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Theoretical Issues in the Application of Bayesian Data Assimilation in Context of Meteorology, Part 1: Bayesian assimilation as a Tikhonov regularization

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For improving or updating the knowledge of atmospheric or oceanic state, observational data are assimilated into numerical evolution models. This is performed, most of the time, following a Bayesian framework to compromise, like Kalman filter, between observation errors and model errors. This article is a preliminary discussion about the structure of the theory, in particular the pivotal definition of a background error covariance matrix. The well known difficulties associated with the practical implementation and the so called catastrophic filter divergence are addressed in a companion paper.

Geophysical Bayesian assimilation may be seen as a Tikhonov regularization, the background error covariance matrix corresponding to the regularizing term. Tikhonov regularization was originally developed to stabilize overdetermined inverse problems against measurement errors. However, Geophysical assimilation is always strongly underdetermined. This changes totally the role of the regularizing term: instead of stabilizing the estimation, it determines its main features. The derivation of the matrix becomes, accordingly, essential. It is shown here that the traditional definition of the background error covariance matrix and its presumed dependence on earlier information raises practical difficulties. These difficulties are not compatible with the simplifications generally assumed. They are also not compatible with a practical implementation of Bayesian assimilation.

Keywords: Assimilation of data, meteorology, Bayesian statistics

1. Introduction

Data assimilation is one of the key tools of modern meteorology and oceanography, hereafter termed jointly as geosciences. Data assimilation designates any technique used to combine the observations with a model in view of improving or updating knowledge of the real state of the system. Here, the word "state" designates the field, through given region and time interval, of one or several parameters such as wind speed, temperature, moisture. In past decades, Bayesian theory has been well established, in the form of 3D-VAR, 4D-VAR and other Kalman Filter (KF) variations.

Operational meteorology and oceanography have seen an extraordinary development with the relatively recent ability to exploit daily an enormous amount of data from sophis-

ticated sensors to infer the state of the earth and accurately predict weather for several days and often weeks. A non-specialist would certainly imagine data assimilation has reached maturity. He might suppose that further achievements could now only be sought marginally by increasing the computational power and refining the numerical methods.

That it is not so is seen from many works (e.g. Bannister (2008 a & b), Li et al. (2009 a & b), Singh et al. (2011), Pinnington et al. (2016), Waller et al. (2016), Howes et al. (2017)) about the background error covariance matrix (becm), pivotal in the Bayesian framework. The becm is still a commonly discussed issue for its (i) subjective elicitation, (ii) huge size requiring simplifications or (iii) generation from a huge system of equations supposedly relating the matrix to earlier information. So far, all schemes proposed eventually diverge, which is interpreted as a numerical artifact due to inappropriate simplifications. The debate is accordingly focussed on simplifications and stabilizing procedures. It is proposed to highlight these issues and identify the origin of the difficulties in this and a companion article, hereafter referred to as part 1 and part 2 respectively.

This article examines the theoretical framework and the definition of a becm. Sections 2 to 5 prepare the discussion held more conclusively in section 6. Section 2 introduces notations with a short reminder about least squares, a basic but insufficient technique. Section 3 addresses Tikhonov regularization to highlight (i) the specific features of data assimilation as an underdetermined compared to overdetermined inverse problem (ii) the prevailing importance of the regularizing term, corresponding to background errors. Section 4 exposes how the cost function is associated with Baye's rule for conditional probabilities. Section 5 describes how the determination of the becm is currently addressed, between adhoc choices and the tentative derivation from earlier information using Kalman filter. The well known conceptual and practical difficulties are reminded. Section 6 discusses the relevance of the earlier information as an input to becm definition. It starts with an important question: why does the Bayesian framework receive that much support in meteorology inspite of the failure of all simplified numerical implementations? The reasons found are essentially implicit or tacit.

2. Data assimilation or ill-posed inverse problem

(a) Statement of the problem

A system is described using a finite-dimensional ambient space \mathcal{D} and a state function $s : \mathcal{D} \rightarrow \mathbb{R}^l$, l being a positive integer. The state s belongs to a Hilbert space \mathcal{S} of functions with sufficient regularity; a Hilbert space is just a vector space associated with a scalar product and complete for the resulting norm or distance. In meteorological applications, the ambient space has the form $\mathcal{D} = \Omega \times T$ in which Ω denotes the atmosphere or a part of it and T a time interval. The state s describes fields through \mathcal{D} of such physical parameters as pressure, temperature, wind, moisture, emissions of trace species into the atmosphere.

The state s of the system is known only through a finite number of observations $\mu_1, \mu_2, \dots, \mu_n$ also jointly denoted as $\vec{\mu}$ in vector form. The relationship between the measurements and the state is described in terms of a measurement operator $\mathcal{H} : \mathcal{S} \rightarrow \mathbb{R}^n$ and measurement errors. In practice, \mathcal{H} may be nonlinear but will generally be linearized during the assimilation procedure.

$$\vec{\mu} = \mathcal{H}s + \vec{r} \tag{2.1}$$

The measurement or observation errors may be decomposed as:

$$\vec{r} = \vec{r}_r + \vec{r}_d \quad (2.2)$$

into a representativity error \vec{r}_r associated with the limited representativity of the measurement model and an instrumental error \vec{r}_d associated with the limited accuracy of the detectors.

The inverse problem of determining s from observations $\vec{\mu}$ is *well-posed* if the information in $\vec{\mu}$ is non redundant and allows to fully identify s from equation 2.1 up to measurement errors. In this case, \mathcal{S} has dimension the number n of measurements and \mathcal{H} has full rank n . The inverse problem is *ill-posed* otherwise. Ill-posedness essentially consists of two opposite situations. The inverse-problem is overdetermined if the information contained in $\vec{\mu}$ is in excess for identifying s : the dimension of \mathcal{S} must be finite, less than n . The inverse problem is underdetermined if the complete identification of s is not feasible: the dimension of \mathcal{S} is larger than n , possibly infinite. In atmosphere and ocean sciences, such underdetermined inverse problem is called *data assimilation*.

Overdeterminacy is of course associated with redundancy in the measurements. Redundancy may exist as well in the underdetermined inverse problem: this possibility is essentially theoretical and of little practical interest. Thus, for the sake of simplicity, the underdetermined problems considered hereafter are taken as non-redundant.

(b) Least squares

Considering the uncertainty in equation 2.1 associated with the error term, a natural idea for estimating s is to minimise some distance $d(\vec{\mu}, \mathcal{H}s)$ between the observed and predicted measurements. If the distance is Euclidean, associated with a matrix \mathbf{G} , symmetric, positive definite, this amounts to minimise the cost function:

$$\mathcal{J}(s) = (\vec{\mu} - \mathcal{H}s)^\top \mathbf{G} (\vec{\mu} - \mathcal{H}s) \quad (2.3)$$

If \mathbf{G} is taken as the $n \times n$ identity matrix \mathbf{I}_n , then $\mathcal{J}(s) = \sum_{i=1}^n (\mu_i - (\mathcal{H}s)_i)^2$ which explains the name of *least squares* associated with the technique. However, choosing \mathbf{G} as \mathbf{I}_n implies that all measurements are paid the same attention. This is inappropriate if the accuracy in the various measurements is very different. Therefore, if the covariance matrix $\mathbf{R} = \overline{\vec{r}\vec{r}^\top}$ of the measurement errors is known, it is recommended to choose $\mathbf{G} = \mathbf{R}^{-1}$ (Gauss-Markov theorem).

3. Tikhonov regularization

Least squares computations often return an estimate with irregular and non-physical patterns. These are generally regarded as numerical instabilities associated with an ill-conditioning of the inverse problem. Tikhonov regularization was originally introduced as a remedy to this ill-conditioning. An important aim of the present section is to show that this interpretation of estimate irregularities should be limited to the overdetermined inverse problem. The clarification is important in the context of Bayesian assimilation of data currently used in geophysics to retrieve the state of the earth from a few measurements. This assimilation is characterized by a Tikhonov type cost function derived from error statistics (see section 4), but the inverse problem is usually strongly underdetermined.

(a) *Tikhonov cost function*

Tikhonov regularization corresponds to the following modification of the least squares cost function (equation 2.3):

$$\mathcal{J}_\lambda(s) = \lambda^2(s, \mathcal{L}s) + (\bar{\mu} - \mathcal{H}s)^\top \mathbf{G}(\bar{\mu} - \mathcal{H}s) \quad (3.1)$$

in which the regularizing term $\lambda^2(s, \mathcal{L}s)$ is a scalar product derived from the scalar product (\cdot, \cdot) of \mathcal{S} as a Hilbert space using a linear operator $\mathcal{L} : \mathcal{S} \rightarrow \mathcal{S}$ and a positive modulating parameter λ . If \mathcal{S} is infinite-dimensional, \mathcal{L} should be so chosen that \mathcal{H} be continuous for the regularizing scalar product. Under this condition, it will be possible to define an adjoint operator $\mathcal{H}_\mathcal{L}^*$.

Hereafter, \mathcal{S} will be rather supposed to be finite-dimensional. This simplifies the analysis of the inverse problem. One should nevertheless keep in mind that real systems are commonly infinite-dimensional and discretized results should remain consistent when the resolution is increased arbitrarily. Thus, if $\mathcal{S} = \mathbb{R}^N$ is finite-dimensional, a linear or linearized \mathcal{H} is necessarily continuous and may be described by a $n \times N$ matrix

$$\mathcal{H}s = \mathbf{H}s \quad \text{with} \quad \mathbf{H} = \begin{bmatrix} h_1^\top \\ \vdots \\ h_n^\top \end{bmatrix} \quad \text{so that} \quad \mu_i = h_i^\top s + r_i \quad (3.2)$$

in which h_i is the adjoint state determining, based on the trivial scalar product of \mathbb{R}^n and up to an error, the value of the i^{th} measurement. The regularizing scalar product in \mathcal{S} may as well be described with a symmetric, positive definite matrix:

$$\mathcal{H}s = \mathbf{H}s, \quad (s, \mathcal{L}s') = s^\top \mathbf{L}s' \quad (3.3)$$

The cost function (equation 3.1) is written as:

$$\mathcal{J}_\lambda(s) = \lambda^2 s^\top \mathbf{L}s + (\bar{\mu} - \mathbf{H}s)^\top \mathbf{G}(\bar{\mu} - \mathbf{H}s) \quad (3.4)$$

Tikhonov regularization has been studied mostly for the overdetermined problems to avoid numerical instabilities. However, in case of underdetermined problem, the unphysical patterns of the least square estimate are not essentially related to numerical instabilities. This is explained hereafter.

(b) *Exact expressions for the estimation*

Two equivalent descriptions may be obtained for the states minimizing the least-square cost function $\mathcal{J} = \mathcal{J}_0$ (equation 2.3) and Tikhonov cost function \mathcal{J}_λ (equation 3.1). The first one is of huge interest for the overestimated case. The second is more useful to the underestimated case.

The first description involves the singular value decomposition of the measurement operator \mathcal{H} . This is explained in appendix A based on the work by Hansen (1992). Let r denote the rank of \mathcal{H} . For $i = 1, 2, \dots, r$ there exist left singular vectors $m_i \in \mathbb{R}^n$, right singular vectors $s_i \in \mathcal{S} = \mathbb{R}^N$ and singular values in decreasing order $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r \geq 0$ such that:

$$s_0 = \sum_{i=1}^r \frac{\bar{\mu}^\top \mathbf{G} \bar{m}_i}{\sigma_i} s_i, \quad s_\lambda = \sum_{i=1}^r \frac{\sigma_i (\bar{\mu}^\top \mathbf{G} \bar{m}_i)}{\sigma_i^2 + \lambda^2} s_i \quad (3.5)$$

An alternative description, equation 3.6, is obtained (appendix B) using the adjoint measurement operator $\mathcal{H}_{\mathcal{L}}^* : \mathbb{R}^n \rightarrow \mathcal{S}$ such that $\bar{\alpha}^\top \mathcal{H}(s) = (\mathcal{H}_{\mathcal{L}}^* \bar{\alpha})^\top \mathbf{L}s$ for all $\bar{\alpha} \in \mathbb{R}^n$, $s \in \mathcal{S}$. The definition of $\mathcal{H}_{\mathcal{L}}^*$ involves the scalar product with matrix \mathbf{L} in \mathcal{S} , but a classical convenience leads to utilise in the measurement space the usual scalar product with identity matrix instead of \mathbf{G} . In order to rewrite expression B.2 in finite-dimensional matrix form, \mathcal{H} and $\mathcal{H}_{\mathcal{L}}^*$ are described by the $n \times N$ matrix \mathbf{H} and $N \times n$ matrix $\mathbf{H}_{\mathcal{L}}^*$ respectively:

$$s_0 = \mathbf{H}_{\mathcal{L}}^* (\mathbf{H}\mathbf{H}_{\mathcal{L}}^*)^{-1} \vec{\mu}, \quad s_\lambda = \mathbf{H}_{\mathcal{L}}^* (\mathbf{H}\mathbf{H}_{\mathcal{L}}^* + \lambda^2 \mathbf{G}^{-1})^{-1} \vec{\mu}, \quad \text{with } \mathbf{H}_{\mathcal{L}}^* = \mathbf{L}^{-1} \mathbf{H}^\top \quad (3.6)$$

For $\lambda > 0$, \mathcal{J}_λ is strictly convex, its minimum s_λ is unique with equivalent expressions 3.5 and 3.6. By continuity for vanishing λ , these expressions are also equivalent regarding s_0 with the following two restrictions.

First, in the underdetermined case, $\mathcal{J} = \mathcal{J}_0$ is convex but not strictly convex and thus, s_0 is just one among infinitely many other minimizing states.

Second, the $n \times n$ matrix $\mathbf{H}\mathbf{H}_{\mathcal{L}}^*$ has its rank bounded by the rank of \mathbf{H} less than N . In the overdetermined case ($n > N$) the matrix is not invertible. $\mathbf{H}\mathbf{H}_{\mathcal{L}}^*$ is invertible only in the non-redundant underdetermined case.

To conclude this section, observe that s_0 and s_λ , regardless of the regularisation parameter λ , belong to the same estimation vector space, the range of $\mathcal{H}_{\mathcal{L}}^*$ denoted as:

$$\mathcal{S}_e = \text{Range } \mathcal{H}_{\mathcal{L}}^* \quad (3.7)$$

This is seen immediately from expressions 3.6. This is seen as well from expressions 3.5 after deducing from the definition of the singular value decomposition $\sigma_i = \vec{m}_i^\top \mathbf{G} \mathcal{H} s_i$ and then $s_i = \frac{1}{\sigma_i} \mathcal{H}_{\mathcal{L}}^* (\vec{m}_i)$. The result 3.7 has different consequences for the overdetermined and underdetermined inverse problems.

(c) Infinitesimal regularization

Among all states minimizing \mathcal{J} , s_0 (equation 3.5, 3.6) additionally minimizes $\|s_0\| = \sqrt{s_0^\top \mathbf{L} s_0}$. Indeed, the functional defined in the measurement space \mathbb{R}^n by $\bar{\alpha} \rightarrow \bar{\alpha}^\top \mathbf{G} \bar{\alpha}$ is strictly convex. Therefore, $\mathcal{J}(s_0 + s') = \mathcal{J}(s_0)$ leads to $(\mathcal{H}s')^\top \mathbf{G} \mathcal{H}s' = 0$ and $\mathcal{H}s' = 0$ implying that s' is orthogonal to \mathcal{S}_e . Since $s_0 \in \mathcal{S}_e$, one deduces $\|s_0 + s'\|^2 = \|s_0\|^2 + \|s'\|^2$.

This suggests s_0 might be regarded as a regularized estimation minimizing a Tikhonov functional \mathcal{J}_λ for λ infinitely small. Such interpretation is further supported by the facts, seen in section 3b that $s_0 = \lim_{\lambda \rightarrow 0} s_\lambda$ and s_0 is in the same estimation space \mathcal{S}_e as all s_λ .

(d) Overdetermined inverse problem

The inverse problem is overdetermined when the rank r of the $n \times N$ operator \mathcal{H} coincides with the dimension N of the state space $\mathcal{S} = \mathbb{R}^N$. Notice that (1) the left singular vectors s_1, s_2, \dots, s_N form a basis of \mathcal{S} and (2) the linear function $\vec{\mu} \rightarrow s_0$ (equation 3.5) is one to one. The estimation space extends to the whole space: $\mathcal{S}_e = \mathcal{S}$. Thus, s_0 is the only solution to the problem of minimizing \mathcal{J} (equation 2.3). As such, s_0 depends on \mathbf{G} , not on \mathbf{L} . This might seem in contradiction with the expression 3.5 of s_0 because the singular value decomposition depends on both \mathbf{G} and \mathbf{L} .

The expression of s_0 highlights two difficulties associated with the least squares technique. First, the coefficients of the modes with small eigenvalues are sensitive to the measurement errors. Second, the number of modes coincides with the dimension N of the

state space \mathcal{S} that can be very large in applications. This large number increases the risk of having relatively small singular values. For instance, Hansen et al. (2006) describe the difficulty of restoring a clear N -pixel digital image (the state) from the raw image obtained using n detectors (the measurements) both blurred and noisy. Even if the blurring process is perfectly known and theoretically invertible, the non regularized inversion is unexploitable. The minimisation of \mathcal{J} using noisy observations is expected to deliver a poor estimate affected by non physical features and irregularities.

In the regularized estimate s_λ (equation 3.5), the unstable modes, corresponding to singular values smaller than λ , are filtered out. The regularization of Tikhonov enables to obtain a smoother estimate. Hansen (1992) has clearly shown the interest of regularization for the overdetermined problem and proposed his criterion of the L-curve for optimally choosing the regularizing parameter λ .

The validity of the above discussion does not extend to the underdetermined inverse problem.

(e) Underdetermined inverse problem

A first consequence of underdeterminacy is that s_0 (equation 3.6) is not the only state minimizing the least square cost function \mathcal{J} (equation 2.3). Infinitely many other states minimize \mathcal{J} and s_0 is just a particular solution in terms of the adjoint operator \mathcal{H}_L^* . If the scalar product in \mathcal{S} is changed, so are \mathcal{H}_L^* and the estimation space $\mathcal{S}_e = \text{Range } \mathcal{H}_L^*$ (equation 3.7). Unlike in overdetermined case, \mathcal{S}_e is a proper linear subspace of \mathcal{S} .

On the other hand, when the cost function is regularized as \mathcal{J}_λ , its minimum s_λ is unique and well defined. One might accordingly consider that Tikhonov regularization has two advantages: (1) damping the unstable modes and (2) avoiding the underdeterminacy. The situation is not that simple.

The number n of modes is less than $N = \dim \mathcal{S}$. In practice, especially in atmospheric or oceanic sciences, \mathcal{S} has infinite dimension and even after discretization, n , the number of independent measurements, is negligible compared to N . The difficulties associated, in the overdetermined case (section d), with a large number of modes, are avoided. The computation of s_0 from equation 3.6 is simple. The matrix $\mathbf{H}\mathbf{H}_L^* = \mathbf{H}\mathbf{L}^{-1}\mathbf{H}^T$ is computed relatively easily. Its matrix coefficients may be regarded as $(\mathbf{H}\mathbf{H}_L^*)_{ij} = h_i^T \mathbf{L}^{-1} h_j$ of the states h_i (equation 3.2). Underdetermined problems correspond to complex systems observed using rare detectors distributed in view of avoiding redundancy. If the monitoring network is well designed, the diagonal coefficients are large compared to off-diagonal ones, the matrix is well conditioned. Tikhonov regularization, from this point of view, is not required.

This does not mean that the estimate is smooth and regular. However, irregularities in the underdetermined problem have specific causes that are not under the control of Tikhonov regularization. The states h_i adjoint to the measurements are generally singular or strongly peaked corresponding to respective detector location. As linear combinations of these, s_0 and s_λ display the similar singularities or peaks irrespective of any regularization. These non-physical features can be removed only by choosing the estimation space \mathcal{S}_e i.e. the scalar product utilized in \mathcal{S} . It is accordingly of interest to discuss the particular choice advocated by atmospheric data assimilation based on Bayesian arguments.

4. Bayes' rule and Kalman filter

The previous section stressed the importance, for the underdetermined inverse problem, of the scalar product utilized in the state space \mathcal{S} . This raises a question: how to choose it? The present section describes how this question is addressed in the Bayesian framework of geosciences. The framework is statistical in nature. The inverse problem is solved by compromising between the reliability of the measurements and the reliability of a forecasted background state. The cost function associated with the compromise is a regularised Tikhonov function. The section contains no new result. It is a purely mathematical presentation of statistical assumptions and logical consequences from which the Bayesian framework is drawn. This is the ground for the later discussion about the concrete choice of the regularizing product in this framework.

(a) Conditional probabilities

Let Ω be a sample set with probability measure P , i.e. $P(\Omega) = 1$. Let A and B be two events from Ω , i.e. two measurable subsets with respective probabilities $P(A)$, $P(B)$. The conditional probability of A given that B is true is defined as $P(A|B) = \frac{P(A \cap B)}{P(B)}$, in which the symbol \cap denotes the intersection. Baye's rule is the following well known identity derived immediately from this definition:

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)} \quad (4.1)$$

The events are defined to be statistically independent if $P(A|B) = P(A)$ or, equivalently, $P(B|A) = P(B)$.

There is also a version of this theorem for probability densities. Let a and b be two random variables with probability densities $p_1(a)$, $p_2(b)$. The probability of intersection is replaced by a joint probability density $p_J(a, b)$. The conditional density of a when the other variable is b is defined as $p(a | b) = \frac{p_J(a, b)}{p_2(b)}$. Baye's rule immediately generalizes as a consequence of this definition:

$$p(a | b) = \frac{p(b | a)p_1(a)}{p_2(b)} \quad (4.2)$$

The variables are statistically independent when $p(a | b) = p_1(a)$ for all b .

(b) State and measurement vector as random variables

The Bayesian assimilation of data is based on the idea that the state s and the observation vector $\vec{\mu}$ are random variables. A forecast state s^b , called the background, is always assumed. The departure $s - s^b$ from the true state is called the background error and the departure of observed from expected measurements, $\Delta\vec{\mu} = \vec{\mu} - \mathcal{H}s^b$, is called the innovation. Putting s as a and $\vec{\mu}$ as b , expression 4.2 becomes:

$$p(s | \vec{\mu}) = \frac{p(\vec{\mu} | s)p_1(s)}{p_2(\vec{\mu})} \quad (4.3)$$

The terms in this expression are interpreted as follows:

- $p_1(s)$ is the probability density of the state prior to the observations

- $p(s | \vec{\mu})$ is the probability density of the state posterior to the observations $\vec{\mu}$
- $p(\vec{\mu} | s)$ is the probability density of the observations when the state is s , which is in fact understood as the probability density of the observation error $\vec{\mu} - \mathcal{H}s$ (equations 2.1, 2.2)
- $p_2(\vec{\mu})$ is the probability $\vec{\mu}$ had to be observed prior to its effective observation; in equation 4.3, this term acts mainly as a normalising coefficient so that its knowledge is generally considered unessential (see coefficient c_o in equation 4.5).

The following assumptions or remarks are added to proceed from this juncture. They are generally formulated based on a discretisation of the state, which amounts to suppose that $N = \dim \mathcal{S}$ is finite.

First, the density $p_1(s)$ of the state is taken as Gaussian with the background state s^b as mean; $s - s^b$ is the background error. The $N \times N$ covariance matrix \mathbf{P} of this density is called the background error covariance matrix (becm).

Second, the random variable $\vec{\mu}$ decomposes as $\vec{\mu} = \mathcal{H}s + \vec{r}$ (equation 2.1) in which $\vec{r} = \vec{r}_r + \vec{r}_d$ (equation 2.2) is a measurement error due to imperfect detectors (\vec{r}_d) and model (\vec{r}_r). It is generally assumed that s and \vec{r} are independent Gaussian variables. Then, the conditional density of $\vec{\mu}$ when the state s reduces to a density $p(\vec{\mu} | s) = p(\vec{r})$ with a $n \times n$ covariance matrix \mathbf{R} independent of s .

$$p_1(s) = \frac{e^{-\frac{1}{2}(s-s^b)^\top \mathbf{P}^{-1}(s-s^b)}}{(2\pi \det \mathbf{P})^{\frac{N}{2}}}, \quad p(\vec{\mu} | s) = \frac{e^{-\frac{1}{2}(\vec{\mu}-\mathcal{H}s)^\top \mathbf{R}^{-1}(\vec{\mu}-\mathcal{H}s)}}{(2\pi \det \mathbf{R})^{\frac{n}{2}}} \quad (4.4)$$

Equation 4.3 may now be written:

$$p(s | \vec{\mu}) = c_o e^{-\frac{1}{2}\mathcal{F}(s)} \quad \text{with} \quad \mathcal{F}(s) = (s - s^b)^\top \mathbf{P}^{-1}(s - s^b) + (\vec{\mu} - \mathcal{H}s)^\top \mathbf{R}^{-1}(\vec{\mu} - \mathcal{H}s) \quad (4.5)$$

in which $c_o = p_2(\vec{\mu})^{-1} (2\pi \det \mathbf{P})^{-\frac{N}{2}} (2\pi \det \mathbf{R})^{-\frac{n}{2}}$ is a constant since $\vec{\mu}$ is fixed corresponding to the observations. Notice that \mathcal{F} can be reformulated using the background error $s - s^b$ and innovation $\Delta\vec{\mu} = \vec{\mu} - \mathcal{H}(s^b)$,

$$\mathcal{F}(s) = (s - s^b)^\top \mathbf{P}^{-1}(s - s^b) + (\Delta\vec{\mu} - \mathcal{H}(s - s^b))^\top \mathbf{R}^{-1}(\Delta\vec{\mu} - \mathcal{H}(s - s^b)) \quad (4.6)$$

with $\Delta\vec{\mu} = \vec{\mu} - \mathcal{H}s^b$

which allows to recognize it as a Tikhonov type functional.

Remark: The assumption that s and \vec{r} are statistically independent is questionable. Suppose, to simplify, the measurement model is linear. Then, if the state s is changed to $2s$, the observed measurement vector $\vec{\mu} = \mathcal{H}s + \vec{r}_r + \vec{r}_d$ is changed to $\vec{\mu}' = 2\mathcal{H}s + 2\vec{r}_r + \vec{r}_d$, i.e. the representativity error is certainly doubled. The statistics of the instrumental error \vec{r}_d may vary too, for instance due to detector saturation. Thus, the above assumption is acceptable if the background error $s - s^b$ is not too large. Otherwise, the error statistics around the unknown real state s could not be estimated based on s^b .

(c) *Optimal estimation and posterior distribution*

The optimal estimator of s posterior to the observations, also called the analysed state, is generally intended, given some scalar product $\langle \cdot, \cdot \rangle$ in \mathcal{S} , as the state s^a minimizing the expectable quadratic distance $\int \langle s^a - s, s^a - s \rangle dp(s | \vec{\mu})$ to the real unknown state. Owing to the quadratic nature of $\mathcal{F}(s)$ with respect to s (equation 4.5), the posterior probability density $p(s | \vec{\mu})$ is Gaussian. This implies the following additional properties of s^a (i) it coincides with the conditional mean after the observations (unbiased estimator), (ii) it is the state most probable maximizing $p(s^a | \vec{\mu})$ and (iii) it is same for any choice of a scalar product in \mathcal{S} .

Since \mathcal{F} (equation 4.5) is convex, the state s^a minimizing it is solution to the gradient equation $\partial\mathcal{F}(s^a) = 0$, i.e. $s^a - s^b = (\mathbf{P}^{-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H})^{-1} \mathbf{H}^T \mathbf{R}^{-1} \Delta \vec{\mu}$ which, after a simple but tedious computation, is shown equivalent to :

$$s^a = s^b + \mathbf{P} \mathbf{H}^T (\mathbf{H} \mathbf{P} \mathbf{H}^T + \mathbf{R})^{-1} \Delta \vec{\mu} \quad (4.7)$$

This expression is just a finite-dimensional version of the equation B.2 for s_λ , in which the regularizing scalar product in \mathcal{S} is described by \mathbf{P}^{-1} . To verify that the conditional probability density (equation 4.5) is Gaussian, let's rewrite it with the origin shifted to s^a . Since $\mathcal{F}(s^a + s) = \mathcal{F}(s^a) + \partial\mathcal{F}(s^a) \cdot s + s^T (\mathbf{P}^{-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H}) s$ in which $\partial\mathcal{F}(s^a) = 0$, one obtains:

$$p(s^a + s | \vec{\mu}) = c_1 e^{-\frac{1}{2} s^T (\mathbf{P}^{-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H}) s} \quad (4.8)$$

in which $c_1 = c_0 e^{-\frac{1}{2} \mathcal{F}(s^a)}$ is a constant. Since this density (equation 4.8) is Gaussian, its maximum s^a (equation 4.7) is indeed the best estimator of s once $\vec{\mu}$ has been observed. The following is known as the *gain matrix* transforming the innovation $\Delta \vec{\mu} = \vec{\mu} - \mathcal{H}(s^b)$ into a state correction.

$$\mathbf{K} = \mathbf{P} \mathbf{H}^T (\mathbf{H} \mathbf{P} \mathbf{H}^T + \mathbf{R})^{-1} \quad (4.9)$$

From expression 4.8, the analysis error covariance matrix \mathbf{P}' is read as:

$$\mathbf{P}' = (\mathbf{P}^{-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H})^{-1} \quad (4.10a)$$

$$= \mathbf{P} - \mathbf{P} \mathbf{H}^T (\mathbf{H} \mathbf{P} \mathbf{H}^T + \mathbf{R})^{-1} \mathbf{H} \mathbf{P} \quad (4.10b)$$

The equivalence of 4.10a and 4.10b corresponds to Woodbury formula (lemma **D1**). The form 4.10a better shows that \mathbf{P}' is positive; it is privileged in geosciences. The form 4.10b shows that \mathbf{P}' corresponds to smaller errors; it is privileged in the mathematical literature.

In the geophysical literature, the update of the state directly from expression 4.7 is termed *optimal interpolation*. However, this update is generally achieved by minimizing the cost function \mathcal{F} . This is equivalent. The minimization process is termed *variational assimilation*.

(d) *Statistical interpretation of Tikhonov cost function*

The functional $\mathcal{F}(s)$ (equation 4.5) is of regularized Tikhonov type (equation 3.1) with two terms. The measurement errors are weighted according to their covariance matrix. The regularizing term, essential as explained in section 2e, corresponds to the scalar product in \mathcal{S} chosen as $\|s\|_{\mathbf{P}}^2 = s^T \mathbf{P}^{-1} s$. The cost function may be regarded as a balance between the information associated with the background forecast and the information obtained from the measurements. A relatively small becm \mathbf{P} indicates a high reliability of the forecast s^b whereas a relatively small \mathbf{R} indicates a requirement for fitting the state to the observations.

The description 3.7 of the estimation space may now be seen as a mere application of a projection theorem formulated in the field of stochastic optimal estimation (e.g. Anderson & Moore, 1979, ch. 5). This result may be traced back to Kalman (1960).

The statistical interpretation of Tikhonov cost function leads to the question: how to determine \mathbf{P} and \mathbf{R} ? The background error covariance matrix \mathbf{P} is not observed directly. There are difficulties as well with the covariance matrix \mathbf{R} of the measurement errors $\vec{r} = \vec{r}_d + \vec{r}_r$. Calibrating the instrumental error \vec{r}_d from the detectors may seem easy. However, the model error \vec{r}_r is also not observed directly and, most often in climatological sciences, it is prevailing compared to the instrumental error.

(e) *System representation*

Baye's rule and analysis equations 4.7, 4.10 can be applied recursively. Consider a system evolving through successive states s_k , $k = 0, 1, 2, \dots$, in a finite-dimensional $\mathcal{S} = \mathbb{R}^N$, observed through measurements $\vec{\mu}_k \in \mathbb{R}^{n_k}$ according to noisy equations:

$$s_{k+1} = \mathcal{E}_k s_k + e_k \quad (4.11a)$$

$$\vec{\mu}_k = \mathcal{H}_k s_k + \vec{r}_k \quad (4.11b)$$

Suppose (i) both dynamical and measurement operators $\mathcal{E}_k, \mathcal{H}_k$ are linear, the errors e_k, \vec{r}_k are (ii) Gaussian and independent with covariance matrices $\mathbf{Q}_k, \mathbf{R}_k$ and (iii) sequentially independent of e_l, \vec{r}_l for $k \neq l$. Equations 4.11 are then written in the following matrix form. For later convenience, the noises are described using the convention of control theory:

$$s_{k+1} = \mathbf{E}_k s_k + \mathbf{M}_k \epsilon_k \quad (4.12a)$$

$$\vec{\mu}_k = \mathbf{H}_k s_k + \mathbf{N}_k \epsilon_k \quad (4.12b)$$

in which \mathbf{E}_k (size $N \times N$), \mathbf{H}_k (size $n_k \times N$) are the dynamical and measurement matrices, ϵ_k is a Gaussian noise with the identity of dimension $N + n_k$ as covariance matrix, \mathbf{M}_k (size $N \times (N + n_k)$), \mathbf{N}_k (size $n_k \times (N + n_k)$) are related to the covariance matrices \mathbf{Q}_k (size $N \times N$), \mathbf{R}_k (size $n_k \times n_k$) as:

$$\mathbf{M}_k = \left[\sqrt{\mathbf{Q}_k} \mid 0 \right], \quad \mathbf{N}_k = \left[0 \mid \sqrt{\mathbf{R}_k} \right] \quad (4.13)$$

The independent dynamical and measurement noises have covariance matrices described as:

$$\mathbf{Q}_k = \mathbf{M}_k \mathbf{M}_k^\top, \quad \mathbf{R}_k = \mathbf{N}_k \mathbf{N}_k^\top, \quad \text{with } \mathbf{M}_k \mathbf{N}_k^\top = 0 \quad (4.14)$$

(f) *Kalman filter*

If the distribution of s_0 prior to observations is Gaussian, with mean s_0^b and becm \mathbf{P}_0 , a recursive analysis may be initiated. This analysis (equations 4.7, 4.10) is conveniently formulated in terms of successive background states $s_0^b, s_1^b, s_2^b, \dots$ with:

$$s_{k+1}^b = \mathcal{E}_k s_k^a \quad (4.15)$$

in matrix form: $s_{k+1}^b = \mathbf{E}_k s_k^a$. This corresponds to the evolution of s_k^a expected in mean from equation 4.11a or 4.12a. The noise in this equation and the noise in s_k^a with becm \mathbf{P}'_k ,

posterior at t_k , combine to provide the noise in s_{k+1}^b with becm \mathbf{P}_{k+1} , prior at t_{k+1} :

$$s_{k+1}^b = \mathbf{E}_k [s_k^b + \mathbf{P}_k \mathbf{H}_k^\top (\mathbf{H}_k \mathbf{P}_k \mathbf{H}_k^\top + \mathbf{R}_k)^{-1} \Delta \vec{\mu}_k] \quad (4.16a)$$

$$\mathbf{P}_{k+1} = \mathbf{E}_k (\mathbf{P}_k^{-1} + \mathbf{H}_k^\top \mathbf{R}_k^{-1} \mathbf{H}_k)^{-1} \mathbf{E}_k^\top + \mathbf{Q}_k \quad (4.16bi)$$

$$= \mathbf{E}_k (\mathbf{P}_k - \mathbf{P}_k \mathbf{H}_k^\top (\mathbf{H}_k \mathbf{P}_k \mathbf{H}_k^\top + \mathbf{R}_k)^{-1} \mathbf{H}_k \mathbf{P}_k) \mathbf{E}_k^\top + \mathbf{Q}_k \quad (4.16bii)$$

The innovation and gain matrix, such that $s_{k+1}^b = \mathbf{E}_k s_k^b + \mathbf{K}_{k+1} \Delta \vec{\mu}_k$, are now:

$$\Delta \vec{\mu}_k = \vec{\mu}_k - \mathbf{H}_k s_k^b, \quad \mathbf{K}_{k+1} = \mathbf{E}_k \mathbf{P}_k \mathbf{H}_k^\top (\mathbf{H}_k \mathbf{P}_k \mathbf{H}_k^\top + \mathbf{R}_k)^{-1} \quad (4.3)$$

The recursive scheme 4.16 is that of Kalman filter. The equation 4.16b for the becm is a discrete time Riccati equation; the two forms are derived from counterparts in equation 4.10. Notice that this equation is independent from equation 4.16a so that the successive becms are independent of the observations. The invertibility of \mathbf{R}_k implies that of $\mathbf{H}_k \mathbf{P}_k \mathbf{H}_k^\top + \mathbf{R}_k$.

(g) Extended Kalman filter

Most systems considered in geosciences are non-linear: they are described by such system as 4.11, but either the dynamical models \mathcal{E}_k or the measurement models \mathcal{H}_k are non-linear. Non-linear assimilation is considerably more difficult and less mature than linear assimilation. A common strategy consists of linearising around the successive background states s_k^b to rewrite the system in the form 4.12 and iterate based on equations 4.16. This non-linear generalization is called extended Kalman filter. Several differences must be stressed between the linear and non-linear cases.

First, when the dynamical and measurement models are linear, the model matrices \mathbf{E}_k , \mathbf{H}_k and the covariance matrices $\mathbf{Q}_k = \mathbf{M}_k \mathbf{M}_k^\top$, $\mathbf{R}_k = \mathbf{N}_k \mathbf{N}_k^\top$ depend only on step k . In the non-linear case, they additionally depend on the estimated state s_k^b . The becm update equation 4.16b is no longer independent from the state update equation 4.16a.

Second, it is very unlikely that the noises e_k , \vec{r}_k of non-linear equations 4.11 be Gaussian, even more unlikely that, in the linearised equations 4.12, $\mathbf{M}_k e_k = e_k + \mathcal{E}_k s_k - \mathbf{E}_k s_k$, $\mathbf{N}_k \vec{r}_k = \vec{r}_k + \mathcal{H}_k s_k - \mathbf{H}_k s_k$ be Gaussian and independent. Thus, the estimator $s_{k+1}^b = \mathbf{E}_k s_k^a$ obtained from equation 4.16a to maximize the approximate posterior probability density, is suboptimal (does not minimize the expectable quadratic distance to the real state) and biased (does not coincide with the conditional mean). Similarly, \mathbf{P}_{k+1} obtained from equation 4.16b, cannot be regarded as the updated becm.

5. Background statistics in geosciences

Operational meteorology and oceanography extensively utilize numerical models to reproduce the dynamics of the real earth. Owing to the limited representativity, the state simulated must be regularly readjusted with observations. This readjustment is an inverse problem. The state is generally a space or space-time field of one or more parameters such as pressure, temperature, wind and moisture, current and salinity, pollutant concentration. The space state is in principle infinite-dimensional and a proper discretization requires more than hundred elements in each horizontal direction, more than ten in the vertical

direction. The discretized dimension of at least 10^5 is larger by several orders of magnitudes than the number of measurements available. The inverse problem of fitting a model is definitely underdetermined.

The Bayesian framework is most commonly utilized to combine the information from the model with the information from the observation. A comprehensive description of the theory may be found in (Fletcher, 2017). The Bayesian framework addresses the underdetermined inverse problem as a statistical compromise between a forecasted background state and the observations. The compromise is based on Baye's rule described in sections 4a-c. The pivotal point in Bayesian theory of inverse problems is the choice, considered a subjective matter of expert's opinion, of the background error statistics called the *Bayesian priors*. This choice is done, based on Gaussian assumption, in the form of a background error covariance matrix (becm) \mathbf{P} . This leads to a Tikhonov type cost-function with the consequences examined in section 3.

The objective or subjective nature of probabilities is a philosophical debate among statisticians. A detailed account is provided in the book of Lad (1996). The definition of a subjective probability density, conform to this debate, is found in the work of Tarantola (1987) that had a great influence in the development of data assimilation for geosciences: *By "subjective" is meant that it represents the knowledge of an individual, obtained using rigorous scientific (objective) methods, but that this knowledge may vary from individual to individual because each may possess different data sets.* Geoscientists are predisposed to welcome this subjective point of view: subjectivity is deeply rooted in our quasi-instinctive approach to the chaotic weather phenomena. The development of meteorology as a modern science in the 19th century is relatively recent. Even then and until now, as nicely explained by Daley (1991), a part of subjectivity has been preserved in the work of meteorological analysts to build synoptic charts and interpret the available observations.

The present section describes how subjective Bayesian inference has been implemented in geosciences, with theoretical and practical difficulties. The simplest adhoc elicitation of the Bayesian priors according to expert's opinion is still widely used. A more rigorous derivation, corresponding to Tarantola's requirement, is based on a sequential processing of earlier information using Kalman filter like techniques, namely 3DVar and 4DVar. In practice, owing to the enormous size of the becm, these techniques are always implemented in a very simplified form such as the ensemble Kalman filter.

For determining the Bayesian priors, i.e. \mathbf{P} , the question is now: how to formulate a sensible opinion in terms of a statistical law? The solution proposed by meteorologists and oceanologists is based on their particular need for data assimilation. This section describes the procedure associated with the claim that expert's opinion, in the form of a becm, may be derived from earlier measurements. It is important to stress, however, that this procedure remains purely theoretical because the practical computations are insurmountable. Adhoc assumptions (section 5b) or techniques (section 5d) are introduced to obtain the satisfactory results.

(a) *Difficulties with the elicitation of the background error covariance matrix*

The weakness with the Bayesian framework most discussed at least for the last two decades is the elicitation of the Bayesian statistical priors in the form of a becm, properly defined for finite-dimensional discretized problems. The main three difficulties are as follows (e.g. Bannister, 2008a):

- (i) The true state needed to measure background error is unknown.

- (ii) Only one error state is available between one true and one background states whereas a large population is needed to deduce statistics.
- (iii) Meteorological systems are continuous in nature, a reasonable discretization necessarily involves a huge number N of elements. The size of the becm, $N \times N$, is so enormous that it cannot even be stored on computing machines available currently.

Difficulties i and ii are fundamental. The algorithm 4.16 is the theoretical core of the techniques that have been proposed to overcome them (Bannister, 2008b) and compute the becm from earlier information when available. The algorithm encounters however the difficulty iii that is practical but yet insurmountable. In spite of considerable efforts made in defining appropriate numerical schemes, the reliable computation of the becm is still discussed and yet out of reach.

(b) *Adhoc choice of the background error covariance matrix*

The underlying assumption of the Bayesian theory is that the becm is a matter of expert's opinion based on scientific principles, past studies, earlier measurements i.e. any earlier information. It may happen that no earlier information is available in which case an adhoc choice must be made to form the becm. When earlier information is available, a procedure is described to construct the becm (section 5 f). However it is not computationally feasible so that, even in this case, becm is formed from adhoc simplifications. The simple and most common adhoc choice of a matrix diagonal or proportional to identity (e.g. Wu et al., 2008; Bocquet et al., 2011) amounts to ignore background error correlations. It is therefore strongly debated (e.g. Singh et al., 2011; Pinnington et al., 2016). Another common choice uses a correlation length from empirical expressions to account for the degree of correlation between the discrete elements of the model (Evensen, 2007, chap. 12). The parameters are adjusted in such a way that the results be satisfactory.

(c) *Derivation from earlier information: 3DVar and 4DVar*

Most often, in geosciences, the data to be analysed are part of a flow. The large amount of analogous data, often accumulated during years, is called a climatology. The recursive scheme 4.16 applies and provides a background error covariance matrix for present. The scheme is generally considered a tool for the expert to draw his opinion from the earlier information.

The situation at successive times t_k , $k = 0, 1, \dots$ is described by equations 4.11 or 4.12 defined in section 4f. When a time t_k comes to present, the following operations are done, respectively analysis and forecast:

- *analysis*: the state at t_k , forecasted as s_k^b , is improved as s_k^a by comparing, for the measurements in the interval $[t_{k-1}, t_k]$, the values expected $\mathcal{H}_k s_k^b$ and observed $\vec{\mu}_k$.
- *forecast*: the state s_k^a analysed at t_k is propagated along $[t_k, t_{k+1}]$ using the dynamical model to provide a forecast $s_{k+1}^b = \mathcal{E}_k s_k^a$ for the next step of assimilation.

Currently, this strategy is implemented with two main variants called 3DVar and 4Dvar.

In 3DVar, $s_k^b(\vec{x})$, $s_k^a(\vec{x})$ are functions of the geometric coordinates only: the state in the sense of the inverse problem corresponds to the state of the atmosphere at time t_k . The background state $s_k^b(\vec{x})$ at t_k is derived from $s_{k-1}^a(\vec{x})$ at t_{k-1} , used as initial condition and propagated till t_k by the dynamical model.

In 4DVar, $s_k^b(\vec{x}, t)$, $s_k^a(\vec{x}, t)$ are additionally functions of $t \in [t_{k-1}, t_k]$: the state in the sense of the inverse problem corresponds to the whole evolution or trajectory of the system in the assimilation window. The background state $s_k^b(\vec{x}, t)$ is forecasted for the whole window $[t_{k-1}, t_k]$ using the evolution model there with $s_{k-1}^a(\vec{x}, t_{k-1})$ as initial condition.

The 4DVar approach is deemed more accurate as it takes into account the dynamics of the system in the assimilation window. The larger computational cost of 4DVar is due to the minimization of the cost function in a state space including the time dimension.

The practical implementation of 3DVar and 4DVar raises difficulties. First, as already mentioned, the size of the becm is enormous. Second, in the covariance matrix \mathbf{R}_k of measurement errors, it is difficult to evaluate the part due to model representativity because of the problems already described in section 5a for the becm. As a matter of fact, Desroziers et al. (2005) evaluate \mathbf{R}_k coupled to \mathbf{P}_k . Third, 3DVar or 4DVar both require a dynamical model error covariance matrix \mathbf{Q}_k the evaluation of which is again bothered by the problems in section 5a. The common option of considering the dynamical model as perfect, i.e. $\mathbf{Q}_k = 0$, called *strong-constraint 3 or 4DVar*, is clearly not satisfactory (Howes et al. 2017). In this article, in order to focus on the difficulties with the becm, it is simply assumed that \mathbf{R}_k , \mathbf{Q}_k are given. The implementation of Kalman filter in operational weather prediction is possible only under strong simplifications. The most popular of such simplified implementations is the ensemble Kalman filter.

(d) *Ensemble Kalman filter : a simplified approach*

Ensemble Kalman filter is a popular technique of simplified approximate resolution of equations 4.16. This is a Monte Carlo technique, described e.g. by Evensen (2007). An ensemble of states $\{s_{01}^b, s_{02}^b, \dots, s_{0q}^b\}$ is taken as a sample from the initial probability distribution with becm \mathbf{P}_0 . By applying the first equation 4.16a state by state, it is transformed into an ensemble $\{s_{11}^b, s_{12}^b, \dots, s_{1q}^b\}$ from the posterior probability distribution with becm \mathbf{P}_1 .

More precisely at t_0 , once true observations $\vec{\mu}_0$ have been obtained, model measurements are computed as $\{\mathcal{H}_0 s_{01}^b + \vec{r}_{d01}, \mathcal{H}_0 s_{02}^b + \vec{r}_{d02}, \dots, \mathcal{H}_0 s_{0q}^b + \vec{r}_{d0q}\}$ in which \vec{r}_{d0i} , $i = 1, 2, \dots, q$, are independent draws from the known distribution of the instrumental error. The representativity error \vec{r}_{r0i} due to the measurement model is implicitly sampled in the computation of the $\mathcal{H}_0 s_{0i}^b$. Similarly, once the analysed states $\{s_{01}^a, s_{02}^a, \dots, s_{0q}^a\}$ have been computed, the forecast ensemble is deduced using the dynamical model, i.e. $s_{1i}^b = \mathcal{E}_0 s_{0i}^a$ which implicitly includes the errors due to the evolution model.

There is a problem however: numerical implementations eventually show *catastrophic filter divergence*. Geoscientists interpret this as a numerical artifact liable to correction procedures. They argue that the limited number of states leads to systematic errors in the becm: overestimation of the off-diagonal terms and underestimation of the diagonal ones. The off-diagonal overestimation (Anderson, 2001; Hamill et al., 2001) is equivalent to spurious correlations between distant regions. This is taken care of by a technique called *localization* reducing the extent of the adjoint functions away from the detectors. The diagonal underestimation (Whitaker and Hamill, 2002) is taken care of by a technique called *covariance inflation*, introduced by Anderson & Anderson (1999). Before assimilating new observations, the ensemble members are modified by increasing their deviation from ensemble mean with a given inflation factor (Li, 2009; Miyoshi 2011). The combination of localization and inflation allows to reach satisfactory results and this is interpreted as a

validation of the proposed divergence mechanism. These arguments will be examined in the companion article, part 2.

The conception of more robust numerical schemes is actively debated in the literature. Indirectly, this amounts to presume that the filter should theoretically not diverge. However, the kind of non-divergence that is expected is never made explicit. This situation is further explored in the next section 6 showing that tacit assumptions are associated with the use of earlier information described above (section 5c).

6. Underlying assumptions in the use of earlier information

The vagueness of the researchers using Bayesian approach in defining the expected non-divergence of Kalman filter is not surprising. The filter output (s_k^b, \mathbf{P}_k) for growing k is not characterized so much in terms of convergence than stability. The estimated state s_k^b is not expected to converge as it is distributed statistically around a true state s_k^{tr} ; in addition, this true state may vary depending on k . The becm \mathbf{P}_k is also not expected to converge; it may vary with k as it is sensitive to the variations of the dynamical and measurement models with weather conditions and detectors arrangement. In the non-linear case, the models additionally depend on the estimated state.

As detailed below, a careful reading of the literature suggests that the presumed non-divergence is composed of two distinct mathematical concepts: (i) the true convergence of \mathbf{P}_k to a limit with a statistically consistent evolution of the estimated state and, more subtly, (ii) the stability with respect to initial conditions.

(a) Convergence of background error statistics, ergodicity

The fact that a true convergence $\lim_{k \rightarrow \infty} \mathbf{P}_k = \mathbf{P}_\infty$ is expected may be deduced from the ergodic assumption usually associated with Kalman filter to determine the background error statistics. The assumption and its role are described e.g. by Bouttier & Courtier (1999): *In general, the only way to estimate statistics is to assume that they are stationary over a period of time and uniform over a domain so that one can take a number of error realizations and make empirical statistics.* These authors are dealing with difficulty i from section 5a, namely $s_k^b - s_k^{tr}$ is the only error state underlying in the k^{th} step of Kalman filter, insufficient to diagnose \mathbf{P}_k . As reminded in introduction of the present section 6, in principle the background statistics and \mathbf{P}_k are expected to vary depending on time and on the true state with its distribution in space. One may however assume that the background statistics are independent of the time and true state: this is the ergodic assumption with respect to both time and space. This assumption is reasonable in particular for the steady linear systems. It allows to consider all successive error states $s_k^b - s_k^{tr}$ are drawn from the same statistics with the almost same becm $\mathbf{P}_k \approx \mathbf{P}$ for all k . Visibly, Bouttier & Courtier and many authors after them suppose that the filter provides approximations of \mathbf{P} of increasing and converging quality thanks to the step-by-step accumulation of error states, all related to the same statistics. This conclusion contains another hidden presumption.

(b) Stability with respect to the initial conditions

Geoscientists tacitly presume that the filter is *stable with respect to the initial conditions*: if two filters, fed with the same sequence of measurements and models, are initiated with different inputs (s_0, \mathbf{P}_0) and (s'_0, \mathbf{P}'_0) , the filtering distributions converge to each other

i.e. $\lim_{k \rightarrow \infty} \mathbf{P}_k - \mathbf{P}'_k = 0$. This property is paid a lot more attention than convergence by the mathematicians studying Kalman filter. It means that the filter forgets the initial inputs and their subjectivity. If the filter would simply transfer the subjectivity of an initial \mathbf{P}_0 to present, it would not be worth the costly preprocessing of a climatology. The expert would rather provide his present opinion directly.

(c) *Dependence on earlier information*

In other words, the researchers using Bayesian approach in geosciences tacitly presume that after some time steps, the becm meets an objective reality depending only on the sequence of observations. The objective nature of the becm is accepted by various researchers (Bannister, 2008a; Waller et al., 2016). These authors all claim that the becm accounts for the earlier information and varies not or little with time.

The recursive scheme 4.16 is definitely considered an objective method to help expert's subjective opinion. Bannister (2008a) describes other strategies for measuring the becm based on earlier information, which is called the 'calibration step'. This becm is then input to scheme 4.16. So, the scheme and its presumed convergence are pivotal for meeting Tarantola's fundamental requirement (section 5). This is probably the reason why the *catastrophic filter divergence* is considered an artifact not undermining the theoretical importance for weather assimilation of Kalman filter in the form of 3DVar or 4DVar. In fact, Kelly et al (2015) have suggested that *catastrophic filter divergence* is a rigorous property of the filter regardless of any simplification. This is the point of view developed in the present work, based however on different arguments. First of all, it is useful to further examine the claim that becm is determined by earlier information.

(d) *Relevance of the earlier information: ergodicity*

As already explained, the complete filter equations are unpracticable (section 5a). So, after a theoretical reference to the filtering of earlier observations, an adhoc becm is commonly chosen as a substitute for the resolution. The justifications never refer to the measurements to be effectively analysed (section 5b), in particular the number and location of the sensors. However, these elements are essential.

If the becm \mathbf{P} is deduced without direct reference to the present measurements, these can always be so chosen that the estimated correction $s^a - s^b$ be arbitrarily irregular. To see this, let h_1, h_2, \dots, h_n be a family of n independent states in the form of column vectors in order to compose the measurement matrix according to equation 3.2. The correction (eq. 4.7) is a linear combination of $\mathbf{P}h_1, \mathbf{P}h_2, \dots, \mathbf{P}h_n$. Since \mathbf{P} is invertible, the h_i 's may be so chosen that the $\mathbf{P}h_i$'s are arbitrarily irregular.

Notice that an adhoc choice of \mathbf{P} proportional to identity (section 5b) is not reasonable. Most often, the sensors are extremely small compared to the atmospheric or oceanic domain. At the location \vec{x}_i of the i^{th} sensor, $h_i(\vec{x}_i)$ becomes singular, which in discretized practice means very peaked, and this behaviour would be passed to the correction.

The claim that \mathbf{P} is deduced from earlier information is too general and misleading. It forgets the ergodicity requirement. Bouttier & Courtier (1999) (cf. paragraph 6a) remind that the becm accounts for the earlier information provided that, based on ergodicity, the earlier information accounts for the present situation.

(e) Consequence for Kalman filter

Under the ergodic assumption, the evolution, measurement and covariance error matrices are repeated same at each step. Assume \mathbf{P} is obtained as the converged becm of scheme 4.16, i.e.:

$$\mathbf{P} = \mathbf{E}(\mathbf{P}^{-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H})^{-1} \mathbf{E}^T + \mathbf{Q} \quad (6.1)$$

According to this Riccati equation, \mathbf{P} does depend on the evolution and measurement operators. To see the importance of the measurement operator with matrix \mathbf{H} , suppose the measurement errors are arbitrarily large. Equation 6.1 tendentially becomes:

$$\mathbf{P} = \mathbf{E} \mathbf{P} \mathbf{E}^T + \mathbf{Q} \quad (6.2)$$

As far as geophysical systems are concerned, this Lyapunov equation has no solution. Indeed, the matrix \mathbf{Q} is positive definite since otherwise, \mathbf{E} would be perfect in predicting the evolution of some state. Then, by the discrete-time lemma of Lyapunov (Anderson & Moore, 1979, theorem 2.1), a positive solution of equation 6.2 exists if and only if all N eigenvalues of \mathbf{E} satisfy: $|\lambda_i(\mathbf{E})| < 1$ and this solution is $\mathbf{P} = \sum_{k=0}^{\infty} \mathbf{E}^k \mathbf{Q} (\mathbf{E}^T)^k$. This is not acceptable in geosciences: for large times t_k , \mathbf{E}^k would be a strict contraction finally evolving all states to 0.

This result simply means that, when measurement errors become too large, background errors grow indefinitely just as if there were no measurement at all. It also means that, in equation 6.1, the term $\mathbf{H}^T \mathbf{R}^{-1} \mathbf{H}$ plays an essential role in the possible existence of a solution \mathbf{P} . Such solution, if it exists, is accordingly expected to be tightly related to the detailed arrangement of the sensors. A becm valid for a monitoring network may not be valid for another network or other conditions. This conclusion is not new. In their text, Bouttier & Courtier (1999) wrote, just before the extract quoted in section 6a: *The error statistics (biases and covariances) are functions of the physical processes governing the meteorological situation and the observing network.*

The tight requirement of ergodicity in Kalman filter, with elements \mathbf{E}_k , \mathbf{M}_k , \mathbf{H}_k , \mathbf{N}_k same for all k , is not consistent with practice. In reality, weather conditions vary, a sensor is moved to another location, another sensor is temporarily out of order. The evaluation of a converged becm is not practicable.

7. Conclusions

In recent meteorological developments, the data assimilation methods (3DVar, 4DVar, Ensemble Kalman Filter) have been evolved to successfully improve the model predictions and estimate the true state of atmosphere. These methods of solving an underdetermined inverse problem are embedded within a theoretical framework of Bayesian theory. The observations are utilized to update the knowledge of the state of a system by compromising between the errors contained in these observations and the errors contained in a background state usually forecasted by a model. The present study discusses the important issue of the Bayesian priors in the form of a background error covariance matrix (becm).

The Bayesian cost function has the same structure as a Tikhonov cost function. The background term stands for the Tikhonov regularizing term. The comparison is subjected to remarks. Tikhonov regularization has been developed to minimize the numerical instabilities arising from the overdeterminacy of an inverse problem. On the contrary, the geophysical inverse problems are strongly underdetermined and this changes totally the role of

the regularizing term. The unsatisfactory features in the estimated state are not produced by numerical instabilities. They depend on the regularizing term, i.e. the becm, because choosing the becm secretly amounts to choosing a basis of functions for estimation.

Since the work of Tarantola, the elicitation of background statistics has been ambiguously hesitating between subjective choice and objective deduction. The objective existence of the becm is advocated by an analogy with the Kalman filter to obtain it from an earlier information. This is associated with the ergodic assumption that background statistics do not vary in time and are homogeneously distributed through space. Ergodicity implies that successive background errors are all drawn from the same statistics so that the filter will provide a converged becm. The argument is purely theoretical because in practice, the enormous system of equations must be simplified and *catastrophic filter divergence* occurs eventually. Geoscientists generally consider that divergence is caused by the simplifications which amounts to presuming that the non-simplified filter should converge.

Here it is shown that the classical definition of a becm and its link with earlier information are poorly practicable. The becm is tightly related to the environmental conditions and arrangement of the observing network. Thus, for obtaining a converged becm, these conditions and arrangement should not vary during many filter iterations, which is not realistic. This may account for filter divergence regardless of any simplification. In addition, still owing to the tight dependence on sensor arrangement, the background errors cannot be homogeneously distributed as is commonly assumed. It is just said here that the link between becm and earlier information is poorly practicable, not that it is ill-founded to support the definition of a becm. This link will be further questioned in the companion article, part 2, with a more theoretical examination of the tacit assumption that the non simplified filter should provide a converged becm.

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A. Singular value decomposition

In order to introduce the singular value decomposition of the measurement operator $\mathcal{H} : \mathcal{S} \rightarrow \mathbb{R}^n$, the state space $\mathcal{S} = \mathbb{R}^N$ is assumed of finite dimension N . The present section is derived from a work by Hansen (1992, 2001). The framework of Hansen is a bit different

from that in the present study as (i) he considers a scalar product in \mathcal{S} possibly degenerate with a matrix \mathbf{L} of rank less than N , (ii) he does not introduce a matrix \mathbf{G} as he utilizes in the measurement space the usual l^2 product with identity matrix, (iii) most importantly, he deals with overdetermined problems only. The discussion in this appendix is valid for both overdetermined and underdetermined inverse problems.

Notice that the operator \mathcal{H} , operating on the state s , can be seen as a $N \times n$ matrix and as such, it may as well operate from the left hand side on n -dimensional measurement vectors. A decomposition into left and right singular vectors is introduced accordingly with reference to the scalar products used in \mathbb{R}^n with matrix \mathbf{G} and in \mathbb{R}^N with matrix \mathbf{L} . Let r denote the rank of \mathcal{H} . The singular value decomposition consists of:

- right singular vectors s_1, s_2, \dots, s_r in \mathcal{S} , with norm $s_i^\top \mathbf{L} s_i = 1$, called the *modes*
- left singular vectors $\vec{m}_1, \vec{m}_2, \dots, \vec{m}_r$ in \mathbb{R}^n , with norm $\vec{m}_i^\top \mathbf{G} \vec{m}_i = 1$
- singular values $\sigma_i = \vec{m}_i^\top \mathbf{G} \mathcal{H} s_i$
 - $\sigma_1 = \vec{m}_1^\top \mathbf{G} \mathcal{H} s_1$ maximizes $\vec{m}^\top \mathbf{G} \mathcal{H} s$ among all \vec{m}, s of norms $\vec{m}^\top \mathbf{G} \vec{m} = 1, s^\top \mathbf{L} s = 1$
 - $\sigma_i = \vec{m}_i^\top \mathbf{G} \mathcal{H} s_i$ maximizes $\vec{m}^\top \mathbf{G} \mathcal{H} s$ among all \vec{m}, s of norms $\vec{m}^\top \mathbf{G} \vec{m} = 1, s^\top \mathbf{L} s = 1$ so that $\vec{m}^\top \mathbf{G} \vec{m}_j = 0, s^\top \mathbf{L} s_j = 1, j = 1, 2, \dots, i-1$

As a result of this definition, the singular vectors are orthonormal, $s_i^\top \mathbf{L} s_j = \vec{m}_i^\top \mathbf{G} \vec{m}_j = \delta_{ij}$ and the singular values are non-negative in decreasing order: $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r \geq 0$.

The expression 3.5 for s_λ minimizing \mathcal{J}_λ for given measurements $\vec{\mu}$ is seen by first showing $\mathcal{H} s_i = \sigma_i \vec{m}_i$, then deducing $\partial \mathcal{J}_\lambda(s_\lambda) = 0$ which is sufficient since \mathcal{J}_λ is strictly convex for $\lambda > 0$. The same reasoning holds for s_0 in the overdetermined case as \mathcal{J}_0 is again strictly convex. In the underdetermined case, $\partial \mathcal{J}_0(s_0) = 0$ still holds, but the convexity is not strict and \mathcal{J}_0 has infinitely many minima equivalent to s_0 .

B. Adjoint measurement operator

The notations are same as in section 3. However, in order to better show the generality of the results, the finite dimension is not supposed for \mathcal{S} . The regularizing scalar product accordingly remains with the notation $(s, \mathcal{L} s')$. The measurement operator $\mathcal{H} : \mathcal{S} \rightarrow \mathbb{R}^n$ is supposed linear and continuous for this scalar product.

Definition B.1. : *There exists a linear operator $\mathcal{H}_\mathcal{L}^* : \mathbb{R}^n \rightarrow \mathcal{S}$ called adjoint to \mathcal{H} such that*

$$\forall \vec{\alpha} \in \mathbb{R}^n, \forall s \in \mathcal{S}, \quad \vec{\alpha}^\top \mathcal{H}(s) = (\mathcal{H}_\mathcal{L}^* \vec{\alpha}, \mathcal{L} s) \quad (\text{B.1})$$

For a sake of symmetry between the scalar products with matrix \mathbf{G} in \mathbb{R}^n and operator \mathcal{L} in \mathcal{S} , the adjoint operator might be defined as $\mathcal{H}_{\mathbf{G}\mathcal{L}}^*$ such that $\vec{\alpha}^\top \mathbf{G} \mathcal{H}(s) = (\mathcal{H}_{\mathbf{G}\mathcal{L}}^* \vec{\alpha}, \mathcal{L} s)$. The later developments would not be changed much. In fact, the symmetry is not relevant because both \mathbf{G} and \mathcal{L} describe deviations of the terms in the cost functions \mathcal{J} (equation 2.3) or \mathcal{J}_λ (equation 3.1) from standard products and \mathcal{S} respectively. The definition B.1 of the adjoint operator referred to the standard product in \mathbb{R}^n highlights (equation 3.7) the independence of the estimation space $\text{Range} \mathcal{H}_\mathcal{L}^*$ from \mathbf{G} .

Proof : Since \mathcal{H} is continuous, the linear form $f_{\vec{\alpha}} : s \rightarrow \vec{\alpha}^\top \mathcal{H} s$ is continuous for any

$\vec{\alpha} \in \mathbb{R}^n$. Riesz representation theorem then ensures the existence of $\mathcal{H}_{\mathcal{L}}^* \vec{\alpha} \in \mathcal{S}$ such that $f_{\vec{\alpha}} = (\mathcal{H}_{\mathcal{L}}^* \vec{\alpha}, \mathcal{L} \cdot)$. The linearity is obvious. □

Obviously, $\mathcal{H}_{\mathcal{L}}^*$ has same rank as \mathcal{H} . This rank is N in the overdetermined case. In the underdetermined case, the rank of \mathcal{H} is at most n and exactly n if the measurements are not redundant.

The following expressions are deduced for s_0 and s_λ minimizing the least square and regularized cost functions respectively. The circle \circ denotes the composition:

$$s_0 = \mathcal{H}_{\mathcal{L}}^* \circ (\mathcal{H} \circ \mathcal{H}_{\mathcal{L}}^*)^{-1} \vec{\mu}, \quad s_\lambda = \mathcal{H}_{\mathcal{L}}^* \circ (\mathcal{H} \circ \mathcal{H}_{\mathcal{L}}^* + \lambda^2 \mathbf{G}^{-1})^{-1} \vec{\mu} \quad (\text{B.2})$$

The expression for s_0 is valid only in the non-redundant underdetermined case since only then $\mathcal{H} \circ \mathcal{H}_{\mathcal{L}}^*$ is invertible. In this case, however, the minimum of \mathcal{J} (equation 2.3) is not unique: s_0 given by equation B.2 is just a particular minimum, the only one in $\text{Range } \mathcal{H}_{\mathcal{L}}^*$. The continuity with the expression for s_λ will imply that this s_0 coincides with that described by equation 3.5.

Proof: Let's first show that, in the non-redundant underdetermined case, $\mathcal{H} \circ \mathcal{H}_{\mathcal{L}}^* : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is invertible. Indeed, $\mathcal{H} \circ \mathcal{H}_{\mathcal{L}}^* \vec{\alpha}$ may not vanish if $\vec{\alpha} \neq \vec{0}$ because, in view of equation B.1, $\vec{\alpha}^T \mathcal{H} \circ \mathcal{H}_{\mathcal{L}}^* \vec{\alpha} = (\mathcal{H}_{\mathcal{L}}^* \vec{\alpha}, \mathcal{L} \mathcal{H}_{\mathcal{L}}^* \vec{\alpha})$. Since $\mathcal{H}_{\mathcal{L}}^*$ has rank n , $\mathcal{H}_{\mathcal{L}}^* \vec{\alpha}$ may not vanish implying $(\mathcal{H}_{\mathcal{L}}^* \vec{\alpha}, \mathcal{L} \mathcal{H}_{\mathcal{L}}^* \vec{\alpha}) > 0$.

Thus, on the one hand, $\mathcal{H}_{\mathcal{L}}^* \circ (\mathcal{H} \circ \mathcal{H}_{\mathcal{L}}^*)^{-1} \vec{\mu}$ is well defined in $\text{Range } \mathcal{H}_{\mathcal{L}}^*$ and $\mathcal{H} \circ \mathcal{H}_{\mathcal{L}}^* \circ (\mathcal{H} \circ \mathcal{H}_{\mathcal{L}}^*)^{-1} \vec{\mu} = \vec{\mu}$. On the other hand, the solution to the inverse problem $\mathcal{H} s_0 = \vec{\mu}$ is unique in $\text{Range } \mathcal{H}_{\mathcal{L}}^*$. This implies the first identity B.2.

The expression for s_λ is valid for both the overdetermined and underdetermined cases. Indeed, $\mathcal{H} \circ \mathcal{H}_{\mathcal{L}}^* + \lambda^2 \mathbf{G}^{-1}$ is always invertible because (i) as deduced from the first part of the proof, $\mathcal{H} \circ \mathcal{H}_{\mathcal{L}}^*$ is non-negative and (ii) \mathbf{G} is positive definite and so is \mathbf{G}^{-1} . The differential of the cost function is: $\partial \mathcal{J}_\lambda(s) \cdot s' = 2\lambda^2 (s, \mathcal{L} s') + 2(\mathcal{H} s)^T \mathbf{G} s' - 2\vec{\mu}^T \mathbf{G} s'$. Substituting s_λ from equation B.2 for s and using equation B.1, one gets after elementary transformations: $\partial \mathcal{J}_\lambda(s_\lambda) \cdot s' = 0$ for all $s' \in \mathcal{S}$. Since \mathcal{J}_λ is obviously a strictly convex function, this characterizes s_λ . □