## Introduction to Data Assimilation

## Learning Objectives

Following this lecture, students will be able to:

- Distinguish between sequential and continuous data assimilation.
- Define model-state vectors, observation vectors, forward operators, innovations, and analysis residuals.
- Derive the least-squares formulation for one-dimensional data assimilation.
- Extend the one-dimensional data assimilation framework to multiple dimensions.


## Fundamental Principles of Data Assimilation

As defined previously, data assimilation is the process by which observations are assimilated to update a first guess for the initial conditions that is typically drawn from a short-range (1-6 h) model forecast. Data assimilation methods seek to obtain the best-possible estimate of the initial atmospheric state while, hopefully but not necessarily intrinsically, satisfying an appropriate atmospheric balance condition. Using a short-range numerical model forecast as the first guess enables atmospheric phenomena on scales of those resolved by the model grid and larger to be partially represented in the initial conditions (e.g., a warm-start initialization). It also allows for approximate initial conditions to be available in locations where few or no observations exist.

Data assimilation involves modifying the first guess based on an observation's characteristics. Consider the assimilation of a wind observation in the core of an upper-tropospheric jet streak. This observation should first update the kinematic fields at the observation's location. However, because most atmospheric fields are continuous, we know that this observation is closely related to the kinematic fields at other nearby locations (both horizontally and vertically). Likewise, as the atmosphere typically approximates some sort of balance, this observation is also closely related to the thermodynamic fields at its location and other nearby locations (also both horizontally and vertically). Thus, this observation should also update these other fields. How it does so, however, significantly varies between assimilation techniques.

Further, data assimilation methods should update the first guess more in locations of higher data density than in locations of lower data density. In the former, the observations provide a tighter constraint upon the 'true' values of the relevant model variables, whereas in the latter the 'true' values of the relevant model variables are less certain. In other words, the first guess forms the basis for the initial conditions in the absence of observations to the contrary.

There are two categories of data assimilation: sequential and continuous. With sequential data assimilation methods (Figs. 1 and 2), observations are assimilated in batches at a single analysis time. For instance, all observations valid at a time deemed sufficiently close to the model's initialization time (typically within $+/-30-60 \mathrm{~min}$ ) are assimilated as if they were taken at the initialization time.

Given a reasonable estimate for the resolved-scale kinematic fields, time-to-space conversion can be used to identify where a given observation would have been taken if it were taken at 0000 UTC, thus allowing for observations to be assimilated at their 'correct' locations.

Sequential data assimilation methods are typically known as cycled methods, with the cycling interval reflecting how frequently observations are assimilated to update the first guess for the initial conditions.


Figure 1. Flowchart of sequential data assimilation. Observations centered on a given analysis time are used to update the first guess for the initial conditions obtained from a previous model forecast valid at the analysis time. Figure reproduced from Warner (2011), their Fig. 6.5.


Figure 2. Sequential data assimilation as manifest in operational numerical weather prediction. Observations centered on a given analysis time are binned and assimilated at a fixed analysis time (e.g., 0000 UTC, 0600 UTC, 1200 UTC, or 1800 UTC) to obtain updated initial conditions. Figure reproduced from Warner (2011), their Fig. 6.6b.

By contrast, continuous data assimilation methods (Fig. 3) assimilate observations at the times at which they are valid. As compared to sequential methods, continuous methods more frequently update the first guess, but do so using fewer observations since they are not all lumped into a single assimilation time. Forecasts launched from initial conditions updated using continuous methods can theoretically be launched at any time; however, in practice, forecasts are typically launched only at synoptic times (i.e., when the most observations are available for assimilation). Continuous methods are more computationally intensive than are sequential methods, and as a result most (but not all) operational data assimilation systems are sequential in nature.


Figure 3. Continuous data assimilation as manifest in operational numerical weather prediction. Observations are assimilated as they are received. In this example, forecasts are launched every 6 h, though they may be launched more or less frequently. Figure reproduced from Warner (2011), their Fig. 6.6a.

## Definitions

Before we consider the data assimilation problem, whether in one or many dimensions, we wish to first introduce some common terms encountered in the data assimilation literature. These include the following:

- State vector $(\vec{x})$ : the vector that defines the simulated atmospheric state. It and the other vectors noted below contain all model variables at all model grid points at a given time.
- True state vector $\left(\overrightarrow{x_{t}}\right)$ : the best-possible representation of the atmospheric state on the model grid. Discretizing the atmosphere onto a discrete model grid and the errors associated with doing so keep the true state vector from matching reality.
- Perfect state vector $\left(\overrightarrow{x_{p}}\right)$ : the unknowable reality.
- Background $\left(\overrightarrow{x_{b}}\right)$ : the first-guess estimate of the initial atmospheric state.
- Analysis $\left(\overrightarrow{x_{a}}\right)$ : the post-assimilation estimate of the simulated atmospheric state; i.e., an updated background.

Each of these vectors are of dimension $n$, where $n$ is equal to the product of the number of model grid points and the number of model variables. Note that boldface and vector notation are equivalently used to refer to vector quantities throughout the remainder of this document.

Ideally, $\mathbf{x a}_{\mathbf{a}}=\mathbf{x t}$. This is generally not feasible, however, due to observing-network limitations (e.g., observation density, observation precision, representativeness errors, etc.). Instead, we seek to minimize the error in $\mathbf{x}$, i.e.,

$$
\overrightarrow{x_{t}}-\overrightarrow{x_{a}} \approx 0
$$

The analysis and background are related to each other by an analysis increment $\delta x$, i.e.,

$$
\overrightarrow{x_{a}}=\overrightarrow{x_{b}}+\delta x \approx \overrightarrow{x_{t}}
$$

As we will demonstrate shortly, the analysis increment is dependent on characteristics of the observations, namely their specific values and error characteristics.

- Observation vector $(\vec{y})$ : a vector of dimension $p$ (equaling the number of observations) of all observations to be assimilated.

Data assimilation starts by comparing the background $\mathbf{x}$ to the observations $\mathbf{y}$. This is done in observation space, meaning that it is done at the locations of the observations for the variables represented by the observations. This requires the use of a...

- Forward/transform operator $(\vec{H}(\vec{x})$ ): an operator to transform a model field $\mathbf{x}$ to observation space. In its simplest form, where the observed variable is a model variable, the forward operator is a spatial interpolation operator. More commonly, however, it also invokes retrieval algorithms to convert a model variable to the observed quantity.
- Innovation $\left(\vec{y}-\vec{H}\left(\overrightarrow{x_{b}}\right)\right.$ ): the difference between the observations and the background. It is an estimate of the needed correction to the background state. This is equal to $\delta x$, except in observation (rather than model) space.
- Analysis residual $\left(\vec{y}-\vec{H}\left(\overrightarrow{x_{a}}\right)\right.$ ): the difference between the observations and the analysis (transformed into observation space).

The analysis will depart from the observations in the absence of perfect observations of every variable at every location on the model grid. Instead, we seek to minimize the analysis residual,

$$
\vec{y}-\vec{H}\left(\overrightarrow{x_{a}}\right) \approx 0
$$

This is the observation space equivalent to minimizing the error in the analysis $\mathbf{x}_{\mathrm{a}}$ relative to the true state $\mathbf{x}_{\mathrm{t}}$.

## One-Dimensional Statistical Framework for Data Assimilation

We now wish to develop a one-dimensional statistical framework for data assimilation. To do so, we use a form of linear regression known as least-squares estimation.

Consider the temperature in Milwaukee with a true value of $T_{t}$. There are two estimates of this temperature: the background or first-guess value $T_{b}$ and the observed value $T_{o}$. Both are imperfect measurements of $T_{t}$, with a background error $\varepsilon_{b}$ and observational error $\varepsilon_{o}$. The background error may be drawn from climatology, whereas the observational error is typically specified empirically based on instrument characteristics and the expected representativeness of the observation.

To obtain the analysis temperature $T_{a}$, we wish to optimally combine $T_{b}$ and $T_{o}$ based on their individual error characteristics. We start by defining $T_{b}$ and $T_{o}$ relative to $T_{t}$ :

$$
T_{b}=T_{t}+\varepsilon_{b} \quad T_{o}=T_{t}+\varepsilon_{o}
$$

In other words, each estimate is equal to $T_{t}$ plus the error in the estimate.
We assume that errors in $T_{b}$ and $T_{o}$ are random, assuming unbiased methods to obtain $T_{b}$ and $T_{o}$. We also assume that we know or can estimate the background and observational errors $\varepsilon b$ and $\varepsilon_{o}$.

Recall that the sample variance can be defined generically as:

$$
\sigma^{2}=\frac{\sum(x-\mu)^{2}}{N-1}
$$

Here, $x$ is some estimate of the variable being considered. In this application, $x$ can be viewed as analogous to either $T_{b}$ or $T_{o}$. In statistical terms, $\mu$ is the mean of the variable being considered. In this application, $\mu$ can be viewed as analogous to $T_{t} . N$ defines the population size, or number of estimates $x$. There can be one or many such estimates. The variance defines the mean squared error and, for unbiased methods for $x$ and $\mu$, can be expressed as:

$$
\sigma^{2}=E\left((x-\mu)^{2}\right)
$$

where the expected value $E()$ is analogous to the mean of an infinitely sampled discrete random variable. This holds here, except that our estimates $x$ are finite in number.

With this information, we can write:

$$
\begin{aligned}
& \sigma_{b}^{2}=E\left(\left(T_{b}-T_{t}\right)^{2}\right)=E\left(\varepsilon_{b}^{2}\right) \\
& \sigma_{o}^{2}=E\left(\left(T_{o}-T_{t}\right)^{2}\right)=E\left(\varepsilon_{o}^{2}\right)
\end{aligned}
$$

where we have used the definitions for $\varepsilon_{b}$ and $\varepsilon_{o}$ given above to obtain the final expressions. Note that errors in the background and observations are said to be uncorrelated, such that:

$$
E\left(\varepsilon_{o} \varepsilon_{b}\right)=0
$$

The least-squares best fit of $T_{b}$ and $T_{o}$, defining the analysis $T_{a}$, is given by:

$$
T_{a}=a_{b} T_{b}+a_{o} T_{o} \quad \text { where } a_{b}+a_{o}=1
$$

This represents the optimal linear combination of $T_{b}$ and $T_{o}$, where $a_{b}$ and $a_{o}$ represent the weights applied to $T_{b}$ and $T_{o}$, respectively. We choose these weights to minimize the mean squared error of $T_{a}$, defined by $\sigma_{a}^{2}$, i.e.,

$$
\sigma_{a}^{2}=E\left(\left(T_{a}-T_{t}\right)^{2}\right)
$$

This expression can be expanded by substituting for both $T_{a}$ and $T_{t}$, noting that $T_{t}=a_{b} T_{t}+a_{o} T_{t}$ (a decomposition of $T_{t}$ solely for algebraic purposes):

$$
\begin{aligned}
E\left(\left(T_{a}-T_{t}\right)^{2}\right) & =E\left(\left(\left(a_{b} T_{b}+a_{o} T_{o}\right)-\left(a_{b} T_{t}+a_{o} T_{t}\right)\right)^{2}\right) \\
& =E\left(\left(a_{o}\left(T_{o}-T_{t}\right)+a_{b}\left(T_{b}-T_{t}\right)\right)^{2}\right)
\end{aligned}
$$

The second step above simply involves grouping like $a_{o}$ and $a_{b}$ terms. Noting that $T_{o}-T_{t}$ is equal to $\varepsilon_{o}$ and that $T_{b}-T_{t}$ is equal to $\varepsilon b$, we obtain:

$$
\sigma_{a}^{2}=E\left(\left(a_{o} \varepsilon_{o}+a_{b} \varepsilon_{b}\right)^{2}\right)
$$

If we expand this, we obtain:

$$
\sigma_{a}^{2}=E\left(\left(a_{o} \varepsilon_{o}\right)^{2}+2 a_{o} a_{b} \varepsilon_{o} \varepsilon_{b}+\left(a_{b} \varepsilon_{b}\right)^{2}\right)
$$

However, we stated earlier that errors in the observations and background are uncorrelated. Thus, the $2 a_{o} a_{b \varepsilon} \varepsilon_{o} b$ term (involving the product of these errors) is zero. Since $E(a+b)=E(a)+e(b)$, we can write:

$$
\sigma_{a}^{2}=E\left(\left(a_{o} \varepsilon_{o}\right)^{2}+\left(a_{b} \varepsilon_{b}\right)^{2}\right)=E\left(\left(a_{o} \varepsilon_{o}\right)^{2}\right)+E\left(\left(a_{b} \varepsilon_{b}\right)^{2}\right)=a_{o}^{2} \sigma_{o}^{2}+a_{b}^{2} \sigma_{b}^{2}
$$

We applied the definitions of both $\sigma_{o}^{2}$ and $\sigma_{b}^{2}$ to obtain this final expression. Consequently, this expression indicates that the analysis error variance is given by a linear combination of the observation and background error variances.

Recall that we are trying to find the $a_{o}$ and $a_{b}$ that minimize the mean squared error in $T_{a}\left(\sigma_{a}^{2}\right)$. Let $a_{o}=k$, such that $a_{b}=1-k$, where $k$ is the optimal weighting factor. Substituting, we obtain:

$$
\sigma_{a}^{2}=k^{2} \sigma_{o}^{2}+(1-k)^{2} \sigma_{b}^{2}
$$

Calculus gives us a means of obtaining an expression that minimizes $\sigma_{a}^{2}$ relative to the optimal weighting factor $k$. By definition, $\sigma_{a}^{2}$ is minimized when its first partial derivative with respect to $k$ is equal to zero, i.e.,

$$
\frac{\partial \sigma_{a}^{2}}{\partial k}=0
$$

Plugging in to this expression, we obtain:

$$
\frac{\partial \sigma_{a}^{2}}{\partial k}=\frac{\partial}{\partial k}\left(k^{2} \sigma_{o}^{2}+(1-k)^{2} \sigma_{b}^{2}\right)=0
$$

The expansion of $(1-k)^{2}$ is given by $k^{2}-2 k+1$. Thus, we obtain:

$$
\frac{\partial}{\partial k}\left(k^{2} \sigma_{o}^{2}+k^{2} \sigma_{b}^{2}-2 k \sigma_{b}^{2}+\sigma_{b}^{2}\right)=2 k \sigma_{o}^{2}+2 k \sigma_{b}^{2}-2 \sigma_{b}^{2}=0
$$

Solving for $k$, we obtain:

$$
k=\frac{\sigma_{b}^{2}}{\sigma_{o}^{2}+\sigma_{b}^{2}}
$$

In other words, $k$ is equal to the background error variance divided by the total error variance, representing the observational plus background error variances. $k$ will be relatively large where the uncertainty in the background is large relative to the uncertainty in the observations, whereas $k$ will be relatively small where the uncertainty in the background is small relative to the uncertainty in the observations.

Recall that $k$ is the coefficient on $\sigma_{o}^{2}$ in the definition of $\sigma_{a}^{2}$. Thus, observations are given more weight when $k$ is large whereas the background is given more weight when $k$ is small. Because of the definitions for $T_{a}$ and $k$ given earlier, we can write:

$$
T_{a}=a_{b} T_{b}+a_{o} T_{o}=(1-k) T_{b}+k T_{o}=T_{b}+k\left(T_{o}-T_{b}\right)
$$

In other words, the analysis temperature $T_{a}$ is equal to the background temperature $T_{b}$ plus an optimally weighted innovation (reflecting the departure of the background from the observation, noting that no transform is needed between model and observation space in this 1-D example). The weighted innovation $k\left(T_{o}-T_{b}\right)$ is equal to the analysis increment.

We can plug in for $k$ in the above:

$$
T_{a}=a_{b} T_{b}+a_{o} T_{o}=(1-k) T_{b}+k T_{o}=\left(1-\frac{\sigma_{b}^{2}}{\sigma_{o}^{2}+\sigma_{b}^{2}}\right) T_{b}+\frac{\sigma_{b}^{2}}{\sigma_{o}^{2}+\sigma_{b}^{2}} T_{o}
$$

However, because $a_{o}+a_{b}=1$,

$$
\left(1-\frac{\sigma_{b}^{2}}{\sigma_{b}^{2}+\sigma_{o}^{2}}\right)=\frac{\sigma_{o}^{2}}{\sigma_{b}^{2}+\sigma_{o}^{2}}
$$

Thus, we obtain:

$$
T_{a}=\frac{\sigma_{o}^{2}}{\sigma_{o}^{2}+\sigma_{b}^{2}} T_{b}+\frac{\sigma_{b}^{2}}{\sigma_{o}^{2}+\sigma_{b}^{2}} T_{o}
$$

The analysis temperature $T_{a}$ depends on the background and observation error variances. The background temperature $T_{b}$ gets larger weight where the observation error variance is large, whereas the observation temperature $T_{o}$ gets larger weight where the background error variance is large. Thus, accurately specifying the observation and background error variances is crucial to obtaining the best-possible estimate for the analysis temperature $T_{a}$.

The observation error variance is typically specified relative to instrument error characteristics, typical magnitudes for representativeness error, and typical uncertainties associated with the use of a retrieval algorithm (if applicable). Specification of the background error variance is far more challenging and is discussed in more detail later.

Recall that $\sigma_{a}^{2}=k^{2} \sigma_{o}^{2}+(1-k)^{2} \sigma_{b}^{2}$. Plug in to this expression for $k$ to obtain:

$$
\sigma_{a}^{2}=\left(\frac{\sigma_{b}^{2}}{\sigma_{b}^{2}+\sigma_{o}^{2}}\right)^{2} \sigma_{o}^{2}+\left(\frac{\sigma_{o}^{2}}{\sigma_{b}^{2}+\sigma_{o}^{2}}\right)^{2} \sigma_{b}^{2}=\frac{\left(\sigma_{b}^{2}\right)^{2} \sigma_{o}^{2}+\left(\sigma_{o}^{2}\right)^{2} \sigma_{b}^{2}}{\left(\sigma_{b}^{2}+\sigma_{o}^{2}\right)^{2}}
$$

The numerator of this expression can be rewritten as $\left(\sigma_{b}^{2}+\sigma_{o}^{2}\right) \sigma_{b}^{2} \sigma_{o}^{2}$. Thus,

$$
\sigma_{a}^{2}=\frac{\sigma_{o}^{2} \sigma_{b}^{2}}{\left(\sigma_{b}^{2}+\sigma_{o}^{2}\right)}
$$

Applying the definition for $k$, we can write:

$$
\sigma_{a}^{2}=k \sigma_{o}^{2} \quad \text { or, equivalently, } \quad \sigma_{a}^{2}=(1-k) \sigma_{b}^{2}
$$

Because $k \leq 1$, this means that the analysis error variance is smaller than or equal to either the observation or background error variance! For a multi-dimensional problem, this implies that the spread across the ensemble analyses will be smaller than the spread in either the observations or the ensemble backgrounds.

We can also state this in terms of the precision, or the inverse variance. Take the inverse of the relationship for $\sigma_{a}^{2}$ to obtain:

$$
\frac{1}{\sigma_{a}^{2}}=\frac{\left(\sigma_{b}^{2}+\sigma_{o}^{2}\right)}{\sigma_{b}^{2} \sigma_{o}^{2}}=\frac{1}{\sigma_{o}^{2}}+\frac{1}{\sigma_{b}^{2}}
$$

Here, the precision of the analysis is equal to the sum of the precisions of the background and observations. Estimates with less error in the background and observations have higher precision. Combining two good estimates results in a very good (in theory, at least) analysis estimate!

Least-squares minimization is one common approach to data assimilation and is used in many Kalman filter implementations (e.g., the ensemble adjustment Kalman filter in NCAR's Data

Assimilation Research Toolkit). A closely related approach is given by cost-function minimization, which is often used by variational data assimilation. Here, we wish to find the analysis that minimizes the combined squared errors in $T_{o}$ and $T_{b}$, each as weighted by the precision of their measurements.

We define the combined squared error in terms of a cost function $J(T)$ as follows:

$$
J(T)=J\left(T_{o}\right)+J\left(T_{b}\right)=\frac{1}{\sigma_{o}^{2}}\left(T-T_{o}\right)^{2}+\frac{1}{\sigma_{b}^{2}}\left(T-T_{b}\right)^{2}
$$

Note that this is expressed relative to a generic $T$ and not to $T_{t}$ or $T_{a}$. The cost in the observations or the background is relatively small when $T \approx T_{o}$ or $T_{b}$ and/or when the precision of the observations or background is relatively large. These characteristics are illustrated in Fig. 4.


Figure 4. Schematic of $J\left(T_{o}\right), J\left(T_{b}\right)$, and the total cost function $J(T)$ relative to $T$ and $J$. The cost functions $J\left(T_{o}\right)$ and $J\left(T_{b}\right)$ are minimized where $T-T_{o}=0$ and $T-T_{b}=0$, respectively. (Note that the representation of $J\left(T_{o}\right)$ above is formally not accurate at $T=T_{o}$.) The total cost function $J(T)$ is simply equal to the sum of the two cost functions. The analysis temperature is defined as the temperature where the cost function is minimized with respect to temperature, which can be determined by finding where the first partial derivative equals zero. Figure reproduced from Warner (2011), their Fig. 6.7.

We wish to minimize the cost function $J\left(T_{a}\right)$ with respect to the analysis temperature, i.e.,

$$
\frac{\partial J\left(T_{a}\right)}{\partial T_{a}}=0
$$

This enables us to obtain an expression the analysis temperature $T_{a}$. For completeness, note that:

$$
J\left(T_{a}\right)=\frac{1}{\sigma_{o}^{2}}\left(T_{a}-T_{o}\right)^{2}+\frac{1}{\sigma_{b}^{2}}\left(T_{a}-T_{b}\right)^{2}=\frac{1}{\sigma_{o}^{2}}\left(T_{a}^{2}+T_{o}^{2}-2 T_{a} T_{o}\right)+\frac{1}{\sigma_{b}^{2}}\left(T_{a}^{2}+T_{b}^{2}-2 T_{a} T_{b}\right)
$$

Thus, we obtain:

$$
\frac{\partial J\left(T_{a}\right)}{\partial T_{a}}=\frac{1}{\sigma_{o}^{2}}\left(2 T_{a}-2 T_{o}\right)+\frac{1}{\sigma_{b}^{2}}\left(2 T_{a}-2 T_{b}\right)=0
$$

Grouping $T_{a}$ terms and dividing through by a common factor of 2, we obtain:

$$
\frac{T_{a}}{\sigma_{o}^{2}}+\frac{T_{a}}{\sigma_{b}^{2}}=\frac{T_{o}}{\sigma_{o}^{2}}+\frac{T_{b}}{\sigma_{b}^{2}}
$$

Operate on the left-hand side to obtain:

$$
\frac{T_{a}\left(\sigma_{b}^{2}+\sigma_{o}^{2}\right)}{\sigma_{o}^{2} \sigma_{b}^{2}}=\frac{T_{o}}{\sigma_{o}^{2}}+\frac{T_{b}}{\sigma_{b}^{2}}
$$

Isolate $T_{a}$ and simplify to obtain:

$$
T_{a}=\frac{\sigma_{o}^{2} \sigma_{b}^{2}}{\left(\sigma_{b}^{2}+\sigma_{o}^{2}\right)}\left(\frac{T_{o}}{\sigma_{o}^{2}}+\frac{T_{b}}{\sigma_{b}^{2}}\right)=\left(\frac{\sigma_{b}^{2}}{\sigma_{b}^{2}+\sigma_{o}^{2}}\right) T_{o}+\left(\frac{\sigma_{o}^{2}}{\sigma_{b}^{2}+\sigma_{o}^{2}}\right) T_{b}=k T_{o}+(1-k) T_{b}
$$

This is identical to that obtained from the least-squares minimization problem described above, albeit coming at the problem from a slightly different starting point. Differences in how each are implemented for multidimensional problems lead to non-identical results in practice.

## Data Assimilation in Multiple Dimensions

In one dimension, the observation and background error variances determine the weighting given to the observation when assimilating it to update the background. In other words, they influence the magnitude of the analysis increment, i.e.,

$$
T_{a}=T_{b}+k\left(T_{o}-T_{b}\right)=T_{b}+\frac{\sigma_{b}^{2}}{\sigma_{o}^{2}+\sigma_{b}^{2}}\left(T_{o}-T_{b}\right)
$$

In the multidimensional problem, they also influence the analysis increment's spread. This is manifest as (1) updates to the same variable at other locations, (2) updates to different variables at the same location, and (3) updates to different variables at other locations. To first order, the spread of the analysis increment is a function of the (mathematical, though also ideally physical) relationship, as manifest via their covariance, between the updated variable and other variables
or locations. It is crucially dependent on accurately specifying the background error covariance matrix.

The multidimensional analog to the background error variance $\sigma_{b}^{2}$ is the background error covariance matrix $\mathbf{B}$. The background error covariance matrix translates information from an innovation vector $\vec{y}-\vec{H}\left(\overrightarrow{x_{b}}\right)$ into a spatially varying analysis increment $\delta \vec{x}$ and applies it to the background to minimize the analysis error. This is the same conceptual framework as in one dimension, except with the added dimensionality.

In the one-dimensional problem, the background error variance $\sigma_{b}^{2}$ is defined as:

$$
\sigma_{b}^{2}=E\left(\varepsilon_{b}^{2}\right)=\overline{\left(x_{b}-x_{t}\right)^{2}}
$$

Similarly, the multi-dimensional background error covariance matrix $\mathbf{B}$ is defined as:

$$
\vec{B}=\overline{\left(\overrightarrow{x_{b}}-\overrightarrow{x_{t}}\right)\left(\overrightarrow{x_{b}}-\overrightarrow{x_{t}}\right)^{T}}
$$

Equivalently, if the background errors are unbiased, the true state can be approximated by the mean of some collection of background estimates (such as that provided by an ensemble), i.e., $x_{t}=\overline{x_{b}}$. Thus, the above expressions can be rewritten as:

$$
\begin{aligned}
& \sigma_{b}^{2}=E\left(\varepsilon_{b}^{2}\right)=\overline{\left(x_{b}-\overline{x_{b}}\right)^{2}} \\
& \vec{B}=\overline{\left(\overrightarrow{x_{b}}-\overrightarrow{\overline{x_{b}}}\right)\left(\overrightarrow{x_{b}}-\overrightarrow{\bar{x}_{b}}\right)^{T}}
\end{aligned}
$$

In the above, $T$ denotes the transpose of the matrix. The background error covariance matrix is an $n \mathrm{x} n$ square matrix, recalling that $n$ is the product of the number of grid points and the number of model variables. The diagonal of $\mathbf{B}$ is populated by the error variances for a given background estimate at a given location. The off-diagonal terms of $\mathbf{B}$ are populated by the covariances between errors in two separate background estimates. For the case where $n=3$, i.e., three variables at one grid point or three grid points for a single variable, $\mathbf{B}$ takes the form:

$$
\vec{B}=\left[\begin{array}{ccc}
\operatorname{var}\left(e_{1}\right) & \operatorname{cov}\left(e_{2}, e_{1}\right) & \operatorname{cov}\left(e_{3}, e_{1}\right) \\
\operatorname{cov}\left(e_{1}, e_{2}\right) & \operatorname{var}\left(e_{2}\right) & \operatorname{cov}\left(e_{3}, e_{2}\right) \\
\operatorname{cov}\left(e_{1}, e_{3}\right) & \operatorname{cov}\left(e_{2}, e_{3}\right) & \operatorname{var}\left(e_{3}\right)
\end{array}\right]
$$

where $e \#=x_{b, \#}$, or the background estimate of variable \#.

As stated before, the specification of the covariance terms defines both the spread of and the weight given to analysis increments. The variance terms define the weight given to analysis increments only for the variable being updated at the location that it is updated.

How is the background error covariance matrix specified? There exist two primary approaches that are used to do so:

- Flow-dependent: Consider an ensemble of short-range numerical forecasts valid at some analysis time. These comprise the background estimates. For unbiased background estimates, the true state can be approximated by this ensemble's mean. Departures of the ensemble estimates from the ensemble mean define $\mathbf{B}$. This specification is implicitly flow-dependent (i.e., the covariances are likely to be larger following the flow) and is explicitly temporally varying. See Fig. 5 for an idealized example.
- Flow-independent: Consider a climatology of short-range numerical forecasts valid at a common lead time (e.g., 6 h ). These comprise the background estimates. The true state can then be approximated by their mean if we crudely assume that these estimates are unbiased. Departures of the short-range forecasts from their climatological-mean errors define $\mathbf{B}$. This specification is explicitly flow-independent (i.e., the covariances become smaller uniformly away from the location and variable being considered). See Fig. 6 for an idealized example. A version of this method was operationally used by NCEP for many years.

Most data assimilation systems employ some means of localization to place an upper bound on the outward spread of the analysis increment to avoid spurious updates that may arise from small non-physical covariances (e.g., 500 hPa temperature near Milwaukee to the 850 hPa zonal wind over Antarctica, as one hypothetical example) whether flow-independent or flow-dependent methods are used to specify B. Specifying an innovation influence (or covariance) of zero beyond a certain radius in Figs. 5 and 6 is an illustrative example of localization.


Figure 5. The hypothetical spatial spread of the innovation, defining the analysis increment, for a flow-dependent specification of the background error covariance matrix. In this example, the background errors are better correlated following the large-scale westerly flow, and thus the analysis increment's decay away from the observation location is non-isotropic (i.e., less rapid following the flow and more rapid perpendicular to the flow). Figure reproduced from Warner (2011), their Fig. 6.9b.


Figure 6. The hypothetical spatial spread of the innovation for a flow-independent specification of the background error covariance matrix. The analysis increment is maximized at the location of the observation and decays isotropically (uniformly in all directions) independent of the largescale flow. Figure reproduced from Warner (2011), their Fig. 6.9a.

For completeness, we present the multidimensional analogs to the other variables defined for the one-dimensional data assimilation problem:

- Observation error covariance matrix ( $\mathbf{R}$ ): the multidimensional analog to $\sigma_{o}^{2}$.

Typically, it is assumed that any two observation errors are uncorrelated, such that the covariance terms of this matrix are all zero. Thus, $\mathbf{R}$ is a diagonal matrix of dimension $p$ $\mathrm{x} p$, where $p$ is equal to the number of observations, and is comprised only of error variances.

- Analysis error covariance matrix (A): the multidimensional analog to $\sigma_{a}^{2}$.
- Forecast error covariance matrix (Q): the multidimensional analog to the forecast error variance $\sigma_{f}^{2}=E\left(\varepsilon_{f}^{2}\right)=E\left(\left(T_{f}-T_{t}\right)^{2}\right)$, where subscripts of $f$ denote forecast quantities.
- Weighting matrix (K): the multidimensional analog to $k$, defining both the weight and spread of analysis increments.

These definitions allow us to state, without formally deriving them, the analogous expressions for the analysis and optimal weight in the multidimensional problem. Recall that the analysis for the one-dimensional problem was expressed as:

$$
T_{a}=T_{b}+k\left(T_{o}-T_{b}\right)
$$

In the multidimensional problem, the analogous expression is:

$$
\overrightarrow{x_{a}}=\overrightarrow{x_{b}}+\vec{K}\left(\vec{y}-\vec{H}\left(\overrightarrow{x_{b}}\right)\right)
$$

Here, the analysis state is equal to the background state plus the weighted innovations, defined as the observations minus the transformed background estimates. Note that the transformation of the innovation back to model space is implicit to the above formulation.

Recall that the weight for the one-dimensional problem was expressed as:

$$
k=\frac{\sigma_{b}^{2}}{\sigma_{o}^{2}+\sigma_{b}^{2}}
$$

In the multidimensional problem, the analogous expression is:

$$
\vec{K}=\frac{\vec{B} \vec{H}^{T}}{\vec{H} \vec{B} \vec{H}^{T}+\vec{R}}
$$

Here, the weighting matrix is equal to the ratio of the background error covariance matrix to the sum of the background and observation error covariance matrices. The $\mathbf{H}$ and $\mathbf{H}^{\mathbf{T}}$ are transform operators between model and observation space.

