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ABSTRACT

If the coefficient matrix in the general Gauss-Markov linear model is ill-conditioned, then the solution is very sensitive to perturbations. For such problems, we propose to add Tikhonov regularization to the model, and we show that this actually stabilizes the solution and decreases its variance. We also give a numerically stable algorithm for computing the regularized solution efficiently.

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1. Introduction

This paper is concerned with the *general Gauss-Markov linear model* $A\,x + \varepsilon = b$, where $A \in \mathbb{R}^{m \times n}$ $(m \ge n)$ and $b \in \mathbb{R}^m$ are known, $x \in \mathbb{R}^n$ is an unknown vector to be estimated, and $\varepsilon \in \mathbb{R}^m$ is a random vector with zero mean and variance-covariance matrix $V(\varepsilon) = s^2 BB^T$ with $B \in \mathbb{R}^{m \times p}$ $(m \ge p)$. The best linear unbiased estimator of x in this model is the solution to the following constrained least-squares problem:

$$\min \|u\|_2 \quad \text{subject to} \quad A\,x + B\,u = b\ . \tag{1}$$

Here, we have introduced the vector $u \in \mathbb{R}^p$ such that $\varepsilon = B\,u$, where u has variance-covariance matrix $V(u) = s^2 I_p$ and where I_p is the identity matrix. The model (1) was introduced by Paige [10], and computational algorithms can be found in [7,9,11]. A more detailed analysis of (1) in terms of the generalized SVD is also given by Paige [12], while Björck [1, Section 23] extended this analysis to the case when both A and B may be rank deficient. However, the case when the problem (1) is ill-conditioned, for example if A or B is ill-conditioned, has not been given much attention and, according to Paige [10], needs further work. The present paper is a step in this direction.

First, a word about our notation: $\|\cdot\|$ denotes the matrix and vector 2-norm, I_p is the identity matrix of order p, and A^+ denotes the pseudoinverse of A.

Let us consider the sensitivity of the solution to (1) to perturbations of the right-hand side b. Let e denote the perturbation, and let $\tilde{x}$ denote the perturbed solution. Then the following approximate error bound follows from [10, Eq. (46)]:

$$\|x - \tilde{x}\| \le \|A^+\|^{-1} (1 + \|B\| / \|(Q^T B)^+\|)\, \|e\|\ , \tag{2}$$

where the columns of Q form an orthonormal basis for the null space of A^T. We immediately see that if A is ill-conditioned then x may be very sensitive to perturbations. This is also clear from the analysis in [12] since we can always expect trouble when dividing by the small generalized singular values of (A, B). Eq. (2) shows that a small $\|(Q^T B)^+\|$ also indicates trouble.

In this paper we investigate the case where A is ill-conditioned while B is well-conditioned. To overcome the problems associated with the ill-conditioned A we suggest to add Tikhonov regularization to the problem (1) (Tikhonov regularization is discussed in e.g. [3] and [1, Section 26]). Thus, we propose the following *regularized Gauss-Markov problem*

$$\min \{\, \|u\|^2 + \lambda^2 \|C\,x\|^2 \,\} \quad \text{subject to} \quad A\,x + B\,u = b\ . \tag{3}$$

Here, for simplicity, we assume that B and C have full rank,

$$A \in \mathbb{R}^{m\times n} \; , \quad B \in \mathbb{R}^{m\times p} \; , \quad C \in \mathbb{R}^{q\times n} \; , \quad \mathrm{rank}(B) = p \le m \; , \quad \mathrm{rank}(C) = q \le n \le m \; . \tag{4a}$$

We also assume that

$$\mathrm{rank}\begin{bmatrix} A \\ C \end{bmatrix} = n \tag{4b}$$

which guarantees that the *regularized solution* x_λ to (3) is unique for any $\lambda > 0$. Notice that we make no assumption about the rank of A since this in not important in connection with Tikhonov regularization, cf. e.g. [4]. Typically, we will take C to be the identity matrix I_n or a well-conditioned discrete approximation to some derivative operator to ensure that the solution x_λ is sufficiently 'smooth'. The quantity λ is the *regularization parameter* which controls the weight given to minimization of $\|C\,x\|$ relative to minimization of $\|u\|$.

We know that the regularized solution x_λ to (3) is no longer an unbiased estimator (which is in fact the case for any regularized solution). However, inspired by the success of adding regularization to ill-conditioned least-squares problems, we feel that x_λ has other nice properties (cf. Section 3) that make it useful in connection with general Gauss-Markov linear models with ill-conditioned coefficient matrix A.

The paper is organized as follows. In Section 2 we introduce the restricted SVD and apply it as a tool for analyzing the model (3), and in Section 3 we use these results to describe the properties of the regularized solution x_λ. In Section 4 we briefly discuss the discrete Picard condition as it applies to the regularized problem (3). Finally, in Section 5 we present a numerically stable algorithm for solving (3) efficiently.

2. An RSVD analysis of the regularized Gauss-Markov problem

We notice first that if $p < m$ then $\min\{\, \|B^+(A\,x - b)\|^2 + \lambda^2\, \|C\,x\|^2 \,\}$ is *not* a valid formulation of (3), and we can therefore not base our analysis of (3) on Van Loan's S,T-singular values [13]. The proper tool to analyze (3) is the *restricted SVD* (RSVD) of (A, B, C) due to Zha [14]:

Theorem 1. *Let A, B and C satisfy the assumptions in Eqs. (4a) and (4b). Then there exist nonsingular matrices $X \in \mathbb{R}^{n\times n}$, $Z \in \mathbb{R}^{m\times m}$ and orthogonal matrices $U \in \mathbb{R}^{p\times p}$, $V \in \mathbb{R}^{q\times q}$ such that*

$$Z^T A\, X = \Sigma \quad , \quad Z^T B\, U = M \quad , \quad V^T C\, X = N \tag{5}$$

where Σ, M and N are pseudo-diagonal matrices with nonnegative elements in the following structure:

$$\Sigma = \begin{array}{cc} \begin{bmatrix} \Sigma_A & 0 & 0 & 0 \\ 0 & I_j & 0 & 0 \\ 0 & 0 & I_k & 0 \\ 0 & 0 & 0 & I_l \\ 0 & 0 & 0 & 0 \end{bmatrix} & \begin{matrix} s \\ j \\ k \\ l \\ u \end{matrix} \\ \begin{matrix} t & j & k & l \end{matrix} & \end{array} \quad , \quad M = \begin{array}{cc} \begin{bmatrix} I_s & 0 \\ 0 & 0 \\ 0 & I_k \\ 0 & 0 \\ 0 & 0 \end{bmatrix} & \begin{matrix} s \\ j \\ k \\ l \\ u \end{matrix} \\ \begin{matrix} s & k \end{matrix} & \end{array} \quad , \quad N = \begin{array}{cc} \begin{bmatrix} I_t & 0 & 0 & 0 \\ 0 & I_j & 0 & 0 \end{bmatrix} & \begin{matrix} t \\ j \end{matrix} \\ \begin{matrix} t & j & k & l \end{matrix} & \end{array} \tag{6}$$

and where

$$\Sigma_A = \operatorname{diag}(\sigma_1, \ldots, \sigma_r) \in \mathbb{R}^{s \times t} \quad , \quad \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r \geq 0 \quad , \quad r = \min\{s, t\} \; . \tag{6a}$$

The dimensions of the submatrices are

$$\begin{array}{lll} j = r_{ab} + q - r_{abc} & k = n + p - r_{abc} & l = r_{abc} - p - q \\ s = r_{abc} - n & t = r_{abc} - r_{ab} & u = m - r_{ab} \end{array} \tag{7}$$

in which $r_{ab} = \operatorname{rank}(A, B)$ *and* $r_{abc} = \operatorname{rank} \begin{pmatrix} A & B \\ C & 0 \end{pmatrix}$.

Proof. The proof of the RSVD as well as the notation is from [14, Theorem 4.2] with the simplifications imposed by our assumptions in (4a) and (4b). □

Remark. In [5] it is shown that if A is ill-conditioned and C is well-conditioned, and if $A = \hat{U} \hat{\Sigma} \hat{X}^{-1}$, $C = \hat{V} \hat{M} \hat{X}^{-1}$ is the generalized SVD of (A, C), then $\hat{\Sigma}$ is ill-conditioned while $\hat{M}$ and $\hat{X}$ are well-conditioned. Using this result in the constructive proof for the RSVD [14], which consists of a sequence of generalized SVD's, it follows immediately that if A is ill-conditioned and both B and C are well-conditioned, then Σ is ill-conditioned while X and Z are well-conditioned.

Inserting the RSVD into (3) and using the fact that the 2-norm is invariant under orthogonal transformations, we immediately obtain the equivalent problem

$$\min \{ \|\bar{u}\|^2 + \lambda^2 \|N \bar{x}\|^2 \} \qquad \text{subject to} \qquad \Sigma \bar{x} + M \bar{u} = \bar{b} \tag{8}$$

where we have defined the transformed vectors $\bar{u} = U^T u$, $\bar{x} = X^{-1} x$ and $\bar{b} = Z^T b$. At this point, it is convenient to partition the matrices X and Z column-wise and to partition the vectors $\bar{x}$, $\bar{u}$ and $\bar{b}$ element-wise according to the partitioning in (6),

$$X = [X_t, X_j, X_k, X_l] \quad , \quad Z = [Z_s, Z_j, Z_k, Z_l, Z_u] \tag{9a}$$

$$\bar{x} = \begin{bmatrix} \bar{x}_t \\ \bar{x}_j \\ \bar{x}_k \\ \bar{x}_l \end{bmatrix} \quad , \quad \bar{u} = \begin{bmatrix} \bar{u}_s \\ \bar{u}_k \end{bmatrix} \quad , \quad \bar{b} = \begin{bmatrix} \bar{b}_s \\ \bar{b}_j \\ \bar{b}_k \\ \bar{b}_l \\ \bar{b}_u \end{bmatrix} . \tag{9b}$$

The equality constraints in (8) then take the following simpler form:

$$\begin{array}{rcl} \Sigma_A\, \bar{x}_t + \bar{u}_s = \bar{b}_s & \qquad \bar{x}_k + \bar{u}_k = \bar{b}_k & \\ \bar{x}_j = \bar{b}_j & \qquad \bar{x}_l = \bar{b}_l & \qquad 0 = \bar{b}_u \end{array} \tag{10}$$

We immediately see that *consistency* of the model (3), i.e. the requirement that the right-hand side b belongs to the range of the matrix (A, B), corresponds to requiring that $\bar{b}_u = 0$. Using the results in (10), the minimization problem in (8) can now be written as

$$\min \left\{ \left\| \begin{bmatrix} \bar{b}_s \\ \bar{b}_k \end{bmatrix} - \begin{bmatrix} \Sigma_A & 0 \\ 0 & I_k \end{bmatrix} \begin{bmatrix} \bar{x}_t \\ \bar{x}_k \end{bmatrix} \right\|^2 + \lambda^2 \left\| \begin{bmatrix} \bar{x}_t \\ \bar{b}_j \end{bmatrix} \right\|^2 \right\} . \tag{11}$$

The minimum is obtained for $\bar{x}_k = \bar{b}_k$ and $\bar{x}_t$ being the solution to

$$\min \{ \|\Sigma_A\, \bar{x}_t - \bar{b}_s\|^2 + \lambda^2 \|\bar{x}_t\|^2 \}$$

which is a discrete regularization problem in standard form and with the unique solution given by

$$\bar{x}_t = F_\lambda \Sigma_A^+ \bar{b}_s \tag{12}$$

where we have defined $F_\lambda = \mathrm{diag}(f_i) \in \mathbb{R}^{t \times t}$ with diagonal elements

$$f_i = \frac{\sigma_i^2}{\sigma_i^2 + \lambda^2} \quad , \quad i = 1, \ldots, t \; . \tag{13}$$

For more details about discrete standard-form regularization, cf. e.g. [4]. Notice that all parts of the solution $\bar{x}$ are determined from Eqs. (10) and (11). If the matrix $\begin{bmatrix} A \\ C \end{bmatrix}$ does not have full rank, then there will also be a non-estimable (arbitrary) part of the solution.

The solution x_λ to (3), as a function of λ, can thus be written as

$$x_\lambda = X \begin{bmatrix} F_\lambda \Sigma_A^+ & 0 & 0 & 0 & 0 \\ 0 & I_j & 0 & 0 & 0 \\ 0 & 0 & I_k & 0 & 0 \\ 0 & 0 & 0 & I_l & 0 \end{bmatrix} Z^T b \;=\; X_t F_\lambda \Sigma_A^+ Z_s^T b + X_j Z_j^T b + X_k Z_k^T b + X_l Z_l^T b \; . \tag{14}$$

In particular, if $q = n$ then $k + l = 0$ such that the last two terms in (14) vanish. In general, we have $x_\lambda \to x_o = X\, \Sigma^+ Z^T b$ for $\lambda \to 0$. Note that the matrix $X\, \Sigma^+ Z^T$ is not a weighted pseudoinverse of A as defined by Eldén [2].

3. Some properties of the regularized solution

We shall now describe some of the nice features of the regularized solution x_λ to (3). First of all, we see that if A has any small σ_i, reflecting the ill-conditioning af A, then the norm of the unregularized solution $x_o = X\,\Sigma^+ Z^T b$ may be very large because of the division by these small σ_i. For the same reason, x_o is very sensitive to perturbations of b. Consider now the first term in the expression (14) for the regularized solution x_λ:

$$X_t\, F_\lambda \Sigma_A^+ Z_s^T b = \sum_{i=1}^{r} \frac{\sigma_i^2}{\sigma_i^2+\lambda^2}\,\frac{z_i^T b}{\sigma_i}\, x_i \ .$$

This is the only term where small σ_i occur. We immediately see from this expression that by choosing a suitable regularization parameter λ somewhere between σ_r and σ_1, we are able to 'filter out' the contributions to x_λ corresponding to the small σ_i via the matrix F_λ. In this way, we can use λ to control the norm and the sensitivity of x_λ, at the expense of neglecting a (small) part of the information in the right-hand side b. This is, in fact, completely analogous to regularization of least-squares problems [4].

Next, we prove that the regularized problem (3) is indeed better conditioned than the original problem (1). For simplicity, we restrict the perturbations to the right-hand side.

Theorem 2. *Let the perturbed right-hand side be $\bar b = b + e$, let $\bar x_\lambda$ denote the corresponding perturbed solution, and let x_o and $\bar x_o$ denote the solutions for $\lambda = 0$. If $\sigma_r \le \lambda \le \sigma_1$, then*

$$\frac{\|x_\lambda - \bar x_\lambda\|}{\|x_\lambda\|} \le \frac{\|\Sigma\|}{\min\{2\lambda, 1\}}\ \kappa(X)\,\kappa(Z)\,\frac{\|e\|}{\|b_\lambda\|} \tag{15}$$

$$\frac{\|x_o - \bar x_o\|}{\|x_o\|} \le \frac{\|\Sigma\|}{\sigma_r}\ \kappa(X)\,\kappa(Z)\,\frac{\|e\|}{\|b_o\|} \ . \tag{16}$$

Here, $\|\Sigma\| = \max\{\sigma_1, 1\}$, $b_\lambda = A\,x_\lambda$, $b_o = A\,x_o$, and $\kappa(X)$ and $\kappa(Z)$ are the condition numbers of X and Z, respectively.

Proof. The relations $\|b_\lambda\| = \|A\,x_\lambda\| \le \|Z^{-1}\|\,\|\Sigma\|\,\|X^{-1}\|\,\|x_\lambda\|$ and $\|x_\lambda - \bar x_\lambda\| \le \|X\|\max\{\|F_\lambda \Sigma_A^+\|, 1\}\,\|Z\|\,\|e\|$ give

$$\frac{\|x_\lambda - \bar x_\lambda\|}{\|x_\lambda\|} \le \kappa(X)\,\|\Sigma\|\,\max\{\|F_\lambda \Sigma_A^+\|, 1\}\,\kappa(Z)\,\frac{\|e\|}{\|b_\lambda\|} \ .$$

It is straightforward to show that $\|F_\lambda \Sigma_A^+\| = \max\{f_i/\sigma_i\} = \max\{\sigma_i/(\sigma_i^2+\lambda^2)\} \le 1/(2\lambda)$ such that $\max\{\|F_\lambda \Sigma_A^+\|, 1\} = 1/\min\{2\lambda, 1\}$, and since $\|\Sigma\| = \max\{\|\Sigma_A\|, 1\} = \max\{\sigma_1, 1\}$, this yields (15).

Eq. (16) is derived analogously by using that $||x_o - \bar{x}_o|| \le ||X||\,||\Sigma^+||\,||Z||\,||e||$ and that $||\Sigma^+|| = \sigma_r^{-1}$. □

Remark. Theorem 2 shows that the condition number κ_λ associated with (3) satisfies

$$\kappa_\lambda \equiv \lim_{||e|| \to 0} \sup \frac{||x_\lambda - \bar{x}_\lambda||}{||x_\lambda||} \le \frac{||\Sigma||}{\min\{2\lambda, 1\}}\, \kappa(X)\, \kappa(Z)\,. \tag{17}$$

The key point here is that Theorem 2 shown that it is always possible to choose λ such that x_λ is much less sensitive to perturbations than x_o. Thus, we can say that for appropriate regularization parameter λ, (3) is better conditioned that (1).

Another important property of introducing regularization in (3) is that it decreases the variance of the solution x_λ, compared to the variance of the solution x_o to (1) without regularization. Since the variance-covariance matrix associated with $\overline{u} = U^T u$ is $V(\overline{u}) = s^2 I_p$, it is easy to show that the variance-covariance matrix $V(\overline{x}_r)$ associated with the regularized solution vector $\overline{x}_r$ is

$$V(\overline{x}_r) = s^2 (F_\lambda \Sigma_A^+)^2\,. \tag{18}$$

We readily see that if λ is chosen suitably somewhere between σ_r and σ_1, then the elements of this matrix are numerically much smaller than those of the variance-covariance matrix $s^2(\Sigma_A^+)^2$ corresponding to $\lambda = 0$.

In this discussion we have not considered the 'smoothness' of x_λ. We feel that such an analysis can be performed in analogy with that in [5]. For example, we know that the null space of C, which is spanned by the columns of X_k and X_l, is always 'smooth' (in the sense, few zero crossings) when C is a discrete approximation to a derivative operator — thus ensuring that the component $X_k Z_k^T b + X_l Z_l^T b$ in x_λ (14) is also 'smooth'. However, we were not able to derive any results about the 'smoothness' of the columns of the submatrices X_t and X_j.

4. The discrete Picard condition

Of course, the introduction of regularization in (3) changes the solution x_λ compared to the unregularized solution to (1). The purpose of this section is to investigate the difference between these solutions. In this connection, notice that if A does not have full rank then the solution to (1) is not unique: the general solution can always be written as the estimable part of the solution plus an arbitrary amount of the non-estimable part of the solution [12]. For $\lambda \to 0$, the regularized solution x_λ converges to a member of this general solution (but not necessarily to the estimable part; we can only guarantee this if $\mathrm{rank}(A) = n$). It is therefore correct to compare the regularized solution $\boldsymbol{x}_\lambda$ to the solution $\boldsymbol{x}_o = X\, \Sigma^+ Z^T \boldsymbol{b}$ obtained from Eq. (14) by setting $\lambda = 0$.

An analysis of the *regularization error* $\boldsymbol{x}_o - \boldsymbol{x}_\lambda$ for general A, B, C and $\boldsymbol{b}$ is probably not possible. Instead, we use the same technique as in [4,6]: we assume a very simple (but still realistic) 'model' of the right-hand side and determine the conditions in which the regularization error is guaranteed to be small. Our 'model' here is

$$z_i^T b \;=\; \begin{cases} \sigma_i^\alpha & , \quad i = 1,\dots,r \\ \sigma_p^\alpha & , \quad i = r{+}1,\dots,s \end{cases} \quad , \qquad \alpha \ge 0\,. \tag{19}$$

The parameter α controls the decay of the $z_i^T \boldsymbol{b}$ relative to the decay of the corresponding σ_i, in such a way that the $z_i^T b$ decay faster to zero than the σ_i for $\alpha > 1$. A direct analysis of $\boldsymbol{x}_o - \boldsymbol{x}_\lambda$ is very difficult, so we multiply by the well-conditioned matrix X^{-1} and consider instead $X^{-1}(\boldsymbol{x}_o - \boldsymbol{x}_\lambda)$:

Theorem 3. *Let* $\boldsymbol{x}_o = X\, \Sigma^+ Z^T \boldsymbol{b}$ *be defined as the solution* $\boldsymbol{x}_\lambda$ *(14) with* $\lambda = 0$, *and let the right-hand side* $\boldsymbol{b}$ *satisfy Eq. (19). If* $\sigma_r \le \lambda \le \sigma_1$, *then*

$$\frac{\|X^{-1}(\boldsymbol{x}_o - \boldsymbol{x}_\lambda)\|}{\|X^{-1}\boldsymbol{x}_o\|} \le \begin{cases} \sqrt{r}\; (\sigma_1/\sigma_r)^{1-\alpha} & , \quad 0 \le \alpha < 1 \\ \sqrt{r}\; (\lambda/\sigma_1)^{\alpha-1} & , \quad 1 \le \alpha < 3 \\ \sqrt{r}\; (\lambda/\sigma_1)^2 & , \quad \alpha \ge 3\,. \end{cases} \tag{20}$$

Proof. We have $\|X^{-1}(\boldsymbol{x}_o - \boldsymbol{x}_\lambda)\| = \|(\Sigma_A^+ - F_\lambda \Sigma_A^+) Z_s^T \boldsymbol{b}\| = \|(I_t - F_\lambda)\Sigma_A^+ Z_s^T \boldsymbol{b}\| \le \sqrt{r}\, \|(I_t - F_\lambda)\Sigma_A^+ Z_s^T \boldsymbol{b}\|_\infty = \sqrt{r} \max\{(1-f_i)\sigma_i^{\alpha-1}\}$. Here, $(1-f_i)\sigma_i^{\alpha-1} = \lambda^2(\sigma_i^2+\lambda^2)^{-1}\sigma_i^{\alpha-1} = \lambda^2\phi(\sigma_i)$, where we have defined $\phi(\sigma) \equiv \sigma^{\alpha-1}/(\sigma^2+\lambda^2)$. It is easy to show the following:

For $0 \le \alpha < 1$: $\phi(\sigma)$ is decreasing, such that

$$\lambda^2\phi(\sigma) \le \lambda^2\phi(\sigma_r) = \frac{\lambda^2}{\sigma_r^2+\lambda^2}\,\sigma_r^{\alpha-1} \le \sigma_r^{\alpha-1}\,,$$

For $1 \le \alpha < 3$: $\phi(\sigma)$ has its maximum at $\sigma^2 = \lambda^2(\alpha-1)/(3-\alpha)$, and

$$\lambda^2\phi(\sigma) \le \frac{\lambda^2}{\lambda^2(\alpha-1)/(3-\alpha)+\lambda^2}\left[\frac{\alpha-1}{3-\alpha}\lambda^2\right]^{\frac12(\alpha-1)} = \frac{3-\alpha}{2}\left[\frac{\alpha-1}{3-\alpha}\right]^{\frac12(\alpha-1)}\lambda^{\alpha-1}$$

$$= \tfrac12(\alpha-1)^{\frac12(\alpha-1)}(3-\alpha)^{\frac12(3-\alpha)}\lambda^{\alpha-1} \le \lambda^{\alpha-1}\,,$$

For $\alpha \ge 3$: $\phi(\sigma)$ is increasing, such that

$$\lambda^2 \phi(\sigma) \le \lambda^2 \phi(\sigma_1) = \frac{\lambda^2}{\sigma_1^2 + \lambda^2}\, \sigma_1^{\alpha-1} \le \lambda^2 \sigma_1^{\alpha-3} .$$

Now, let Σ_o denote Σ (6a) with the three identity matrices replaced by 0. Then $\|Z_s^T \boldsymbol{b}\| = \|\Sigma_o\, X^{-1} \boldsymbol{x}_o\|$ $\le \|\Sigma_A\|\, \|X^{-1}\boldsymbol{x}_o\| = \sigma_1 \|X^{-1}\boldsymbol{x}_o\|$. From the definition (19) of $\boldsymbol{b}$ we also have $\|Z_s^T \boldsymbol{b}\| \ge \|Z_s^T \boldsymbol{b}\|_\infty = \sigma_1^\alpha$. Thus, $1/\|X^{-1}\boldsymbol{x}_o\| \le 1/\sigma_1^{\alpha-1}$. Together, these formulas lead to Eq. (20). □

Not surprisingly, we see that in order to ensure a small upper bound for the regularization error, we must require that the coefficients $|z_i^T b|$ decay to zero *faster* that the σ_i. We also see that the faster the decay, the better $\boldsymbol{x}_\lambda$ approximates $\boldsymbol{x}_o$. Following the idea in [6] we are then lead to the following definition of the *discrete Picard condition* for the regularized Gauss-Markov problem (3):

Definition 4. The discrete Picard condition (DPC). *The right-hand side b in (3) satisfies the DPC if, for all numerically nonzero σ_i, the coefficients $|z_i^T b|$ in average decay to zero faster than the σ_i.*

If the underlying, unperturbed right-hand side in (3) does not satisfy the DPC, then there is no point in trying to solve (3) at all, because $\boldsymbol{x}_\lambda$ does not approximated the true solution $\boldsymbol{x}_o$ for any value of λ. If, on the other hand, the unperturbed right-hand side $\boldsymbol{b}$ satisfies the DPC, and if the given $\tilde{\boldsymbol{b}} = \boldsymbol{b} + \boldsymbol{e}$ (which is contaminated with errors) is not completely dominated by the errors $\boldsymbol{e}$, then $\tilde{\boldsymbol{b}}$ actually satisfies the DPC for $i \le K$, where K is determined by the magnitude and the statistical distribution of the errors. Hence, if we choose $\lambda \simeq \sigma_K$, then the effect of regularization is to dampen the contributions to $\boldsymbol{x}_\lambda$ corresponding to the small $\sigma_i < \lambda$. In other words, we can regard the addition of regularization to the linear model as a means for producing a slightly perturbed model that is guaranteed to satisfy the DPC, thus ensuring that the regularized solution $\boldsymbol{x}_\lambda$ is a meaningful estimator. For more details and how to implement a check for satisfaction of the DPC in practice, cf. [6].

5. A numerical algorithm

In this section we describe an algorithm for computing the unique regularized solution $\boldsymbol{x}_\lambda$ to (3). It is easy to see that (3) can be reformulated as

$$\min \left\| \begin{bmatrix} \lambda C & 0 \\ 0 & I_p \end{bmatrix} \begin{bmatrix} x \\ u \end{bmatrix} \right\| \quad \text{subject to} \quad [A, B] \begin{bmatrix} x \\ u \end{bmatrix} = b$$

which is a simple equality-constrained linear least-squares problem. Algorithms such as those described in [8], especially the null-space method [8, Chapter 20], can be applied directly to solve the above problem. However, as also pointed out in [10] (which is in the setting of general Gauss-Markov linear models without regularization), such an approach does not treat $\boldsymbol{x}$, $\boldsymbol{u}$, A, B and C separately and in turn can not take advantage of any special structure of the problem. The following algorithm tries to take these aspects into account, and is inspired by the work of Paige [10,11]. The algorithm requires that the assumptions (4a) and (4b) be satisfied.

Step 1. Make a QR decomposition of B so that $B = Q \begin{bmatrix} B_1 \\ 0 \end{bmatrix}$, where $B_1 \in \mathbb{R}^{p \times p}$ is upper triangular and nonsingular. Let

$$Q^T [A, b] = \begin{array}{c} \begin{bmatrix} A_1 & b_1 \\ A_2 & b_2 \end{bmatrix} \end{array} \begin{array}{l} p \\ m-p \end{array} . \tag{21}$$

Step 2. Make the following decomposition of A_2:

$$A_2 U = \begin{array}{c} [\; 0 \;,\; A_{22} \;] \\ \begin{array}{cc} n-i & i \end{array} \end{array} m-p$$

so that U is orthogonal and $A_{22} \in \mathbb{R}^{(m-p) \times i}$ is of full column rank i. Let

$$\begin{bmatrix} A_1 \\ C \end{bmatrix} U = \begin{array}{c} \begin{bmatrix} A_{11} & A_{12} \\ C_1 & C_2 \end{bmatrix} \\ \begin{array}{cc} n-i & i \end{array} \end{array} \quad \text{and} \quad U^T \boldsymbol{x} = \begin{bmatrix} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \end{bmatrix} \begin{array}{l} n-i \\ i \end{array} . \tag{22}$$

Then $\begin{bmatrix} A_{11} \\ C_1 \end{bmatrix}$ is of full column rank.

Step 3 (including consistency check). Make a QR decomposition of A_{22} such that $A_{22} = Q_1 \begin{bmatrix} \tilde{A}_{22} \\ 0 \end{bmatrix}$ where $\tilde{A}_{22} \in \mathbb{R}^{i \times i}$ is upper triangular and nonsingular, and let $Q_1^T b_2 = \begin{bmatrix} b_2^{(1)} \\ b_2^{(2)} \end{bmatrix}$, with $b_2^{(1)} \in \mathbb{R}^i$. Then the regularized general Gauss-Markov linear model is consistent only if $b_2^{(2)} = \mathbf{0}$. In this case,

$$\boldsymbol{x}_2 = \tilde{A}_{22}^{-1} b_2^{(1)} . \tag{23}$$

After some manipulation, we obtain the following ordinary least-squares problem, which only involves the component $\boldsymbol{x}_1$:

$$\min \left\| \begin{bmatrix} \lambda C_1 \\ B_1^{-1} A_{11} \end{bmatrix} \boldsymbol{x}_1 - \begin{bmatrix} \lambda C_2 \boldsymbol{x}_2 \\ B_1^{-1} (b_1 - A_{12} \boldsymbol{x}_2) \end{bmatrix} \right\| . \tag{24}$$

Step 4. The observation here is that we do not need to explicitly compute the matrix products involving B_1^{-1} in order to solve the above problem, and this enhances the numerical stability of the algorithm. In fact, (24) is equivalent to the 'standard' problem described in [11] with

$$\tilde{y} = \begin{bmatrix} \lambda C_2 x_2 \\ b_1 - A_{12} x_2 \end{bmatrix} \quad , \quad \tilde{C} = \begin{bmatrix} \lambda C_1 \\ A_{11} \end{bmatrix} \quad \text{and} \quad \tilde{B} = \begin{bmatrix} I & 0 \\ 0 & B_1 \end{bmatrix} .$$

We only need to choose orthogonal $\tilde{P}$ and $\tilde{Q}$ such that

$$\tilde{Q}^T [\ \tilde{C}\ ,\ \tilde{y}\ ,\ \tilde{B}\ ] \begin{bmatrix} I & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \tilde{P} \end{bmatrix} = \begin{array}{c} \left[\begin{array}{ccccc} R & \tau & R_1 & r & R_{12} \\ 0 & \eta & 0 & \rho & w^T \\ 0 & 0 & 0 & 0 & R_2 \end{array} \right] n-i \\ \begin{array}{ccccc} n-i & 1 & n-i & 1 & \end{array} \end{array} \tag{25}$$

where R, R_1 and R_2 are upper triangular and nonsingular. Now, if we let

$$\tilde{P}^T u = v = \begin{array}{c} \begin{bmatrix} v_1 \\ \mu \\ v_2 \end{bmatrix} \end{array} \begin{array}{l} n-i \\ 1 \\ p+q-(n-i)-1 \end{array}$$

then x_1 can be obtained by solving the following nonsingular upper triangular linear system

$$\begin{bmatrix} R & r \\ 0^T & \rho \end{bmatrix} \begin{bmatrix} x_1 \\ \mu \end{bmatrix} = \begin{bmatrix} \tau \\ \eta \end{bmatrix} . \tag{26}$$

For details, see [11].

Step 5. The unique solution is given by

$$x_\lambda = U \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} . \tag{27}$$

We now give some more details about the factorization of Eq. (25). Since $\tilde{B}$ is block diagonal, we can employ this in the reduction step. In order to illustrate the situation, we give below a low-dimension example with $p = q = n - i + 1 = 3$. We first use a QR decomposition to transform $[\lambda C_1, \lambda C_2 x_2]$ to upper triangular form. Since the first block of $\tilde{B}$ is an identity matrix, the effect of this transformation can be compensated by multiplying u by the orthogonal matrix, so that at the initial stage we have

$$\left([\tilde{C}\ ,\ \tilde{y}\ ],\ \tilde{B} \right) = \left(\begin{bmatrix} \times & \times & \times \\ & \times & \times \\ & & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix} , \begin{bmatrix} \times & & & & & \\ & \times & & & & \\ & & \times & & & \\ & & & \times & \times & \times \\ & & & & \times & \times \\ & & & & & \times \end{bmatrix} \right) .$$

We can now reduce the leftmost matrix $[\tilde{C}, \tilde{y}]$ to triangular form, while maintaining the triangular form of the rightmost matrix $\tilde{B}$, by a sequence of left and right Givens transformations. Fig. 1 below illustrates how to eliminate the first column of the lower part of the first matrix. The same procedure can be continued in a similar way until we obtain the decomposition in (25). Throughout, $\rightarrow$ shows the two rows or columns involved in the Givens transformation, and $\circ$ indicates the element being annihilated.

$$
\begin{array}{c}\rightarrow\\ \\ \\ \\ \\ \rightarrow\end{array}
\begin{bmatrix} \times & \times & \times \\ & \times & \times \\ & & \times \\ \times & \times & \times \\ \times & \times & \times \\ \circ & \times & \times \end{bmatrix}
\begin{bmatrix} \times & & & & & \\ & \times & & & & \\ & & \times & & & \\ & & & \times & \times & \times \\ & & & & \times & \times \\ & & & & & \times \end{bmatrix}
\qquad
\begin{bmatrix} \times & \times & \times \\ & \times & \times \\ & & \times \\ \times & \times & \times \\ \times & \times & \times \\ & \times & \times \end{bmatrix}
\begin{array}{c}
\begin{bmatrix} \times & & & & & \times \\ & \times & & & & \\ & & \times & & & \\ & & & \times & \times & \times \\ & & & & \times & \times \\ \circ & & & & & \times \end{bmatrix} \\
\begin{matrix} \uparrow & & & & & \uparrow \end{matrix}
\end{array}
$$

$$
\begin{array}{c}\rightarrow\\ \\ \\ \\ \rightarrow\\ \\ \end{array}
\begin{bmatrix} \times & \times & \times \\ & \times & \times \\ & & \times \\ \times & \times & \times \\ \circ & \times & \times \\ & \times & \times \end{bmatrix}
\begin{bmatrix} \times & & & & & \times \\ & \times & & & & \\ & & \times & & & \\ \times & & & \times & \times & \times \\ \times & & & & \times & \times \\ & & & & & \times \end{bmatrix}
\qquad
\begin{bmatrix} \times & \times & \times \\ & \times & \times \\ & & \times \\ \times & \times & \times \\ & \times & \times \\ & \times & \times \end{bmatrix}
\begin{array}{c}
\begin{bmatrix} \times & & & & \times & \times \\ & \times & & & & \\ & & \times & & & \\ \times & & & \times & \times & \times \\ \circ & & & & \times & \times \\ & & & & & \times \end{bmatrix} \\
\begin{matrix} \uparrow & & & & \uparrow & \end{matrix}
\end{array}
$$

$$
\begin{array}{c}\rightarrow\\ \\ \\ \rightarrow\\ \\ \\ \end{array}
\begin{bmatrix} \times & \times & \times \\ & \times & \times \\ & & \times \\ \circ & \times & \times \\ & \times & \times \\ & \times & \times \end{bmatrix}
\begin{bmatrix} \times & & & & \times & \times \\ & \times & & & & \\ & & \times & & & \\ \times & & & \times & \times & \times \\ & & & & \times & \times \\ & & & & & \times \end{bmatrix}
\qquad
\begin{bmatrix} \times & \times & \times \\ & \times & \times \\ & & \times \\ & \times & \times \\ & \times & \times \\ & \times & \times \end{bmatrix}
\begin{array}{c}
\begin{bmatrix} \times & & & \times & \times & \times \\ & \times & & & & \\ & & \times & & & \\ \circ & & & \times & \times & \times \\ & & & & \times & \times \\ & & & & & \times \end{bmatrix} \\
\begin{matrix} \uparrow & & & \uparrow & & \end{matrix}
\end{array}
$$

Figure 1. The first steps in reducing the leftmost matrix to triangular form while maintaining the triangular form of the rightmost matrix.

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