Chapter 2
Representation of the Physical System

Abstract The core problems of estimation approaches to data assimilation problems lie in the generic discrete stochastic dynamic model of the system components and the generic discrete stochastic model of the observations. Thus, the first step in the mathematical formulation of the analytical problem is the definition of the work space, data quality and the model used to represent the system dynamics. This chapter deals with the estimation problem, the representativeness of the model and the Optimal Estimation techniques. A special attention is also devoted to explaining why the data assimilation is an inverse problem.

2.1 The Observational System and Errors

The core problems of estimation approaches to data assimilation problems lie in the generic discrete stochastic dynamic model of the system components and in the generic discrete stochastic model of the observations. Discrete dynamics are assumed as given and the difference between the discrete dynamics and the governing continuum dynamics is accounted for by model error represented by stochastic forcing. Since the system state is considered discretely whereas it is the continuum state that should be observed, the observation model includes a representativeness error term as well as a measurement error term.

Although the applicable equations imply that a continuous "initial condition" field description is sufficient to define the values of the field for all future time, the uncertainty of the synoptic reconstruction, caused by finite sampling density and inaccurate measurements, suggests that continuity stems from a previous analysis may assist in defining the present distribution of values. The analyst utilizes this principle intuitively by inspecting the current array of data for patterns previously identified [1].

As a natural consequence the design of observation and data collection system for analysis and prediction of physical fields needs to be oriented toward periodic simultaneous measurements throughout the medium under investigation. The analysis consists of a reconstruction of the continuous spatial field, or a dense grid

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representation of the same, to which the dynamic equations of motion are applied in order to extrapolate into future time.

Thus the first step in the mathematical formulation of the analytical problem is the definition of the work space. The goal is to find a true state vector that is the projection of the infinite dimensional space of the field vector to the finite dimensional space of its numerical representation.

In dynamic meteorology and related disciplines, the forecasts of physical field variables and the mathematical models of field dynamics are expressed by a system of nonlinear partial differential equations PDEs whose prognostic state variables at time t_k is the vector $\mathbf{x}_k$.

Assuming the governing PDEs to be well-posed in the sense of Hadamard there is a unique solution operator or time dependent propagator $\mathbf{g}$ that yields the solution $\mathbf{x}_k$ given the solution $\mathbf{x}_{k-1}$ at an earlier time interval $t_k - t_{k-1}$. Omitting the time index t_k, from now on represented by the index k, we have:

$$\mathbf{x}_k = \mathbf{g}(\mathbf{x}_{k-1}) \tag{2.1}$$

for $k = 1, 2, 3 \ldots$. It is a faithful representation of the dynamics of the system under investigation.

This system could be stochastically forced, for example through uncertain boundary conditions or also be internally forced by stochastic free parameters estimated during the course of data assimilation, for example by physical parameterization. If the presentation parameters and forcing are considered fixed the propagator $\mathbf{g}$ is deterministic.

Since the numerical representation is defined through a discretization process, one has a discretized version $\mathbf{x}_k^d$ of Eq. 2.1 by the discrete propagator $\mathbf{f}$. How these vector components relate to the real state depend on the choice of discretization, which is mathematically equivalent to a choice of basis.

$$\mathbf{x}_k^d = \mathbf{f}(\mathbf{x}_{k-1}^d), \tag{2.2}$$

for $k = 1, 2, 3 \ldots$, where the superscript d means discrete.

Since the reality is more complex than what can be represented by a state vector, one must distinguish between reality itself and the best possible representation of reality, which one denotes as the *true* state at the time of the analysis. Thus we define a discrete *true* state vector $\mathbf{x}^t$ of dimension n, based on the available observation $t_1, t_2, \ldots$, that is the representation of the discrete state on a continuum state.

$$\mathbf{x}_k^t \equiv \mathbf{\Pi}\mathbf{x}_k \tag{2.3}$$

where $\mathbf{\Pi}$ is an operator mapping, in a proper manner, the discrete space on continuous space. The *true* state is still unknown since $\mathbf{x}_k$ is unknown and also the initial condition $\mathbf{x}_0$ and the propagator $\mathbf{g}$ are unknown.

Using the previously defined operators and applying the operator $\mathbf{\Pi}$ on both side of Eq. 2.1 and adding and subtracting $\mathbf{f}(\mathbf{x}^t_{k-1})$ we obtain the discrete evolution of the equation for $\mathbf{x}^t_k$

$$\mathbf{x}^t_k = \mathbf{f}(\mathbf{x}^t_{k-1}) + \mathbf{e}^t_{k-1} \tag{2.4}$$

where $\mathbf{f}$ is the discrete propagator that resides in our numerical solution and the forcing term $\mathbf{e}^t_{k-1}$ is the model error from time t_{k-1} to t_k that is:

$$\mathbf{e}^t_k = \mathbf{\Pi}\mathbf{g}(\mathbf{x}_k) - \mathbf{f}(\mathbf{\Pi}\mathbf{x}_k) \tag{2.5}$$

that is appropriate to be represented as a stochastic perturbation because:

- is state-dependent;
- its dependence on unknown $\mathbf{\Pi}$ renders it, from a deterministic point of view, unknowable;
- is small provided $\mathbf{f}$ approximates $\mathbf{g}$.

Let us now explore the observed data on the basis of the *true* state $\mathbf{x}^t_k$. Le us define a continuous observing vector obtained by a number of time dependent observations, with their errors, made at time t_k where $k = 1, 2, 3, \ldots$. If the error is additive we can write:

$$\mathbf{x}^{obs}_k = \mathbf{h}^c_k(\mathbf{x}_k) + \mathbf{e}^m_k \tag{2.6}$$

Here $\mathbf{h}^c_k$ is the continuum forward observation operator and $\mathbf{e}^m_k$ is the measurement error, considered stochastic, whose mean is: $\hat{\mathbf{e}}^m_k \equiv E[\mathbf{e}^m_k]$. $E[\cdot]$ is the expectation operator.[1]

The observation operator can be considered linear when the state variables are directly observed, as in case devices located in ground measurement stations and radiosondes and non linear when data come from remotely sensed devices that require proper integro-differential algorithms to be interpreted.

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[1]The expectation of a random variable is defined as the sum of all values the random variable may take, each weighted by the probability with which the value is taken. In term of formula the expectation of $E[x]$ is given by:

$$E[x] = \int_{-\infty}^{+\infty} x f(x) dx \tag{2.7}$$

This is also called mean value of x or first moment. A second moment is given by the quantity $E[x^2] = \int_{-infty}^{+infty} x^2 f(x) dx$. The variance of a random variable is the mean squared deviation of the random variable from its mean; it is $\sigma^2 = E[x^2] - E[x]^2$. Another important concept is the statistical correlation between random variables that is given by the covariance, which is the expectation of the product of the deviations of two random variables from their means:

$$E[(x - E[x])(y - E[y])] = E[xy] - E[x]E[y] \tag{2.8}$$

that is a measure of bias, and its covariance matrix $\mathbf{R}_k \equiv E[(\mathbf{e}^m_k - \hat{\mathbf{e}}^m_k)(\mathbf{e}^m_k - \hat{\mathbf{e}}^m_k)^T]$.

Let us now formulate the stochastic dynamic model adding and subtracting $\mathbf{h_k}(\mathbf{x}_k^t)$ from the relation (2.6) taking into account the discrete *true* state $\mathbf{x}_k^t = \mathbf{\Pi x}_k$. Then the discrete observation model is obtained by:

$$\mathbf{x}_k^{obs} = \mathbf{h_k}(\mathbf{x}_k^t) + \mathbf{e}_k^{obs} \tag{2.9}$$

where $\mathbf{h}_k$ is the discrete forward operator acting on $\mathbf{x}_k^t$ and $\mathbf{e}^{obs} \equiv \mathbf{e}_k^r + \mathbf{e}_k^m$ is the total observation error. The measurement error is $\mathbf{e}_k^m$ while the representativeness error (see Lorenc [2]) $\mathbf{e}_k^r$ is given by the difference between the representation of the continuum forward model and formulating the model error discretely, that is:

$$\mathbf{e}_k^r = \mathbf{e}_k^r(\mathbf{x}_k) \equiv \mathbf{h}_k^c(\mathbf{x}_k) - \mathbf{h}_k(\mathbf{\Pi x}_k). \tag{2.10}$$

The impact of this error on our system will be more clear when we address the initialization problem in the next paragraph.

2.1.1 The Estimation Problem

Since our goal is to study a physical system described by the vector state $\mathbf{x}_k^t$ and since this vector is unknown, one assumes that the best estimation of the system is given by the state vector $\mathbf{x}_k^b$, where b stands for background, denoting the a priori or background estimate of the true state before the analysis is carried out, valid at the same time. This vector is the result of the data assimilation or statistical analysis performed earlier. By Eq. 2.9 the observations performed on the system bring new information through the operator $\mathbf{h}_k$. One assumes the statistics of the observation error are known up to the second order moments. When new observations are available we can improve the analysis obtaining our estimation $\mathbf{x}_k^a$ with its error. The suffix a means analysis.

In geophysics it is usual to define the a priori estimate as forecast/background and the posterior estimate as analysis.

Let us now explore the background and analysis errors. The background error is defined as:

$$\mathbf{e}_k^b = \mathbf{x}_k^b - \mathbf{x}_k^t \tag{2.11}$$

it reflects the discrepancy between the a priori estimate and the unknown truth. It is considered stochastic the mean of which is $\hat{\mathbf{e}}^b = E[\mathbf{e}_k^b]$. The background error covariance is: $\mathbf{B} = E[(\mathbf{e}_k^b - \hat{\mathbf{e}}_k^b)(\mathbf{e}_k^b - \hat{\mathbf{e}}_k^b)^T]$. The analysis error is defined as:

$$\mathbf{e}_k^a = \mathbf{x}_k^a - \mathbf{x}_k^t \tag{2.12}$$

It defines the difference between the analysis process and the truth; the related analysis error covariance is: $\mathbf{A} = E[(\mathbf{e}_k^a - \hat{\mathbf{e}}_k^a)(\mathbf{e}_k^a - \hat{\mathbf{e}}_k^a)^T]$ with its mean given by: $\hat{\mathbf{e}}^a = E[\mathbf{e}_k^a]$. All matrices are symmetric and positive.

2.1.2 The Linear Hypothesis

In order to understand if we can linearize our system we need to analyze the role played by the representativeness error in the model. If we write the representativeness error adding and subtracting $\mathbf{h}_k^c(\mathbf{\Pi x}_k)$ to the relation (2.10)

$$\mathbf{e}_k^r = \mathbf{h}_k^c(\mathbf{x}_k) - \mathbf{h}_k(\mathbf{\Pi x}_k) + \mathbf{h}_k^c(\mathbf{\Pi x}_k) - \mathbf{h}_k^c(\mathbf{\Pi x}_k), \tag{2.13}$$

we can split the representativeness error into the sum of two parts, $\mathbf{e}_k^{'}$ and $\mathbf{e}_k^{''}$ giving:

$$\begin{aligned} \mathbf{e}_k^{'} &\equiv \mathbf{h}_k^c(\mathbf{x}_k) - \mathbf{h}_k^c(\mathbf{\Pi x}_k) \\ \mathbf{e}_k^{''} &\equiv \mathbf{h}_k^c(\mathbf{\Pi x}_k) - \mathbf{h}_k(\mathbf{\Pi x}_k), \end{aligned} \tag{2.14}$$

where $\mathbf{e}_k^{''}$ can be all depending on our integration interpolation formulas and is easy to solve, while $\mathbf{e}_k^{'}$ depending on the scale variability of $\mathbf{x}_k$ could dominate the measurement error, as happens in a highly variable field. This can be more clarified if we use a linear approximation of $\mathbf{e}_k^{'}$, for instance applying the first order Taylor expansion to $\mathbf{h}_k^c$ obtaining:

$$\mathbf{e}_k^{'} = \mathbf{H}_k^c(\mathbf{I} - \mathbf{\Pi})\mathbf{x}_k \tag{2.15}$$

where $\mathbf{H}_k^c$ is:

$$\mathbf{H}_k^c = \left.\frac{\partial \mathbf{h}_k^c(\mathbf{x}_k)}{\partial \mathbf{x}}\right|_{\mathbf{x}=\mathbf{\Pi x_k}}, \tag{2.16}$$

that operates on the unresolved portion of $(\mathbf{I} - \mathbf{\Pi})\mathbf{x}_k$ of the continuum state $\mathbf{x}_k$. $\mathbf{H}_k^c$ is a tangent linear operator or Jacobian matrix of a non linear operator. If we define the linear operator as $\mathbf{H}$ we can write $\mathbf{H}_k^c = \mathbf{H}$

Thus the vector of observations $\mathbf{y}$ is related with the observation operator $\mathbf{H}(\mathbf{x})$ and the observation error as $\mathbf{e}$ by:

$$\mathbf{y} = \mathbf{H}\mathbf{x}^t + \mathbf{e}. \tag{2.17}$$

Let us estimate now, with a reasonable assumption, that $\mathbf{x}^a$ is a linear combination of all available information given by the $n \times n$ matrix $\mathbf{L}$ and $n \times p$ matrix where $\mathbf{K}$ is the linear operator, we have:

$$\mathbf{x}^a = \mathbf{L}\mathbf{x}^b + \mathbf{K}\mathbf{y} \tag{2.18}$$

Given the observation Eq. 2.17 we obtain that the estimate error of the analysis is:

$$\begin{aligned} \mathbf{x}^a - \mathbf{x}^t &= \mathbf{L}(\mathbf{x}^b - \mathbf{x}^t + \mathbf{x}^t) + \mathbf{K}(\mathbf{H}\mathbf{x}^t + \mathbf{e}) - \mathbf{x}^t \\ \mathbf{e}^a &= \mathbf{L}\mathbf{e}^b + \mathbf{K}\mathbf{e} + (\mathbf{L} + \mathbf{K}\mathbf{H} - \mathbf{I})\mathbf{x}^t. \end{aligned} \tag{2.19}$$

If we assume the errors and observations are unbiased, the related expectations are $E[\mathbf{e}] = 0$ and $E[\mathbf{e}^b] = 0$ and thus $E[\mathbf{e}^a] = (\mathbf{L} + \mathbf{KH} - \mathbf{I})E[\mathbf{x}^t]$. On the contrary if there is a bias, it is always possible to diagnose it and subtract its value from the total observation errors to make the corrected error unbiased. If we postulate that:

$$\mathbf{L} = \mathbf{I} - \mathbf{KH}, \tag{2.20}$$

as sufficient but not necessary condition, we have:

$$\begin{aligned} \mathbf{x}^a &= (\mathbf{I} - \mathbf{KH})\mathbf{x}^b + \mathbf{Ky} \\ \mathbf{x}^a &= \mathbf{x}^b + \mathbf{K}(\mathbf{y} - \mathbf{Hx}^b), \end{aligned} \tag{2.21}$$

where the difference $[\mathbf{y} - \mathbf{Hx}^b]$ is called innovation and $\mathbf{K}$ is a weight or gain computed on the estimated statistical error covariances of the forecast and the observations. It gives the additional information brought in by the observation compared to background. The error covariance matrix obtained from the innovation vector is called information matrix. Since the operator $\mathbf{K}$ is linear, the analysis is a linear interpolation, as was for example in the first Cressman [3] interpolation.

Once we have computed the optimal gain matrix $\mathbf{K}$ we need to compute the error covariance or posterior error matrix $\mathbf{P}^a$.

Using the notation already introduced for the error we have:

$$\mathbf{e}^a = \mathbf{e}^b + \mathbf{K}(\mathbf{e} - \mathbf{He}^b) \tag{2.22}$$

As previously we assume the errors and observations are unbiased so that the covariance analysis matrix is $\mathbf{P}^a = E[(\mathbf{e}^a)(\mathbf{e}^a)^T]$. Remembering the error covariance background matrix $\mathbf{P}^b$ and error covariance observation matrix $\mathbf{R}$ and the relation (2.20) we have:

$$\begin{aligned} \mathbf{P}^a &= E[(\mathbf{e}^a)(\mathbf{e}^a)^T] \\ &= E[(\mathbf{e}^b + \mathbf{K}(\mathbf{e} - \mathbf{He}^b))(\mathbf{e}^b + \mathbf{K}(\mathbf{e} - \mathbf{He}^b))^T] \\ &= E[(\mathbf{Le}^b + \mathbf{Ke})(\mathbf{Le}^b + \mathbf{Ke})^T] \\ &= E[\mathbf{Le}^b(\mathbf{e}^b)^T\mathbf{L}^T] + E[\mathbf{Ke}(\mathbf{e})^T\mathbf{K}^T] \\ &= \mathbf{LP}^b\mathbf{L}^T + \mathbf{KRK}^T \\ &= (\mathbf{I} - \mathbf{KH})\mathbf{P}^b(\mathbf{I} - \mathbf{KH})^T + \mathbf{KRK}^T \end{aligned} \tag{2.23}$$

that is the posterior error.

In order to obtain an optimal estimation, we minimize the trace of the analysis error covariance given by (2.23). Remembering $Trace[\mathbf{P}^b] = Trace[\mathbf{P}^b]^T$ and $Trace[\mathbf{R}] = Trace[\mathbf{R}]^T$, expanding the relation (2.23) we have:

$$Trace[\mathbf{P}^a] = Trace[\mathbf{P}^b] + Trace[\mathbf{KHP}^b\mathbf{H}^T\mathbf{K}^T] - 2Trace[\mathbf{P}^b\mathbf{H}^T\mathbf{K}^T] + Trace[\mathbf{KRK}^T] \tag{2.24}$$

Following Bouttier and Courtier [4] we have a continuous differentiable scalar function of the coefficient of $\mathbf{K}$ whose first order derivative in $\mathbf{K}$ of the difference $Trace[\mathbf{P}^a](\mathbf{K}+\mathbf{L}) - Trace[\mathbf{P}^a](\mathbf{K})$, where $\mathbf{L}$ is an arbitrary test matrix, is:

$$\begin{aligned}\frac{d[Trace[\mathbf{P}^a]]\mathbf{L}}{d\mathbf{K}} &= 2Trace[\mathbf{KHP}^b\mathbf{H}^T\mathbf{L}^T] - 2Trace[\mathbf{P}^b\mathbf{H}^T\mathbf{L}^T] + 2Trace[\mathbf{KRL}^T] \\ &= 2Trace[\mathbf{KHP}^b\mathbf{H}^T\mathbf{L}^T - \mathbf{P}^b\mathbf{H}^T\mathbf{L}^T + \mathbf{KRL}^T] \\ &= 2Trace\{[\mathbf{K}(\mathbf{HP}^b\mathbf{H}^T + \mathbf{R}) - \mathbf{P}^b\mathbf{H}^T]\mathbf{L}^T\}\end{aligned} \tag{2.25}$$

The last line shows that the derivative is zero for any choice of $\mathbf{L}$ if $(\mathbf{HP}^b\mathbf{H}^T + \mathbf{R})\mathbf{K}^T - \mathbf{P}^b\mathbf{H} = 0$ that is equivalent to:

$$\mathbf{K} = \mathbf{P}^b\mathbf{H}^T(\mathbf{HP}^b\mathbf{H}^T + \mathbf{R})^{-1} \tag{2.26}$$

because $(\mathbf{HP}^b\mathbf{H}^T + \mathbf{R})$ is assumed invertible.

The estimate of $\mathbf{x}^a$ and $\mathbf{P}^a$ are called **Best Linear Unbiased Estimator, BLUE**. **BLUE**, because $\mathbf{H}$ is linear through $\mathbf{K}$ and $\mathbf{L}$, without bias through the first step of derivation and optimal through the second derivation.

2.1.3 Optimal Estimation

Now we need to improve our knowledge of the state $\mathbf{x}^a$ taking into account the two available sources of information: the model and observations. There are two ways to combine observations with the model:

- the observations $\mathbf{y}$ may be interpolated between the observational data which can be sparse in time and space subjected to constraints provided by the model;
- we want to reduce the uncertainties of model $\mathbf{H}$ on the input $\mathbf{x}$, under the constrains of the measurements.

We define a cost function $\mathcal{J}$ that is a measure of the distance between the observations and model.

$$\mathcal{J}(\mathbf{x}) = ||\mathbf{y} - \mathbf{H}(\mathbf{x})||^2, \tag{2.27}$$

with $||\cdot||$ the norm two. Since we need to balance each component through the confidence in the measurement we can access to the a priori estimate or background information. In this way we introduce a compromise between the observations given by the observation and the information given by background value. Then the cost function can be defined as

$$\mathcal{J}(\mathbf{x}) = \alpha \times ||\mathbf{y} - \mathbf{H}(\mathbf{x})||^2 + \beta \times ||\mathbf{x} - \mathbf{x}^b||^2. \tag{2.28}$$

α and β are the weight given to the confidence in the observations and background. Those parameters can be defined empirically or analytically, knowing the background and observation errors.

A simple example drawn by Bouttier and Courtier [4] based on temperature and related error variance shows that the cost function terms which have a quadratic form tend to pull the analysis $\mathbf{x}^a$ toward the background $\mathbf{x}^b$ and the observation $\mathbf{y}$, respectively. In this case $\mathbf{x}^a$ makes $\mathcal{J}(\mathbf{x})$ as small as possible, given the computational constraints.

The quadratic form (2.28) can be written in matrix form as:

$$\mathcal{J}(\mathbf{x}) = \frac{1}{2}\{(\mathbf{y} - \mathbf{H}(\mathbf{x}))^T \mathbf{R}^{-1}(\mathbf{y} - \mathbf{H}(\mathbf{x})) + (\mathbf{x} - \mathbf{x}^b)^T (\mathbf{P}^b)^{-1}(\mathbf{x} - \mathbf{x}^b)\}, \quad (2.29)$$

where $\mathbf{y}$ is the vector of observation of length k; $\mathbf{x}^b$ is a vector of background of length j and $\mathbf{P}^b$ is the background error covariance matrix of rank $j \times j$ and $\mathbf{R}$ is the observation error covariance matrix of rank $k \times k$. $\mathbf{H}$ is the linear forward interpolation operator.

The optimal solution, i.e. the analysis $\mathbf{x}^a$ that is closest to the *true* state $\mathbf{x}^t$, in an *r.m.s.* sense, requires the minimum:

$$\mathcal{J}(\mathbf{x}) \xrightarrow{x} min \quad (2.30)$$

It demands the first derivative, the gradient, of the cost function with respect to its variable $\mathbf{x}$ at the analysis $\mathbf{x}^a$ be equal zero

$$\nabla \mathcal{J}(\mathbf{x}^a) = \left.\frac{d\mathcal{J}}{d\mathbf{x}}\right|_{\mathbf{x}^a} = 0 \quad (2.31)$$

Under our linear assumption, we have:

$$(\mathbf{P}^b)^{-1}(\mathbf{x}^a - \mathbf{x}^b) - \mathbf{H}^T \mathbf{R}^{-1}[\mathbf{y} - \mathbf{H}(\mathbf{x}^a)] = 0 \quad (2.32)$$

Adding and subtracting $\mathbf{y} - \mathbf{H}(\mathbf{x}^b)$ we obtain:

$$(\mathbf{P}^b)^{-1}(\mathbf{x}^a - \mathbf{x}^b) - \mathbf{H}^T \mathbf{R}^{-1}[\mathbf{y} - \mathbf{H}(\mathbf{x}^b)] - \mathbf{H}^T \mathbf{R}^{-1}[\mathbf{H}(\mathbf{x}^a) - \mathbf{H}(\mathbf{x}^b)] = 0 \quad (2.33)$$

Rearranging this equation and applying again the linear assumption, we have:

$$\begin{aligned} 0 &= (\mathbf{P}^b)^{-1}(\mathbf{x}^a - \mathbf{x}^b) - \mathbf{H}^T \mathbf{R}^{-1}[\mathbf{y} - \mathbf{H}(\mathbf{x}^b)] - \mathbf{H}^T \mathbf{R}^{-1}\mathbf{H}(\mathbf{x}^a - \mathbf{x}^b) \\ \mathbf{x}^a - \mathbf{x}^b &= ((\mathbf{P}^b)^{-1} + \mathbf{H}^T \mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T \mathbf{R}^{-1}[\mathbf{y} - \mathbf{H}(\mathbf{x}^b)] \end{aligned} \quad (2.34)$$

The analysis state $\mathbf{x}^a$ is called optimal because is closest in a root mean square sense to the *true* state $\mathbf{x}^t$. The equivalence of this relation with relation (2.21) can also be

shown applying the Sherman-Woodbury-Morrinson equation.[2] In fact, remembering that $\mathbf{K}$ is given by the relation (2.26) we have:

$$\begin{aligned}\mathbf{K} &= \mathbf{P}^b\mathbf{H}^T(\mathbf{H}\mathbf{P}^b\mathbf{H}^T + \mathbf{R})^{-1} \\ &= ((\mathbf{P}^b)^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}((\mathbf{P}^b)^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})\mathbf{P}^b\mathbf{H}^T(\mathbf{H}\mathbf{P}^b\mathbf{H}^T + \mathbf{R})^{-1} \\ &= ((\mathbf{P}^b)^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}(\mathbf{H}^T + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}\mathbf{P}^b\mathbf{H}^T)(\mathbf{H}\mathbf{P}^b\mathbf{H}^T + \mathbf{R})^{-1} \\ &= ((\mathbf{P}^b)^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}(\mathbf{R} + \mathbf{H}\mathbf{P}^b\mathbf{H}^T)(\mathbf{H}\mathbf{P}^b\mathbf{H}^T + \mathbf{R})^{-1} \\ &= ((\mathbf{P}^b)^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}. \end{aligned} \tag{2.36}$$

The equivalence can be useful because sometime the inversion of the $((\mathbf{P}^b)^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}$ is more costly than the matrix $\mathbf{R} + \mathbf{H}\mathbf{P}^b\mathbf{H}^T$.

Summarizing we have:

$$\begin{aligned}\mathbf{x}^a &= \mathbf{x}^b + \mathbf{K}[\mathbf{y} - \mathbf{H}(\mathbf{x}^b)] \\ \mathbf{W} &= \mathbf{P}^b\mathbf{H}^T[\mathbf{R} + \mathbf{H}\mathbf{P}^b\mathbf{H}^T]^{-1}. \end{aligned} \tag{2.37}$$

With respect to the relaxation method Optimal Interpolation is an intermittent assimilation methods. It is used at synoptic times, that is the instant of standard meteorological time. The difference of $\mathbf{K}$ gain with respect to the Kalman gain is that the background error covariance matrix $\mathbf{P}_k^b$ is specified rather than predicted. In optimal estimation the element of $\mathbf{P}_k^b$ is based on statistical evaluations and dynamic constraints. For the state vector $\mathbf{r}(\lambda, \psi, \phi)$ at a certain instant, the error covariance matrix $\mathbf{P}^b$ is:

$$\mathbf{P}^b = E[\mathbf{e}(\mathbf{r}_i)\mathbf{e}^T(\mathbf{r}_j)] \tag{2.38}$$

where $\mathbf{e}(\mathbf{r}) = \mathbf{x}^b(\mathbf{r}) - \mathbf{x}^t(\mathbf{r})$ is the forecast error with $\mathbf{x}^t(\mathbf{r})$ represents the true value of the state vector and $\mathbf{x}^b(\mathbf{r})$ is the forecast state vector. Therefore we can decompose $\mathbf{P}^b$ as

$$\mathbf{P}^b(\mathbf{r}_i, \mathbf{r}_j) \equiv \begin{vmatrix} \mathbf{P}^{b|\lambda\lambda} & \mathbf{P}^{b|\lambda\psi} & \mathbf{P}^{b|\lambda\phi} \\ \mathbf{P}^{b|\psi\lambda} & \mathbf{P}^{b|\psi\psi} & \mathbf{P}^{b|\psi\phi} \\ \mathbf{P}^{b|\phi\lambda} & \mathbf{P}^{b|\phi\psi} & \mathbf{P}^{b|\phi\phi} \end{vmatrix}$$

where $\mathbf{P}^{b|\cdot\cdot}$ are the cross-covariance functions defined in analogy to (2.38).

It is a simplification of the algebraic calculation of the gain matrix. The first of the Eq. (2.37) is solved through the inversion, the matrix $\mathbf{K}$ is simplified assuming that only the most forthcoming observations determine the analysis increment. For each of the variables of the model the increment of the analysis is given from the corresponding $\mathbf{K}$ for the vector of deviations of the background value $[\mathbf{y} - \mathbf{H}(\mathbf{x}^b)]$.

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[2] Sherman-Morrison-Woodbury formula is:

$$(\mathbf{A} + \mathbf{U}\mathbf{C}\mathbf{V})^{-1} = \mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{V}(\mathbf{C}^{-1} + \mathbf{V}\mathbf{A}^{-1}\mathbf{V})^{-1}\mathbf{V}\mathbf{A}^{-1}, \tag{2.35}$$

where all matrices have they correct size.

Bouttier, and Courtier [4] provide the fundamental assumptions and procedures to be followed.

The fundamental hypothesis of optimal interpolation (OI) is that: for each variable of the model, just some observations are important to determine the increase of the analysis. From this it follows that:

1. for each variable of the model $\mathbf{x}(i)$ choose a small number of observations p_i using an empirical policy of selection;
2. form the corresponding p_i list of deviations of the background data $[\mathbf{y} - \mathbf{H}(\mathbf{x}^b)]_i$, of the errors background covariance matrix, between the variables of the model $x(i)$ and the state of the model interpolated in points p_i namely the p_i coefficients of the ith row of $\mathbf{P}^b\mathbf{H}$ and $(p_i \times p_i)$ covariance submatrix of the errors observations and background formed by $\mathbf{H}\mathbf{P}^b\mathbf{H}^T$ and $\mathbf{R}$ for selected observations;
3. invert the positive-definite matrix $(p_i \times p_i)$ formed from $[\mathbf{R} + \mathbf{H}\mathbf{P}^b\mathbf{H}^T]$ for selected observations (e.g. using Cholesky Factorizazion methods or LU);
4. multiply it by the ith row of $\mathbf{P}^b\mathbf{H}$ to get the $\mathbf{K}$ row required.

In Optimal Interpolation it is necessary that $\mathbf{P}^b$ is a matrix that can be easily applied to a pair of observed value and model variables or to a pair of observed variables. The simplicity of the OI collides with the disadvantage that there is no consistency between small and large scales and that $\mathbf{H}$ must be linear.

2.1.4 Minimization Methods of Cost Functions

There are several methods to minimize the cost function including the most relevant below. If the cost function is quadratic and convex, its solution is unique. In general, however, $\mathcal{J}$ exhibits several minima. In such a case the problem is more difficult to solve, even though there are some algorithms among which we select conjugate gradient and quasi-Newton methods.

The minimization algorithms start from an initial point $\mathbf{x}_0$ and construct a sequence $\mathbf{x}_k$ which converges to a local minimum. At each step k one determines a direction $\mathbf{d}_k$ to define the next point of the sequence. Then the problem of minimization of multivariable functions is usually solved by determining a search direction vector $\mathbf{d}_k$ and solve it as a linear minimization problem. If $\mathbf{x}_k$ is the vector containing the variables to be determined and $\mathbf{d}_k$ is the vector of search direction, at each iteration step the minimization problem of a function $\mathbf{f}$ is formulated so as to find the step size λ that minimizes $\mathbf{f}(\mathbf{x} + \lambda\mathbf{d}_k)$, where λ is a positive and real number. At the next iteration, $\mathbf{x}$ is replaced by $\mathbf{x}_k + \lambda_k\mathbf{d}_k$ and a new search direction is determined.

The conjugate gradient method is an algorithm for finding the nearest local minimum of a function which uses conjugate directions for descending. Two vectors $\mathbf{u}$ and $\mathbf{v}$ are said to be conjugate, with respect to a matrix $\mathbf{A}$, if

$$\mathbf{u}^T\mathbf{A}\mathbf{v} = 0, \tag{2.39}$$

where **A** is the Hessian matrix of the cost function. In Press et al's book [5] there are two conjugate gradient methods by Fletcher-Reeves and Polak-Ribière.

These algorithms calculate the mutually conjugate directions of search with respect to the Hessian matrix of the cost function directly from the function and the gradient evaluations, but without the direct evaluation of the Hessian matrix. The new search direction $\mathbf{d}_{k+1}$ is determined by using

$$\mathbf{d}_{k+1} = -\mathbf{g}_{k+1} + \lambda_k \mathbf{d}_k, \tag{2.40}$$

where $\mathbf{d}_k$ is the previous search direction, $\mathbf{g}_{k+1}$ is the local gradient at iteration step $k+1$ that is determined by the Fletcher-Reeves equation

$$\lambda_k = \frac{\mathbf{g}_{k+1} \cdot \mathbf{g}_{k+1}}{\mathbf{g}_k \cdot \mathbf{g}_k} \tag{2.41}$$

and the Polak-Ribière equation

$$\lambda_k = \frac{(\mathbf{g}_{k+1} - \mathbf{g}_k) \cdot \mathbf{g}_{k+1}}{\mathbf{g}_k \cdot \mathbf{g}_k}. \tag{2.42}$$

If the vicinity of the minimum has the shape of a long, narrow valley, the minimum is reached in far fewer steps than would be the case using the steepest descent method, which makes use of the inverse of the local gradient as the search direction. The line minimization to find the step size λ that minimizes $\mathbf{f}(\mathbf{x} + \lambda \mathbf{d}_k)$ at every iteration step can be done by using the Golden Section Search Algorithm [5].

For the problem of minimizing a multivariable function quasi-Newton methods are also widely used. These methods involve the approximation of the Hessian, or its inverse, matrix of the function. The LBFGS (Limited memory-Broyden-Fletcher-Goldfarb-Shanno) method is basically a method to approximate the Hessian matrix in the quasi-Newton method of optimization. It is a variation of the standard BFGS method, which is given by (Nocedal [6], Byrd et al. [7])

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \lambda_k \mathcal{H}_k \mathbf{g}_k, \quad k = 1, 2, 3 \ldots \tag{2.43}$$

where λ_k is a step length, $\mathbf{g}_k$ is the local gradient of the cost function, and $\mathcal{H}_k$ is the approximate inverse Hessian matrix which is updated at every iteration by means of the formula

$$\mathcal{H}_{k+1} = \mathbf{V}_k^T \mathcal{H}_k \mathbf{V}_k + \rho_k \mathbf{s}_k \mathbf{s}_k^T \tag{2.44}$$

where

$$\rho_k = \frac{1}{\mathbf{q}^T \mathbf{s}_k} \tag{2.45}$$

and

$$\mathbf{V}_k = \mathbf{I} - \rho_k \mathbf{q}\mathbf{s}_k^T \tag{2.46}$$

$$\mathbf{s}_k = \mathbf{s}_{k+1} - \mathbf{s}_k \tag{2.47}$$

and

$$\mathbf{q}_k = \mathbf{g}_{k+1} - \mathbf{g}_k \tag{2.48}$$

Using this method, instead of storing the matrices $\mathcal{H}_k$, one stores a certain number of pairs $\{\mathbf{s}_k, \mathbf{q}_i\}$ that define them implicitly. The product of $\mathcal{H}_k \mathbf{g}_k$ is obtained by performing a sequence of inner products involving $\mathbf{g}_k$ and the most recent vector pairs $\{\mathbf{s}_k, \mathbf{q}_i\}$ to define the iteration matrix.

2.1.5 Some Properties of Estimation

1. The innovation and the analysis residue $\mathbf{y} - \mathbf{H}\mathbf{x}^a$ are unbiased.
   As consequence of the linearity of the observation operator and absence of bias of the analysis error $\mathbf{e}^a$ the analysis residue is unbiased. In fact:

   $$\mathbf{y} - \mathbf{H}\mathbf{x}^a = \mathbf{H}\mathbf{x}^t + \mathbf{e} - \mathbf{H}\mathbf{x}^a = \mathbf{H}\mathbf{e}^a - \mathbf{e} \tag{2.49}$$

   and we can conclude $E[\mathbf{y} - \mathbf{H}\mathbf{x}^a] = 0$. Since the background error is unbiased also the innovation error is also unbiased

   $$\mathbf{y} - \mathbf{H}\mathbf{x}^b = \mathbf{H}\mathbf{x}^t + \mathbf{e} - \mathbf{H}\mathbf{x}^b = \mathbf{H}\mathbf{e}^b - \mathbf{e}, \tag{2.50}$$

   from which $E[\mathbf{y} - \mathbf{H}\mathbf{x}^b] = 0$.
2. The analysis and analysis error are orthogonal.
   Calculate the covariance matrix

   $$\mathbf{C} = E[\mathbf{x}^a (\mathbf{e}^a)^T]. \tag{2.51}$$

   Assuming the background satisfies

   $$E[\mathbf{x}^b (\mathbf{e}^b)^T] = 0 \tag{2.52}$$

   means the background and its error are uncorrelated. From Eq. 2.21 we have

   $$\mathbf{x}^a = \mathbf{x}^b + \mathbf{K}(\mathbf{y} - \mathbf{H}\mathbf{x}^b) = \mathbf{x}^b + \mathbf{K}(-\mathbf{H}\mathbf{e}^b - \mathbf{e}). \tag{2.53}$$

Then, recalling (2.22)

$$\begin{aligned}\mathbf{C} &= E[(\mathbf{x}^b + \mathbf{K}(-\mathbf{H}\mathbf{e}^b - \mathbf{e}))((\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{e}^b - \mathbf{K}\mathbf{e}^T] \\ &= -\mathbf{K}\mathbf{H}\, E[\mathbf{e}^b(\mathbf{e}^b)^T](\mathbf{I} - \mathbf{K}\mathbf{H})^T + \mathbf{K}\, E[\mathbf{e}\mathbf{e}^T]\mathbf{K}^T \\ &= \mathbf{K}[\mathbf{H}\mathbf{P}^b(-\mathbf{I} - \mathbf{K}\mathbf{H})^T + \mathbf{R}\mathbf{K}^T]. \end{aligned} \tag{2.54}$$

If the analysis is optimal, we have $-\mathbf{H}\mathbf{P}^b(\mathbf{I} - \mathbf{K}\mathbf{H})^T + \mathbf{R}\mathbf{K}^T = 0$, so $\mathbf{C} = 0$ and the estimate $\mathbf{x}^a$ and its error $\mathbf{e}^a$ are orthogonal.

2.1.6 Estimation of the quality of analysis

An important step in the process of assimilation is to be able to estimate the quality of the analysis. In fact in a sequential analysis it is useful to know the level of reliability of the analysis because it helps to specify the background error covariance matrix for later analysis. If the background is a forecast then as we have seen the errors are a combination of the errors of the model and those of the analysis that evolve in time according to dynamic model as it is also seen using of the algorithm of Kalman filter.

The word quality means reliability and it is estimated through the value of the covariance matrix of the error of the analysis $\mathbf{P}^a$. The process by which we estimate the quality of the analysis is closely linked to the cost or penalty function and its gradient. Recalling the relation (2.29) and (2.31), the second derivative or Hessian of the cost function derived two times around x that the control variable is:

$$\bigtriangledown \bigtriangledown \mathcal{J}(x) = 2((\mathbf{P}^b)^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}) \tag{2.55}$$

Introducing the true state x^t of the model into the (2.31) we have:

$$\begin{aligned} 0 &= (\mathbf{P}^b)^{-1}(\mathbf{x}^a - \mathbf{x}^t + \mathbf{x}^t - \mathbf{x}^a) - \mathbf{H}^T\mathbf{R}^{-1}(\mathbf{y} - \mathbf{H}(\mathbf{x}^t) + \mathbf{H}(\mathbf{x}^t) - \mathbf{x}^a) \\ &= (\mathbf{P}^b)^{-1}(\mathbf{x}^a - \mathbf{x}^t) - \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}(\mathbf{x}^t - \mathbf{x}^a) - (\mathbf{P}^b)^{-1}(\mathbf{x}^b - \mathbf{x}^t) + \mathbf{H}^T\mathbf{R}^{-1}(\mathbf{y} - \mathbf{H}(\mathbf{x}^t)). \end{aligned} \tag{2.56}$$

Thus

$$((\mathbf{P}^b)^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})(\mathbf{x}^a - \mathbf{x}^t) = (\mathbf{P}^b)^{-1}(\mathbf{x}^b - \mathbf{x}^t) + \mathbf{H}^T\mathbf{R}^{-1}(\mathbf{y} - \mathbf{H}(\mathbf{x}^t)). \tag{2.57}$$

Multiplying the right side of this equation by its transposed and taking into account of the Eq. 2.23 and computing the expectation we have:

$$\begin{aligned} &((\mathbf{P}^b)^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})\mathbf{P}^a((\mathbf{P}^b)^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^T \\ &\quad = (\mathbf{P}^b)^{-1}\mathbf{P}^b(\mathbf{P}^b)^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{R}\mathbf{R}^{-1}\mathbf{H} \qquad (2.58) \\ &+[(\mathbf{P}^b)^{-1}\mathbf{H}^T\mathbf{R}^{-1}\overline{(\mathbf{x}^b - \mathbf{x}^t)^T(\mathbf{y} - \mathbf{H}(\mathbf{x}^t)} + (\mathbf{P}^b)^{-1}\mathbf{R}^{-1}\overline{(\mathbf{x}^b - \mathbf{x}^t)(\mathbf{y} - \mathbf{H}(\mathbf{x}^t)^T}. \qquad (2.59) \end{aligned}$$

Assuming the background error and those due to the observation are uncorrelated, by simplifying we obtain:

$$((\mathbf{P}^b)^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})\mathbf{P}^a((\mathbf{P}^b)^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^T = ((\mathbf{P}^b)^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}). \quad (2.60)$$

Removing the zero component we have:

$$\mathbf{P}^a = ((\mathbf{P}^b)^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1} \quad (2.61)$$

By definition, the Hessian is given by (2.55) and:

$$\mathbf{P}^a = \frac{1}{2}[\bigtriangledown \bigtriangledown \mathcal{J}(x)]^{-1} \quad (2.62)$$

or inversely

$$\bigtriangledown \bigtriangledown \mathcal{J}(x) = \frac{1}{2}(\mathbf{P}^a)^{-1} \quad (2.63)$$

The matrix $(\mathbf{P}^a)^{-1}$ is called information matrix.

2.2 Variational Approach: 3-D VAR and 4-D VAR

The basic principle of the $3D - Var$ is to avoid explicitly calculating the gain matrix and make its inversion using a minimization procedure of the cost function $\mathcal{J}$. In this case the solution of the Eq. (2.29) is obtained iteratively doing various evaluations of the equation and its gradient to get the minimum using a suited descent algorithm. The minimization is obtained limiting the number of iterations and stipulating that the norm of the gradient $\parallel \bigtriangledown \mathcal{J}(s^a) \parallel$ decreases by a predefined amount, during minimization this is an intrinsic measure of how close the analysis is to the optimal value rather than the starting point of minimization.

When the observations are distributed over time the approach $3D - Var$ is generalized to the approach $4D - Var$. The equations are the same provided the operators are generalized including a forecasting model that allows comparison the state of the model with the observations at a time k defined.

In a given time interval the cost function to be minimized is the same of the $3D - Var$ but with a difference related to the operator H and R that are subject to a partial trajectory, i.e. the k ranges from $k - 1$ to k. Thus according to the relation given by Lorenc [2]:

$$\mathcal{J} = \frac{1}{2}\left\{\sum_{t=0}^{N}[\mathbf{y}_k - \mathbf{H}_k(\mathbf{x}_t)]^T\mathbf{R}_k^{-1}[\mathbf{y}_k - \mathbf{H}_k(\mathbf{x}_k)]\right\} + \frac{1}{2}[\tilde{\mathbf{x}} - \mathbf{x}_0^b]^T(\mathbf{P}^b)^{-1}[\tilde{\mathbf{x}} - \mathbf{x}_0^b], \quad (2.64)$$

where $\tilde{\mathbf{x}}$ is at zero time forecast produced by the data assimilation for $k < k_0$. $\mathbf{P}^b$ is the covariance matrix of the errors while $k = 0$; $\mathbf{x}_0^b$ is a value of $\tilde{\mathbf{x}}$ before the first iteration of the descent algorithm. The second term on the right it is thought to force the forecast $\mathbf{x}_0^b$ towards the prediction before $\tilde{\mathbf{x}}$ to reduce the time discontinuity. In the classical receipt (see [8]) the assimilation issue $4D - Var$ is subject to a strong constraint such that the sequence of model states $\mathbf{x}_t$ must be a solution of the equation:

$$\mathbf{x}_k = \mathbf{M}_{0\to k}(\mathbf{x}) \quad \forall k \tag{2.65}$$

where $\mathbf{M}_{0\to k}$ is a forecasting model from the starting time to k. $4D-Var$ is a problem of nonlinear optimization difficult to solve unless in the following two hypotheses: causality and tangent linear.

1. Causality
   The forecast model can be expressed as the product of intermediate forecasting steps, that reflect the randomness of nature. The integration of a prognostic model starts with the initial condition $\mathbf{x}_0 = \mathbf{x}$ so that $\mathbf{M}_0$ is the identity. Thus indicating with $\mathbf{M}_k$ the step of forecasting from $k-1$ to k we have $\mathbf{x}_t = \mathbf{M}_k\mathbf{x}_{k-1}$ and by recurrence:
   $$\mathbf{x}_k = \mathbf{M}_k\mathbf{M}_{k-1}...\mathbf{M}_1\mathbf{x}_1. \tag{2.66}$$

2. Tangent linear
   The cost function can be squared assuming that the operator $\mathbf{M}$ can be linearized, that is:
   $$\mathbf{y}_k - \mathbf{H}_k\mathbf{M}_{0\to k}(x) \approx \mathbf{y}_k - \mathbf{H}_t\mathbf{M}_{0\to k}(\mathbf{x}^b) - \mathbf{H}_k\mathbf{M}_{0\to k}(\mathbf{x} - \mathbf{x}^b), \tag{2.67}$$
   where $\mathbf{M}$ is the tangent linear model, i.e. the differential of $\mathbf{M}$.

These two assumptions simplify the problem of minimizing an unconstrained quadratic function which is numerically much easier to solve. The second term of the cost function (2.64) is no more complicated than that is in $3D - Var$. The evaluation of the first term $\mathcal{J}_o$ requires N integrations of the forecasting model from the time of the analysis at each observation time k and more for the calculation of the gradient.

The evaluation of the cost function and its gradient require an integration model from $k = 0$ at the value N and the use of integration with adjoint operators performed with the transpose of the tangent linear model of temporal operators $\mathbf{M}$.[3] The minimization of the cost function and its gradient is carried out according to the following procedure:

[3]The adjoint operators have been introduced to reduce the size and the number of multiplication of matrices and to be able to calculate the cost function. Algebraically means replace a set of matrices with their transposed, hence the name of *adjoint* techniques.

1. estimate $\mathbf{x}_k = \mathbf{M}_k \mathbf{M}_{k-1} ... \mathbf{M}_1 x_1$;
2. normalized discrepancies $\mathbf{d}_k = \mathbf{R}_k^{-1}(\mathbf{y}_k - \mathbf{H}_k[\mathbf{x}_k])$ that are stored
3. the contribution of the first part of cost function $\mathcal{J}_{ok} = (\mathbf{y} - \mathbf{H}_k[\mathbf{x}_k])^T \mathbf{d}_k$
4. and finally $\mathcal{J}_o = \sum_{t=0}^{N} \mathcal{J}_{ok}(\mathbf{x})$.

In order to compute $\nabla \mathcal{J}_o$ we need to factorize:

$$\begin{aligned} -\frac{1}{2}\nabla \mathcal{J}_o &= -\frac{1}{2}\sum_{k=0}^{N} \nabla \mathcal{J}_{ok} \\ &= \sum_{k=0}^{N} \mathbf{M}_1^T ... \mathbf{M}_k^T \mathbf{H}_k^T \mathbf{d}_k \\ &= \mathbf{H}_0^T \mathbf{d}_0 + \mathbf{M}_k^T [\mathbf{H}_1^T \mathbf{d}_1 + \mathbf{M}_1^T [\mathbf{H}_2^T \mathbf{d}_2 + .. \mathbf{H}_n^T \mathbf{d}_n]...]. \end{aligned} \tag{2.68}$$

This equation needs to be evaluated using the following algorithm.

1. initialize the adjoint variable $\tilde{\mathbf{x}} = 0$
2. for each step $k-1$ the variable $\tilde{\mathbf{x}}_{k-1}$ is obtained adding the adjoint forcing $\mathbf{H}_k^T \mathbf{d}_k$ to $\tilde{\mathbf{x}}_k$ and performing the adjoint integration by multiplying the result for $\mathbf{M}_k^T$, i.e. $\tilde{\mathbf{x}}_{k-1} = \mathbf{M}_k^T (\tilde{\mathbf{x}}_k + \mathbf{H}_k^T \mathbf{d}_k)$
3. at the end of recurrent the adjoint value $\tilde{\mathbf{x}}_0 = -\frac{1}{2}\mathcal{J}_o(\mathbf{x})$ gives the required result.

2.3 Assimilation as an Inverse Problem

Before showing why the assimilation is an inverse problem let us introduce the concept of well and ill posed problem in the sense of Hadamard. Given and operator $\mathbf{A}$, we wish to solve the following system of equations

$$\mathbf{g} = \mathbf{A}\mathbf{f}. \tag{2.69}$$

By Hadamard [9] e Hilbert e Courant [10] it is a well-posed problem when:

1. a solution exists;
2. the solution is only determined by the input parameters (forcing, boundary conditions, initial conditions);
3. depends continually on input parameters and it is stable ($\mathbf{A}^{-1}$ continuous).

When the conditions 2 and/or 3 are not satisfied the problem is ill-posed. In finite dimension, existence and uniqueness can be imposed and stability follows, however, the discrete problem of underlying ill-posed problem become ill-conditioned and the singular value of $\mathbf{A}$ decay to zero.

2.3.1 An Illustrative Example

Let us now apply the approach to a simplified model or toy model representing the sea circulation in a well defined ocean basin (Bennet [11]):

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = F, \tag{2.70}$$

with dimension between $0 \leq x \leq L$ in the time interval $0 \leq t \leq T$ where c is a known positive constant. Let $F = F(x,t)$ be the forcing field. An initial condition is given by:

$$u(x,0) = I(x), \tag{2.71}$$

where $I(x)$ is specified. The boundary conditions are:

$$u(0,t) = B(t), \tag{2.72}$$

where $B(t)$ is defined. In order to evaluate the uniqueness of the solution we assume F, I e B have two solutions u_1 and u_2. Defining the difference $v = u_1 - u_2$ we have:

$$\frac{\partial v}{\partial t} + c\frac{\partial v}{\partial x} = 0, \tag{2.73}$$

with the boundary conditions and initial conditions respectively of $v(x,0) = 0$ and $v(0,t) = 0$. The solution can be obtained using the methods of characteristics by which Partial Differential Equations (PDEs) are reduced to Ordinary Differential Equation (ODEs). The characteristic equations are:

$$\begin{aligned} \frac{dx}{ds} &= c \\ \frac{dt}{ds} &= 1. \end{aligned} \tag{2.74}$$

The PDE that has been transformed into ODE is

$$\frac{du}{ds} = 0 \tag{2.75}$$

On the basis of the initial condition and the boundary conditions the solution is:

$$u(x,t) = 0 \tag{2.76}$$

and then $u_1(x,t) = u_2(x,t)$ showing the solution is unique.

Let us now verify the other two points of the well-posed conditions. Using the Green function one defines $G = G(x, t, \zeta, \tau)$

$$-\frac{\partial G}{\partial s} - c\frac{\partial G}{\partial x} = \delta(x - \zeta)\delta(t - \tau) \tag{2.77}$$

where δ is the Dirac's delta with $0 \leq \zeta \leq L$ and $0 \leq \tau \leq T$. The boundary conditions for $0 \leq x \leq L$ are $G(L, t, \zeta, \tau) = 0$ and for $0 \leq t \leq T$ are $G(x, T, \zeta, \tau) = 0$.

The solution is:

$$u(x,t) = \int_0^T d\tau \int_0^L d\zeta G(\zeta, \tau, x, t)F(\zeta, \tau) + \int_0^L d\zeta G(\zeta, 0, x, t)I(\zeta) + \int_0^T d\tau G(0, \tau, x, t)B(\tau) \tag{2.78}$$

that is an explicit solution for the forward model. Relation (2.78) indicates u depends on F, I, B with continuity and if they change of a $\mathcal{O}(\mathbf{e})$, u also consequently changes. Furthermore the request is that $I(0) = B(0)$ otherwise u discontinues along $x = ct$ for all ts. On the basis of such evaluation one can deduce the model is well posed.

Let us see what happens to the forward model when we introduce the information for the field $u(x, t)$ of the circulation model proposed. This information consist of imperfect observations around at an isolated point in space and time. The direct model becomes indeterminate and cannot be solved with a smooth function and therefore must be considered an ill-posed problem that must be resolved through a *best fit* weighted with all the information we hold.

Let us assume to collect a M number of measurements (observations, data, etc. ..) of u, in our basin with $0 \leq x \leq L$, during the time cruise $0 \leq t \leq T$. The data are collected in x_i, t_i with $0 \leq i \leq M$ and will be indicated by the recorded value u_i and its error as:

$$u_i = u(x_i, t_i) + e_i, \tag{2.79}$$

where $\mathbf{e}_i$ is the measurement error and $u(x_i, t_i)$ is the true value. Since the boundary conditions and the initials conditions are affected by errors the equation should be written taking into account the error f on the forcing F.

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = F + f, \tag{2.80}$$

with

$$u(x, 0) = I(x) + i(x) \tag{2.81}$$

and

$$u(0, t) = B(t) + b(t). \tag{2.82}$$

The problem is now to obtain a unique solution for each choice of $F + f$, $I + i$ and $B + b$. This can be done by looking for the field $\hat{u} = \hat{u}(x_i, t_i)$ that minimizes errors.

One will try the minimum of the function $\mathcal{J}$ cost or penalty function where one also has introduced the error standard deviations of the "a priori" functions: W_i for the model, W_b for the boundary conditions and W_o for the observations.

$$\mathcal{J} = \mathcal{J}[u] = W_f \int_0^T dt \int_0^L f(x,t)^2 dx + W_i \int_0^L i(x)^2 dx + W_b \int_0^T b(t)^2 dt + w \sum_{m=1}^{M} e_i^2, \tag{2.83}$$

where W_f, W_i, W_b and w are the positive weights. The cost function $\mathcal{J}[u]$ is a number for each choice of the entire field u. Rewriting (2.83) and highlighting the explicit dependence of m, b, o and, e_i from F, I, B and u_i, we have:

$$\mathcal{J}(u) = W_f \int_0^T dt \int_0^L \{\frac{\partial u}{dt} + c\frac{\partial u}{\partial x} - F\}^2 dx + W_i \int_0^L \{u(x,0) - I(x)\}^2 dx + W_b \int_0^T \{u(0,t) - B(t)\}^2 dt + w \sum_{m=1}^{M} \{u(x_i,t_i) - u_i\}^2, \tag{2.84}$$

the solution of which can be obtained using the calculation of variations as reported in Appendix, both for the solution with weak constraint and strong constraints. Since $\mathcal{J}$ is quadratic in u, it is non negative and the local extremum must be the global minimum [11].

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