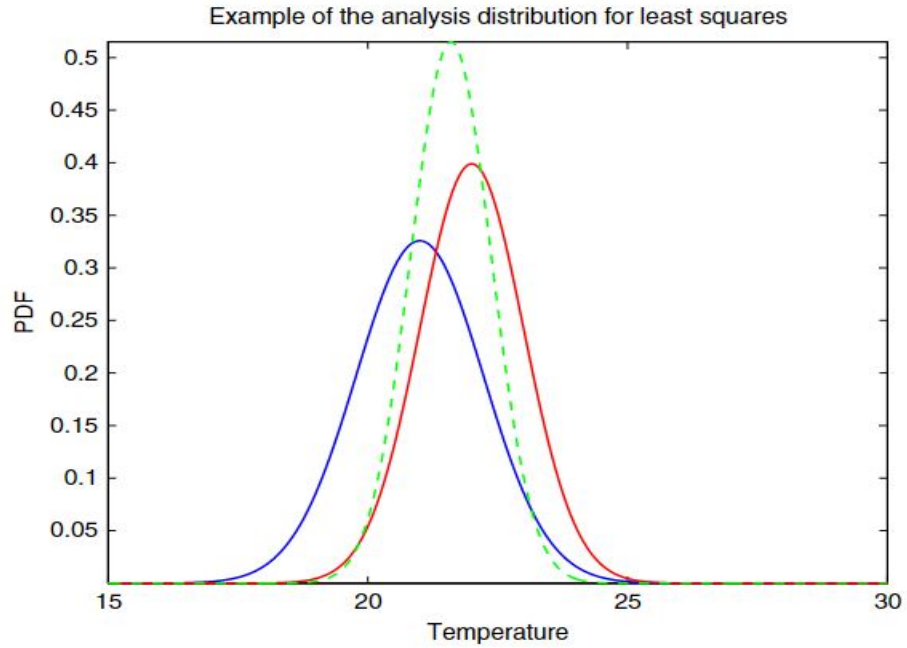

FIG. 15.2
Plot of the background (blue), observational (red), and analysis (green) distributions from a least squares approach.

15.4.2 MULTIDIMENSIONAL LEAST SQUARES

We now move on to the multiple dimension problem where instead of a scalar prior estimate, we now have a vector that is denoted x_b, where the b refers to the **background**. This vector can be viewed as representing the complete state of a numerical model at some time, where the elements of x_b may be grid point values, spherical harmonic coefficients, but also where the vector's elements do not represent only one physical attribute, i.e., not just temperature but temperature, winds, sea surface temperature, soil moisture, salinity, magma density, etc.

We now introduce the vector of observations y which contains observations, both direct and indirect, at different locations to the grid points, and of different variables. Therefore, we need to be able to match the background state to these locations and in terms of these observations. To formalize this we introduce the **observation/forward operator**, which can be a nonlinear operator, and is denoted by $h(x)$. This means that $h(x)$ can be compared to y, where the $h(x)$ represents the **model equivalent** of y.

For the time being we are going to assume that the observation operator does not introduce any errors, so that

$$h(x_t) = y_t, \tag{15.39}$$

where x_t is vector of the true states, and y contains the true values of the observed quantities.

As with the scalar case, we now seek an analysis that is a linear combination of the background and the observations, which in a matrix vector form is

$$x_a = \mathbf{F}x_b + \mathbf{G}h(x_b) + \mathbf{K}y + c, \tag{15.40}$$

where **F**, **G**, and **K** are matrices to be determined, and **c** is an unknown vector.

If we assume that $\boldsymbol{h}$ is linear, then we can look for a linear unbiased estimate as we did for the scalar case. If, however, $\boldsymbol{h}$ is nonlinear, then we require that error-free inputs, that is to say, $\boldsymbol{x}_b = \boldsymbol{x}_t$ and $\boldsymbol{y} = \boldsymbol{y}_t$, produce error-free analysis, that is to say, $\boldsymbol{x}_a = \boldsymbol{x}_t$, which then implies

$$\boldsymbol{x}_t = \mathbf{F}\boldsymbol{x}_t + \mathbf{G}\boldsymbol{h}(\boldsymbol{x}_t) + \mathbf{K}\boldsymbol{h}(\boldsymbol{x}_t) + \boldsymbol{c}. \tag{15.41}$$

We require the expression in (15.41) to hold for all true states, including the case where $\boldsymbol{x}_t = \mathbf{0}$, which then implies that $\boldsymbol{c} = \mathbf{0}$. This in turn implies that

$$\mathbf{F}\boldsymbol{x}_t + \mathbf{G}\boldsymbol{h}(\boldsymbol{x}_t) = \mathbf{I}\boldsymbol{x}_t - \mathbf{K}\boldsymbol{h}(\boldsymbol{x}_t), \tag{15.42}$$

and therefore we can see that the expression in (15.42) can only hold if $\mathbf{F} = \mathbf{I}$ and $\mathbf{G} = -\mathbf{K}$. Therefore, the analysis equation for this situation is

$$\boldsymbol{x}_a = \boldsymbol{x}_b + \mathbf{K}(\boldsymbol{y} - \boldsymbol{h}(\boldsymbol{x}_b)). \tag{15.43}$$

We now need to determine what the matrix $\mathbf{K}$ is. If we recall from the scalar case we had that

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

which is similar in appearance to the matrix equation in (15.43), and therefore, the $\mathbf{K}$ matrix plays a role of the weights given to the observations as well as handling the information of the transformations between the **observation space** and **model space**. The matrix $\boldsymbol{K}$ is referred to as the **gain matrix**.

We now introduce the definition of the errors for the multidimensional analysis error along with the multidimensional versions of the background and observation errors as

$$\boldsymbol{\varepsilon}_a \equiv \boldsymbol{x}_a - \boldsymbol{x}_t, \tag{15.44a}$$

$$\boldsymbol{\varepsilon}_b \equiv \boldsymbol{x}_b - \boldsymbol{x}_t, \tag{15.44b}$$

$$\boldsymbol{\varepsilon}_o \equiv \boldsymbol{y} - \boldsymbol{y}_t. \tag{15.44c}$$

The next step is to make the assumption that the errors are small, which then enables us to linearize the observation operator about the background state, and then have a linear model for the error. This implies that

$$\boldsymbol{h}(\boldsymbol{x}_b) = \boldsymbol{h}(\boldsymbol{t}_b) + \mathbf{H}\boldsymbol{\varepsilon}_b + \mathcal{O}\left(\boldsymbol{\varepsilon}_b^2\right), \tag{15.45}$$

where $\mathbf{H}$ is the Jacobian of the observation operator, defined as

$$\mathbf{H}_{ij} = \frac{\partial h_i(\boldsymbol{x}_b)}{\partial x_j}, \tag{15.46}$$

where $i = 1, 2, \ldots, N_o$ and $j = 1, 2, \ldots, N$, where N_o is the number of observations and N is the number of entries in $\boldsymbol{x}$.

We now substitute the expressions for the errors from (15.44a) to (15.44c) into the analysis equation and use the property that $\boldsymbol{h}(\boldsymbol{x}_t) = \boldsymbol{y}_t$, which then results in the following equation to the first order of

$$\boldsymbol{\varepsilon}_a = \boldsymbol{\varepsilon}_b + \mathbf{K}(\boldsymbol{\varepsilon}_o - \mathbf{H}\boldsymbol{\varepsilon}_b). \tag{15.47}$$

We now assume again that the mean errors have be removed so that $\mathbb{E}[\boldsymbol{\varepsilon}_b] = \mathbb{E}[\boldsymbol{\varepsilon}_o] = \mathbf{0}$; given this information, we see from (15.47) that $\mathbb{E}[\boldsymbol{\varepsilon}_a] = 0$.

As we are now seeking a statistical weight, we recall the definition for a multivariate distribution as

$$\mathbb{C} = \mathbb{E}\left[(x_i - \bar{x}_i)\left(x_j - \bar{x}_j\right)\right], \tag{15.48}$$

and we recall that covariances matrices are symmetric and positive definite matrices.

We return to the analysis error equation (15.47), which we can rewrite in the following form,

$$\boldsymbol{\varepsilon}_a = (\mathbf{I} - \mathbf{KH})\,\boldsymbol{\varepsilon}_b + \mathbf{K}\boldsymbol{\varepsilon}_o. \tag{15.49}$$

The next step is to form the **analysis error covariance matrix** which is obtained by taking the expectation of the product of the vector of analysis error with its transpose, which is referred to as an **outer product**, therefore we have

$$\begin{aligned}
\mathbb{E}\left[\boldsymbol{\varepsilon}_a \boldsymbol{\varepsilon}_a^T\right] &= \mathbb{E}\left[((\mathbf{I} - \mathbf{KH})\,\boldsymbol{\varepsilon}_b + \mathbf{K}\boldsymbol{\varepsilon}_o)((\mathbf{I} - \mathbf{KH})\,\boldsymbol{\varepsilon}_b + \mathbf{K}\boldsymbol{\varepsilon}_o)^T\right], \\
&= (\mathbf{I} - \mathbf{KH})\,\mathbb{E}\left[\boldsymbol{\varepsilon}_b \boldsymbol{\varepsilon}_b^T\right](\mathbf{I} - \mathbf{KH})^T + (\mathbf{I} - \mathbf{KH})\,\mathbb{E}\left[\boldsymbol{\varepsilon}_b \boldsymbol{\varepsilon}_o^T\right]\mathbf{K}^T \\
&\quad + \mathbf{K}\mathbb{E}\left[\boldsymbol{\varepsilon}_o \boldsymbol{\varepsilon}_b^T\right](\mathbf{I} - \mathbf{KH})^T + \mathbf{K}\mathbb{E}\left[\boldsymbol{\varepsilon}_o \boldsymbol{\varepsilon}_o^T\right]\mathbf{K}^T.
\end{aligned} \tag{15.50}$$

As with the scalar case, we assume that there is no correlation between the background errors and the observational errors. This then simplifies (15.50) to

$$\mathbb{E}\left[\boldsymbol{\epsilon}_a \boldsymbol{\epsilon}_a^T\right] = (\mathbf{I} - \mathbf{KH})\,\mathbb{E}\left[\boldsymbol{\epsilon}_b \boldsymbol{\epsilon}_b^T\right](\mathbf{I} - \mathbf{KH})^T + \mathbf{K}\mathbb{E}\left[\boldsymbol{\epsilon}_o \boldsymbol{\epsilon}_o^T\right]\mathbf{K}^T, \tag{15.51}$$

where we can see that the expression in (15.51) is similar to the scalar version we derived earlier, i.e., $\sigma_a^2 = (1-\alpha)^2\sigma_b^2 + \alpha^2\sigma_o^2$. Thus, we see that the $\mathbf{K}$ matrix in (15.51) is equivalent to α in the scalar case, where we showed that the value of α was chosen so as to minimize the variance.

However, we have to address how we minimize the variance in a multidimensional situation. We have seen from Chapter 4 that the covariance matrices contain the variances of the variable in their diagonal entries. This implies that it is possible to define the minimum variance analysis as that which minimized the sum of the diagonal elements of the analysis error covariance matrix. It is possible to obtain a function of the diagonal entries of a matrix through its *trace*, which we shall denote as Tr. We recall that for the scalar case we were able to obtain the expression for the minimum variance analysis by setting $\frac{d\sigma_a^2}{d\alpha} = 0$. For the multidimensional case we do something similar, but with respect to the trace of the analysis covariance matrix as

$$\frac{\mathrm{Tr}\left(\mathbb{E}\left[\boldsymbol{\epsilon}_a \boldsymbol{\epsilon}_a^T\right]\right)}{\partial \mathbf{K}} = \mathbf{0}. \tag{15.52}$$

In order to apply the derivative in (15.52) to the expression we have for the analysis error covariance matrix in (15.50), we require the following identities for the derivative of the trace of the product of matrices:

$$\frac{\mathrm{Tr}\left(\mathbf{K}\mathbf{A}\mathbf{K}^T\right)}{\partial \mathbf{K}} = {}^T\left(\mathbf{A}+\mathbf{A}^T\right),$$
$$\frac{\mathrm{Tr}\left(\mathbf{K}\mathbf{A}\right)}{\partial \mathbf{K}} = \mathbf{A}^T,$$
$$\frac{\mathrm{Tr}\left(\mathbf{A}\mathbf{K}^T\right)}{\partial \mathbf{K}} = \mathbf{A}.$$

Substituting these properties into (15.52) acting on (15.50) results in

$$\frac{\mathrm{Tr}\left(\mathbb{E}\left[\boldsymbol{\varepsilon}_a\boldsymbol{\varepsilon}_a^T\right]\right)}{\partial \mathbf{K}} = 2\mathbf{K}\left(\mathbf{H}\mathbb{E}\left[\boldsymbol{\varepsilon}_b\boldsymbol{\varepsilon}_b^T\right]\mathbf{H}^T + \mathbb{E}\left[\boldsymbol{\varepsilon}_o\boldsymbol{\varepsilon}_o^T\right]\right) - 2\mathbb{E}\left[\boldsymbol{\varepsilon}_b\boldsymbol{\varepsilon}_b^T\right]\mathbf{H}^T = \mathbf{0}. \tag{15.53}$$

Rearranging (15.53) and factorizing leads to the expression for $\mathbf{K}$ as

$$\mathbf{K} = \mathbb{E}\left[\boldsymbol{\varepsilon}_b\boldsymbol{\varepsilon}_b^T\right]\mathbf{H}^T\left(\mathbf{H}\mathbb{E}\left[\boldsymbol{\varepsilon}_b\boldsymbol{\varepsilon}_b^T\right]\mathbf{H}^T + \mathbb{E}\left[\boldsymbol{\varepsilon}_o\boldsymbol{\varepsilon}_o^T\right]\right)^{-1}. \tag{15.54}$$

The expression in (15.54) is for the optimal gain matrix which is called the **Kalman gain matrix**; we shall see why in Chapter 19. We can see that the appearance of the optimal expression for $\mathbf{K}$ in (15.54) is quite similar in appearance to that of the scalar case, where we have $\alpha = \frac{\sigma_b^2}{\sigma_b^2+\sigma_o^2}$.

The method that we have used to obtain the expressions for the minimum variance estimates is the **weighted least sum of squares** approach. If we had not had the α or the $\mathbf{K}$ terms, then that would be the method of **least sum of squares**.

Before we move on to nonlinear least squares theory, we introduce some standardized notation for the different covariance matrices in (15.54) as set out in [149]:

$$\mathbf{P}^a \equiv \mathbb{E}\left[\boldsymbol{\varepsilon}_a \boldsymbol{\varepsilon}_a^T\right], \quad \mathbf{P}^b \equiv \mathbb{E}\left[\boldsymbol{\varepsilon}_b \boldsymbol{\varepsilon}_b^T\right], \quad \mathbf{R} = \mathbb{E}\left[\boldsymbol{\varepsilon}_o \boldsymbol{\varepsilon}_o^T\right], \tag{15.55}$$

where $\mathbf{P}^a$ is the **analysis error covariance matrix**, $\mathbf{P}^b$ is the **background error variance matrix** and $\mathbf{R}$ is the **observation error covariance matrix**. **Note:** in most variational data assimilation derivation the background error covariance is usually approximated and is denoted by $\mathbf{B}$.

Exercise 15.3. *Show that the Kalman gain matrix can also be defined as*

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

Quote comes from Tarantola and Valette where they state that:

The aim of physical sciences is to discover the minimal set of parameters which completely describes physical systems and the laws relating the values of these parameters to the results of any set of measurements on the system

Definition 15.4. If given some information on the values of the set of parameter, we try to use a theoretical relationship in order to obtain information on the values of some measurable quantity; this is solving a **direct/forward** problem.

If given some information on the values of some measured quantities, we try to use a theoretical relationship in order to obtain information on the values of the set of parameters; this is solving an **inverse** problem [151].

15.6 OPTIMAL (OPTIMUM) INTERPOLATION/STATISTICAL INTERPOLATION/ANALYSIS CORRECTION

Given the statistical and probability theory from the last section, we now move on to the last of the set of non-variational-based data assimilation schemes. The reason there are three names in the title of this section is that optimal interpolation, which was originally derived in the Soviet Union by Gandin in 1963, translated into English in 1965 [4], is often not considered as actually being an optimal interpolation. In fact the actual name for this method is **optimum interpolation**.

Statistical interpolation is the phase coined by Dr. Roger Daley in his very good book "*Atmospheric Data Analysis*," [157] but also in his publications [158]. The final name, analysis correction (AC) comes from a permutation of optimum interpolation theory that lead to the operational implementation at the United Kingdom's Meteorological Office [159]. In this section we shall present all three different formulations, but we shall state that it is quite difficult to obtain a copy of Gandin's book. However, there is a good derivation along with an explanation of the practical aspect of the optimum interpolation method in a paper by Alaka and Elvander in 1972 [160]. It is the derivation from [160] that we summarize here.

15.6.1 DERIVATION OF THE OPTIMUM INTERPOLATION FROM ALAKA AND ELVANDER [160]

Let $\mathbf{r}_i = \mathbf{r}_0, \mathbf{r}_1, \ldots, \mathbf{r}_n$ denote a set of independent vectors defining the location of points in a sampling space. Next we consider a function $f(\mathbf{r})$ whose sampled values $\hat{f}_i = \hat{f}_1, \hat{f}_2, \ldots, \hat{f}_n$ have errors $\varepsilon_i = \varepsilon_1, \varepsilon_2 \ldots, \varepsilon_n$, so that

$$\hat{f}_i = f_i + \varepsilon_i. \tag{15.126}$$

The problem then is to determine the values of f_0 at some location $\mathbf{r}_0$ from the measured values $\hat{f}_i$. We now let f_0' and f_i' denote the deviations of f_0 and f_i from their respective mean states, which then allows us to express f_0' in terms of the following linear combination:

$$f_0' = \sum_{i=1}^{n} (f_i' + \varepsilon_i) P_i + I_0, \tag{15.127}$$

in which P_i are the weighting factors and I_0 is the errors in determining f_0' by interpolating from $\hat{f}_i$.

We now define the mean square interpolating error as being given by

$$\epsilon = \bar{I}_0^2 = \overline{\left(\sum_{i=1}^{n} (f_i' + \varepsilon_i) P_i - f_0' \right)^2}, \tag{15.128}$$

We now make the standard assumption that the random (background) errors, ε_i, are independent of the true values of the measured quantities, which means that $\overline{\varepsilon_i f_i'} = 0$, and that they are unrelated to each other, which implies that

$$\overline{\varepsilon_i \varepsilon_j} = \begin{cases} 0 & i \neq j, \\ \sigma_{\varepsilon_i}^2 & i = j, \end{cases} \tag{15.129}$$

where in [160] $\sigma_{\varepsilon_i}^2$ is the mean-square random observation errors. The assumptions above imply that the random errors do not affect the values of the true covariances, but inflate the true variances σ_i^2 by an amount $\sigma_{\varepsilon_i}^2$.

Given the assumptions above, we can rewrite (15.128) as

$$\epsilon = \sum_{i=1}^{n} \sum_{j=1}^{n} \overline{\hat{f}_i' \hat{f}_j'} P_i P_j + \sum_{i=1}^{n} \sigma_{\varepsilon_i}^2 P_i^2 - 2 \sum_{i=1}^{n} \overline{\hat{f}_i' f_0'} P_i + \sigma_0^2. \tag{15.130}$$

The **optimum** weights, p_i, corresponding to a minimum value of ϵ, are obtained by setting

$$\frac{\partial \epsilon}{\partial P_i} = 0. \tag{15.131}$$

As we saw in the linear regression section, (15.131) forms the set of linear equations

$$\sum_{j=1}^{n} \overline{\hat{f}_i' \hat{f}_j'} p_j + \sigma_{\varepsilon_i}^2 p_i = \overline{\hat{f}_i' f_o'}, \quad i = 1, 2, \ldots, n. \tag{15.132}$$

If we now denote the minimum of the mean-square error, ϵ_{min}, by E, then combining (15.130) and (15.132), we obtain

$$E = \sigma_0^2 - \sum_{i=1}^{n} \overline{\hat{f}_i' f_o'} p_i. \tag{15.133}$$

Definition 15.6 (Homogeneity of Variances). Homogeneity of variances assumes that the dependent variables exhibit equal levels of variance across the range of predictor variables. This is also true for the covariances and is referred to as the **homogeneity of covariances**.

Definition 15.7 (Isotropic). A covariance is said to be **isotropic** if it is uniform in all directions. This implies that the values are the same even under a rotation of the points.

We now assume the two properties defined above for the variances (homogeneous) and for the covariances (homogeneous and isotropic). This enables us to write (15.132) as

$$\sum_{j=1}^{n} \mu_{i,j} pj + \lambda_i^2 p_i = \mu_{0,i}, \quad \text{for } i = 1, 2, \ldots, n, \tag{15.134}$$

and (15.133) as

$$E = \sigma^2 \left(1 - \sum_{i=1}^{n} \mu_{0,i} p_i \right), \tag{15.135}$$

where

$$\mu_{i,j} = \frac{\overline{\hat{f}_i' f_j'}}{\sigma^2},$$

is the autocorrelation coefficient between values of the function at locations $\mathbf{r}_i$ and $\mathbf{r}_j$, while

$$\mu_{0,j} = \frac{\overline{\hat{f}_0' f_i'}}{\sigma^2},$$

is the autocorrelation coefficient between values of the function at $\mathbf{r}_0$ and $\mathbf{r}_i$, and finally

$$\lambda_i^2 = \frac{\sigma_{\varepsilon_i}^2}{\sigma^2}.$$

For us to be able to effectively minimize the root mean square interpolation error through the procedure just described, we require accurate estimates of the random errors, the variance, and the autocorrelations functions. We have already assumed that the variances are homogeneous, and that the covariances are homogeneous and isotropic. Therefore, to determine the root mean square random error, σ_{ε_i}, we assume a structure function, β, to be homogenous and isotropic. Under these assumptions, this function depends only on $\boldsymbol{\rho} = \mathbf{r}_i - \mathbf{r}_j$, which is the distance between observation pairs located at $\mathbf{r}_i$ and $\mathbf{r}_j$. Therefore,

$$\beta(\boldsymbol{\rho}) = \overline{\left(f_i' - f_j'\right)^2}. \tag{15.136}$$

Now it is stated in Alaka and Elvander that the estimated structure function, $\hat{\beta}(\boldsymbol{\rho})$, is related to the true function $\beta(\boldsymbol{\rho})$ through

$$\hat{\beta}(\boldsymbol{\rho}) = \beta(\boldsymbol{\rho}) + 2\sigma_\varepsilon^2, \tag{15.137}$$

but they reference Chapter 2 from Gandin's book as their source for (15.137).

Alaka and Elvander then state a procedure to obtain estimates for $2\sigma_\varepsilon$ term as that of fitting a curve to the computed structure function $\beta(\boldsymbol{\rho})$ plotted against distance $\boldsymbol{\rho}$ and extrapolating the curve until it intersect the axis of $\beta(\boldsymbol{\rho})$ at $\boldsymbol{\rho} = \mathbf{0}$. It is then stated that the value of σ_ε^2 will comprise of both the random measurement errors and the aliasing errors inherent in the observations.

Determining the autocorrelation functions

Under the assumption of homogeneity and isotropy for the autocorrelations, the μ is function of distance ρ between observation pairs and as such can be written as $\mu(\rho) = \frac{\overline{f_i' f_j'}}{\sigma^2}$.

However, in [160] the authors state that when they plotted the autocorrelations then the results contained scatter which was a result of the anisotropy and non-homogeneity of the true autocorrelations. To smooth these non-conforming autocorrelations, the points were divided into 100 km segments, with the middle of these intervals stored in the vector $\boldsymbol{d}$, and then given the number of points in each interval N_i, they use the following function:

$$\mu(d) = \sum_{i=1}^{n} \hat{\mu}(\rho_i) \frac{N_i \left(\frac{1}{2} + \frac{1}{2}\cos\frac{\pi(\rho_i - d)}{100}\right)}{\sum_{j=1}^{n} N_j \left(\frac{1}{2} + \frac{1}{2}\cos\frac{\pi(\rho_i - d)}{100}\right)}, \tag{15.138}$$

where ρ_i denoted the distance between the pairs of stations used in the calculations.

The values $\mu(d)$ obtained through (15.138) were then fitted to the empirical curve of the form

$$\mu(\rho) = \left(Ae^{-B\rho^c} + 1 - A\right)\cos D\rho. \tag{15.139}$$

We have recreated the four plots of the autocorrelations of the zonal winds from [160] at 850 and 200 mb in January and July in Fig. 15.4. We can see that they detected seasonal changes as well as changes with respect to height. The determining of autocorrelation and variances is a task that still affects the performance of the data assimilation schemes today.

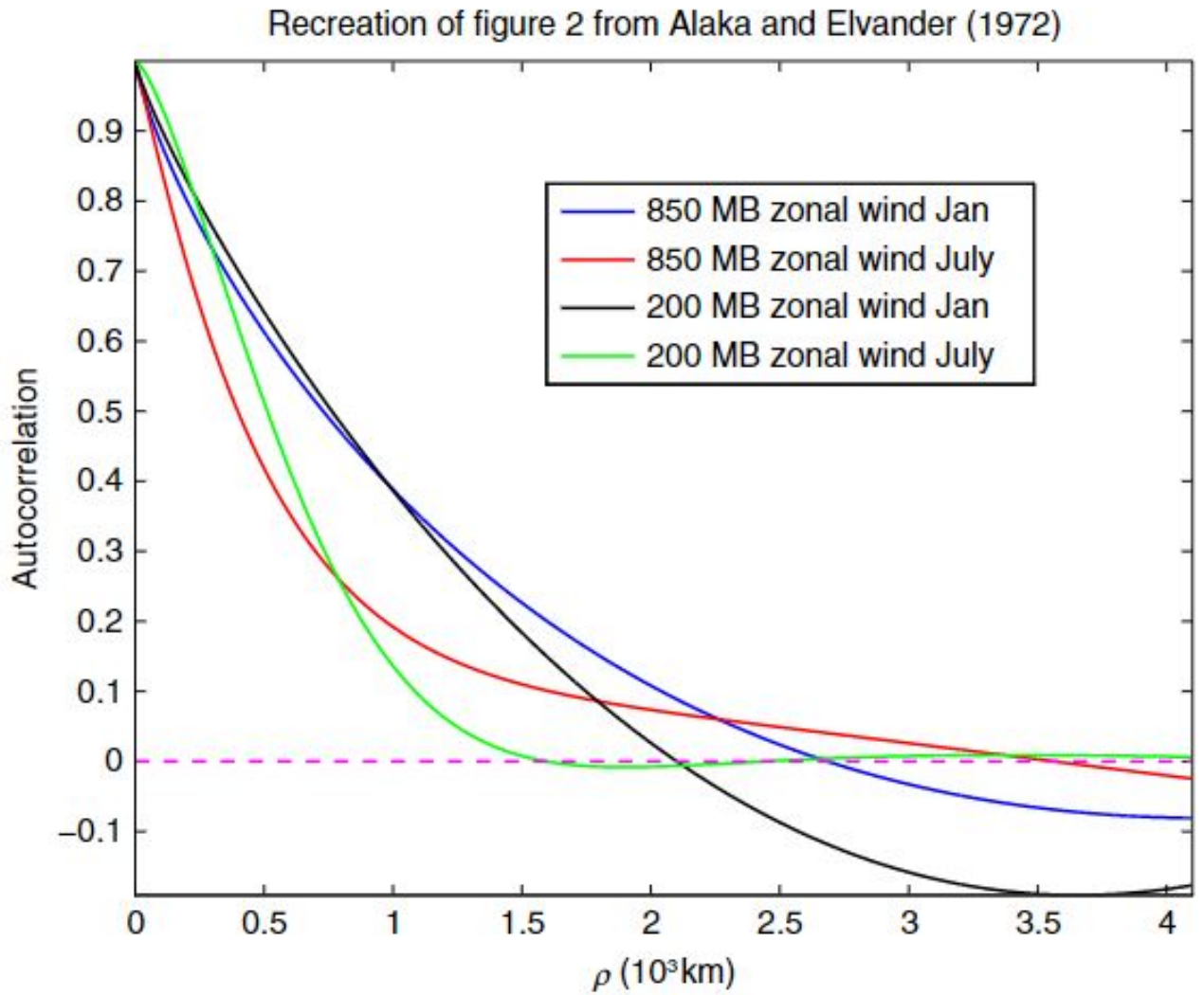

FIG. 15.4

Recreation of the autocorrelation plots from Alaka and Elvander (1972) for the zonal winds at 850 and 200 mb in January and July.

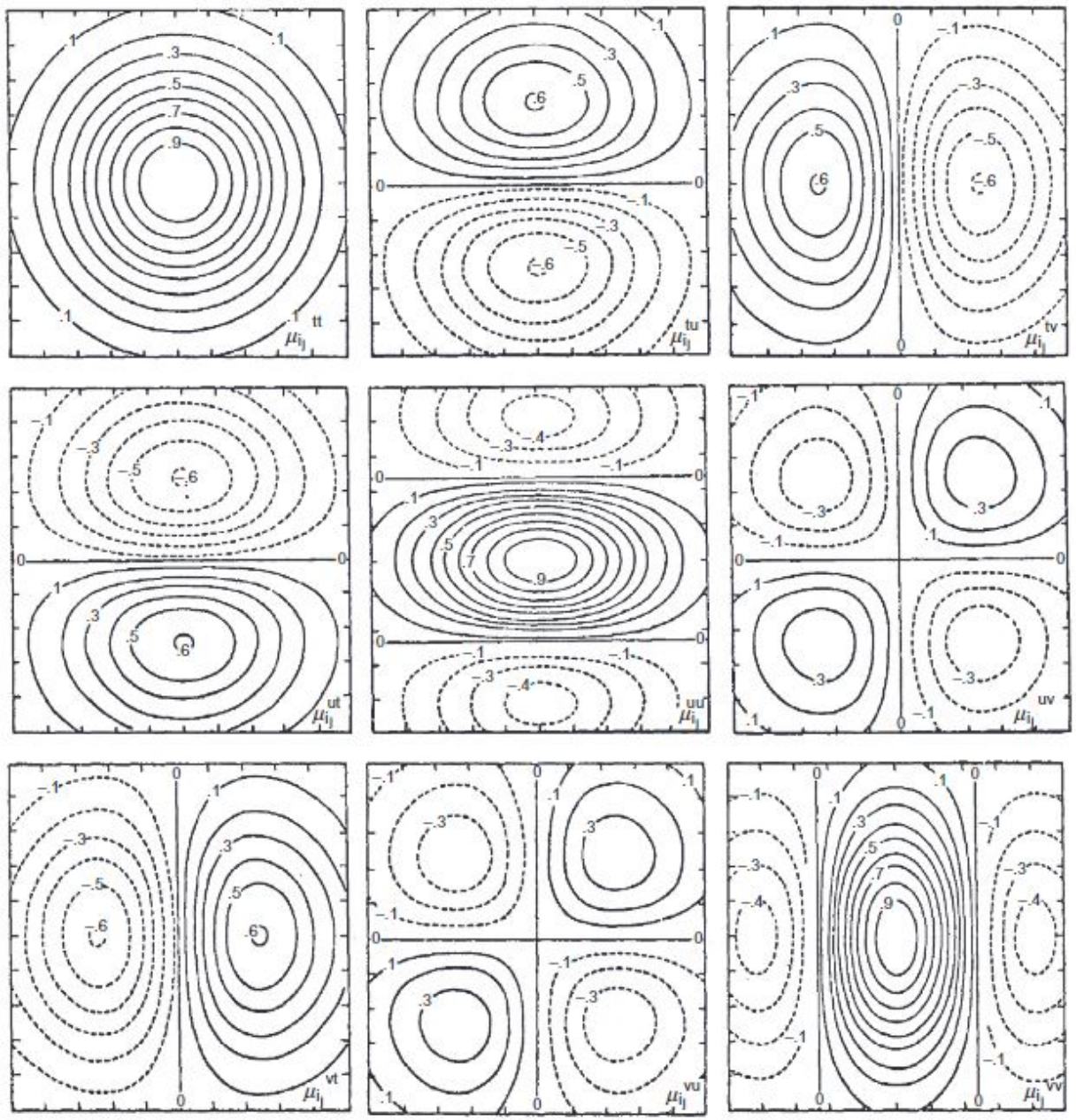

FIG. 15.7

Copy of figure 1 from Bergman (1979), [161] of the isopath of lateral correlation functions.

VARIATIONAL DATA ASSIMILATION

16

CHAPTER OUTLINE

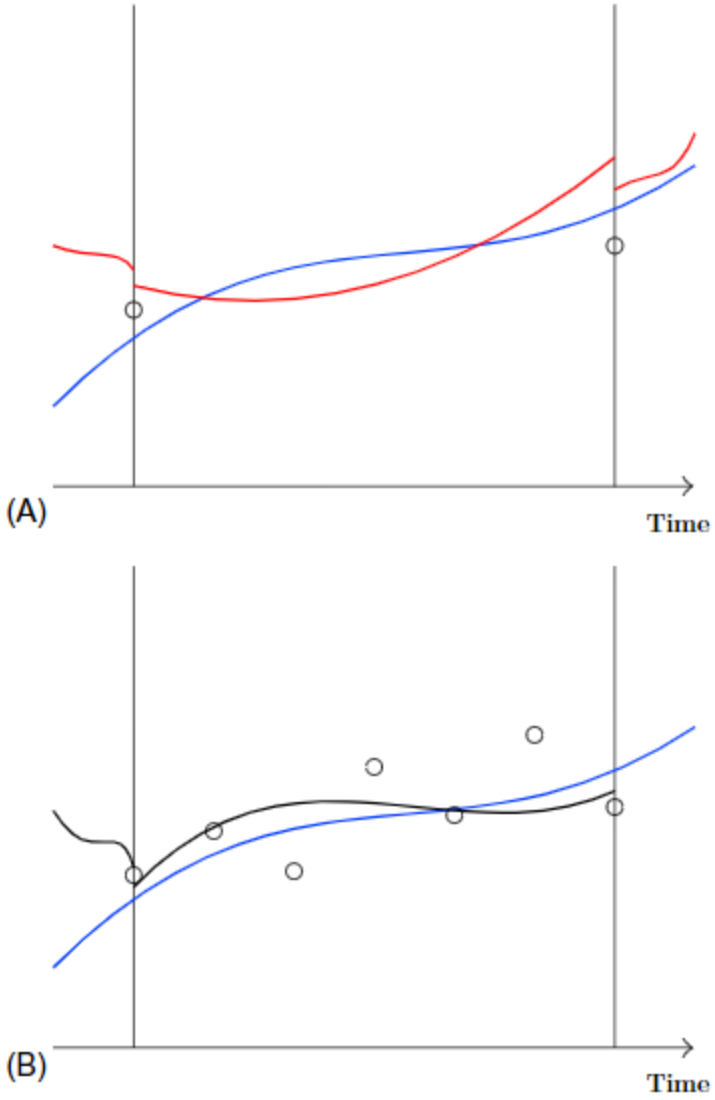

FIG. 16.1

(A) Schematic of filtering, where the blue line is the true trajectory, the red line is the 3D VAR trajectory, and the circles are the observations at the analysis times. (B) Schematic of smoothing where the blue line is the true trajectory, the black line is the 4D VAR smoothed trajectory, and the circles are observations throughout the window.

16.1 SASAKI AND THE STRONG AND WEAK CONSTRAINTS

In the previous chapter we introduced the different statistical-based schemes that were used for data assimilation before the introduction of the variational-based schemes. The emphasis here is on the statistical component. All of the various schemes, successive corrections, Barnes scheme, optimum interpolation, and analysis correction were based on minimizing a form of sum of squares, which for a linear Gaussian case is equivalent to finding the state that has the minimum variance. At the same time as the development of these scheme, there was an approach based upon calculus of variations being developed by **Yoshikazu Sasaki**.

Sasaki wrote a series of papers advocating that the variational principle could be used to form an objective analysis for numerical weather prediction [169–174]. The two fundamental papers associated with Sasaki's work are: *An Objective Analysis Based Upon Variational Methods* [170] and *Some Basic Formalisms in Numerical Variational Analysis* [172]; it is the latter paper that we shall briefly summarize here.

The starting point for the calculus of variational approach, which we shall refer to as just variational from here on, is to define the functional, J, as

$$\delta J = \delta \sum_{\Omega} \sum_{i} \left(\tilde{\alpha}_i (\varphi_i - \tilde{\varphi})^2 + \alpha_i (\nabla_t \varphi_i)^2 \right) = 0, \tag{16.1}$$

where δ is the variational operator, φ_i is the analyzed field, $\tilde{\varphi}_i$ is the observation, ∇_t is the local change in a finite-difference form, $\tilde{\alpha}_i$ and α_i are predetermined weights, and Ω is the domain in time t and space x_1, x_2, x_3. Sasaki refers to the first term in (16.1) as a condition used for minimizing the variance of the difference between the observed and analyzed values. The second term is a simple low pass filter in frequency. (16.1) is solved with the dynamical constraint such as those given by the primitive equations. It is possible to write these constraints in the form

$$\nabla_t \varphi_i = F_i \left(\varphi_i, \varphi_j, \nabla_{x_k} \varphi_i, \nabla_{x_k} \varphi_j \right), \tag{16.2}$$

where F_i is a given function and ∇_{xk} represents the space derivative with respect to x_k for $k = 1, 2, 3$.

The functional that is defined in (16.1) is quadratic and therefore the associated stationary value of J becomes the minimum. As we saw in both the calculus of variation and the optimal control chapters, Chapters 5 and 7, respectively, the solution of (16.1) is obtained through solving the Euler, or the Euler-Lagrange, equations after the substitution of (16.2) into (16.1). Sasaki state that the disadvantage of this approach is that it is only for an instantaneous field and the functional does not describe explicitly the **time variations**.

This disadvantage can be overcome by taking the following approaches. The first is an orthodox approach and is written as

$$\delta J = \delta \sum_{\Omega} \sum_{i} \left(\tilde{\alpha} \left(\varphi_i - \tilde{\varphi}_j \right)^2 + \lambda_i G_i \left(\varphi_i, \varphi_j \nabla_t \varphi_i, \nabla_{x_k} \varphi_i, \nabla_{x_k} \varphi_j \right) \right) = 0, \tag{16.3}$$

where G_i represents a prognostic or diagnostic equation and λ_i is the Lagrange multiplier. The Euler equation derived from (16.3) will include $\nabla_t \varphi_i$ and $\nabla_t \lambda_i$. It is noted here in [172] that the solution of the Euler equation requires a considerable amount of effort to solve numerically.

An alternative approach is to formulate the functional as

$$\delta J = \delta \sum_{\Omega} \sum_{i} \left(\tilde{\alpha}_i \left(\varphi_i - \tilde{\alpha}_i \right)^2 + \alpha_i G_i^2 \right) = 0, \tag{16.4}$$

where α_i is a predetermined weight. We should note that G_i is linear in (16.3) and quadratic in (16.4), and that the coefficient of the G term is the Lagrange multiplier in (16.3), but is a weight in (16.4). Because of these differences with the coefficients of G, we obtain the following two conditions:

$$G = 0, \tag{16.5a}$$

$$G \neq 0, \tag{16.5b}$$

from (16.3) and (16.4), respectively. Sasaki refers to formalism that results in (16.5a) as the **strong constraint**, and to the formalism that leads to (16.5b) as the **weak constraint**. We refer the reader to [172] for an example with the one-dimensional advection equation for the differences these two approaches form. However, we shall introduce loose definitions of what strong and weak constraint mean:

Definition 16.1. Strong constraint: This is the constraint where the analyzed solution to (16.3) must satisfy the discrete model exactly. The strong constraint is also stated as the **perfect model** assumption. This is also referred to as the case where there is **no model error**.

Definition 16.2. Weak constraint: This is the constraint where the analyzed solutions to (16.4) **does not** have to satisfy the discrete model equations exactly. The weak constraint is also stated as the **imperfect model** assumption. This is also referred to as the case where there **is model error**.

16.2 THREE-DIMENSIONAL DATA ASSIMILATION

From the 1986 paper by Andrew Lorenc [5], we have that the general starting point for the derivation of the 3D VAR cost function is to consider the problem of finding the set of initial states so that the subsequent forecast is the *best* possible. Due to the problem of the forecast being imperfect, we have to try to compensate by introducing observations. Therefore, let the state vector be $\boldsymbol{x}$, where $\boldsymbol{x} = (x_1, x_2, \ldots, x_N)^T$, and N is the total number of state variables, and the observational vector, $\boldsymbol{y}$, where $\boldsymbol{y} = \left(y_1, y_2, \ldots, y_{N_o}\right)^T$, and N_o represents the number of observations with $N_o \ll N$.

We now require a relationship between the model states, $\boldsymbol{x}$ and the observations, $\boldsymbol{y}$. This relationship is given by

$$\boldsymbol{y} = \boldsymbol{h}(\boldsymbol{x}), \tag{16.6}$$

where $\boldsymbol{h}(\boldsymbol{x})$ is a vector of nonlinear interpolations from the model states to the observations given by

$$\boldsymbol{h}(\boldsymbol{x}) = \begin{pmatrix} h_1(x_1, x_2, \ldots, x_N) \\ h_2(x_1, x_2, \ldots, x_N) \\ \vdots \\ h_{N_o}(x_1, x_2, \ldots x_N) \end{pmatrix}. \tag{16.7}$$

If the relationship between the observation and the model state variables is linear, for example, an average or a linear interpolation, then $\mathbf{h}$ is a matrix vector multiplication, $\mathbf{H}\boldsymbol{x}$, where $\mathbf{H}$ is a linear rectangular matrix of dimensions $N_o \times N$. This then gives us the problem, according to Lorenc, of finding the "best" $\boldsymbol{x}$ that inverts (16.6) for a given $\boldsymbol{y}^o$, where $\boldsymbol{y}^o$ is the physical observation which contain errors.

The method to set up this problem is to consider a Bayesian probability approach, where Bayes' theorem states that the posterior probability of an event A occurring, given that event B is known to have occurred, is proportional to the prior probability of A, multiplied by the probability of B occurring given that A is known to have occurred:

$$P(A \mid B) \propto P(B \mid A) P(A). \tag{16.8}$$

In the case that we are interested, we have that A is the event that $\boldsymbol{x} = \boldsymbol{x}_t$ and that B is the event $\boldsymbol{y} = \boldsymbol{y}^o$. This then enables us to write (16.8) as

$$P\left(\boldsymbol{x} = \boldsymbol{x}_t | \boldsymbol{y} = \boldsymbol{y}^o\right) \propto P\left(\boldsymbol{y} = \boldsymbol{y}^o | \boldsymbol{x} = \boldsymbol{x}_t\right) P\left(\boldsymbol{x} = \boldsymbol{x}_t\right), \tag{16.9}$$

where the superscript t represents the "true" solution and o represents observed value. Thus (16.9) defines an N-dimensional PDF, which is denoted as $P_a(\boldsymbol{x})$, where a represents the analysis. Lorenc then tells us that the "best" estimate, $\boldsymbol{x}_a$, is either the mean of $P_a(\boldsymbol{x})$,

$$\boldsymbol{x}_a = \int \boldsymbol{x} P_a(\boldsymbol{x})\, d\boldsymbol{x}, \tag{16.10}$$

or the mode, which is

$$\boldsymbol{x}_a = \boldsymbol{x} \text{ such that } P_a(\boldsymbol{x}) \text{ is maximum.} \tag{16.11}$$

As we mentioned earlier, the mean and the mode are the minimum variance and the maximum likelihood states, respectively.

16.2.1 GAUSSIAN FRAMEWORK

We now consider the probability, $P(\boldsymbol{x} = \boldsymbol{x}_t)$, that represents our knowledge about $\boldsymbol{x}$ before the observations are taken. This can be considered as an error, $\boldsymbol{\varepsilon}_b$, which we define as

$$\boldsymbol{\varepsilon}_b \equiv \boldsymbol{x} - \boldsymbol{x}_b, \tag{16.12}$$

where $\boldsymbol{x}_b$ represents the background state, and thus we are considering deviations away from this state, and has a probability $P_b(\boldsymbol{x} - \boldsymbol{x}_b)$, which will be defined soon, once the rest of the problem is set up.

The observational error can be written in terms of two parts [5]. The first part is due to instrumental errors and the other is in the representativeness error. We shall consider these as one entity as the total observational error. This then enables us to write the conditional part of the probability of (16.9) as

$$P(\boldsymbol{y} = \boldsymbol{y}^o | \boldsymbol{x} = \boldsymbol{x}_t) = P_o(\boldsymbol{y}^o - \boldsymbol{h}(\boldsymbol{x})), \tag{16.13}$$

which is the observational error, $\boldsymbol{\varepsilon}_o$. We have assumed that the observational and the background errors are independent, which is an acceptable assumption [5], and is made in most data assimilation schemes. Combining (16.12) and (16.13) enables us to write (16.9) as

$$P_a(\boldsymbol{x}) = P_o(\boldsymbol{y}^o - \boldsymbol{h}(\boldsymbol{x}))\, P_b(\boldsymbol{x} - \boldsymbol{x}_b) \equiv P_o(\boldsymbol{\varepsilon}_o)\, P_b(\boldsymbol{\varepsilon}_b). \tag{16.14}$$

We now define these probabilities in terms of a multivariate Gaussian, MG, distributions such that $\boldsymbol{\varepsilon}_o \sim MG(\mathbf{0}, \mathbf{R})$ in other words the observational errors are multivariate Gaussian distributed with mean $\mathbf{0}$ and covariance matrix $\mathbf{R}$. The background errors are such that $\boldsymbol{\varepsilon}_b \sim MG(\mathbf{0}, \mathbf{B})$; that is to say that the background errors are also multivariate Gaussian distributed,with the same mean vector, but with covariance matrix $\mathbf{B}$. These distributions are then defined as

$$P_b(\boldsymbol{\varepsilon}_b) \propto \exp\left\{-\frac{1}{2}\boldsymbol{\varepsilon}_b^T B^{-1} \boldsymbol{\varepsilon}_b\right\} \equiv \exp\left\{-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}_b)^T \mathbf{B}^{-1}(\boldsymbol{x} - \boldsymbol{x}_b)\right\}, \tag{16.15}$$

$$P_o(\boldsymbol{\varepsilon}_o) \propto \exp\left\{-\frac{1}{2}\boldsymbol{\varepsilon}_o^T R^{-1} \boldsymbol{\varepsilon}_o\right\} \equiv \exp\left\{-\frac{1}{2}(\boldsymbol{y}^o - \boldsymbol{h}(\boldsymbol{x}))^T \mathbf{R}^{-1}(\boldsymbol{y}^o - \boldsymbol{h}(\boldsymbol{x}))\right\}. \tag{16.16}$$

Therefore substituting (16.15) and (16.16) into (16.9) yields

$$P_a(\boldsymbol{x}) \propto \exp\left\{-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}_b)^T \mathbf{B}^{-1}(\boldsymbol{x} - \boldsymbol{x}_b) - \frac{1}{2}(\boldsymbol{y}^o - \boldsymbol{h}(\boldsymbol{x}))^T \mathbf{R}^{-1}(\boldsymbol{y}^o - \boldsymbol{h}(\boldsymbol{x}))\right\}. \tag{16.17}$$

To maximize P_a is the equivalent of minimizing $-\ln$ of (16.17). This then gives us our nonlinear cost function, J, as

$$J(\boldsymbol{x}) = \frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}_b)^T \mathbf{B}^{-1}(\boldsymbol{x} - \boldsymbol{x}_b) + \frac{1}{2}(\boldsymbol{y}^o - \boldsymbol{h}(\boldsymbol{x}))^T \mathbf{R}^{-1}(\boldsymbol{y}^o - \boldsymbol{h}(\boldsymbol{x})). \tag{16.18}$$

If we consider an unconstrained minimization method, such as the nonlinear conjugate gradient or quasi-Newton methods, to find the minimum of (16.18), then we require the Jacobian and the Hessian of (16.18). The Jacobian vector of (16.18) can easily be verified as

$$\frac{\partial J}{\partial \boldsymbol{x}} \equiv \mathbf{B}^{-1}(\boldsymbol{x}-\boldsymbol{x}_b) - \mathbf{H}^T\mathbf{R}^{-1}(\boldsymbol{y}-\boldsymbol{h}(\boldsymbol{x})), \tag{16.19}$$

where $\mathbf{H}$ is defined as

$$\mathbf{H} = \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{x}}, \tag{16.20}$$

and is the Jacobian matrix of $\boldsymbol{h}$ with dimensions $N_o \times N$ and $\dfrac{\partial J}{\partial \boldsymbol{x}}$ has dimensions $N \times 1$ where we have dropped the superscript o for the rest of the chapter as we are now just dealing with the physical observations.

For the Hessian of (16.18) we present this componentwise, but be aware that these entries are components that form a series of matrix multiplications. Thus the components of the Hessian matrix are given by

$$\frac{\partial^2 J}{\partial x_i \partial x_j} \equiv \left[\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}\right]_{ij} - \left[\mathbf{G}_i\mathbf{R}^{-1}(\boldsymbol{y}-\boldsymbol{h}(\boldsymbol{x}))\right]_j, \tag{16.21}$$

where G is the Hessian of $\boldsymbol{h}$ with

$$\mathbf{G}_i \equiv \frac{\partial}{\partial x_i}\left(\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{x}}\right). \tag{16.22}$$

Therefore the dimensions of the full Hessian matrix of J is $N_o \times N$ and where there are N of the G_i matrices with $i = 1, 2, \ldots, N$ and $j = 1, 2, \ldots, N_o$.

Everything that we have presented above is for what is referred to as the **full field** formulation. However, while Lorenc does not introduce incremental VAR in [5], he does linearize the problem. The linearization is associated with the observation operator $\boldsymbol{h}(\boldsymbol{x})$, which is based on being able to approximate the observation operator at the true state by the observation operator at the background state plus a small perturbation. This then implies that

$$\boldsymbol{h}(\boldsymbol{x}_a) = \boldsymbol{h}(\boldsymbol{x}_b) + \mathbf{H}\delta\boldsymbol{x}, \tag{16.23}$$

where $\mathbf{H}$ is the Jacobian of the observation operator, and where we are assuming that $\boldsymbol{x}_a$ is the state that minimizes J and is given as the nonlinear solution to

$$\mathbf{0} = \mathbf{H}^T(\mathbf{O}+\mathbf{F})^{-1}(\boldsymbol{y}-\boldsymbol{h}(\boldsymbol{x}_a)) + \mathbf{B}^{-1}(\boldsymbol{x}_b - \boldsymbol{x}_a). \tag{16.24}$$

We now assume that the linearization in (16.23) is valid in the entire range of probable values of $\boldsymbol{x}$ in the region of $\boldsymbol{x}_b$, as such there is an explicit solution can be found by evaluating $\boldsymbol{h}$ at $\boldsymbol{x} = \boldsymbol{x}_b$ and then rewriting (16.23) as

$$\boldsymbol{h}(\boldsymbol{x}_a) = \boldsymbol{h}(\boldsymbol{x}_b) + \mathbf{H}(\boldsymbol{x}_b - \boldsymbol{x}_a). \tag{16.25}$$

Through substituting (16.25) into (16.24), it can be shown that the following solutions are equivalent:

$$\boldsymbol{x}_a = \boldsymbol{x}_b + \left(\mathbf{B}\mathbf{H}^T(\mathbf{O}+\mathbf{F})^{-1}\mathbf{H} + \mathbf{I}\right)^{-1}\mathbf{B}\mathbf{H}^T(\mathbf{O}+\mathbf{F})^{-1}(\boldsymbol{y} - \boldsymbol{h}(\boldsymbol{x}_b)), \tag{16.26a}$$

$$\boldsymbol{x}_a = \boldsymbol{x}_b + \mathbf{B}\mathbf{H}^T(\mathbf{O}+\mathbf{F})^{-1}\left(\mathbf{H}\mathbf{B}\mathbf{H}^T(\mathbf{O}+\mathbf{F})^{-1} + \mathbf{I}\right)^{-1}(\boldsymbol{y} - \boldsymbol{h}(\boldsymbol{x}_b)), \tag{16.26b}$$

$$\boldsymbol{x}_a = \boldsymbol{x}_b + \mathbf{B}\mathbf{H}^T\left(\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{O} + \mathbf{F}\right)^{-1}(\boldsymbol{y} - \boldsymbol{h}(\boldsymbol{x}_b)). \tag{16.26c}$$

Finally, in the derivation section of [5], Lorenc refers to the *expected analysis error covariance for this linearized Gaussian case* as given by

$$\langle(\boldsymbol{x}_a - \boldsymbol{x}_b)(\boldsymbol{x}_a - \boldsymbol{x}_b)^T\rangle = \mathbf{B} - \mathbf{B}\mathbf{H}^T\left(\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{O} + \mathbf{F}\right)^{-1}\mathbf{H}\mathbf{B}. \tag{16.27}$$

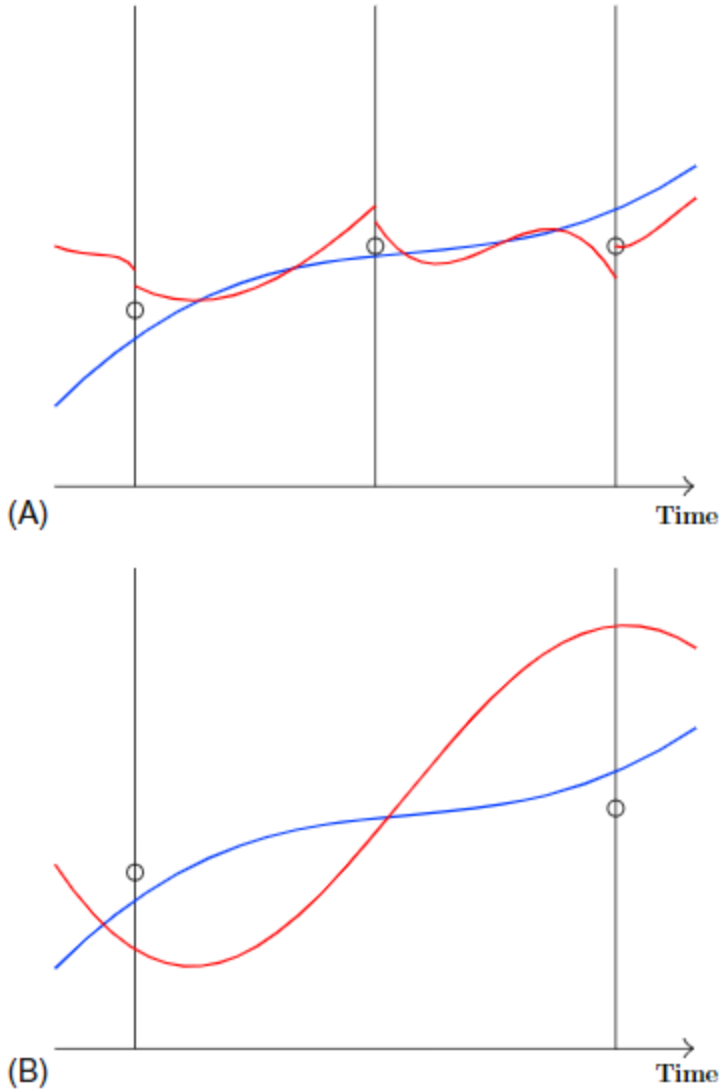

FIG. 16.2

(A) Schematic of 3D VAR filtering when the cycling length is short enough to control model error, where the blue line is the true trajectory and the red lines are the 3D VAR analysis trajectories. (B) Schematic of 3D VAR filtering when the cycling length is too long to control model error, where the blue line is the true state and the red line is the 3D VAR analysis trajectory, and the circles are observations. The circles are observations.

TANGENT LINEAR MODELING AND ADJOINTS

13

CHAPTER OUTLINE

13.1.1 DERIVATION OF THE LINEARIZED MODEL

If we consider a general nonlinear initial value problem denoted by

$$y_i = \mathcal{M}(x_1, x_2, \ldots, x_N), \tag{13.2}$$

where N is the total number of grid points in the numerical grid, the x_js are the discrete model variables, for $j = 1, 2, \ldots, N$, and the y_is are the output from the numerical model, then what we may be seeking in various applications of data assimilation are answers to the questions of: how does $x\left(t^{n+1}\right)$ change with respect to $x_i\left(t^n\right)$? and when we are analyzing the output y_i, then what features in x_j caused this? It is possible to attempt to quantify answers to these two questions by considering tangent linear models and the adjoint model.

To derive the linearized model, we start by expressing the x_js as either a background, or reference state, and a perturbation such that

$$x_j = \bar{x}_j + \delta x_j. \tag{13.3}$$

We are trying to ascertain how the nonlinear model is affected by the perturbation to the state, x_j, which can be approximated through considering the difference between the outputs from $y(\bar{x} + \delta x)$ and $y(\bar{x})$. We have plotted the situation just described in Fig. 13.1, where we see that we can approximate the change in the output δy through a tangent approximation. Mathematically we can express the gradient as

$$\frac{dy}{dx} \approx \frac{\delta y_i}{\delta x_i} \Rightarrow \delta y_i \approx \left(y_i(\bar{x} + \delta x) - y_i(\bar{x})\right) \delta x_i. \tag{13.4}$$

We now substitute the nonlinear model for y in (13.4), and expand the nonlinear model about the reference state to obtain

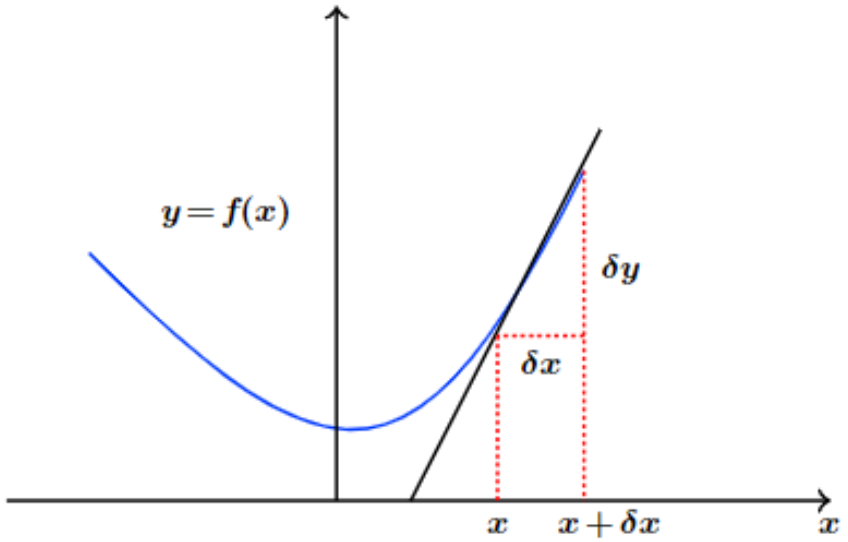

FIG. 13.1

Schematic of the additive tangent linear approximation to the function $f(x)$.

$$\delta y_i = y_i(\bar{x} + \delta x) - y_i(\bar{x}) = \mathcal{M}(\bar{x}_1 + \delta x_1, \bar{x}_2 + \delta x_2, \ldots, \bar{x}_N + \delta x_N) - \mathcal{M}(\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_N),$$

$$= \mathcal{M}(\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_N) + \frac{\partial \bar{y}_i}{\partial x_1}\delta x_1 + \frac{\partial \bar{y}_i}{\partial x_2}\delta x_2 + \cdots - \mathcal{M}(\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_N),$$

$$\delta y_i = \sum_j^N \left(\overline{\frac{\partial y_i}{\partial x_j}}\right) \delta x_j. \tag{13.5}$$

The expression in (13.5) is the **tangent linear model**, which is quite often abbreviated to TLM, and it gives an approximation for the growth of the perturbations, δx_j, $j = 1, 2, \ldots, N$. The tangent linear model enables us to address the question of how y_i changes with respect to x_j, for $j = 1, 2, \ldots, N$ and $i = 1, 2, \ldots, M$, where M is the number of time steps the numerical model has taken.

13.1.2 ADJOINTS

We now consider how to address the second question of linking the behavior in y_i to x_j. We start by introducing a scalar measure of the outputs

$$J = J\left(\mathbf{y}\left(\mathbf{x}\right)\right). \tag{13.6}$$

We next expand (13.6) through a Taylor series, which then leads to a change in the measure, δJ, as

$$\delta J = \sum_{i=1}^{M} \frac{\partial \bar{J}}{\partial y_i} \delta y_i, \tag{13.7}$$

but we can also consider variations with respect to the x_js, which results in

$$\delta J = \sum_{j=1}^{N} \frac{\partial \bar{J}}{\partial x_j} \delta x_j, \tag{13.8}$$

where (13.7) and (13.8) are **equal when both functions are linear**.

It is (13.8) that is of interest here, as it depends on the perturbation inputs. Given how we defined J as a function of a function, it is possible to differentiate through the chain rule to obtain estimates for $\frac{\partial \bar{J}}{\partial x_j}$ as

$$\frac{\partial \bar{J}}{\partial x_j} = \sum_{i=1}^{M} \left(\overline{\frac{\partial y_i}{\partial x_j}} \right) \frac{\partial \bar{J}}{\partial y_i}. \tag{13.9}$$

An important and arguably very powerful property of (13.9) is that it enables us to integrate the future time gradient, or sensitivities, **backwards** to the initial time.

The first feature to notice here is that the tangent linear model sums the terms $\frac{\partial y_i}{\partial x_j}$ over the js, while the summation in (13.9) is over the is. To help keep track of the different terms here, we shall now use matrix-vector notation. First let the matrix $\mathbf{M}$ be defined as

$$\mathbf{M}_{i,j} \equiv \frac{\partial y_i}{\partial x_j}, \tag{13.10}$$

then for the tangent linear model we see that we are summing over the columns of $\mathbf{M}$, while for the model given by (13.9) we are summing over the rows of $\mathbf{M}$. From the rules of matrix-vector multiplication and introducing the vectors δy and δx, we can write (13.5) as

$$\delta y = \mathbf{M} \delta x. \tag{13.11}$$

We can then also write (13.9) as

$$\frac{\partial J}{\partial x} = \mathbf{M}^T \frac{\partial J}{\partial y}. \tag{13.12}$$

The matrix $\mathbf{M}$ as defined in (13.10) is referred to as either the **resolvent** of the tangent linear model, or as the **Jacobian** of the nonlinear model. Given the definition for the resolvent, it is possible to write the perturbation to the nonlinear model as

$$\mathcal{M}(\bar{x} + \delta x) = \mathcal{M}(\bar{x}) + \mathbf{M} \delta x, \tag{13.13}$$

13.1.4 TEST OF THE TANGENT LINEAR AND ADJOINTS MODELS

There are a series of tests that can be applied to verify if the derivation and the coding of the tangent linear and adjoint models are correct. If we consider the tangent linear model first, then we have shown that if we have a nonlinear $\mathcal{M}(x)$, and $\mathbf{M}$ is the tangent linear model, then for small perturbations δx we have

$$\mathcal{M}(x + \delta x) - \mathcal{M}(x) \approx \mathbf{M}\gamma\delta x.$$

If we now define the relative error as

$$E_R = \frac{\mathcal{M}(x + \gamma\delta x) - \mathcal{M}(x)}{\mathbf{M}\gamma\delta x}, \tag{13.22}$$

now if the tangent linear approximation is a good approximation, then as $\gamma \to 0$ we should have that the relative error should tend to zero.

If we now consider the adjoint model, then we have the following identity for the tangent linear and adjoint model

$$\langle \mathbf{M}\delta x, \mathbf{M}\delta x \rangle = \left\langle \delta x, \mathbf{M}^T\mathbf{M} \right\rangle, \tag{13.23}$$

for an inner product, $\langle \cdot, \cdot \rangle$, and any δx. This is a mechanism to test the accuracy of the adjoint calculation.

The third measure to ascertain the accuracy of the adjoint derivation and coding is through the **gradient test**. If we recall that we have a functional associated with the adjoint given by J, then the gradient of J is ∇J, and it is possible to check that the gradient of the functional has been coded correctly through the identity

$$\Psi(\alpha) = \frac{J(x + \alpha h) - J(x)}{\alpha h^T \nabla J(x)} = 1 + O(\alpha), \tag{13.24}$$

where h is a vector of unit length which is often taken to be $\frac{\nabla J(x)}{\|\nabla J(x)\|_2}$. Therefore, for some values of α away from the accuracy of the machine precision, if the gradient is accurate then we would expect the function $\Psi(\alpha)$ to be approximately 1.

16.3 FOUR-DIMENSIONAL DATA ASSIMILATION

The earliest form of the mathematical ideas behind modern 4D VAR appears in Lewis and Derber [89]. The approach described in [89] is to find the minimum of the cost function

$$J(\boldsymbol{x}(t_0)) = \frac{1}{2}\sum_{i=0}^{t_a} \langle \mathbf{W}(t_i)(\boldsymbol{x}(t_i) - \boldsymbol{x}_b(t_i)), \boldsymbol{x}(t_i) - \boldsymbol{x}_b(t_i)\rangle, \tag{16.28}$$

where t_a is the analysis time, $\mathbf{W}$ is a *weight* matrix that can be changed depending on known accuracies, the expression $\langle \cdot, \cdot \rangle$ is the inner product operator, $\boldsymbol{x}_b$ is the output from a numerical model which has been started by some set of initial conditions, $\boldsymbol{x}_{b,0}$ and $\boldsymbol{x}$ is the analyses that has come from a simpler version of data assimilation, i.e., optimum interpolation (OI). The problem is to seek the initial conditions that minimize the weighted squared differences between the original analysis from the OI scheme at several times and the coincident solutions to the numerical model. Note: In later formulations $\mathbf{W}$ becomes the background error covariance matrix, $\mathbf{B}$.

The minimum of (16.28) is found through its gradient, ∇J, with respect to the initial conditions. To find the minimum of (16.28), an adjoint approach is used. This approach starts by considering the first-order change to (16.28) from a small perturbation, $\boldsymbol{x}'(t_0)$, about the initial conditions $\boldsymbol{x}(t_0)$. Therefore, J' is the first-order change in the functional and is related to the directional derivative in $\boldsymbol{x}'(t_0)$ by

$$J' = \langle \nabla J, \boldsymbol{x}'(t_0) \rangle. \tag{16.29}$$

Substituting the information from (16.28) into (16.29) and introducing a linearized perturbation model, the reader is referred to [89] for more details about this, and through using the property of adjoints,

$$\langle \boldsymbol{x}, \mathbf{A}\boldsymbol{y} \rangle = \langle \mathbf{A}^T \boldsymbol{x}, \boldsymbol{y} \rangle, \tag{16.30}$$

then the gradient can be expressed as

$$\nabla J = \sum_{i=0}^{t_a} \left(\left[\prod_{k=0}^{K_i} \mathbf{D}^T(t_0 + k\Delta t) \right] \hat{\boldsymbol{x}}_i(t_i) \right), \tag{16.31}$$

where $\mathbf{D}$ is the matrix containing the coefficient of the discrete approximation to the linearized perturbation equation and K_i represents the total number of time steps from t_0 to t_i, where $i = 1, 2, \ldots, K$, and K is the total number of time steps to t_a.

The extension of the adjoint techniques from Lewis and Derber (1985) to an observational-based approach appears in Le Demit and Talagrand [178]. The approach in [178] is based upon calculus of variations techniques and optimal control theory. The starting point in [178] is the state vector, $\boldsymbol{x}$, that is defined in time by the equation

$$\frac{d\boldsymbol{x}}{dt} = \mathcal{M}(\boldsymbol{x}), \tag{16.32}$$

where $\mathcal{M}$ is a continuous nonlinear model operator acting on $\boldsymbol{x}$.

It is assumed that there are sets of observations at different times, denoted by $\boldsymbol{y}(t_1), \boldsymbol{y}(t_2), \ldots, \boldsymbol{y}(t_a)$. Given these observations, it is possible to define a functional in terms of the observations as

$$J(\boldsymbol{x}(t)) = \sum_{i=1}^{t_a} \langle \boldsymbol{x}(t_i) - \boldsymbol{y}(t_i), \boldsymbol{x}(t_i) - \boldsymbol{y}(t_i) \rangle . \tag{16.33}$$

However, there is the problem that the observations do not exactly match the state vector and therefore the gradient of (16.33) cannot be assumed to be exactly zero.

As in [89], it is the initial conditions to (16.32), such that (16.33) is minimized, that are required. To achieve this goal we take the first variation of (16.33) with respect to a small perturbation to the initial conditions, $\delta\boldsymbol{x}(t_0)$. Following the techniques summarized above with the continuous perturbation equation given by

$$\frac{d\delta\boldsymbol{x}}{dt} = \mathbf{A}(t)\,\delta\boldsymbol{x}, \tag{16.34}$$

where (16.34) is started from initial conditions $\delta\boldsymbol{x}(t_0)$ and

$$\mathbf{A}(t) = \frac{\partial \boldsymbol{\mathcal{M}}(\boldsymbol{x}(t))}{\partial \boldsymbol{x}(t)}$$

is the Jacobian matrix of the model equations, then the gradient is given by

$$\nabla J = 2 \sum_{i=0}^{t_a} \mathbf{L}^*(t_i, t_0)(\boldsymbol{x}(t_i) - \boldsymbol{y}(t_i)), \tag{16.35}$$

where the property that (16.34) is a linear equation for $\delta\boldsymbol{x}$ has been used, and therefore the solution at $t = t_i$ depends linearly on $\delta\boldsymbol{x}(t_0)$. The linear operator in (16.35) is referred to as the **resolvent** between t_0 and t_i and is denoted by $\mathbf{L}(t, t_0)$ and $\mathbf{L}^*(t_i, t_0)$ is its **adjoint** as we saw in the last chapter.

The more advance observation operator version of (16.33) appears in Talagrand [179], where the cost function is defined by

$$J\left(\boldsymbol{x}\left(t\right)\right)=\frac{1}{2}\sum_{i=1}^{t_a}\left\langle \boldsymbol{y}-\boldsymbol{h}\left(\boldsymbol{x}\left(t_i\right)\right),\boldsymbol{y}\left(t_i\right)-\boldsymbol{h}_i\left(\boldsymbol{x}\left(t_i\right)\right)\right\rangle . \tag{16.36}$$

Given that the observation operator is a function of the model state at t_i, then a discrete version of the dynamical model equations is required, which is

$$\boldsymbol{x}_{i+1}=\boldsymbol{x}_i+\Delta t\boldsymbol{\mathcal{M}}_{0,i}\left(\boldsymbol{x}_i\right). \tag{16.37}$$

To find the minimum of (16.36), then we require the first variations of (16.36) and (16.37) with respect to the initial conditions to (16.37). By using the techniques summarized above, as well as the adjoint property (16.30), we obtain the following expression for the Jacobian of (16.36), given (16.37) as

$$\nabla_{\boldsymbol{x}_0}J=\sum_{i=0}^{t_a}\left(\mathbf{I}+\Delta t\mathbf{M}_0^*\right)\left(\mathbf{I}+\Delta t\mathbf{M}_{0,1}^*\right)\ldots\left(\mathbf{I}+\Delta t\mathbf{M}_{0,i-1}^*\right)\mathbf{H}_i^*\left(\boldsymbol{h}_i\left(\boldsymbol{x}_i\right)-\boldsymbol{y}_i\right), \tag{16.38}$$

where

$$\mathbf{H}_i=\frac{\partial\boldsymbol{h}_i\left(\boldsymbol{x}_i\right)}{\partial\boldsymbol{x}_i},\quad \mathbf{M}_i=\frac{\partial\boldsymbol{\mathcal{M}}_{0,i}\left(\boldsymbol{x}_0\right)}{\partial\boldsymbol{x}_i}$$

are the tangent linear models of the observation operator and the nonlinear model, respectively, and * is the adjoint operator.

$$J(\boldsymbol{x}_0) = \frac{1}{2}(\boldsymbol{x}_0 - \boldsymbol{x}_{b,0})^T \mathbf{B}^{-1}(\boldsymbol{x}_0 - \boldsymbol{x}_{b,0}) + \frac{1}{2}\sum_{i=1}^{t_a}(\boldsymbol{y}_i - \boldsymbol{h}_i(\mathcal{M}_{0,i}(\boldsymbol{x}_0)))^T \mathbf{R}_i^{-1}(\boldsymbol{y}_i - \boldsymbol{h}_i(\mathcal{M}_{0,i}(\boldsymbol{x}_0))). \quad (16.39)$$

The reason to include the background, a priori information is because the problem is ill-posed if we are just considering the fit to the observations as an inverse problem [151,175], as there are not enough observations to constrain all of the degrees of freedom and as such there is not a unique solution.

The nonlinear solution to (16.39) is identified through finding the zero of the Jacobian of (16.39) which can easily be shown to be

$$\nabla_{\boldsymbol{x}_0} J = \mathbf{B}^{-1}(\boldsymbol{x}_0 - \boldsymbol{x}_b) - \sum_{i=1}^{t_a} \mathbf{H}_i^T \mathbf{M}_{0,t_i}^T \mathbf{R}_i^{-1} \mathbf{d}_i = \mathbf{0}, \quad (16.40)$$

where $\mathbf{d}_i \equiv (\boldsymbol{y}_i - \boldsymbol{h}_i(\mathcal{M}_{0,i}(\boldsymbol{x}_0)))$ is referred to as either the *innovation*, or the **departure vector**.

Another way of writing (16.40), and the more practical method for coding a **full field 4D VAR** system, is as

$$\nabla_{\boldsymbol{x}_0} J = \mathbf{B}^{-1}(\boldsymbol{x}_0 - \boldsymbol{x}_b) - \mathbf{M}_1^T \times \left(\mathbf{H}_1\mathbf{d}_1 + \mathbf{M}_2^T\left(\mathbf{H}_2\mathbf{d}_2 + \mathbf{M}_3\left(\cdots + \mathbf{M}_{N_o-1}^T\left(\mathbf{H}_{N_0-1}^T + \mathbf{M}_{N_o}^T\mathbf{H}_{N_o}^T\mathbf{d}_{N_o}\right)\right)\cdots\right)\right), \quad (16.41)$$

where in (16.41) we are moving the innovation at time k back to time $k-1$, and then adding on the scaled innovations $\mathbf{H}_{k-1}^T\mathbf{d}_{k-1}$ to $\mathbf{M}_{k,k-1}^T\mathbf{H}_k^T\mathbf{d}_k$ and so on back to the initial time of the window. Therefore, through programming the gradient in this approach, we see that we only have to evaluate the adjoint of the tangent linear model once through the whole window rather than for each innovation and then collecting their sums at time t_0.

Therefore, in a four-dimensional variational system we are seeking the initial conditions, but we could also be seeking adjusted model parameters as well as bias corrections to the observations, at the start of the assimilation window, given a set of observations through that window. (See Fig. 16.3 for an illustration of the assimilation windows.)

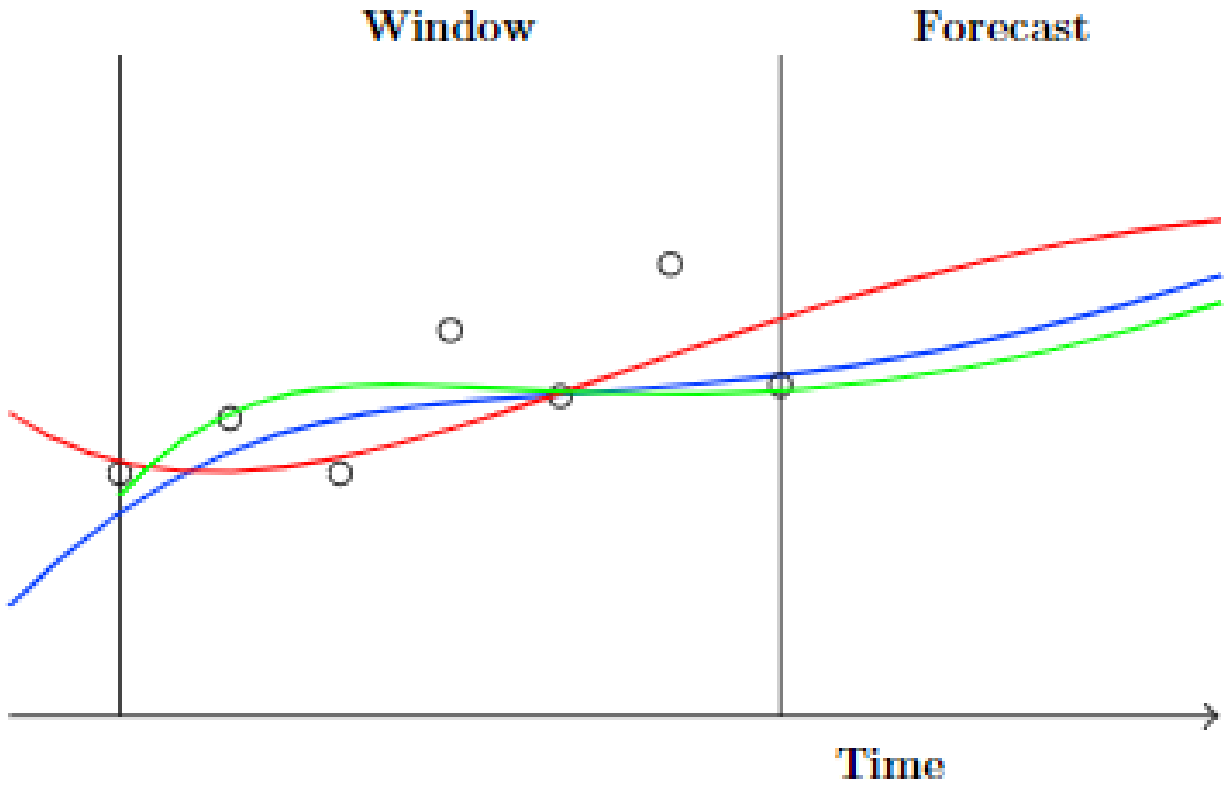

FIG. 16.3

Schematic of 4D VAR smoothing, where the blue line is the true solution, the red line is the forecast from the previous analysis time and is the background state, and the green line is the analysis trajectory filtering when the cycling length is short enough to control model error, and the circles are observations.

Incremental Variational Data Assimilation

In full field 3D VAR we have to minimize the cost function

$$J\left(\boldsymbol{x}^t\right) = \frac{1}{2}\left(\boldsymbol{x}^t - \boldsymbol{x}_b\right)^T \mathbf{B}^{-1}\left(\boldsymbol{x}^t - \boldsymbol{x}_b\right) + \frac{1}{2}\left(\boldsymbol{y} - \boldsymbol{h}\left(\boldsymbol{x}^t\right)\right)\mathbf{R}^{-1}\left(\boldsymbol{y} - \boldsymbol{h}\left(\boldsymbol{x}^t\right)\right). \quad (16.43)$$

If we look at (16.43) then we see that the only nonlinear term is the observation operator. Therefore, we are going to apply the tangent linear approximation to the observation operator as

$$\boldsymbol{h}\left(\boldsymbol{x}^t\right) \approx \boldsymbol{h}\left(\boldsymbol{x}_b\right) + \mathbf{H}\delta\boldsymbol{x},$$

where **H** is again the tangent linear approximation to the observation operator as we have used in the optimum interpolation and the full field 3D VAR schemes. Now if we notice that the background term in (16.42) is our definition for the increment, then we are able to redefine (16.43) as a cost function for the increment $\delta\boldsymbol{x}$ as

$$J\left(\delta\boldsymbol{x}\right) = \frac{1}{2}\left(\delta\boldsymbol{x}\right)^T \mathbf{B}^{-1}\left(\delta\boldsymbol{x}\right) + \frac{1}{2}\left(\boldsymbol{y} - \boldsymbol{h}\left(\boldsymbol{x}_b\right) + \mathbf{H}\delta\boldsymbol{x}\right)^T \mathbf{R}^{-1}\left(\boldsymbol{y} - \boldsymbol{h}\left(\boldsymbol{x}_b\right) + \mathbf{H}\delta\boldsymbol{x}\right). \quad (16.44)$$

Now the problem becomes to find the increment, $\delta\boldsymbol{x}^a$, such that (16.44) is minimized. As always this requires us finding the zeros, hopefully only one, of (16.44). Therefore, differentiating (16.44) with respect to $\delta\boldsymbol{x}$ yields

$$\begin{aligned} \mathbf{B}^{-1}\delta\boldsymbol{x} - \mathbf{H}^T\mathbf{R}^{-1}\left(\mathbf{d}_b - \mathbf{H}\delta\boldsymbol{x}\right) &= \mathbf{0}, \\ \Rightarrow \left(\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}\right)\delta\boldsymbol{x} &= \mathbf{H}^T\mathbf{R}^{-1}\mathbf{d}_b, \end{aligned} \quad (16.45)$$

where $\mathbf{d}_b$ is the background innovation, $\boldsymbol{y} - \boldsymbol{h}\left(\boldsymbol{x}_b\right)$. Therefore we have to iteratively find the value of $\delta\boldsymbol{x}$ such that it is possible to invert the matrix equation in (16.45). We should note here that we are not updating the background innovation; this is the slight difference to the equation that we identified from Tarantola and Valette [150] that we said was the nonlinear updated version of incremental 3D VAR. Therefore, to make (16.45) equivalent to a rearrangement of (15.84) we would have to update $\mathbf{d}_b$ with the increment added to $\boldsymbol{x}_b$ and evaluate $\boldsymbol{h}$ and as such $\mathbf{d}_b$. This is not done on each iteration, but in some implications of incremental VAR it is done at a certain stage or stages and this process is referred to as the **inner and outer loops**. We shall go into some details about the inner and outer loops in the next section; but first we move on to incremental 4D VAR.

$$\boldsymbol{x}_0^t = \boldsymbol{x}_{b,0} + \delta\boldsymbol{x}_0 \Rightarrow \delta\boldsymbol{x}_0 = \boldsymbol{x}_0^t - \boldsymbol{x}_{b,0}. \tag{16.46}$$

Thus, we need to find a way to linearize the full field 4D VAR cost function

$$J\left(\boldsymbol{x}_0^t\right) = \frac{1}{2}\left(\boldsymbol{x}_0^t - \boldsymbol{x}_{b,0}\right)^T \mathbf{B}_0^{-1}\left(\boldsymbol{x}_0^t - \boldsymbol{x}_{b,0}\right) + \frac{1}{2}\sum_{i=1}^{N_o}\left(\boldsymbol{y}_i - \boldsymbol{h}_i\left(\mathcal{M}_{0,i}\left(\boldsymbol{x}_0^t\right)\right)\right)^T \mathbf{R}_i^{-1}\left(\boldsymbol{y}_i - \boldsymbol{h}\left(\mathcal{M}_{0,i}\left(\boldsymbol{x}_0^t\right)\right)\right), \tag{16.47}$$

with respect to (16.46). The answer is to first apply the tangent linear approximation that we used for the observation operator in the incremental 3D VAR derivation, but first we apply the tangent linear approximation to the nonlinear numerical model as

$$\mathcal{M}_{0,i}\left(\boldsymbol{x}_0^t\right) \approx \mathcal{M}_{0,i}\left(\boldsymbol{x}_{b,0}\right) + \mathbf{M}_{0,i}\delta\boldsymbol{x}_0. \tag{16.48}$$

However, before we are able to implement (16.48) we have to notice that we have to apply a tangent linear approximation to the composite of two functions. Therefore, in general we have

$$f\left(g\left(x^t\right)\right) = f\left(g\left(x_b + \delta x\right)\right) \approx f\left(g\left(x_b\right)\right) + f'\left(g\left(x_b\right)\right) g'\left(x_b\right)\delta x. \tag{16.49}$$

Given (16.49), then for our application of 4D VAR, we have

$$\begin{aligned} f &= \boldsymbol{h}_i \\ g &= \mathcal{M}_{0,i}\left(\boldsymbol{x}_0^t\right), \\ f' &= \mathbf{H}_i, \\ g' &= \mathbf{M}_{0,i}. \end{aligned}$$

Thus, if we defined the ith innovation vector as $\mathbf{d}_{b,i} \equiv \boldsymbol{y}_i - \left(\mathcal{M}_{0,i}\left(\boldsymbol{x}_{b,0}\right)\right)$, then we can linearize (16.47) as

$$J\left(\delta\boldsymbol{x}_0\right) = \frac{1}{2}\left(\delta\boldsymbol{x}_0\right)^T \mathbf{B}_0^{-1}\left(\delta\boldsymbol{x}_0\right) + \frac{1}{2}\sum_{i=1}^{N_o}\left(\mathbf{d}_{b,i} - \mathbf{H}_i\mathbf{M}_{0,i}\delta\boldsymbol{x}_0\right)^T \mathbf{R}_i^{-1}\left(\mathbf{d}_{b,i} - \mathbf{H}_i\mathbf{M}_{0,i}\delta\boldsymbol{x}_{b,0}\right). \tag{16.50}$$

Therefore, we are now seeking the increment to the initial conditions that minimized (16.50). Thus we require the zeros of the Jacobian of (16.50) with respect to the perturbation to the initial conditions. The Jacobian of (16.50) can easily be shown to be

$$\nabla_{\delta \boldsymbol{x}_0} J = \mathbf{B}_0^{-1} \delta \boldsymbol{x}_0 - \sum_{i=1}^{N_o} \mathbf{M}_{0,i}^T \mathbf{H}_i^T \mathbf{R}_i^{-1} \left(\mathbf{d}_{b,i} - \mathbf{H}_i \mathbf{M}_{0,i} \delta \boldsymbol{x}_0 \right) = \mathbf{0}. \tag{16.51}$$

To be able to solve for the zeros of (16.51) we again have to apply an iterative solver for the inverse of the matrix-vector equation; however, the difference between the full field and the incremental versions of 4D VAR is that now we are only having to evolve the increment throughout the assimilation window which we assume follows the tangent linear approximation we introduced in Chapter 13, so long as the increment is sufficiently small so that the resolvent does describe its evolution throughout the assimilation window. This is an important feature to note as this now puts a constraint on the window length. We now require the window length to be of a sufficient size such that the tangent linear approximation holds.

16.4.3 INNER AND OUTER LOOPS

As we mentioned over the last two subsections, when we are implementing, or running, incremental VAR then we can take advantage of the coarseness of the spatial resolution of the small increment to reduce the cost of running the tangent linear and adjoint models. We now introduce the loose definition of the inner and outer loops in incremental VAR.

Definition 16.4 (Inner Loop). The inner loop refers to a lower spatial resolution, and possible temporal resolution with respect to incremental 4D VAR, that an iterative minimization scheme for finding the minimum of the cost function is run.

Definition 16.5 (Outer Loop). The outer loop refers to a higher-order spatial and temporal resolution, where the nonlinear trajectory of the model in the case of incremental 4D VAR, and the observation operators and hence the innovations are updated, here this is the case for both incremental 3D and 4D VAR. Note: The iterative scheme is not normally evaluated at this higher resolution. Normally only the nonlinear trajectories and innovations are updated at this resolution.

FIG. 16.4

Schematics of different possible configurations for the resolution of the inner and outer loops in 3D VAR.

SUBCOMPONENTS OF VARIATIONAL DATA ASSIMILATION

17

CHAPTER OUTLINE

17.3.1 ERROR MODELING FUNCTIONS

In this subsection we shall consider a few different functions that have been used to determine the structure and the decorrelation lengths in different atmospheric and ocean operational numerical prediction centers over the last 30 years. We have seen some of the approaches in the optimal interpolation chapter as this is a requirement of these systems, but for the OI schemes we are only determining over a finite area, while in the VAR schemes we are solving globally.

Autoregressive models

The first auto regressive model that we present is the **second-order auto-regressive** model, or SOAR for short. This function is defined by

$$c_{n,m} = (1 + |\Delta\omega|)\, e^{-|\delta\omega|}, \tag{17.139}$$

where here we are defining this model in the vertical and as such $\delta\omega = -\int_{z_m}^{z_n} L(z)^{-1}\, dz$ and that $L(z)$ is a local vertical length scale that is a function of pressure.

In the horizontal direction, the SOAR model is defined as

$$c_b^h(s_{nm}, L_{nm}) = \left(1 + \frac{s_{nm}}{L_{nm}}\right) e^{-\frac{s_{nm}}{L_{nm}}}, \tag{17.140}$$

where s_{nm} is some form of distance measure between points on the type of grid being considered, and L_{nm} is the decorrelation length in that specific horizontal direction. A **third-order auto-regressive**, or **TOAR**, as stated in [225], can be defined as

$$F(c, r) = (1 + \alpha)^{-1} \left(f(c, r) + \alpha f\left(\frac{c}{N}, r\right)\right), \tag{17.141}$$

where

$$f(c,r) = \left(1 + cr + \frac{c^2 r^2}{c}\right) e^{-cr}, \tag{17.142}$$

and

$$L_c = \sqrt{\left(\frac{3(1+\alpha)}{1+\frac{\alpha}{N^2}}\right)} c^{-1}, \tag{17.143}$$

where L_c is the correlation length scale and c is inversely related to this length scale. It is also stated in [225] that is possible to fit the covariance model to the wind fields from the function for the covariance for the geopotential height in (17.141) as

$$F'(c,r) = \left(1 + \frac{\alpha}{N^2}\right)^{-1} \left(f'(c,r) + \frac{\alpha}{N^2} f'\left(\frac{c}{N}, r\right)\right), \tag{17.144a}$$

$$f'(c,r) = (1 + cr) e^{-cr}, \tag{17.144b}$$

where in [225] the values for α is 0.2 and for N is 3.

Gaussian

An alternative to the auto-regressive models in the vertical is to fit a Gaussian for the decorrelation which is given by

$$c_{n,m} = e^{-\frac{(\Delta\omega)^2}{2}}. \tag{17.145}$$

The reason why people may not use the Gaussian and prefer the SOAR approach is due to the slope, effectively the dropoff of the correlations as a function of distance. We can see from Fig. 17.3 that there is a subtle difference between the two approach where the Gaussian allows for a longer dropoff, whereas for the SOAR approximation, this model does not allow as far a correlation as the Gaussian approach does.

The horizontal version of the Gaussian model for the correlation is given by

$$c_b^h(s_{nm}, L_{nm}) = e^{-\left(\frac{s_{nm}}{L_{nm}}\right)^2}. \tag{17.146}$$

Compact spline

The covariance model here comes from [226], where this a function of compact support that goes identically to zero with its first two derivatives at some finite distance, which is denoted as $2c$. If we let $c = \left(\frac{10}{3}\right)^{\frac{1}{2}}$ and $r = \frac{s_{nm}}{cL_{nm}}$, therefore the correlation model in the horizontal is given by

$$c_b^h = -\frac{r^5}{4} + \frac{r^4}{2} + \frac{5r^4}{8} - \frac{5r^2}{3} + 1, \qquad 0 \le r \le 1, \tag{17.147a}$$

$$= \frac{r^5}{12} - \frac{r^4}{2} + \frac{5r^3}{8} + \frac{5r^2}{3} - 5r + 4 - \frac{2}{3r}, \qquad 1 < r \le 2, \tag{17.147b}$$

$$= 0, \qquad r > 2. \tag{17.147c}$$

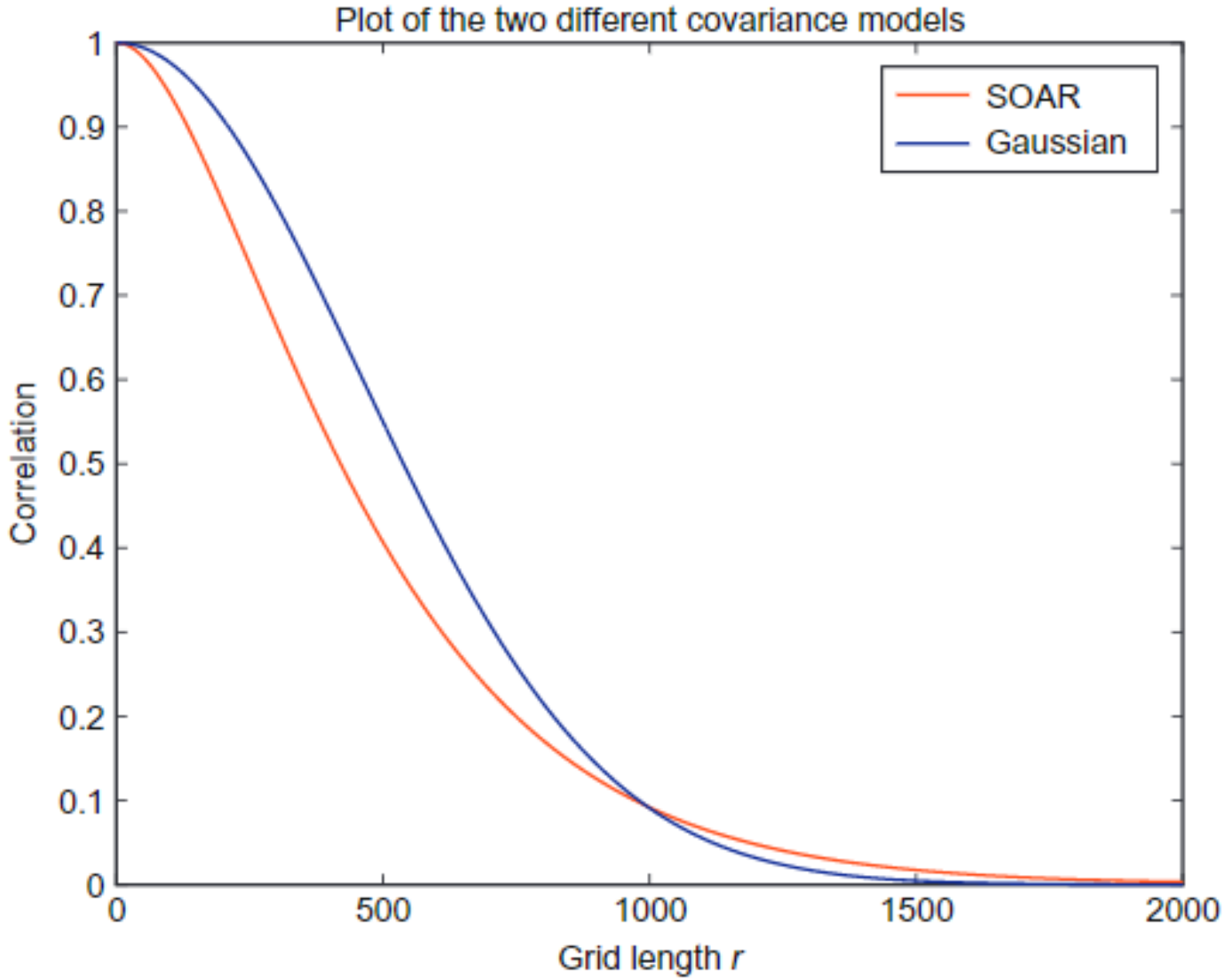

FIG. 17.3

Plot of the SOAR and the Gaussian correlation functions.