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A note on preconditioning weighted linear least squares, with consequences for weakly-constrained variational data assimilation

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Abstract

The effect of preconditioning linear weighted least-squares using an approximation of the model matrix is analyzed, showing the interplay of the eigenstructures of both the model and weighting matrices. A small example is given illustrating the resulting potential inefficiency of such preconditioners. Consequences of these results in the context of the weakly-constrained 4D-Var data assimilation problem are finally discussed.

Keywords: linear least-squares, preconditioning, data assimilation, weakly-constrained 4D-Var, earth sciences.

1 Introduction

Solving weighted linear least-squares problems, that is optimization problem of the form

$$\min_{x \in \mathbb{R}^n} \frac{1}{2} \|Ax - b\|^2_{W^{-1}} \tag{1.1}$$

(with $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$ and $W \in \mathbb{R}^{m \times m}$ symmetric positive-definite), is an ubiquitous problem in applied mathematics (see [1, 10, 15] for an introduction to this domain and its vast literature), in particular when modelling in the presence of uncertainties in the data and/or the model itself. The particular application which motivates this paper is the solution of the weakly-constrained 4D-Var problem in data assimilation [18, 19, 20, 21], a mathematical formulation used, among others, for weather forecasting [13, 16, 9, 2] and oceanography [4].

It is well-known that the solution of (1.1) is given by solution of the system of "normal equations"

$$(A^T W^{-1} A)x = A^T W^{-1} b. \tag{1.2}$$

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In many applications of interest (such as data assimilation in the earth sciences), this system can be so large that the use of factorizations becomes impractical, and one is then led to applying iterative methods, such as Krylov methods [17]. However, these methods typically require preconditioning for achieving computational efficiency, often in the context of parallel computing. Building preconditioners for general symmetric positive-definite matrices has been widely investigated over the years (and is out of the scope of the present study). It is however fair to say that the choice of a good preconditioner is often far from easy and typically relies on experience and on the details of the problem at hand. When the matrix to precondition is that of the system of normal equations (1.2) and W is known, one might consider that a reasonable preconditioner may be obtained by using a suitable approximation of the matrix A.

The purpose of this short paper is to show why this strategy may sometimes be ineffective. While practitioners have been aware of the difficulty for some time (see [7, 8, 12, 14] for example), a formal analysis, and hence a complete understanding, has been missing so far. A first step in this direction was made by Braess and Peisker in [3], where they showed (in a slighly different context) that, if A is square, symmetric and positive-definite, and if W is the identity matrix, then preconditioning A^2 (which corresponds to unweighted symmetric least-squares) using the square of an approximation of A as a preconditioner might lead to a situation worse than not preconditioning at all, unless A and its preconditioner commute. Our objective is to elaborate further and to provide an analysis for the case where A need not be symmetric nor positive-definite while still requiring that A be square and nonsingular. As it turns out, this framework is general enough to cover our application in data assimilation.

The paper is organized as follows. Section 2 proposes the main analysis and relevant theorem, while a small illustrative numerical example is presented in Section 3. The consequences of our analysis for the weakly-constrained 4D-Var data assimilation are then discussed in Section 4 and some conclusions finally drawn in Section 5.

2 Preconditioning weighted linear least squares

Let the non-singular matrix $\tilde{A} \in \mathbb{R}^{n\times n}$ be an approximation (in a sense yet to be defined) of $A \in \mathbb{R}^{n\times n}$. Then the inverse of the matrix

$$P = \tilde{A}^T W^{-1} \tilde{A} \tag{2.1}$$

may be used to construct a preconditioner for the system (1.2), yielding

$$P^{-1}(A^T W^{-1} A)x = P^{-1} A^T W^{-1} b = (\tilde{A}^{-1} W \tilde{A}^{-T}) A^T W^{-1} b. \tag{2.2}$$

The condition number of the preconditioned system matrix $A_p = (\tilde{A}^{-1} W \tilde{A}^{-T})(A^T W^{-1} A)$ – and thus the "quality" of the preconditioner P – naturally depends on the approximation $\tilde{A}$ and the weight matrix W. A trivial (but useless) choice is $\tilde{A} = A$, resulting in the condition number of A_p being equal to 1.

We now show that $\sigma((\tilde{A}^{-1} W \tilde{A}^{-T})(A^T W^{-1} A))$, the spectrum of the preconditioned system matrix, is bounded by a function of the error of $\tilde{A}$ as an approximation of A and the condition number of the matrix W.

Theorem 2.1 Let $(A, \tilde{A}) \in \mathbb{R}^{n\times n} \times \mathbb{R}^{n\times n}$ be non singular matrices, and let W be a symmetric positive-definite matrix in $\mathbb{R}^{n\times n}$ and let

$$A_p \stackrel{\text{def}}{=} (\tilde{A}^{-1} W \tilde{A}^{-T})(A^T W^{-1} A). \tag{2.3}$$

Then

$$\sigma(A_p) \subset \mathcal{B}\Big(1, (1 + \kappa_2(W))\|E\|_2 + \kappa_2(W)\|E\|_2^2\Big) \tag{2.4}$$

where $E \stackrel{\text{def}}{=} A\tilde{A}^{-1} - I_n$ the approximation error of A by $\tilde{A}$,$\kappa_2(W) = \|W\|_2 \|W^{-1}\|_2$ the condition number of W in the Euclidean norm and $\mathcal{B}(a, r)$ is the closed ball of radius r centered in a .

Proof. We first note that, because $\tilde{A}$ is non singular, the eigenvalues of A_p are identical to the eigenvalues of

$$\begin{aligned} F &= W\tilde{A}^{-T} A^T W^{-1} A \tilde{A}^{-1} \\ &= W(I_n + E^T)W^{-1}(I_n + E) \\ &= I_n + E + WE^T W^{-1} + WE^T W^{-1} E \\ &\stackrel{\text{def}}{=} I_n + G. \end{aligned}$$

Now let (λ, v) be an eigenpair of F, with $\|v\|_2 = 1$. By definition, we have that

$$v^T F v = 1 + v^T G v = \lambda \|v\|_2^2 = \lambda, \tag{2.5}$$

and therefore, using the Cauchy-Schwarz and triangle inequalities, that

$$\lambda \in \mathcal{B}(1, \|G\|_2). \tag{2.6}$$

Now, using $\|E\| = \|E^T\|$,

$$\begin{aligned} \|G\|_2 &= \|E + WE^T W^{-1} + WE^T W^{-1} E\|_2 && (2.7) \\ &\leq \|E\|_2 + \|WE^T W^{-1}\|_2 + \|WE^T W^{-1} E\|_2 && (2.8) \\ &\leq \|E\|_2 + \|W\|_2 \|E^T\|_2 \|W^{-1}\|_2 + \|W\|_2 \|E^T\|_2 \|W^{-1}\|_2 \|E\|_2 && (2.9) \\ &\leq (1 + \kappa_2(W))\|E\|_2 + \kappa_2(W)\|E\|_2^2 && (2.10) \end{aligned}$$

Combining this inequality with (2.6) then gives (2.4). □

It results from this theorem that the condition number of W and the approximation error E interact, and that a large condition number of W then requires the error $\|E\|_2$ to be correspondingly small in order to guarantee a small bound on the eigenvalues of the preconditioned system. Thus the choice of the approximation of the system matrix A, and thus of the preconditioner, should take the weighting matrix W into account, as to ensure that $\kappa(W)\|E\|_2 = \mathcal{O}(1)$.

Following [3], we now define, $\kappa(D, C)$, the condition number of a symmetric positive definite matrix D with respect to a symmetric positive definite matrix C by

$$\kappa(D, C) = \min_{0<\gamma_1<\gamma_2} \frac{\gamma_2}{\gamma_1} \quad \text{subject to} \quad \gamma_1 x^T C x \leq x^T D x \leq \gamma_2 x^T C x \ \text{ for all } \ x \in \mathbb{R}^n. \tag{2.11}$$

The following easy property then follows, where $\lambda_{\min}(M)$ (resp. $\lambda_{\max}(M)$) denotes the smallest (resp. largest) eigenvalue of the matrix M.

Theorem 2.2 Let (D, C) two symmetric positive-definite matrices. Then

$$\kappa(D, C) = \frac{\lambda_{\max}(C^{-1}D)}{\lambda_{\min}(C^{-1}D)}. \tag{2.12}$$

Proof. If $C^{1/2}$ its symmetric square root of C and if $y = C^{1/2}x$, we obtain that, for all $0 < \gamma_1 < \gamma_2$, (2.11) is equivalent to

$$\gamma_1 \|y\|_2^2 \leq y^T C^{-1/2} D C^{-1/2} y \leq \gamma_2 \|y\|_2^2 \quad \text{for all} \quad y \in \mathbb{R}^n.$$

The optimal constant γ_1 (resp. γ_2) is equal to the smallest (resp. largest) eigenvalues of the matrix $C^{-1/2}DC^{-1/2}$ which is also the smallest (resp. largest) eigenvalue of the matrix $C^{-1}D$. □

We now provide an upper bound of the condition number of $A^T W^{-1} A$ with respect to $\tilde{A}^T W^{-1} \tilde{A}$.

Corollary 2.3 Let $(A, \tilde{A}) \in \mathbb{R}^{n\times n} \times \mathbb{R}^{n\times n}$ be non singular matrices, and let W be a symmetric positive-definite matrix. Then, if $E = A\tilde{A}^{-1} - I_n$ is the approximation error of A by $\tilde{A}$, and assuming that

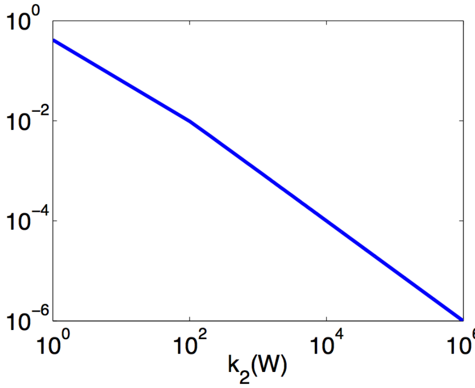
$$\|E\|_2 < \frac{-(1 + \kappa_2(W)) + \sqrt{(1 + \kappa_2(W))^2 + 4\kappa_2(W)}}{2\kappa_2(W)}, \tag{2.13}$$

one has that

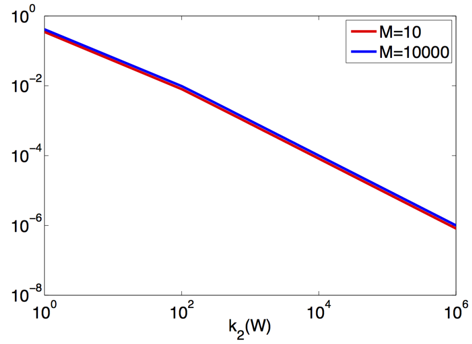
$$\kappa(A^T W^{-1} A, \tilde{A}^T W^{-1} \tilde{A}) \leq \frac{1 + (1 + \kappa_2(W))\|E\|_2 + \kappa_2(W)\|E\|_2^2}{1 - (1 + \kappa_2(W))\|E\|_2 - \kappa_2(W)\|E\|_2^2}.$$

Proof. From Theorem 2.2, one has that $\kappa(A^T W^{-1} A, \tilde{A}^T W^{-1} \tilde{A})$ is the ratio between the largest and smallest eigenvalues of the matrix A_p. Furthermore, the assumption (2.13) guarantees that $1 - (1 + \kappa_2(W))\|E\|_2 - \kappa_2(W)\|E\|_2^2 > 0$. The desired conclusion then follows from the observation that, because of Theorem 2.1, the eigenvalues of the matrix A_p defined in (2.3) all belong to $\mathcal{B}(1, (1 + \kappa_2(W))\|E\|_2 + \kappa_2(W)\|E\|_2^2)$. □

The condition (2.13) has a strong impact on numerical applications. Observe that the upper bound on the error $\|E\|_2$ stated in (2.13) is less than one and tends to zero when $\kappa_2(W)$ grows (see Figure 2 (a)). For instance, a condition number $\kappa_2(W) = 100$ imposes an approximation error of the order of 10^{-2}. Furthermore, if one aims at a preconditioned matrix A_p with a



(a) Upper bound (2.13) on the error $\|E\|_2$ as a function of the condition number of W (logarithmic scales).



(b) Upper bound g on the error $\|E\|_2$ as a function of the condition number of W (logarithmic scales).

condition number bounded above by $M > 0$, then the requirement

$$\kappa(A^T W^{-1} A, \tilde{A}^T W^{-1} \tilde{A}) \leq \frac{1 + (1 + \kappa_2(W))\|E\|_2 + \kappa_2(W)\|E\|_2^2}{1 - (1 + \kappa_2(W))\|E\|_2 - \kappa_2(W)\|E\|_2^2} \leq M$$

results in an upper bound for the approximation error given by

$$\|E\|_2 \leq \frac{-(1 + \kappa_2(W)) + \sqrt{(1 + \kappa_2(W))^2 + 4\kappa_2(W)\frac{M-1}{M+1}}}{2\kappa_2(W)} \stackrel{\text{def}}{=} g(\kappa_2(W), M).$$

The evolution of g with respect to $\kappa_2(W)$ is shown in Figure 2 (b) for two values of M. We note that even relatively large bounds on the condition number of $A^T W^{-1} A$ with respect to $\tilde{A}^T W^{-1} \tilde{A}$ impose small approximation errors, especially when W has a large condition number.

3 A simple illustrative example

We now illustrate the impact of the preconditioners (2.1) on the eigenvalues and condition number of the preconditioned system matrix (2.2) in a very simple case. Let $\alpha \geq 1$ be a parameter corresponding to the condition number of the weight matrix W. We define

$$A = \begin{pmatrix} 1 & 0 \\ \alpha & 1 \end{pmatrix} \quad \text{and} \quad W = \begin{pmatrix} \alpha & 0 \\ 0 & 1 \end{pmatrix}.$$

It can then be verified that the matrices $A^T A$ and $A^T W^{-1} A$ both have their condition numbers tending to infinity when α grows. We now introduce the approximation of A given by

$$\tilde{A} = \begin{pmatrix} 1 & 0 \\ \alpha + 2 & 1 \end{pmatrix}.$$

It is now possible to construct a "good preconditioner" $P^{-1} = \tilde{A}^{-1} \tilde{A}^{-T}$ of the matrix $A^T A$ in the sense that, while the condition number of $A^T A$ goes towards infinity when α grows, the condition number of the matrix A^TA with respect to $\tilde{A}^T\tilde{A}$ is constant. In this specific case, one has $\kappa(A^TA, \tilde{A}^T\tilde{A})$ which is the same as $\kappa_2(\tilde{A}^{-T}(A^TA)\tilde{A}^{-1})$ is approximately equal to 33.9706.

However, the approximation error E associated with this matrix is

$$E = A\tilde{A}^{-1} - I_2 = \begin{pmatrix} 0 & 0 \\ -2 & 0 \end{pmatrix},$$

leading to $\|E\|_2 = 2$. From Theorem 2.1, one then has that the eigenvalues of $A_p = (\tilde{A}^{-1}W\tilde{A}^{-T})(A^TW^{-1}A)$ belong to the closed ball $\mathcal{B}(1, 1+6\alpha)$, which makes it possible for the largest eigenvalue to tend to infinity with α. Indeed, this is is what happens in this example. One has that

$$A_p = \begin{pmatrix} 1-2\alpha^2 & -2\alpha \\ 2\alpha^3+4\alpha^2-2 & 2\alpha^2+4\alpha+1 \end{pmatrix}.$$

It can be shown that the eigenvalues of A_p are $1+2\alpha \pm 2\sqrt{\alpha(\alpha+1)}$, and so the largest one tends to infinity when α grows. Moreover, $\kappa(A^TW^{-1}A, \tilde{A}^TW^{-1}\tilde{A})$, the condition number of $A^TW^{-1}A$ with respect to $\tilde{A}^TW^{-1}\tilde{A}$, therefore also tends to infinity with α.

However, if we now define the approximation of A by

$$\tilde{A} = \begin{pmatrix} 1 & 0 \\ \alpha+\alpha^{-1} & 1 \end{pmatrix},$$

the approximation error then becomes

$$E = \begin{pmatrix} 0 & 0 \\ \alpha^{-1} & 0 \end{pmatrix},$$

leading to $\|E\|_2 = \alpha^{-1}$ and $\kappa_2(W)\|E\|_2 = 1$. Again, Theorem 2.1 says that the eigenvalues of A_p belongs to $\mathcal{B}(1, 1+2\alpha^{-1})$, but now the radius of this ball tends to one when α grows, which results in bounded eigenvalues. This can easily be verified as, in this case,

$$A_p = \begin{pmatrix} 1-\alpha & -1 \\ \alpha^2-\alpha^{-1}+1 & \alpha+\alpha^{-1}+1 \end{pmatrix}.$$

which has two distinct eigenvalues $\frac{1}{2}(2+\alpha^{-1} \pm \sqrt{4\alpha^{-1}+\alpha^{-2}})$ tending to one when α grows, as does $\kappa(A^TW^{-1}A, \tilde{A}^TW^{-1}\tilde{A})$.

4 Application to weakly-constrained data assimilation

We now turn to the implications of the above results for our motivating application, the weakly-constrained 4D variational formulation for data assimilation. In this context, one attempts to fit an initial state x_0 so as to fit observations y_j taken from the evolution of a dynamical model $\mathcal{M}$ over N_{sw} time windows. We refer to [18, 19] for further details and motivation for this formulation, but, for our present purposes, it is enough to know that it involves the (often approximate) solution of the optimization problem

$$\min_{\mathbf{x}\in\mathbb{R}^n} \frac{1}{2}\|x_0 - x_b\|^2_{B^{-1}} + \frac{1}{2}\sum_{j=0}^{N_{sw}} \|\mathcal{H}_j(x_j) - y_j\|^2_{\mathbf{R}_j^{-1}} + \frac{1}{2}\sum_{j=1}^{N_{sw}} \|x_j - \mathcal{M}_j(x_{j-1})\|^2_{\mathbf{Q}_j^{-1}} \tag{4.1}$$

where

- $x = (x_0, x_1, \ldots, x_{N_{sw}})^T \in \mathbb{R}^n$ is the control variable (with $x_j = x(t_j)$),
- x_b is the background given at the initial time (t_0),
- $y_j \in \mathbb{R}^{m_j}$ is the observation vector over a given time interval,
- $\mathcal{H}_j$ maps the state vector x_j from model space to observation space,
- $\mathcal{M}_j$ represents an integration of the numerical model from time t_{j-1} to t_j,
- B, R_j and Q_j are the covariances of the background, observation and model error.

This general unconstrained nonlinear least-squares problem is typically solved by applying the Gauss-Newton algorithm, which iteratively proceeds by linearizing $\mathcal{H}$ and $\mathcal{M}$ at the current iterate and then, again approximately, minimizing the resulting quadratic function. If the operators M_j are the linearized $\mathcal{M}_j$ and H_j are the linearized $\mathcal{H}_j$, then the problem can be expressed in terms of $\delta x = x - x_0$ as

$$\min_{\delta x \in \mathbb{R}^n} \frac{1}{2}\|L\delta x - b\|^2_{D^{-1}} + \frac{1}{2}\|H\delta x - d\|^2_{R^{-1}}$$

where

$$L = \begin{pmatrix} I_n & & & & \\ -M_1 & I_n & & & \\ & -M_2 & I_n & & \\ & & \ddots & \ddots & \\ & & & -M_{N_{sw}} & I_n \end{pmatrix} \tag{4.2}$$

for suitable vectors

$$d = (d_0, d_1, \ldots, d_{N_{sw}})^T \text{ and } b = (b, c_1, \ldots, c_{N_{sw}})^T,$$

and where

$$H = \mathrm{diag}(H_0, H_1, \ldots, H_{N_{sw}}),\ D = \mathrm{diag}(B, Q_1, \ldots, Q_{N_{sw}}) \text{ and } R = \mathrm{diag}(R_0, R_1, \ldots, R_{N_{sw}}).$$

This particular form of the problem is called the "state formulation" and its optimality conditions amount to (approximately) solving linear systems of the form

$$(L^T D^{-1} L + H^T R^{-1} H)\delta x = L^T D^{-1} b + H^T R^{-1} d \tag{4.3}$$

An alternative, called the "forcing formulation", is also possible by rewriting the problem in terms of $\delta p = L\delta x$, but we do not consider it here because it is not amenable to parallel computation. Its conditioning has been studied in [5, 6].

It is traditionally assumed that the term $L^T D^{-1} L$ (called the background term) dominates in the system matrix, which then leads to preconditioners of the form

$$P^{-1} = \tilde{L}^{-1}\, D\, \tilde{L}^{-T}, \tag{4.4}$$

with $\tilde{L}$ an approximation of the matrix L (see (4.2)). This approximation is often built by replacing in L the operators M_j associated with the numerical model by approximations $\tilde{M}_j$. While the matrix-vector product with L can be done in parallel, the preconditioner (4.4) involves $\tilde{L}^{-1}$, whose parallelization potential crucially depends on the choice of the operators $\tilde{M}_j$. Two very simple approximations are commonly chosen in practice: $\tilde{M}_j = 0$ or $\tilde{M}_j = I_n$.

The preconditioned system matrix is then $(\tilde{L}^{-1}D\tilde{L}^{-T})(L^TD^{-1}L+H^TR^{-1}H)$. In what follows, we focus on the preconditioned background term $(\tilde{L}^{-1}D\tilde{L}^{-T})(L^TD^{-1}L)$ and we investigate the consequences of Theorem 2.1 for this matrix.

We first analyse the form of the approximation error $E = L\tilde{L}^{-1} - I_{nN_{sw}}$.

Lemma 4.1 Let L, $\tilde{L}$, M_j, $\tilde{M}_j$ and $E = L\tilde{L}^{-1} - I_{nN_{sw}}$. Then

- if $\tilde{M}_j = 0$, one has that $E = \begin{pmatrix} 0 & & & & \\ -M_1 & 0 & & & \\ & -M_2 & 0 & & \\ & & \ddots & \ddots & \\ & & & -M_{N_{sw}} & 0 \end{pmatrix}$;
- if $\tilde{M}_j = I_n$, one has that $E = \begin{pmatrix} 0 & & & & \\ I_n - M_1 & 0 & & & \\ I_n - M_2 & I_n - M_2 & 0 & & \\ & & \ddots & \ddots & \\ I_n - M_{N_{sw}} & I_n - M_{N_{sw}} & \cdots & I_n - M_{N_{sw}} & 0 \end{pmatrix}$.

Proof. It can be verified that E is block-lower triangular with null blocks on the diagonal. Furthermore, one has that, for all indeces (i,j) such that $1 \le j < i \le N_{sw}+1$,

$$E_{i,j} = \begin{cases} (\tilde{M}_{i-1} - M_{i-1})\tilde{M}_{i-2}\cdots\tilde{M}_j & \text{if } j < i-1, \\ \tilde{M}_{i-1} - M_{i-1} & \text{if } j = i-1, \end{cases}$$

where $E_{i,j} \in \mathbb{R}^{n\times n}$ is the (i,j)-th block of E. The conclusions of the lemma then follow by specializing M_j. $\square$

Using those expressions for the approximation error (of $\tilde{M}_j$ as an approximation of M_j), we may then derive the following conclusions from Theorem 2.1, in terms of $\sigma_{\max}(M_j)$, the largest singular value of the linearized model matrix M_j.

Corollary 4.2 Let L and M_j be defined in (4.2), and let $\tilde{L}$ be the approximation of L defined from $\tilde{M}_j \in \{0, I_n\}$ for $j = 1,\ldots,N_{sw}$. Let $A_p = (\tilde{L}^{-1}D\tilde{L}^{-T})(L^TD^{-1}L)$ be the preconditioned background matrix. Then

$$\sigma(A_p) \subset \mathcal{B}(1, (1+\kappa_2(D))\rho + \kappa_2(D)\rho^2)$$

where

$$\rho = \begin{cases} \max\limits_{j=1,\ldots,N_{sw}} \sigma_{\max}(M_j) & \text{if } \tilde{M}_j = 0 \ \ (j = 1\ldots,N_{sw}), \\ \sqrt{\frac{(nN_{sw}+1)(nN_{sw}+2)}{2}} \left[\max\limits_{j=1,\ldots,N_{sw}} \sigma_{\max}(I_n - M_j)\right] & \text{if } \tilde{M}_j = I_n \ (j = 1,\ldots,N_{sw}). \end{cases}$$

Proof.

1. Consider first the case where $M_j = 0$. From Lemma 4.1, we deduce that $E^T E$ is block diagonal and

$$E^T E = \text{diag}(M_1^T M_1, M_2^T M_2, \cdots, M_{N_{sw}}^T M_{N_{sw}}, 0).$$

This then implies that $\|E\|_2 = \max_{j=1,\ldots,N_{sw}}(\sigma_{\max}(M_j))$ and we can conclude by applying Theorem 2.1.

2. If $M_j = I_n$, then, from Corollary 4.1, one has that $E = ST$ with

$$S = \begin{pmatrix} 0 & & & & \\ I_n - M_1 & 0 & & & \\ & I_n - M_2 & 0 & & \\ & & \ddots & \ddots & \\ & & & I_n - M_{N_{sw}} & 0 \end{pmatrix}$$

and T is the lower triangular matrix with the lower entries equal to one. As in the previous case, one obtains that $\|S\|_2 = \max_{j=1,\ldots,N_{sw}} \sigma_{\max}(I_n - M_j)$. Hence the desired conclusion follows from applying Theorem 2.1, and using the bound

$$\|E\|_2 \leq \|S\|_2 \|T\|_2 \leq \|S\|_2 \|T\|_F = \|S\|_2 \sqrt{\frac{(nN_{sw}+1)(nN_{sw}+2)}{2}}.$$

□

We immediately see that obtaining a well-conditioned matrix A_p requires specific assumptions on the dynamical models within a sub-window. Choosing $\tilde{M}_j = 0$ will work well if the model itself is close to zero, which may be unrealistic in many situations. The choice $\tilde{M}_j = I_n$ is often more sensible if the dynamics of the model may remain limited, especially if the time sub-windows are short. This can be viewed as a motivation to choose N_{sw} large, but one nevertheless should remember that the gain in making the singular value closer to 1 is offset by the dependence on the square root term in part 2 of Corollary 4.2. Obviously, the quality of the preconditioner may improve with the quality of $\tilde{M}_j$ as an approximation of M_j, but it remains challenging to select good approximations which preserve efficient parallel computation of $\tilde{L}^{-1}$ (see [11] for an approach of this question). One should also remember that our analysis merely provides bounds on the conditioning, which are pessimistic by nature, and that the observation term $H^T R^{-1} H$ (which we ignored here) may not always be negligible. The situation is therefore often problem dependent, as has been demonstrated in [12] where very different behaviours (good and bad) were observed for two contrasting data assimilation problems.

5 Conclusions

We have provided a formal analysis of the preconditioning efficiency for nonsingular weighted least-squares, thereby extending previous results by Braess and Peisker [3] and vindicating the numerical experience of several practitioners. We have also specialized the analysis to the state formulation of the weakly-constrained data assimilation problems, an important computational tool in the earth sciences. While the conditioning bounds discussed in this paper remain indicative as all bounds are, they nevertheless provide some guidance on how to construct good parallelizable preconditioners, a task which remains for now a problem-dependent exercize.

References

[1] Å. Björck. *Numerical Methods for Least Squares Problems.* SIAM, Philadelphia, USA, 1996.

[2] M. Bonavita, Y. Trémolet, E. Holm, S. T. K. Lang, M. Chrust, M. Janisková, Ph. Lopeze, P. Laloyaux, P. de Rosnay, M. Fisher, M. Hamrud, and S. English. A strategy for data assimilation. Technical Report 800, ECMWF, 2017.

[3] D. Braess and P. Peisker. On the numerical solution of the biharmonic equation and the role of squaring matrices for preconditioning. *IMA Journal of Numerical Analysis*, 6:393–404, 1986.

[4] E. Di Lorenzo, A. M. Moore, H. G. Arango, B. D. Cornuelle, A. J. Miller, B. Powell, B. S. Chua, and A. F. Bennett. Weak and strong constraint data assimilation in the inverse regional ocean modeling system (ROMS): Development and application for a baroclinic coastal upwelling system. *Ocean Modelling*, 16:160187, 2007.

[5] A. El-Said. *Variational Data Assimilation Problem for Numerical Weather Prediction.* PhD thesis, University of Reading, Reading, UK, 2015.

[6] A. El-Said, N. K. Nichols, and A. S. Lawless. Conditioning of the weak-constraint 4DVAR problem. Technical report, University of Reading, Reading, UK, 2017.

[7] M. Fisher and S. Gürol. Time-parallel algorithms for 4D-Var. Talk at the 6th WMO Data Assimilation Symposium, 2013. Available at `http://das6.umd.edu/program/Daily/slides/1`.

[8] M. Fisher and S. Gürol. Parallelisation in the time dimension of four-dimensional variational data assimilation. *Quarterly Journal of the Royal Meteorological Society*, 143(703):1136–1147, 2017.

[9] M. Fisher, Y. Trémolet, H. Auvinen, D. Tan, and P. Poli. Weak-constrained and long window 4D-Var. Technical Report 655, ECMWF, 2011.

[10] G. H. Golub and C. F. Van Loan. *Matrix Computations.* Johns Hopkins University Press, Baltimore, third edition, 1996.

[11] S. Gratton, S. Gürol, E. Simon, and Ph. L. Toint. Issues in making the weakly-constrained 4D-Var formulation computationally efficient. Oberwolfach Reports 47, 2017.

[12] S. Gratton, S. Gürol, E. Simon, and Ph. L. Toint. On the use of the saddle formulation in weakly constrained 4D-Var data assimilation. arXiv:1709.06383, 2017.

[13] T. Janjić and H. Lange. Weak constrained localized ensemble transform Kalman filter for radar data assimilation. *Geophysical Research Abstracts*, 17(EGU2015-13021), 2015.

[14] T. Janjić and Y. Zhang. Private communication, 2017.

[15] T. Kariya and H. Kurata. *Generalized Least-Squares.* J. Wiley and Sons, Chichester, England, 2004.

[16] M.-S. Lee and D.-K. Lee. An application of a weakly constrained 4dvar to satellite data assimilation and heavy rainfall simulation. *Monthly Weather Review*, pages 2151–2176, 2003.

[17] Y. Saad. *Iterative Methods for Sparse Linear Systems.* PWS Publishing Company, Boston, USA, 1996.

[18] Y. Trémolet. Accounting for an imperfect model in 4D-Var. *Quarterly Journal of the Royal Meteorological Society*, 132(621):2483–2504, 2006.

[19] Y. Trémolet. Model error estimation in 4D-Var. *Quarterly Journal of the Royal Meteorological Society*, 133(626):1267–1280, 2006.

[20] P. A. Vidard, A. Piacentini, and F.-X. Le Dimet. Variational data analysis with control of the forecast bias. *Tellus*, 56A:177–188, 2004.

[21] D. Zupanski. A general weak constraint applicable to operational 4DVAR data assimilation systems. *Monthly Weather Review*, 125, 1997.