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On Instabilities in Data Assimilation Algorithms

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Abstract. Data assimilation algorithms are a crucial part of operational systems in numerical weather prediction, hydrology and climate science, but are also important for dynamical reconstruction in medical applications and quality control for manufactoring processes. Usually, a variety of diverse measurement data are employed to determine the state of the atmosphere or to a wider system including land and oceans. Modern data assimilation systems use more and more remote sensing data, in particular radiances measured by satellites, radar data and integrated water vapor measurements via GPS/GNSS signals. The inversion of some of these measurements are ill-posed in the classical sense, i.e. the inverse of the operator H which maps the state onto the data is unbounded. In this case, the use of such data can lead to significant instabilities of data assimilation algorithms.

The goal of this work is to provide a rigorous mathematical analysis of the instability of well-known data assimilation methods. Here, we will restrict our attention to particular linear systems, in which the instability can be explicitly analyzed. We investigate the three-dimensional variational assimilation and four-dimensional variational assimilation. A theory for the instability is developed using the classical theory of ill-posed problems in a Banach space framework. Further, we demonstrate by numerical examples that instabilities can and will occur, including an example from dynamic magnetic tomography.

1. Introduction

Data assimilation algorithms in combination with the reconstruction of quantities from remote sensing data are important in many areas like *numerical weather prediction* [War11], *oceanic and hydrologic applications* [PX09] as well as *process tomography* (for example using *magnetic tomography* [KKP02], [HKP05], [HPWS05], [HP07], [HPW08], [PW09], [Wan09]) and in cognitive neuroscience [PbG09].

Today, there is a variety of algorithms for data assimilation. There are classical variational approaches (compare [LLD06], [LSK10]) known as three-dimensional variational assimilation (3dVar) and four-dimensional variational assimilation (4dVar). Many data assimilation schemes can be considered as special cases of statistical inversion methods [Jaz70], [KS04], i.e. Bayesian estimation for the case of linear systems [RL00].

In the case of Gaussian errors and Gaussian background distributions for linear systems Bayes' formula leads to the well known *Kalman Filter* [Kal60].

Here, we study data assimilation algorithms as *iterative* or *cycled* schemes. Our viewpoint is driven by the field of inverse problems, which rather than focusing on stochastical properties of the fields under consideration, has placed strong emphasis on the analysis of the ill-posedness of the reconstruction problem.

In fact, using remote sensing data we will find severe instabilities of these algorithms. The origin of this instable behavior may either be due to the nonlinear or chaotic systems dynamics as for examle presented in [CGTU08] or because of the ill-posedness of the observation operator H. The second cause of instability is our key concern in this work.

To provide a thorough analysis we investigate a *dynamic (or cycled) Tikhonov regularization* scheme (compare also [Mar11]), which is a Tikhonov regularization with a dynamic background which is updated by propagating the analysis of the previous step to the next point in time where data are provided. We use the Hilbert spaces X, Y and the discrete time-slices

$$t_0 < t_1 < t_2 < ... < t_k < \dots \tag{1.1}$$

where we consider the system states $x_k \in X$ at time t_k and the corresponding data $y_k \in Y$. They are given via the measurement operator $H : X \to Y$ by

$$y_k = y_k^{(true)} + y^{(\delta)} = Hx_k^{(true)} + y^{(\delta)}, \quad k \in \mathbb{N} \tag{1.2}$$

Let our measurement operator H be *compact* and linear and X be of *infinite dimension*. Then, H cannot have a bounded inverse H^{-1} (c.f. [Kre99 analysis. These systems serve as key examples to prepare the investigation of more complex nonlinear systems. In particular, we will study a constant system and spectrally

b) *Spectrally diagonal systems*, i.e. systems for which the dynamics is given by

$$M_{k+1|k} = U^{-1} D U \tag{2.1}$$

with some orthonormal transformation $U : X \to X$ and a diagonal mapping D. We call a mapping diagonal in an infinite dimensional space, when there is some orthonormal system $\{\varphi_n : n \in \mathbb{N}\}$ such that

$$D\varphi_n = d_n \varphi_n, \quad n \in \mathbb{N}. \tag{2.2}$$

c) *Spectrally expanding systems.* In the case where all d_n satisfy

$$|d_n| \geq q > 1, \quad n \in \mathbb{N}, \tag{2.3}$$

with some constant q we call the system *expanding*.

d) *Spectrally collapsing systems.* These are systems with a representation of type (2.1), (2.2) for which

$$|d_n| \leq q < 1, \quad n \in \mathbb{N} \tag{2.4}$$

with some constant q is satisfied.

We will also be interested in systems for which the columns of U are the singular vectors of the measurement operator H, i.e. $H^* H \varphi_n = \mu_n^2 \varphi_n$ for $n \in \mathbb{N}$. In this case, the complete dynamics of the data assimilation system can be diagonalized by the singular vectors of H.

2.2. Cycled Regularization

Tikhonov regularization is a well-known scheme to solve an ill-posed operator equation of the type $Hx = y$ by minimization of the cost functional

$$J(x) = ||Hx - y||^2 + \alpha ||x||^2. \tag{2.5}$$

To solve such a data equation on successive points in time t_k, we employ a modified regularization term using the b7N1 a;a mo Td [3.662 Td [(Ti18(singular)]Ti18(singular)]Ti18(sin6 Td [(2)]

with

$$R_\alpha = (\alpha I + H^* H)^{-1} H^* . \tag{2.9}$$

starting from some initial state $x_0^{(a)}$. The parameter $\alpha > 0$ is denoted as regularization parameter (compare [CK97] Theorem 4.14). We call (2.8) together with (2.6) the *cycled Tikhonov regularization*.

2.3. Three-dimensional Variational Assimilation (3dVar).

Three-dimensional variational data assimilation (3dVar) is basically a cycled Tikhonov scheme with weighted norms. For this section let us restrict our arguments to the n-dimensional case where $X = \mathbb{R}^n$ with some $n \in \mathbb{N}$ and $Y = \mathbb{R}^m$, $m \in \mathbb{N}$. For some symmetric positive definite matrix W we define the *weighted scalar product*

$$\langle \varphi, \psi \rangle_W := \langle \varphi, W\psi \rangle, \tag{2.10}$$

where $\langle \cdot, \cdot \rangle$ denotes the standard L^2 scalar product in $\mathbb{R}^n$. Given a linear operator $H : X \to Y$, we denote the adjoint operator with respect to the standard scalar products by H' and the adjoint with respect to the weighted scalar products by H^*.

Let B be the covariance matrix for the background system and R the covariance matrix for the measurements. Then the cost function for the *cycled 3dVar* scheme (compare [LLD06] Chapter 20) is given by

$$J_{3dVar}($$

with y_j 2 Y. Then we can write (2.20) as

$$J_{4dVar}(x) := jjx \quad x_0 jj^2_{B \ 1} + jjy \quad Hxjj^2_{R \ 1}; \tag{2.26}$$

which corresponds to (2.11) for one iteration step. Thus, 4dVar for linear systems can be written as a 3dVar algorithm and in a second step as a cycled Tikhonov regularization, such that results for cycled Tikhonov regularization apply both 3dVar and 4dVar.

3. Instability of Variational Data Assimilation

The goal of this section is to carry out the stability analysis for cycled variational assimilation algorithms with ill-posed observation operators, in particular for a cycled Tikhonov regularization (which according to the above arguments then also hold for 3dVar and 4dVar). We will show that all cycled assimilation schemes can exhibit strong instabilities when remote sensing operators are involved.

3.1. Cycled Tikhonov Regularization

We have shown that for linear models choosing appropriate norms the cycled 3dVar or 4dVar can be written as a cycled Tikhonov regularization. Thus, without loss of generality, we can restrict our attention to the update formula (2.8). We denote the true system by $x_k^{(true)}$ with true data $y_k^{(true)} = Hx_k^{(true)}$. The real measured data is assumed to be of the form

$$y_k = Hx_k^{(true)} + y_k^{(\ )}; \quad k \ 2 \ \mathbb{N}: \tag{3.1}$$

Further, for simplicity we study a un8mf f 11.5599(f 11.5599(f 11.5599(f 11.5599(:=0l.26 Td [(3.1.cu5996.11

Theorem 3.2 *Assume that $H : X \to Y$ is a compact injective operator from a Hilbert space X into a Hilbert space Y. Then we have the* pointwise convergence

$$\left(I + \alpha^{-1} H^* H\right)^{-k} \varphi \to 0, \quad k \to \infty \tag{3.12}$$

for every fixed element $\varphi \in X$.

Proof. To show the convergence (3.12) we use $\alpha = 1$ to keep things readable, the general case is carried out analogously. We have

$$\begin{aligned} \left\langle (I + H^* H)\psi, (I + H^* H)\psi \right\rangle &= \|\psi\|^2 + 2\|H\psi\|^2 + \|H^* H\psi\|^2 \\ &> \|\psi\|^2 \end{aligned} \tag{3.13}$$

if $H\psi \neq 0$. If we use $\psi = (I + H^* H)^{-1}\varphi$, we estimate

$$\|(I + H^* H)^{-1}\varphi\| < \|\varphi\|. \tag{3.14}$$

This observation can be generalized. We calculate

$$\left\langle (I + H^* H)^k \psi, (I + H^* H)^k \psi \right\rangle = \|\psi\|^2 + 2k\|H\psi\|^2 + U_k \tag{3.15}$$

with some terms U_k for which we show later that they are positive or zero. As a consequence we obtain

$$\|(I + H^* H)^{-k}\varphi\|^2 + 2k\|H(I + H^* H)^{-k}\varphi\|^2 < \|\varphi\|^2. \tag{3.16}$$

Now, we know that $\psi_k := (I + H^* H)^{-k}\varphi$ is bounded in X. Assume that it is not convergent towards zero. Then there is a weakly convergent subsequence $(\psi_{k_j})_{j \in \mathbb{N}}$, which tends weakly towards $\psi \in X$, $\psi \neq 0$. But now $H\psi_{k_j} \to H\psi$ in X. From (3.16) we then obtain $H\psi = 0$ and thus $\psi = 0$, which is a contradiction to our assumption and shows that (3.12) must be satisfied.

Finally, we need to show that the terms U_k are positive. We use the binomial formula to calculate

$$\begin{aligned} &\left\langle (I + H^* H)^k \psi, (I + H^* H)^k \psi \right\rangle \\ &= \left\langle \sum_{\xi=0}^{k} \binom{k}{\xi} (H^* H)^{\xi} \psi, \sum_{\eta=0}^{k} \binom{k}{\eta} (H^* H)^{\eta} \psi \right\rangle \\ &= \sum_{\xi=0}^{k} \sum_{\eta=0}^{k} \binom{k}{\xi} \binom{k}{\eta} \left\langle (H^* H)^{\xi} \psi, (H^* H)^{\eta} \psi \right\rangle. \end{aligned} \tag{3.17}$$

Each scalar product in (3.17) can be seen to be positive by transforming them into terms of the form

$$\left\langle (H^* H)^l \psi, (H^* H)^l \psi \right\rangle = \|(H^* H)^l \psi\|^2 \tag{3.18}$$

with $l = (\xi + \eta)/2$ for $\xi + \eta$ even or

$$\left\langle (H^* H)^{l+1} \psi, (H^* H)^l \psi \right\rangle = \|H(H^* H)^l \psi\|^2 \tag{3.19}$$

with $l = (\xi + \eta - 1)/2$ for $\xi + \eta$ odd, and the proof is complete.

For H injective we have shown the pointwise convergence $^k e_0 \to 0$ for $k \to \infty$ for any $e_0 \in X$. To fully study the behaviour of e_k we further need to calculate the second term in (3.6) or (3.7), respectively. We need to investigate

$$(I \quad)^{-1} S = (R \ H)^{-1} R \ y^{(\ )}. \tag{3.20}$$

Under the condition that $H \ H$ is invertible, we calculate

$$\begin{aligned} (R \ H)^{-1} R &= \left((\ I + H \ H)^{-1} H \ H \right)^{-1} (\ I + H \ H)^{-1} H \\ &= (H \ H)^{-1} H \ , \end{aligned} \tag{3.21}$$

which is the Moore-Penrose pseudo inverse. Since H and H are compact, in general invertibility is not given, but we obtain invertibility of $R \ H$ on the subspace

$$Z := (\ I + H \ H)^{-1} H \ H(X) \quad Y.$$

We capture the phenomena in the following lemma.

Lemma 3.3 *Assume that H and H are injective. If $y^{(\ )} \in H(X)$, i.e. there is $x^{(\ )} \in X$ such that $y^{(\ )} = Hx^{(\ )}$, then with $S = R \ y^{(\ )}$ we obtain*

$$\sum_{=0}^{k-1} \quad S \to x^{(\ )}, \quad k \to \infty. \tag{3.22}$$

In the case where $y^{(\ )} \notin H(X)$, we have

$$\left\| \sum_{=0}^{k-1} \quad S \right\| \to \infty, \quad k \to \infty. \tag{3.23}$$

Proof. In the case $y^{(\ )} \in H(X)$ we have

weandrethvy3TdI [[)(o)9]TJ/F22 7.971 Tf 10.045 1.64 T6 [(k)]TJ/F25 convergent sequence into a strongly convergent sequence, i.e. $H_{k_j} \to H$. We further have the convergence

$$
\begin{aligned}
(R\ H)\sum_{=0}^{k_j-1} S &= (I\ )\sum_{=0}^{k_j-1} S \\
&= (I\ ^{k_j})S \\
&\to R\,y^{(\,)}, \quad j \to \infty.
\end{aligned}
\tag{3.27}
$$

and

$$
\begin{aligned}
(R\ H)\sum_{=0}^{k_j-1} S &= R\ H_{k_j} \\
&\to R\ H\ , \quad j \to \infty.
\end{aligned}
\tag{3.28}
$$

Since R is boundedly invertible, from (3.27) and (3.28) we obtain the identity $H\ = y^{(\,)}$, i.e. $y^{(\,)}$ is in the images space $H(X)$. This shows that under the condition $y^{(\,)} \notin H(X)$ the sequence $(\ _k)_{k \in \mathbb{N}}$ cannot be uniformly bounded and the proof is complete.

Finally, we summarize our results and apply them to variational data assimilation schemes as a corollary.

Corollary 3.4 (Instability of Assimilation Schemes) *The cycled Tikhonov regularization and thus also the data assimilation schemes 3dVar and 4dVar for a constant model M*

with coefficients $a_{n,k}$. The coefficients of the data vectors y_k at time t_k are defined by

$$y_k = \sum_{n=0}^{\infty} b_{n,k} g_n, \qquad k = 1, 2, \ldots \tag{3.32}$$

According to (3.29) an application of the operators H or H

for $n_0 \to \infty$. Given $\, > 0$ we first choose n_0 such that $\sum_{n=n_0+1}^{\infty} \; {}_n \varphi_n$ is smaller than $=2$ in norm. Then, we choose $k_0 > 0$ such that

$$\sum_{n=1}^{n_0} \quad 1 + \frac{1}{\;} \, {}_n^2 \quad {}^k \quad {}_n \, {}^2 < \frac{\;}{2} \tag{3.47}$$

for $k \quad k_0$. This yields

$$I + \quad {}^1 H \; H \quad {}^k \varphi \quad {}^2 \qquad ; \tag{3.48}$$

thus (3.38) is satisfied for $k \to \infty$. To show (3.39) we employ the trivial identity $I = (I + \quad {}^1 H \; H) \qquad {}^1 H \; H$ to calculate

$$\begin{aligned}
(I + \quad {}^1 H \; H) \; {}^1 \varphi &= (I + \quad {}^1 H \; H) \; {}^1 \quad (I + \quad {}^1 H \; H) \qquad {}^1 H \; H \quad \varphi \\
&= \varphi \quad (I + \quad {}^1 H \; H) \; {}^1 \quad {}^1 H \; H \varphi \\
&= \varphi
\end{aligned} \tag{3.49}$$

for $\varphi \in N(H \; H$

Lemma 3.9 *Let $a, b \in \mathbb{R}$, then we have*

$$|a \quad b|^2 \qquad \frac{|a|^2}{2} \qquad |b|^2 \tag{3.53}$$

Proof.

3.3. Instability for spectrally expanding or collapsing systems

Finally, we will study the behaviour of the error of data assimilation algorithms with a compact observation operator in the case of spectrally expanding or collapsing systems as introduced in (2.1). We start with the spectral update formula (3.35) and use the dynamics introduced in (2.2)

$$a^{(b)}_{n;k+1} = d_n a^{(a)}_{n;k}, \quad k = 0, 1, 2, \dots \tag{3.60}$$

which is spectrally diagonal with respect to the singular system of the observation operator H. In this case the coefficients show an exponential behaviour

$$a^{(true)}_{n;k} = d_n^k a^{(true)}_{n;0}, \quad k = 1, 2, 3, \dots. \tag{3.61}$$

Then, the assimilation (3.35) with data $y_k = Hx_k^{(true)} + y_k^{(\ )}$, $k = 1, 2, 3, \dots$, leads to the update formula

$$a^{(a)}_{n;k+1} = q_n d_n a^{(a)}_{n;k} + (1 - q_n) a^{(true)}_{n;k+1} + (1 - q_n) \frac{b^{(\ )}_{n;k+1}}{\ _n}. \tag{3.62}$$

Note that the true solution is dynamical as well and we need to build this dynamics into our induction formula to study the dynamical evolution of the analysis and the errors.

One key question is how the data error evolves. Here, we assume that the measurements are remote sensing data which are independent of the system

$$= q_n^{k+1} d_n^{k+1} a_{n;0} + (1 \quad q_n^{k+1}) d_n^{k+1} a_{n;0}^{(true)} + \sum_{=0}^{k} q_n d_n \; (1 \quad q_n) \frac{b_n^{(\ )}}{\ _n};$$

which is the desired formula with k replaced by $k+1$. Finally, (3.65) is obtained by standard geometric series, and the proof is complete.

1) The Convergence Case. We can now investigate the asymptotic behavior, where two main situations arise. We have convergent terms in (3.65) if the condition

$$|d_n q_n| = \frac{d_n}{\ + \ _n^2} < 1 \tag{3.66}$$

is satisfied. The condition (3.66) can be rewritten as

$$|d_n| < 1 + \frac{\ _n^2}{\ }; \quad n \in \mathbb{N}. \tag{3.67}$$

The spectral expansion coefficient d

$y = Hx^{(true)} + y^{( )} \in H(X)$ … in Lemma 3.10 that in this … have

$$||x_k^{(a)}|| \to \infty, \quad \ldots \tag{4.1}$$

Further, from (3.37) we deduce that the sp… cient of the analysis … exponentially convergent towards

$$\frac{b_n^{( )}}{\;_n}; \quad n \in \mathbb{N}. \tag{4.2}$$

The spee… onvergence is proportional to

$$\frac{\ldots}{\ldots + \;_n^2}; \quad n \in \mathbb{N}; \tag{4.3}$$

i.e. it is depe… particular mode … 0 for $n \to \infty$ the … is quick for sma… arger.

Figure 3 shows the relative reconstruction error. We see that the error decreases until it reaches a minmum after 11 steps. After that point the sum of the error according to (3.57) takes over and the full system behaves as seen in (3.59). This confirms the evolution given by Lemma 3.10 for a practically relevant example.

5. Summary

We have investigated the instability which can occur when measurements are assimilated into a dynamical system evolution which are linked to the system state φ in an infinite dimensional state space X by a compact measurement operator H. For simple systems we have shown that cycling of standard data assimilation schemes can lead to severe instabilities of the analysis, i.e. small measurement errors accumulate over time and can lead to large analysis errors. We have worked out explicit spectral formulas which show the instable behaviour. Further, numerical results in simple cases and from dynamical magnetic tomography confirm the results. These results are interesting also in seismology and earth sciences.

The systems investigated in this work can be seen as a simple model if the speed of change in the dynamical system is small compared to the frequency of measurements. But if even these quite stable systems can show severe instable behaviour, more general systems are even more likely to show similar behaviour. Subsequent work has already been carried out by Potthast, Moodey, Lawless and van Leeuwen [PMLvL], where dynamical systems M of trace class are investigated. Note that the systems here, in particular the constant system $M = I$, are not of trace class, but trace class systems damp higher modes as it is usually carried out in global atmospheric models. For trace class systems the authors show similar results, but also provide a stable assimilation setup to control the analysis error over time. Further research in this direction is highly interesting to learn more about possible instabilities of operational data assimilation systems, which by causing large forecast error can have a significant impact on many parts of society.

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