

AN EFFICIENT ALGORITHM FOR A BOUNDED ERRORS-IN-VARIABLES MODEL*

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Abstract. We pose and solve a parameter estimation problem in the presence of bounded data uncertainties. The problem involves a minimization step and admits a closed form solution in terms of the positive root of a secular equation.

Key words. least-squares estimation, total least-squares, modeling errors, secular equation

AMS subject classifications. 15A06, 65F05, 65F10, 65F35, 65K10, 93C41, 93E10, 93E24

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1. Introduction. Parameter estimation in the presence of data uncertainties is a problem of considerable practical importance, and many estimators have been proposed in the literature with the intent of handling modeling errors and measurement noise. Among the most notable is the total least-squares (TLS) method [1, 2, 3, 4], also known as orthogonal regression or errors-in-variables method in statistics and system identification [5]. In contrast to the standard least-squares problem, the TLS formulation allows for errors in the data matrix. Its performance may degrade in some situations where the effect of noise and uncertainties can be unnecessarily over-emphasized. This may lead to overly conservative results.

Assume $A \in \mathbf{R}^{m \times n}$ is a given full rank matrix with $m \geq n$, $b \in \mathbf{R}^m$ is a given vector, and consider the problem of solving the inconsistent linear system $A\hat{x} \approx b$ in the least-squares sense. The TLS solution assumes data uncertainties in A and proceeds to correct A and b by replacing them by their projections, \hat{A} and \hat{b} , onto a specific subspace, and by solving the consistent linear system of equations $\hat{A}\hat{x} = \hat{b}$. The spectral norm of the correction $(A - \hat{A})$ in the TLS solution is bounded by the smallest singular value of $\begin{bmatrix} A & b \end{bmatrix}$. While this norm might be small for vectors b that are close enough to the range space of A , it need not always be so. In other words, the TLS solution may lead to situations in which the correction in A is unnecessarily large. Consider, for example, a situation in which the uncertainties in A are very small and, say, A is almost known exactly. Assume further that b is far from the range space of A . In this case, it is not difficult to visualize that the TLS solution will need to modify (A, b) into (\hat{A}, \hat{b}) and may therefore end up with an overly corrected approximant for A , despite the fact that A is almost exact.

These facts motivate us to introduce a new parameter estimation formulation with a bound on the size of the allowable correction to A . The solution of the new

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formulation turns out to involve the minimization of a cost function in an “indefinite” metric, in a way that is similar to more recent works on robust (or H^∞) estimation and filtering (e.g., [6, 7, 8, 9]). However, the cost function considered in our work is more complex and, contrary to robust estimation where no prior bounds are imposed on the size of the disturbances, the problem of this paper shows how to solve the resulting optimization problem in the presence of such constraints. A “closed” form solution to the new optimization problem is obtained in terms of the positive root of a secular equation.

The solution method proposed in this paper proceeds by first providing a geometric interpretation of the new optimization problem, followed by an algebraic derivation that establishes that the optimal solution can in fact be obtained by solving a related “indefinite” regularized problem. The regression parameter of the regularization step is further shown to be obtained from the positive root of a secular equation. The solution involves an SVD step and its computational complexity amounts to $O(mn^2 + n^3)$, where n is the smaller matrix dimension. A summary of the problem and its solution is provided in section 4.7.

2. Problem statement. Let $A \in \mathbf{R}^{m \times n}$ be a given matrix with $m \geq n$ and let $b \in \mathbf{R}^m$ be a given nonzero vector, which are assumed to be linearly related via an unknown vector of parameters $x \in \mathbf{R}^n$,

$$(2.1) \quad b = Ax + v.$$

The vector $v \in \mathbf{R}^m$ explains the mismatch between Ax and the given vector (or observation) b .

We assume that the “true” coefficient matrix is $A + \delta A$ and that we know only an upper bound on the perturbation δA :

$$(2.2) \quad \|\delta A\|_2 \leq \eta,$$

with η being known and where the notation $\|\cdot\|_2$ denotes the 2-induced norm of a matrix argument (i.e., its maximum singular value) or the Euclidean norm of a vector argument. We pose the following optimization problem.

PROBLEM 1. *Given $A \in \mathbf{R}^{m \times n}$, with $m \geq n$, $b \in \mathbf{R}^m$, and a nonnegative real number η , determine, if possible, an \hat{x} that solves*

$$(2.3) \quad \min_{\hat{x}} \min \{ \|(A + \delta A)\hat{x} - b\|_2 : \|\delta A\|_2 \leq \eta \}.$$

It turns out that the existence of a unique solution to this problem will require a fundamental condition on the data (A, b, η) , which we describe in Lemma 3.1. When the condition is violated, the problem will become degenerate. In fact, such existence and uniqueness conditions also arise in other formulations of estimation problems (such as the TLS and H_∞ problems, which will be shown later to have some relation to the above optimization problem). In the H_∞ context, for instance, similar fundamental conditions arise, which when violated indicate that the problem does not have a meaningful solution (see, e.g., [6, 7, 8, 9]).

2.1. Intuition and explanation. Before discussing the solution of the optimization problem we formulated above, it will be helpful to gain some intuition into its significance.

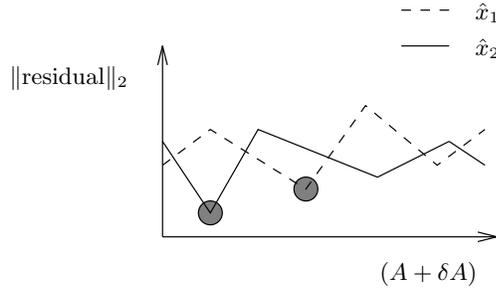


FIG. 2.1. Two illustrative residual-norm curves.

Intuitively, the above formulation corresponds to “choosing” a perturbation δA , within the bounded region, that would allow us to best predict the right-hand side b from the column span of $(A + \delta A)$. Comparing with the TLS formulation, we see that in TLS there is not an a priori bound on the size of the allowable perturbation δA . Still, the TLS solution finds the “smallest” δA (in a Frobenius norm sense) that would allow to estimate b from the column span of $(A + \delta A)$, viz., it solves the following problem [3]:

$$\min_{\delta A, \hat{x}} \left\| \begin{bmatrix} \delta A & (A + \delta A)\hat{x} - b \end{bmatrix} \right\|_F.$$

Nevertheless, although small in a certain sense, the resulting correction δA need not satisfy an a priori bound on its size. The problem we formulated above explicitly incorporates a bound on the size of the allowable perturbations. We may further add that we have addressed a related estimation problem in the earlier work [10], where we have posed and solved a min-max optimization problem; it allows us to guarantee optimal performance in a worst-case scenario. Further discussion, from a geometric point of view, of this related problem and others, along with examples of applications in image processing, communications, and control, can be found in [11].

Returning to (2.3), we depict the situation in Figure 2.1. Any particular choice for \hat{x} would lead to many residual norms,

$$\| (A + \delta A)\hat{x} - b \|_2,$$

one for each possible choice of δA . A second choice for \hat{x} would lead to other residual norms, the minimum value of which need not be the same as the first choice. We want to choose an estimate \hat{x} that minimizes the minimum possible residual norm.

2.2. A geometric interpretation. The optimization problem (2.3) admits an interesting geometric formulation that highlights some of the issues involved in its solution. We explain this by considering a scalar example. For the vector case, see [11].

Assume that we have a unit-norm vector b , $\|b\|_2 = 1$, and that A is simply a column vector, say a , with $\eta \neq 0$. Now problem (2.3) becomes

$$(2.4) \quad \min_{\hat{x}} \left(\min_{\|\delta a\|_2 \leq \eta} \| (a + \delta a)\hat{x} - b \|_2 \right).$$

This situation is depicted in Figure 2.2. The vectors a and b are indicated in thick black lines. The vector a is shown in the horizontal direction and a circle of radius η around its vertex indicates the set of all possible vertices for $a + \delta a$.

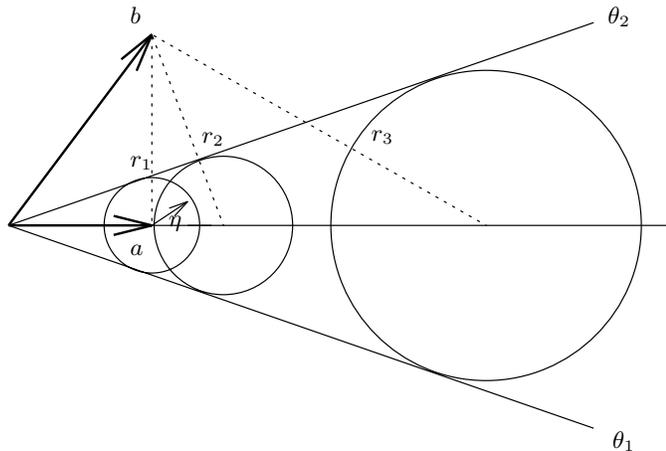


FIG. 2.2. Geometric construction of the solution for a simple example.

For any \hat{x} that we pick, the set $\{(a + \delta a)\hat{x}\}$ describes a disc of center $a\hat{x}$ and radius $\eta\hat{x}$. This is indicated in the figure by the largest rightmost circle, which corresponds to a choice of a positive \hat{x} that is larger than one. The vector in $\{(a + \delta a)\hat{x}\}$ that is the closest to b is the one obtained by drawing a line from b through the center of the rightmost circle. The intersection of this line with the circle defines a residual vector r_3 whose norm is the smallest among all possible residual vectors in the set $\{(a + \delta a)\hat{x}\}$.

Likewise, if we draw a line from b that passes through the vertex of a (which is the center of the leftmost circle), it will intersect the circle at a point that defines a residual vector r_1 . This residual will have the smallest norm among all residuals that correspond to the particular choice $\hat{x} = 1$.

More generally, for any \hat{x} that we pick, it will determine a circle and the corresponding smallest residual is obtained by finding the closest point on the circle to b . This is the point where the line that passes through b and the center of the circle intersects the circle on the side closer to b .

We need to pick an \hat{x} that minimizes the smallest residual norm. The claim is that we need to proceed as follows: we drop a perpendicular from b to the upper tangent line denoted by θ_2 . This perpendicular intersects the horizontal line in a point where we draw a new circle (the middle circle) that is tangent to both θ_1 and θ_2 . This circle corresponds to a choice of \hat{x} such that the closest point on it to b is the foot of the perpendicular from b to θ_2 . The residual indicated by r_2 is the desired solution; it has the minimum norm among the smallest residuals.

3. An equivalent minimization problem. To solve (2.3), we start by showing how to reduce it to an equivalent problem. For this purpose, we note that

$$(3.1) \quad \|(A + \delta A)\hat{x} - b\|_2 \geq \left| \|A\hat{x} - b\|_2 - \|\delta A\hat{x}\|_2 \right|.$$

The lower bound on the right-hand side of the above inequality is a nonnegative quantity and, therefore, the least it can get is zero. This will in turn depend on how big or how small the value of $\|\delta A\|_2$ can be.

For example, if it happens that for all vectors \hat{x} we always have

$$(3.2) \quad \eta\|\hat{x}\|_2 < \|A\hat{x} - b\|_2,$$

then we conclude, using the triangle inequality of norms, that

$$\|\delta A \hat{x}\|_2 \leq \|\delta A\|_2 \|\hat{x}\|_2 \leq \eta \|\hat{x}\|_2 < \|A\hat{x} - b\|_2 .$$

It then follows from (3.1) that, under assumption (3.2), we obtain

$$\begin{aligned} \|(A + \delta A)\hat{x} - b\|_2 &\geq \|A\hat{x} - b\|_2 - \|\delta A\hat{x}\|_2 \\ &\geq \|A\hat{x} - b\|_2 - \|\delta A\|_2 \|\hat{x}\|_2 \\ &\geq \|A\hat{x} - b\|_2 - \eta \|\hat{x}\|_2 . \end{aligned}$$

It turns out that condition (3.2) is the main (and only) case of interest in this paper, especially since we shall argue later that a degenerate problem arises when it is violated. For this reason, we shall proceed for now with our analysis under assumption (3.2) and shall postpone our discussion of what happens when it is violated until later in this section.

Now the lower bound in (3.1) is in fact achievable. That is, there exists a δA for which

$$\|(A + \delta A)\hat{x} - b\|_2 = \|A\hat{x} - b\|_2 - \eta \|\hat{x}\|_2 .$$

To see that this is indeed the case, choose δA as the rank-1 matrix

$$\delta A^o = - \frac{(A\hat{x} - b)}{\|A\hat{x} - b\|_2} \frac{\hat{x}^T}{\|\hat{x}\|_2} \eta .$$

This leads to a vector $\delta A^o \hat{x}$ that is collinear with the vector $(A\hat{x} - b)$. (Note that \hat{x} in the above definition for δA^o cannot be zero since otherwise (3.2) cannot be satisfied. Likewise, $A\hat{x} - b$ cannot be zero. Hence, δA^o is well defined.)

We are therefore reduced to the solution of the following optimization problem.

PROBLEM 2. Consider a matrix $A \in \mathbf{R}^{m \times n}$, with $m \geq n$, a vector $b \in \mathbf{R}^m$, and a nonnegative real number η , and assume that for all vectors \hat{x} it holds that

$$(3.3) \quad \eta \|\hat{x}\|_2 < \|A\hat{x} - b\|_2 \quad (\text{fundamental assumption}).$$

Determine, if possible, an \hat{x} that solves

$$(3.4) \quad \min_{\hat{x}} (\|A\hat{x} - b\|_2 - \eta \|\hat{x}\|_2) .$$

3.1. Connections to TLS and H_∞ -problems. Before solving problem (3.4), we elaborate on its connections with other formulations in the literature that also attempt, in one way or another, to take into consideration uncertainties and perturbations in the data.

First, cost functions similar to (3.4) but with squared distances, say

$$(3.5) \quad \min_{\hat{x}} (\|A\hat{x} - b\|_2^2 - \gamma \|\hat{x}\|_2^2)$$

for some $\gamma > 0$, often arise in the study of indefinite quadratic cost functions in robust or H^∞ estimation (see, e.g., the developments in [8, 9]). The major distinction between this cost and the one posed in (3.4) is that the latter involves *distance* terms

and it will be shown to provide an automatic procedure for selecting a “regularization” factor that plays the role of γ in (3.5).

Likewise, the TLS problem seeks a matrix δA and a vector \hat{x} that minimize the following Frobenius norm:

$$(3.6) \quad \min_{\delta A, \hat{x}} \left\| \begin{bmatrix} \delta A & (A + \delta A)\hat{x} - b \end{bmatrix} \right\|_F^2.$$

The solution of the above TLS problem is well known and is given by the following construction [4, p. 36]. Let $\{\sigma_1, \dots, \sigma_n\}$ denote the singular values of A , with $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n \geq 0$. Let also $\{\bar{\sigma}_1, \dots, \bar{\sigma}_n, \bar{\sigma}_{n+1}\}$ denote the singular values of the extended matrix $\begin{bmatrix} A & b \end{bmatrix}$, with $\bar{\sigma}_i \geq 0$. If $\bar{\sigma}_{n+1} < \sigma_n$, then a unique solution \hat{x} of (3.6) exists and is given by

$$(3.7) \quad \hat{x} = (A^T A - \bar{\sigma}_{n+1}^2 I)^{-1} A^T b.$$

For our purposes, it is more interesting to consider the following interpretation of the TLS solution (see, e.g., [9]). Note that the condition $\bar{\sigma}_{n+1} < \sigma_n$ ensures that $(A^T A - \bar{\sigma}_{n+1}^2 I)$ is a positive-definite matrix, since σ_n^2 is the smallest eigenvalue of $A^T A$. Therefore, we can regard (3.7) as the solution of the following optimization problem, with an indefinite cost function:

$$\min_{\hat{x}} (\|A\hat{x} - b\|_2^2 - \bar{\sigma}_{n+1}^2 \|\hat{x}\|_2^2).$$

This is a special form of (3.5) with a particular choice for γ . It again involves squared distances, while (3.4) involves *distance* terms and it will provide another choice of a γ -like parameter. In particular, compare (3.7) with the expression (4.4) derived further ahead for the solution of (3.4). We see that the new problem replaces $\bar{\sigma}_{n+1}^2$ with a new parameter α that will be obtained from the positive root of a secular (nonlinear) equation.

3.2. Significance of the fundamental assumption. We shall solve (3.4) in the next section. Here, we elaborate on the significance of the condition (3.3). Assume (3.3) is violated at some nonzero point $\hat{x}^{(1)}$, namely¹

$$(3.8) \quad \eta \|\hat{x}^{(1)}\|_2 \geq \|A\hat{x}^{(1)} - b\|_2,$$

and define the perturbation

$$(3.9) \quad \delta A^{(1)} = (A\hat{x}^{(1)} - b) \frac{(\hat{x}^{(1)})^T}{\|\hat{x}^{(1)}\|_2^2}.$$

It is clear that $\delta A^{(1)}$ is a valid perturbation since, in view of (3.8), we have $\|\delta A^{(1)}\|_2 \leq \eta$. But this particular perturbation leads to

$$\begin{aligned} \left\| (A + \delta A^{(1)}) \hat{x}^{(1)} - b \right\|_2 &\geq \left| \|A\hat{x}^{(1)} - b\|_2 - \|\delta A^{(1)} \hat{x}^{(1)}\|_2 \right| \\ &\geq \|A\hat{x}^{(1)} - b\|_2 - \|A\hat{x}^{(1)} - b\|_2 = 0. \end{aligned}$$

That is, the lower limit of zero is achieved for $(\delta A^{(1)}, x^{(1)})$ and $x^{(1)}$ can be taken as a solution to (2.3). In fact, there are many possible solutions in this case. For example,

¹If violation occurs for some zero $\hat{x}^{(1)}$ this means that we must necessarily have $b = 0$, which contradicts our assumption of a nonzero vector b .

once one such $x^{(1)}$ has been found, an infinite number of others can be constructed from it. To verify this claim, assume $x^{(1)}$ is a vector that satisfies (3.8), viz., it satisfies

$$(3.10) \quad \eta \|\hat{x}^{(1)}\|_2 = \|A\hat{x}^{(1)} - b\|_2 + \epsilon,$$

for some $\epsilon \geq 0$. Now assume we replace $x^{(1)}$ by $x^{(2)} = (x^{(1)} + \delta)$ for some vector δ to be determined so as to violate condition (3.3) and, therefore, also satisfy a relation of the form

$$(3.11) \quad \eta \|\hat{x}^{(2)}\|_2 \geq \|A\hat{x}^{(2)} - b\|_2.$$

If such an $x^{(2)}$ can be found, then constructing the corresponding $\delta A^{(2)}$ as in (3.9) would also lead to a solution $(\delta A^{(2)}, x^{(2)})$.

Condition (3.11) requires a choice for the vector δ such that

$$(3.12) \quad \eta \|\hat{x}^{(1)} + \delta\|_2 \geq \|A(\hat{x}^{(1)} + \delta) - b\|_2.$$

But this can be satisfied by imposing the sufficient condition

$$\eta \|x^{(1)}\|_2 - \eta \|\delta\|_2 \geq \|A\hat{x}^{(1)} - b\|_2 + \|A\|_2 \|\delta\|_2,$$

where the left-hand side is the smallest $\eta \|\hat{x}^{(1)} + \delta\|_2$ can get, while the right-hand side is the largest $\|A(\hat{x}^{(1)} + \delta) - b\|_2$ can get. Solving for $\|\delta\|_2$ we see that any vector δ that satisfies

$$\|\delta\|_2 \leq \frac{\epsilon}{\eta + \|A\|_2}$$

will lead to a new vector $\hat{x}^{(2)}$ that also violates (3.3). Consequently, given any single nonzero violation $\hat{x}^{(1)}$, many others can be obtained by suitably perturbing it.

We shall not treat the degenerate case in this paper (nor the case when (3.8) is violated only with equality). We shall instead assume throughout that the fundamental condition (3.3) holds. Under this assumption, the problem will turn out to always have a unique solution.

3.3. The fundamental condition for nondegeneracy. The fundamental condition (3.3) needs to be satisfied for all vectors \hat{x} . This can be restated in terms of conditions on the data (A, b, η) alone. To see this, note that (3.3) implies, by squaring, that we must have

$$(3.13) \quad J(\hat{x}) \triangleq \hat{x}^T (\eta^2 I - A^T A) \hat{x} + 2\hat{x}^T A^T b - b^T b < 0 \text{ for all } \hat{x}.$$

That is, the quadratic form $J(\hat{x})$ that is defined on the left-hand side of (3.13) must be negative for any value of the independent variable \hat{x} . This is possible only if

- (i) the quadratic form $J(\hat{x})$ has a maximum with respect to \hat{x} , and
- (ii) the value of $J(\hat{x})$ at its maximum is negative.

The necessary condition for the existence of a unique maximum (since we have a quadratic cost function) is

$$(3.14) \quad (\eta^2 I - A^T A) < 0,$$

which means that η should satisfy

$$(3.15) \quad \eta < \sigma_{min}(A).$$

Under this condition, the expression for the maximum point \hat{x}_{max} of $J(\hat{x})$ is

$$\hat{x}_{max} = (A^T A - \eta^2 I)^{-1} A^T b.$$

Evaluating $J(\hat{x})$ at $\hat{x} = \hat{x}_{max}$ we obtain

$$J(\hat{x}_{max}) = b^T [A(A^T A - \eta^2 I)^{-1} A^T - I] b.$$

Therefore, the requirement that $J(\hat{x}_{max})$ be negative corresponds to

$$(3.16) \quad b^T [I - A(A^T A - \eta^2 I)^{-1} A^T] b > 0.$$

LEMMA 3.1. *Necessary and sufficient conditions in terms of (A, b, η) for the fundamental relation (3.3) to hold are the following:*

$$(3.17) \quad (\eta^2 I - A^T A) < 0 \quad \iff \quad \eta < \sigma_{min}(A),$$

and

$$(3.18) \quad b^T [I - A(A^T A - \eta^2 I)^{-1} A^T] b > 0.$$

Note that for a well-defined problem of the form (2.3) we need to assume $\eta > 0$ which, in view of (3.17), means that A should be full rank so that $\sigma_{min}(A) > 0$. We therefore assume, from now on, that

A is full rank.

We further introduce the SVD of A :

$$(3.19) \quad A = U \begin{bmatrix} \Sigma \\ 0 \end{bmatrix} V^T,$$

where $U \in \mathbf{R}^{m \times m}$ and $V \in \mathbf{R}^{n \times n}$ are orthogonal and $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_n)$ is diagonal, with

$$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_{n-1} \geq \sigma_n > 0$$

being the singular values of A . We further partition the vector $U^T b$ into

$$(3.20) \quad \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = U^T b,$$

where $b_1 \in \mathbf{R}^n$ and $b_2 \in \mathbf{R}^{m-n}$.

While solving the minimization problem (3.4), we shall first assume that the two smallest singular values of A are distinct and, hence, satisfy

$$\sigma_n < \sigma_{n-1}.$$

Later, in section 4.6, we consider the case in which multiple singular values can occur.

4. Solving the minimization problem. To solve (3.4), we define the non-convex cost function

$$\mathcal{L}(\hat{x}) = \|A\hat{x} - b\|_2 - \eta\|\hat{x}\|_2,$$

which is continuous in \hat{x} and bounded from below by zero in view of (3.3). A minimum point for $\mathcal{L}(\hat{x})$ can occur only at ∞ , at points where $\mathcal{L}(\hat{x})$ is not differentiable, or at points where its gradient, $\nabla\mathcal{L}(\hat{x})$, is 0. In particular, note that $\mathcal{L}(\hat{x})$ is not differentiable only at $\hat{x} = 0$ and at any \hat{x} that satisfies $A\hat{x} - b = 0$. But points \hat{x} satisfying $A\hat{x} - b = 0$ are excluded by the fundamental condition (3.3). Also, we can rule out $\hat{x} = \infty$ since

$$\lim_{\|\hat{x}\|_2 \rightarrow \infty} \mathcal{L}(\hat{x}) = \lim_{\|\hat{x}\|_2 \rightarrow \infty} \|A\hat{x}\|_2 - \eta\|\hat{x}\|_2 \geq (\sigma_n - \eta)\|\hat{x}\|_2 \rightarrow +\infty.$$

Now at points where $\mathcal{L}(\hat{x})$ is differentiable, the gradient of \mathcal{L} is given by

$$\begin{aligned} \nabla\mathcal{L}(\hat{x}) &= \frac{1}{\|A\hat{x} - b\|_2} A^T (A\hat{x} - b) - \frac{\eta}{\|\hat{x}\|_2} \hat{x} \\ &= \frac{1}{\|A\hat{x} - b\|_2} ((A^T A - \alpha I) \hat{x} - A^T b), \end{aligned}$$

where we have introduced the positive real number

$$(4.1) \quad \alpha = \frac{\eta\|A\hat{x} - b\|_2}{\|\hat{x}\|_2}.$$

In view of the fundamental condition (3.3) we see that the value of α is necessarily larger than η^2 ,

$$(4.2) \quad \alpha > \eta^2.$$

Likewise, the Hessian of \mathcal{L} is given by

$$(4.3) \quad \Delta\mathcal{L}(\hat{x}) = \frac{A^T A}{\|A\hat{x} - b\|_2} - \frac{\eta}{\|\hat{x}\|_2} I - \frac{A^T (A\hat{x} - b)(A\hat{x} - b)^T A}{\|A\hat{x} - b\|_2^3} + \eta \frac{\hat{x}\hat{x}^T}{\|\hat{x}\|_2^3}.$$

The critical points of $\mathcal{L}(\hat{x})$ (where the gradient is singular) satisfy

$$A^T (A\hat{x} - b) - \alpha\hat{x} = 0$$

or, equivalently,

$$(4.4) \quad (A^T A - \alpha I) \hat{x} = A^T b.$$

Equations (4.1) and (4.4) completely specify the stationary points of $\mathcal{L}(\hat{x})$. They provide two equations in the unknowns (α, \hat{x}) . We can use (4.4) to eliminate \hat{x} from (4.1) and, hence, obtain an equation in α . Once we solve for α , we can then use (4.4) to determine the solution \hat{x} . The equation we obtain for α will in general be a nonlinear equation and the desired α will be a root of it. The purpose of the discussion in what follows is to show where the root α that corresponds to the global minimizer of \mathcal{L} lies and how to find it.

We know from (4.2) that $\alpha > \eta^2$. We shall soon show that we need only to look for the solution α in the interval $(\eta^2, \sigma_{n-1}^2]$ —see (4.5). (Further analysis later in the

paper will in fact show that α lies within the smaller interval $(\eta^2, \sigma_n^2]$. Hence, the coefficient matrix $(A^T A - \alpha I)$ in (4.4) is always nonsingular except for $\alpha = \sigma_{n-1}^2$ or $\alpha = \sigma_n^2$.

In summary, we see that the candidate solutions \hat{x} to our minimization problem are the following:

1. $\hat{x} = 0$, which is a point at which \mathcal{L} is not differentiable. We shall show that $\hat{x} = 0$ cannot be a global minimizer of \mathcal{L} .
2. Solution(s) (α, \hat{x}) to (4.1) and (4.4) when $(A^T A - \alpha I)$ is invertible. In this case, we will see that α can lie only in the open interval (η^2, σ_n^2) .
3. Solutions (α, \hat{x}) to (4.1) and (4.4) when $(A^T A - \alpha I)$ is singular. We will see that this can happen only for the choices $\alpha = \sigma_{n-1}^2$ or $\alpha = \sigma_n^2$.

The purpose of the analysis in the sequel is to rule out all the possibilities except for one as a global minimum for \mathcal{L} . In loose terms, we shall show that in general a unique global minimizer (α, \hat{x}) exists and that the corresponding α lies in the open interval (η^2, σ_n^2) . Only in a degenerate case, the solution is obtained by taking $\alpha = \sigma_n^2$ and by solving (4.4) for \hat{x} . In other words, the global minimum will be obtained from the stationary points of \mathcal{L} , which is why we continue to focus on them.

The final statement of the solution is summarized in section 4.7.

4.1. Positivity of the Hessian matrix. We are of course interested only in those critical points of \mathcal{L} that are candidates for local minima. Hence, the Hessian matrix at these points must be positive semidefinite.

Since $A^T(A\hat{x} - b) = \alpha\hat{x}$ at a critical point, we conclude from (4.3) that

$$\begin{aligned} \Delta\mathcal{L}(\hat{x}) &= \frac{1}{\|A\hat{x} - b\|_2} (A^T A - \alpha I) + \left(-\frac{\alpha^2}{\|A\hat{x} - b\|_2^3} + \frac{\eta}{\|\hat{x}\|_2^3} \right) \hat{x}\hat{x}^T \\ &= \frac{1}{\|A\hat{x} - b\|_2} (A^T A - \alpha I) + \frac{1}{\|A\hat{x} - b\|_2^3} \left(-\alpha^2 + \frac{\alpha^3}{\eta^2} \right) \hat{x}\hat{x}^T \\ &= \frac{1}{\|A\hat{x} - b\|_2} (A^T A - \alpha I) + \frac{\alpha^2}{\|A\hat{x} - b\|_2^3 \eta^2} (\alpha - \eta^2) \hat{x}\hat{x}^T. \end{aligned}$$

Now observe that the second term is a symmetric rank-1 matrix that is also positive-semidefinite since $\alpha > \eta^2$. Hence, in view of the Cauchy interlacing theorem [3] the smallest eigenvalue of $\Delta\mathcal{L}(\hat{x})$ will lie between the two smallest eigenvalues of the matrix $\frac{1}{\|A\hat{x} - b\|_2} (A^T A - \alpha I)$. This shows that the value of α cannot exceed σ_{n-1}^2 since otherwise the two smallest eigenvalues of $(A^T A - \alpha I)$ will be nonpositive and the Hessian matrix will have a nonpositive eigenvalue.

The above argument explains why we need only to look for α in the interval

$$(4.5) \quad \eta^2 < \alpha \leq \sigma_{n-1}^2.$$

4.2. Solving for \hat{x} and the secular equation. Given that we need only consider values of α in the interval $(\eta^2, \sigma_{n-1}^2]$, we can now solve for \hat{x} using (4.1) and (4.4). Two cases should be considered since the coefficient matrix $(A^T A - \alpha I)$ may be singular for $\alpha = \sigma_n^2$ or $\alpha = \sigma_{n-1}^2$.

I. The case $\alpha \notin \{\sigma_n^2, \sigma_{n-1}^2\}$. From (4.4) we see that among the α 's in the interval (4.5), as long as α is not equal to either σ_n^2 or σ_{n-1}^2 , the critical point \hat{x} associated with α is given uniquely by

$$\hat{x} = (A^T A - \alpha I)^{-1} A^T b \quad \text{for } \alpha \in (\eta^2, \sigma_{n-1}^2] \text{ and } \alpha \neq \sigma_n^2, \sigma_{n-1}^2.$$

Moreover, from (4.1) and (4.4) we see that

$$\mathcal{G}(\alpha) \triangleq \|\hat{x}\|_2^2 - \frac{\eta^2 \|A\hat{x} - b\|_2^2}{\alpha^2} = 0.$$

Substituting for \hat{x} and using the SVD of A to simplify we obtain the equivalent expressions for \hat{x} and $\mathcal{G}(\alpha)$:

$$(4.6) \quad \hat{x} = V(\Sigma^2 - \alpha I)^{-1} \Sigma b_1,$$

$$(4.7) \quad \mathcal{G}(\alpha) = b_1^T (\Sigma^2 - \eta^2 I) (\Sigma^2 - \alpha I)^{-2} b_1 - \frac{\eta^2 \|b_2\|_2^2}{\alpha^2}.$$

Clearly the roots of $\mathcal{G}(\alpha)$ that lie in the interval $(\eta^2, \sigma_{n-1}^2]$ will correspond to critical points that are candidates for local minima. Therefore we will later investigate the roots of $\mathcal{G}(\alpha)$.

II. The case $\alpha = \sigma_n^2$ or $\alpha = \sigma_{n-1}^2$. From (4.4) we see that $\alpha = \sigma_n^2$ or $\alpha = \sigma_{n-1}^2$ can correspond to a critical point \hat{x} only if either $u_n^T b = 0$ (for $\alpha = \sigma_n^2$) or $u_{n-1}^T b = 0$ (for $\alpha = \sigma_{n-1}^2$). Here, $\{u_n, u_{n-1}\}$ denote the columns of U that correspond to $\{\sigma_n, \sigma_{n-1}\}$, i.e., the last two columns of U .

Here we show only how to solve for \hat{x} when $\alpha = \sigma_n^2$. The technique for $\alpha = \sigma_{n-1}^2$ is similar.

From (4.4) it is clear that $\alpha = \sigma_n^2$ is a candidate for a critical point if and only if $u_n^T b = 0$. In this case the associated \hat{x} 's (there may be more than one) satisfy the equations

$$(4.8) \quad (A^T A - \sigma_n^2 I) \hat{x} = A^T b$$

and

$$(4.9) \quad \sigma_n^2 = \eta \frac{\sqrt{\|b_2\|_2^2 + \|\Sigma V^T \hat{x} - b_1\|_2^2}}{\|\hat{x}\|_2}.$$

Now we define $y \triangleq V^T \hat{x}$ and consider the following partitionings:

$$y = \begin{bmatrix} \bar{y} \\ y_n \end{bmatrix}, \quad b_1 = \begin{bmatrix} \bar{b}_1 \\ 0 \end{bmatrix}, \quad \Sigma = \begin{bmatrix} \bar{\Sigma} & 0 \\ 0 & \sigma_n \end{bmatrix}.$$

The quantities \hat{x} and y define each other uniquely and $\|y\|_2 = \|\hat{x}\|_2$.

It follows from (4.8) that

$$(4.10) \quad \bar{y} = (\bar{\Sigma}^2 - \sigma_n^2 I)^{-1} \bar{\Sigma} \bar{b}_1.$$

Substituting this into (4.9) we have

$$\sigma_n^4 = \eta^2 \frac{\|b_2\|_2^2 + \|\bar{\Sigma}^2 (\bar{\Sigma}^2 - \sigma_n^2 I)^{-1} \bar{b}_1 - \bar{b}_1\|_2^2 + \sigma_n^2 y_n^2}{\|\bar{y}\|_2^2 + y_n^2}.$$

Solving for y_n^2 we obtain

$$\begin{aligned} y_n^2 &= -\sigma_n^2 \frac{\bar{b}_1^T (\bar{\Sigma}^2 - \eta^2 I) (\bar{\Sigma}^2 - \sigma_n^2 I)^{-2} \bar{b}_1 - \|b_2\|_2^2 \eta^2 \sigma_n^{-4}}{\sigma_n^2 - \eta^2} \\ &= -\frac{\sigma_n^2}{\sigma_n^2 - \eta^2} \bar{\mathcal{G}}(\sigma_n^2), \end{aligned}$$

where we introduced the function

$$(4.11) \quad \bar{\mathcal{G}}(\alpha) \triangleq \bar{b}_1^T (\bar{\Sigma}^2 - \eta^2 I) (\bar{\Sigma}^2 - \alpha I)^{-2} \bar{b}_1 - \frac{\eta^2 \|b_2\|_2^2}{\alpha^2}.$$

Comparing with the definition (4.7) for $\mathcal{G}(\alpha)$ we see that

$$(4.12) \quad \bar{\mathcal{G}}(\alpha) = \mathcal{G}(\alpha) - (u_n^T b)^2 \frac{\sigma_n^2 - \eta^2}{(\sigma_n^2 - \alpha)^2}.$$

Note that $\mathcal{G}(\alpha) = \bar{\mathcal{G}}(\alpha)$ if $u_n^T b = 0$, which is the case when $\alpha = \sigma_n^2$ is a possibility. Therefore the possible values of y_n are

$$(4.13) \quad y_n = \frac{\sigma_n}{\sqrt{\sigma_n^2 - \eta^2}} \left(\pm \sqrt{-\bar{\mathcal{G}}(\sigma_n^2)} \right).$$

It follows that

$$(4.14) \quad u_n^T b = 0 \quad \text{and} \quad \bar{\mathcal{G}}(\sigma_n^2) \leq 0$$

are the necessary conditions for $\alpha = \sigma_n^2$ to correspond to a stationary double point at

$$(4.15) \quad \hat{x} = V \begin{bmatrix} (\bar{\Sigma}^2 - \sigma_n^2 I)^{-1} \bar{\Sigma} \bar{b}_1 \\ \frac{\sigma_n}{\sqrt{\sigma_n^2 - \eta^2}} \left(\pm \sqrt{-\bar{\mathcal{G}}(\sigma_n^2)} \right) \end{bmatrix}.$$

The global minimum. The purpose of the analysis in the following sections is to show that in general the global minimum is given by (4.6) with the corresponding α lying in the interval (η^2, σ_n^2) . When a root of the secular equation $\mathcal{G}(\alpha)$ in (4.7) does not exist in the open interval (η^2, σ_n^2) , we shall then show that the global minimum is given by (4.15).

4.3. The roots of the secular equation. We have argued earlier in (4.5) that the roots α of $\mathcal{G}(\alpha)$ that may lead to global minimizers \hat{x} can lie in the interval $(\eta^2, \sigma_{n-1}^2]$. We now determine how many roots can exist in this interval and later show that only the root lying in the subinterval (η^2, σ_n^2) corresponds to a global minimum when it exists. Otherwise, we have to use (4.15). The details are given below.

To begin with, we establish some properties of $\mathcal{G}(\alpha)$. From the nondegeneracy assumption (3.3) on the data it follows that $\mathcal{G}(\eta^2) < 0$. Moreover, from the expression (4.7) for $\mathcal{G}(\alpha)$ we see that it has a pole at σ_n^2 provided that $u_n^T b$ is not equal to zero, in which case

$$(4.16) \quad \lim_{\alpha \rightarrow \sigma_n^2} \mathcal{G}(\alpha) = +\infty.$$

Now observe from the expression for the derivative of $\mathcal{G}(\alpha)$,

$$(4.17) \quad \mathcal{G}'(\alpha) = 2 \left(b_1^T (\Sigma^2 - \eta^2 I) (\Sigma^2 - \alpha I)^{-3} b_1 \right) + \frac{\eta^2 \|b_2\|_2^2}{\alpha^3},$$

that $\mathcal{G}'(\alpha) > 0$ for $0 < \alpha < \sigma_n^2$. We conclude from these facts that $\mathcal{G}(\alpha)$ has exactly one root in the open interval (η^2, σ_n^2) . Actually, also since

$$\lim_{\alpha \rightarrow 0^+} \mathcal{G}(\alpha) = -\infty,$$

we conclude that when $u_n^T b \neq 0$, $\mathcal{G}(\alpha)$ has exactly one root in the interval $(0, \sigma_n^2)$ and that this root lies in the subinterval (η^2, σ_n^2) .

When $u_n^T b = 0$, the function $\mathcal{G}(\alpha)$ does not have a pole at σ_n^2 and, hence, (4.16) does not hold. However, by using the still-valid fact that $\lim_{\alpha \rightarrow 0^+} \mathcal{G}(\alpha) = -\infty$ and that $\mathcal{G}'(\alpha) > 0$ over the larger interval $(0, \sigma_{n-1}^2)$, we conclude the following:

1. If $u_{n-1}^T b \neq 0$ then $\lim_{\alpha \rightarrow \sigma_{n-1}^2} \mathcal{G}(\alpha) = +\infty$ and, hence, $\mathcal{G}(\alpha)$ has a unique root in the interval $(0, \sigma_{n-1}^2)$.
2. If we also have $u_{n-1}^T b = 0$, then $\mathcal{G}(\alpha)$ can have at most one root in the interval $(0, \sigma_{n-1}^2)$. The root may or may not exist.

What about the interval $(\sigma_n^2, \sigma_{n-1}^2)$ when $u_n^T b \neq 0$? We now establish that $\mathcal{G}(\alpha)$ can have at most two roots in this interval. For this purpose, we first observe that both $\mathcal{G}(\alpha)$ and $\alpha^2 \mathcal{G}(\alpha)$ have the same number of roots in $(\sigma_n^2, \sigma_{n-1}^2)$ (since we added only a double root at 0). Next we compute the first derivative of $\alpha^2 \mathcal{G}(\alpha)$, obtaining

$$\frac{d}{d\alpha} (\alpha^2 \mathcal{G}(\alpha)) = 2\alpha b_1^T (\Sigma^2 - \eta^2 I) \Sigma^2 (\Sigma^2 - \alpha I)^{-3} b_1.$$

Using this we compute the second derivative obtaining

$$\frac{d^2}{d\alpha^2} (\alpha^2 \mathcal{G}(\alpha)) = 2b_1^T (\Sigma^2 - \eta^2 I) \Sigma^2 (\Sigma^2 + 2\alpha I) (\Sigma^2 - \alpha I)^{-4} b_1.$$

It is clear that the second derivative is strictly positive for nonnegative α . From this we can conclude that $\alpha^2 \mathcal{G}(\alpha)$ and, hence, $\mathcal{G}(\alpha)$ have at most two zeros in $(\sigma_n^2, \sigma_{n-1}^2)$. We have therefore established the following result.

LEMMA 4.1. *The following properties hold for the function $\mathcal{G}(\alpha)$ defined in (4.7):*

1. *When $u_n^T b \neq 0$, the function $\mathcal{G}(\alpha)$ has a single root in the interval (η^2, σ_n^2) and at most two roots in the interval $(\sigma_n^2, \sigma_{n-1}^2)$. We label them as*

$$\eta^2 < \alpha_1 < \sigma_n^2 < \alpha_2 \leq \alpha_3 < \sigma_{n-1}^2.$$

2. *When $u_n^T b = 0$ and $u_{n-1}^T b \neq 0$, the function $\mathcal{G}(\alpha)$ has a unique root in the interval (η^2, σ_{n-1}^2) .*
3. *When $u_n^T b = 0$ and $u_{n-1}^T b = 0$, the function $\mathcal{G}(\alpha)$ has at most one root in the interval (η^2, σ_{n-1}^2) .*

It is essential to remember that the roots α_2 and α_3 may not exist, though they must occur as a pair (counting multiplicity) if they exist.

We now show that α_3 cannot correspond to a local minimum if $\alpha_2 < \alpha_3$, i.e., if the two roots in the interval $(\sigma_n^2, \sigma_{n-1}^2)$ are distinct. Indeed, assume α_2 and α_3 exist. Then from the last lemma it must hold that $u_n^T b \neq 0$ and α_1 must also exist. Hence, we must have $\mathcal{G}'(\alpha_2) < 0$ and $\mathcal{G}'(\alpha_3) > 0$.

If we assume $\alpha_2 < \alpha_3$, we shall use the fact that $\mathcal{G}'(\alpha_3) > 0$ to show that α_3 cannot correspond to a local minimum solution \hat{x} . This will be achieved by showing that the determinant of the Hessian of $\mathcal{L}(\hat{x})$ at α_3 is negative. For this we note that

$$\begin{aligned} \det(\Delta \mathcal{L}(\hat{x})) &= \frac{\det(A^T A - \alpha I)}{\|A\hat{x} - b\|_2^n} \left(1 + \frac{\alpha^2(\alpha - \eta^2)}{\|A\hat{x} - b\|_2^2 \eta^2} \hat{x}^T (A^T A - \alpha I)^{-1} \hat{x} \right) \\ &= \frac{\det(A^T A - \alpha I)}{\|A\hat{x} - b\|_2^{n+2} \eta^2} (\|A\hat{x} - b\|_2^2 \eta^2 + \alpha^2(\alpha - \eta^2) \hat{x}^T (A^T A - \alpha I)^{-1} \hat{x}). \end{aligned}$$

We introduce for convenience the shorthand notation

$$\xi \triangleq \frac{\det(A^T A - \alpha I)}{\|A\hat{x} - b\|_2^{n+2} \eta^2}.$$

Then, using the SVD of A ,

$$\begin{aligned} \det(\Delta\mathcal{L}(\hat{x})) &= \xi \left(\eta^2 \|b_2\|_2^2 + \alpha^3 b_1^T (\Sigma^2 - \eta^2 I) (\Sigma^2 - \alpha I)^{-3} b_1 \right) \\ &= \xi \frac{\alpha^3}{2} \mathcal{G}'(\alpha). \end{aligned}$$

Evaluating at $\alpha = \alpha_3$, and noting that $\det(A^T A - \alpha_3 I) < 0$ and $\mathcal{G}'(\alpha_3) > 0$, we conclude that $\det(\mathcal{L})$ at the \hat{x} corresponding to α_3 is negative. Hence, α_3 cannot correspond to a local minimum.

4.4. Candidates for minima. We can now be more explicit about the candidates for global minimizers of \mathcal{L} , which we mentioned just prior to section 4.1:

1. $\hat{x} = 0$, which corresponds to a point where \mathcal{L} is not differentiable.
2. If α_1 exists, then the corresponding \hat{x} is a candidate. Recall that α is guaranteed to exist if $u_n^T b \neq 0$. It may or may not exist otherwise.
3. If $u_n^T b \neq 0$ and α_2 exists, then the corresponding \hat{x} is a candidate.
4. If $u_n^T b = 0$, then the \hat{x} associated with $\alpha = \sigma_n^2$ is a candidate.
5. If $u_{n-1}^T b = 0$, then the \hat{x} associated with $\alpha = \sigma_{n-1}^2$ is a candidate.

We shall show that item 2 is the global minimizer when α_1 exists. Otherwise, item 4 is the global minimizer.

We start by showing that $\hat{x} = 0$ cannot be the global minimizer of \mathcal{L} . We divide our argument into two cases: $b_1 = 0$ and $b_1 \neq 0$. When $b_1 \neq 0$, we necessarily have $u_i^T b \neq 0$ for some i between 1 and n . Let $z = (u_i^T b / \sigma_i) V e_i$. Then $\mathcal{L}(0) = \|b\|_2$, and

$$\mathcal{L}(z) = \|b - (u_i^T b) u_i\| - \frac{\eta}{\sigma_i} |u_i^T b|.$$

The term $b - (u_i^T b) u_i$ is the error vector due to projecting b onto u_i . Hence,

$$\|b - (u_i^T b) u_i\|^2 = \|b\|^2 - (u_i^T b)^2,$$

and we obtain

$$\mathcal{L}(z) = \sqrt{\|b\|_2^2 - (u_i^T b)^2} - \frac{\eta}{\sigma_i} |u_i^T b|.$$

We conclude that $\mathcal{L}(0) > \mathcal{L}(z)$, and $\hat{x} = 0$ cannot correspond to a global minimum when $b_1 \neq 0$.

Now we consider the case when $b_1 = 0$. Note that by the nondegeneracy assumption we must have $b_2 \neq 0$. Now define again $y = V^T \hat{x}$. Then we can simplify $\mathcal{L}(\hat{x})$ to obtain

$$\mathcal{L}(\hat{x}) = \sqrt{\|b_2\|_2^2 + \|\Sigma y\|_2^2} - \eta \|y\|_2.$$

Choose $\hat{x} = \gamma V e_n$, where $0 < \gamma < \frac{2\|b_2\|_2 \eta}{\sigma_n^2 - \eta^2}$. The following sequence of inequalities then holds:

$$\begin{aligned} \gamma &< \frac{2\|b_2\|_2 \eta}{\sigma_n^2 - \eta^2} \\ \Rightarrow (\sigma_n^2 - \eta^2) \gamma^2 &< 2\|b_2\|_2 \eta \gamma \\ \Rightarrow \|b_2\|_2^2 + \sigma_n^2 \gamma^2 &< \|b_2\|_2^2 + \eta^2 \gamma^2 + 2\|b_2\|_2 \eta \gamma \\ \Rightarrow \sqrt{\|b_2\|_2^2 + \|\Sigma \gamma e_n\|^2} &< \|b_2\|_2 + \eta \gamma \\ \Rightarrow \mathcal{L}(\gamma V e_n) &< \mathcal{L}(0). \end{aligned}$$

Therefore $\hat{x} = 0$ can never be the global minimum.

4.5. Continuation argument. We are now ready to show that if α_1 exists, then the corresponding \hat{x} in (4.6) gives the global minimum. Otherwise, the \hat{x} in (4.15) that corresponds $\alpha = \sigma_n^2$ gives a double global minimum. The proof will be by continuation on the parameter $\beta \triangleq |u_n^T b|^2$.

We use (4.12) to write

$$(4.18) \quad \mathcal{G}(\alpha) = \bar{\mathcal{G}}(\alpha) + \beta \frac{\sigma_n^2 - \eta^2}{(\sigma_n^2 - \alpha)^2}.$$

We also recall from the definition of $\bar{\mathcal{G}}$ in (4.11) that it has a similar expression to that of \mathcal{G} in (4.7), except that the pole of \mathcal{G} at σ_n^2 has been extracted (as shown by (4.18)). Hence, the derivative of $\bar{\mathcal{G}}$ has a form similar to that of the derivative of \mathcal{G} in (4.17) and we can conclude that $\bar{\mathcal{G}}'(\alpha) > 0$ over $(0, \sigma_{n-1}^2)$.

We continue our argument by considering separately the three cases: $\bar{\mathcal{G}}(\sigma_n^2) > 0$, $\bar{\mathcal{G}}(\sigma_n^2) = 0$, and $\bar{\mathcal{G}}(\sigma_n^2) < 0$.

I. $\bar{\mathcal{G}}(\sigma_n^2) > 0$. In this case, and because of (4.14), $\alpha = \sigma_n^2$ cannot correspond to a global minimum. By further noting that $\bar{\mathcal{G}}'(\alpha) > 0$ over $(\sigma_n^2, \sigma_{n-1}^2)$ we conclude that $\bar{\mathcal{G}}(\alpha) > 0$ over $(\sigma_n^2, \sigma_{n-1}^2)$. Hence, using (4.18) we also have that $\mathcal{G}(\alpha) > 0$ over $(\sigma_n^2, \sigma_{n-1}^2)$. Moreover, σ_n^2 is either a pole of $\mathcal{G}(\alpha)$ (when $u_n^T b \neq 0$) or $\mathcal{G}(\sigma_n^2) = \bar{\mathcal{G}}(\sigma_n^2) > 0$ (when $u_n^T b = 0$). Now since $\mathcal{G}(\eta^2) < 0$ and $\mathcal{G}'(\alpha) > 0$ over (η^2, σ_n^2) , we conclude that \mathcal{G} has a unique root in (η^2, σ_n^2) .

In this case the only contenders for global minima over $(0, \sigma_{n-1}^2]$ are $\alpha = \alpha_1$ and $\alpha = \sigma_{n-1}^2$. By an analysis similar to the one in section 4.2 for $\alpha = \sigma_n^2$ it can be shown that a necessary condition for $\alpha = \sigma_{n-1}^2$ to correspond to a global minimum is that

$$(4.19) \quad u_{n-1}^T b = 0, \quad \mathcal{G}(\sigma_{n-1}^2) - (u_{n-1}^T b)^2 \frac{\sigma_{n-1}^2 - \eta^2}{(\sigma_{n-1}^2 - \alpha)^2} \leq 0.$$

These two conditions imply that we must have $\mathcal{G}(\sigma_{n-1}^2) \leq 0$. This result is compatible with the fact that $\mathcal{G}(\alpha) > 0$ over $(\sigma_n^2, \sigma_{n-1}^2)$ only if $\mathcal{G}(\sigma_{n-1}^2) = 0$. This in turn implies from (4.18) that we must have $\bar{\mathcal{G}}(\sigma_{n-1}^2) \leq 0$. This is inconsistent with the facts $\bar{\mathcal{G}}(\sigma_n^2) > 0$ and $\bar{\mathcal{G}}'(\alpha) > 0$ over $(\sigma_n^2, \sigma_{n-1}^2)$.

Therefore, $\alpha = \sigma_{n-1}^2$ cannot correspond to a global minimum and we conclude that the only critical point we need to consider corresponds to the one associated with the unique root of $\mathcal{G}(\alpha)$ in (η^2, σ_n^2) , which must naturally correspond to the global minimum.

In summary, the solution \hat{x} in (4.6) that corresponds to α_1 is the global minimum in this case.

II. $\bar{\mathcal{G}}(\sigma_n^2) = 0$. In this case, and because of (4.14), $\alpha = \sigma_n^2$ can correspond to a global minimum only if $\beta = 0$, in which case we also deduce from (4.18) that $\mathcal{G}(\sigma_n^2) = 0$ since $\mathcal{G} = \bar{\mathcal{G}}$. Hence, σ_n^2 is a root of \mathcal{G} . By using $\mathcal{G}(\eta^2) < 0$ and $\mathcal{G}'(\alpha) > 0$ over (η^2, σ_{n-1}^2) we conclude that \mathcal{G} does not have any other root in (η^2, σ_{n-1}^2) .

Therefore, when $\beta = 0$, the only contenders for global minima over $(0, \sigma_{n-1}^2)$ are $\alpha = \sigma_n^2$ and $\alpha = \sigma_{n-1}^2$. For $\alpha = \sigma_{n-1}^2$ to correspond to a global minimum we saw above that we must necessarily have $\mathcal{G}(\sigma_{n-1}^2) \leq 0$. This is inconsistent with $\mathcal{G}(\sigma_n^2) > 0$ and $\mathcal{G}'(\alpha) > 0$ over (η^2, σ_{n-1}^2) . We thus obtain that the solution \hat{x} in (4.15) that corresponds to σ_n^2 is the global minimizer.

What about the case $\beta \neq 0$? In this case, and because of (4.14), $\alpha = \sigma_n^2$ cannot correspond to a global minimum. By further noting that $\bar{\mathcal{G}}'(\alpha) > 0$ over $(\sigma_n^2, \sigma_{n-1}^2)$

we conclude that $\bar{\mathcal{G}}(\alpha) > 0$ over $(\sigma_n^2, \sigma_{n-1}^2)$. Hence, using (4.18) we also have that $\mathcal{G}(\alpha) > 0$ over $(\sigma_n^2, \sigma_{n-1}^2)$. Moreover, σ_n^2 is now a pole of $\mathcal{G}(\alpha)$ and since $\mathcal{G}(\eta^2) < 0$ and $\mathcal{G}'(\alpha) > 0$ over (η^2, σ_n^2) we conclude that \mathcal{G} has a unique root in (η^2, σ_n^2) . In this case the only contenders for global minima over $(0, \sigma_{n-1}^2)$ are $\alpha = \alpha_1$ and $\alpha = \sigma_{n-1}^2$. By an analysis similar to the one in case I, we can rule out σ_{n-1}^2 .

In summary, we showed the following when $\bar{\mathcal{G}}(\sigma_n^2) \geq 0$:

1. When $u_n^T b \neq 0$, the solution \hat{x} in (4.6) that corresponds to α_1 is the global minimum.
2. When $u_n^T b = 0$, the solution \hat{x} in (4.15) that corresponds to σ_n^2 is the global minimum.

III. $\bar{\mathcal{G}}(\sigma_n^2) < 0$. This is the most complex situation. Let ω be the largest number such that $\sigma_n^2 < \omega \leq \infty$ and $\mathcal{G}(\omega) = \infty$ if $\omega < \infty$ and $\mathcal{G}(\alpha)$ has no poles in the interval (σ_n^2, ω) .

By the given conditions it is obvious from the form of $\mathcal{G}(\alpha)$ that it has two roots in $(\sigma_n^2, \omega]$ for sufficiently small β . Now we find the largest number δ such that for all β in the interval $(0, \delta]$ the function $\mathcal{G}(\alpha)$ has two roots (counting multiplicity) in $(\sigma_n^2, \omega]$. We claim that for $\beta > \delta$ there are no roots of $\mathcal{G}(\alpha)$ in $(\sigma_n^2, \omega]$. To see this we replace β in $\mathcal{G}(\alpha)$ by $\beta = \delta + \nu$, obtaining

$$\mathcal{G}(\alpha) = \bar{\mathcal{G}}(\alpha) + \delta \frac{\sigma_n^2 - \eta^2}{(\sigma_n^2 - \alpha)^2} + \nu \frac{\sigma_n^2 - \eta^2}{(\sigma_n^2 - \alpha)^2},$$

and observe that the term involving ν is strictly positive in the interval $(\sigma_n^2, \omega]$, for strictly positive ν .

We continue our analysis by considering separately two cases: $\beta = 0$ and $\beta \neq 0$.

IIIA. $\beta = 0$. We will show that at $\beta = 0$ ($u_n^T b = 0$), the function \mathcal{L} has a double global minimum at $\alpha = \sigma_n^2$, and that as β is increased this double root at $\alpha = \sigma_n^2$ bifurcates into the two roots α_1 and α_2 , and that $\mathcal{L}(\alpha_1) < \mathcal{L}(\alpha_2)$ when $0 < \beta \leq \delta$.

When $\bar{\mathcal{G}}(\sigma_n^2) < 0$, the function $\bar{\mathcal{G}}(\alpha)$ has exactly one root in $(0, \omega]$. This is because $\bar{\mathcal{G}}(0) \rightarrow -\infty$ and $\bar{\mathcal{G}}'(\alpha) > 0$ in $(0, \omega]$. By using the same proof that we used earlier to show that α_3 cannot correspond to a local minimum we can establish that this root also cannot correspond to minimum. This leaves us with the double stationary points that we computed in (4.15) and which corresponded to $\alpha = \sigma_n^2$. It is an easy matter to verify, using the formula $\mathcal{L}(\hat{x})\eta = (\alpha - \eta^2)\|\hat{x}\|_2$, that both the stationary points yield the same value for \mathcal{L} .

IIIB. $0 < \beta \leq \delta$. We now allow β to increase. Let $y(\beta)$ denote the stationary point \hat{x} corresponding to $\alpha_1(\beta)$. Also, let $z(\beta)$ denote the stationary point \hat{x} corresponding to $\alpha_2(\beta)$. It is easy to see from the form of $\mathcal{G}(\alpha)$ that

$$\lim_{\beta \rightarrow 0^+} \alpha_1(\beta) = \sigma_n^2 = \lim_{\beta \rightarrow 0^+} \alpha_2(\beta)$$

whenever $\bar{\mathcal{G}}(\sigma_n^2) < 0$. Now we will show that

$$\lim_{\beta \rightarrow 0^+} |y_i(\beta)| = |y_i(0)| = |z_i(0)| = \lim_{\beta \rightarrow 0^+} |z_i(\beta)|, \quad 1 \leq i \leq n.$$

First we observe that the result is true for $i \neq n$ directly from formulas (4.4) and (4.10). Next we note that $\bar{\mathcal{G}}(\alpha)$ is continuous at $\alpha = \sigma_n^2$. Therefore

$$\lim_{\beta \rightarrow 0^+} \frac{\sigma_n^2 - \eta^2}{(\sigma_n^2 - \alpha_1(\beta))^2} \beta + \bar{\mathcal{G}}(\sigma_n^2) = \lim_{\beta \rightarrow 0^+} \left(\frac{\sigma_n^2 - \eta^2}{(\sigma_n^2 - \alpha_1(\beta))^2} \beta + \bar{\mathcal{G}}(\alpha_1(\beta)) \right)$$

$$\begin{aligned}
 &= 0 \\
 &= \lim_{\beta \rightarrow 0^+} \frac{\sigma_n^2 - \eta^2}{(\sigma_n^2 - \alpha_2(\beta))^2} \beta + \bar{\mathcal{G}}(\sigma_n^2).
 \end{aligned}$$

Now using formula (4.13) it can be verified that

$$\lim_{\beta \rightarrow 0^+} |y_n(\beta)| = |y_n(0)| = |z_n(0)| = \lim_{\beta \rightarrow 0^+} |z_n(\beta)|.$$

Therefore $\mathcal{L}(y(\beta))$ and $\mathcal{L}(z(\beta))$ are continuous on the interval $[0, \infty)$, with $\mathcal{L}(y(0)) = \mathcal{L}(z(0))$. We now compute the derivative of \mathcal{L} with respect to β at a stationary point. We have already observed that at a stationary point \hat{x} , corresponding to some α , the objective function \mathcal{L} can be simplified $\mathcal{L}(\hat{x})\eta = (\alpha - \eta^2)\|\hat{x}\|_2$. To simplify the derivation we actually take the derivative of $\eta^2 L^2$, which can be expressed as

$$\eta^2 \mathcal{L}^2(\hat{x}) = (\alpha - \eta^2)^2 b_1^T \Sigma^2 (\Sigma^2 - \alpha I)^{-2} b_1$$

for $\alpha \in (\sigma_n, \sigma_{n-1})$. Now we differentiate, obtaining

$$\frac{d}{d\beta} (\eta^2 L^2(\hat{x}(\beta))) = \frac{d\alpha}{d\beta} (\alpha - \eta^2) b_1^T \Sigma^2 (\Sigma^2 - \alpha I)^{-3} (\Sigma^2 - \eta^2 I) b_1 + \frac{(\alpha - \eta^2)^2}{(\sigma_n^2 - \alpha)^2} \sigma_n^2.$$

Now we obtain an expression for $d\alpha/d\beta$ by differentiating $\alpha^2 \mathcal{G}(\alpha(\beta)) = 0$ with respect to β . Doing so we obtain

$$2\alpha b_1^T \Sigma^2 (\Sigma^2 - \eta^2 I) (\Sigma^2 - \alpha I)^{-3} b_1 \frac{d\alpha}{d\beta} + \alpha^2 \frac{\sigma_n^2 - \eta^2}{(\sigma_n^2 - \alpha)^2} = 0.$$

Solving this equation for the term involving $d\alpha/d\beta$ and substituting it into the above equation for $\frac{d}{d\beta} (\eta^2 L^2(x(\beta)))$ we obtain

$$\begin{aligned}
 \frac{d}{d\beta} (\eta^2 L^2(\hat{x}(\beta))) &= -\alpha (\alpha - \eta^2) \frac{\sigma_n^2 - \eta^2}{(\sigma_n^2 - \alpha)^2} + \sigma_n^2 \frac{(\alpha - \eta^2)^2}{(\sigma_n^2 - \alpha)^2} \\
 &= \frac{\alpha - \eta^2}{(\sigma_n^2 - \alpha)^2} (\sigma_n^2 (\alpha - \eta^2) - \alpha (\sigma_n^2 - \eta^2)) \\
 &= \frac{\alpha - \eta^2}{(\sigma_n^2 - \alpha)^2} (\alpha \eta^2 - \sigma_n^2 \eta^2) \\
 (4.20) \qquad \qquad \qquad &= \frac{\alpha - \eta^2}{\alpha - \sigma_n^2} \eta^2.
 \end{aligned}$$

From this expression we can immediately conclude that the smaller root $\alpha_1(\beta)$ decreases the objective function $\mathcal{L}(y(\beta))$, as β increases from 0, and the larger root $\alpha_2(\beta)$ increases the value of the objective function $\mathcal{L}(z(\beta))$, as β increases. Since $\mathcal{L}(y(0)) = \mathcal{L}(z(0))$, we can now conclude that $\mathcal{L}(y(\beta)) \leq \mathcal{L}(z(\beta))$ for all nonnegative β such that $\alpha_2(\beta) < \sigma_{n-1}^2$.

Therefore the choice for global minimum is between $y(\beta)$ and the critical points, if any, corresponding to $\alpha = \sigma_{n-1}^2$. As mentioned before, $\alpha = \sigma_{n-1}^2$ can correspond to a critical point only if condition (4.19) holds.

From the arguments in section 4.3 we know that $\mathcal{G}(\alpha)$ has at most two roots in (σ_n^2, ω) . Therefore it follows that under condition (4.19), $\omega > \sigma_{n-1}^2$. This in turn implies that $\alpha_2(\beta_0) = \sigma_{n-1}^2$ for some $\beta_0 \in (0, \delta]$.

Using condition (4.19) and carrying out an analysis similar to that of (4.15), we can compute the critical point associated with $\alpha = \sigma_{n-1}^2$. From that it is easy to verify that

$$\lim_{\beta \rightarrow \beta_0^-} |z_i(\beta)| = |z_i(\beta_0)|, \quad 1 \leq i \leq n,$$

where $z(\beta_0)$ denotes the critical point associated with $\alpha = \sigma_{n-1}^2$.

Now from the continuation argument for \mathcal{L} it follows that $\mathcal{L}(y(\beta)) \leq \mathcal{L}(y(0)) = \mathcal{L}(z(0)) \leq \mathcal{L}(z(\beta_0))$. Therefore we do not need to consider $\alpha = \sigma_{n-1}^2$ as a possibility for the global minimum.

Furthermore, when $\beta > \delta$ we argued earlier that there are no roots of $\mathcal{G}(\alpha)$ in the interval $(\sigma_n^2, \omega]$. Also, from the above argument it follows that $\alpha = \sigma_{n-1}^2$ cannot correspond to a global minimum.

In summary, the \hat{x} in (4.6) that corresponds to α_1 is the global minimizer.

4.6. Multiple singular values. So far in the analysis we have implicitly ignored the possibility that $\sigma_n = \sigma_{n-1}$. We now discuss how to take care of this possibility. We need only to consider critical points α situated in the interval $(0, \sigma_n^2]$.

Let U_n denote a matrix with orthonormal columns that span the left singular subspace associated with the smallest singular value of A . If $\|U_n^T b\|_2 > 0$, then it follows from (4.4) that $\alpha = \sigma_n^2$ is not a possibility for a critical point. Furthermore $\mathcal{G}(\alpha)$ has a single root in (η^2, σ_n^2) and this must give the global minimum.

If $\|U_n^T b\|_2 = 0$, then either there exists a root of $\mathcal{G}(\alpha)$ in the interval (η^2, σ_n^2) , which corresponds to the global minimum, or there is no such root and $\alpha = \sigma_n^2$ will give rise to multiple global minima, all of which can be calculated by the technique that led to (4.15). The only difference is that \bar{y} in (4.10) will now denote the components of y associated with the right singular vectors perpendicular to the range space of V_n , where V_n is a matrix with orthonormal columns that span the right singular subspace of A corresponding to σ_n . The proofs of these statements are similar to the nonmultiple singular value case.

4.7. Statement of the solution of the optimization problem. We collect in the form of a theorem the conclusions of our earlier analysis.

THEOREM 4.2. *Given $A \in \mathbf{R}^{m \times n}$, with $m \geq n$ and A full rank, a nonzero $b \in \mathbf{R}^m$, and a positive real number η satisfying $\eta < \sigma_{\min}(A)$, assume further that*

$$b^T [I - A(A^T A - \eta^2 I)^{-1} A^T] b > 0.$$

The solution of the optimization problem,

$$(4.21) \quad \min_{\hat{x}} \left(\min_{\|\delta A\|_2 \leq \eta} \|(A + \delta A)\hat{x} - b\|_2 \right),$$

can be constructed as follows:

- *Introduce the SVD of A ,*

$$(4.22) \quad A = U \begin{bmatrix} \Sigma \\ 0 \end{bmatrix} V^T,$$

where $U \in \mathbf{R}^{m \times m}$ and $V \in \mathbf{R}^{n \times n}$ are orthogonal, and $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_n)$ is diagonal, with

$$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n > 0$$

being the singular values of A .

- Partition the vector $U^T b$ into

$$(4.23) \quad \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = U^T b,$$

where $b_1 \in \mathbf{R}^n$ and $b_2 \in \mathbf{R}^{m-n}$.

- Introduce the secular function

$$(4.24) \quad \mathcal{G}(\alpha) = b_1^T (\Sigma^2 - \eta^2 I) (\Sigma^2 - \alpha I)^{-2} b_1 - \frac{\eta^2}{\alpha^2} \|b_2\|_2^2.$$

- Determine the unique positive root $\hat{\alpha}$ of $\mathcal{G}(\alpha)$ that lies in the interval (η^2, σ_n^2) . If it does not exist, then set $\hat{\alpha} = \sigma_n^2$.
- Then
 1. If $\hat{\alpha} < \sigma_n^2$, the solution \hat{x} is unique and is given by (4.6) or, equivalently,

$$\hat{x} = (A^T A - \hat{\alpha} I)^{-1} A^T b.$$

2. If $\hat{\alpha} = \sigma_n^2$ and $\sigma_n < \sigma_{n-1}$, then two solutions exist that are given by (4.15). Otherwise, if A has multiple singular values at σ_n , then multiple solutions exist and we can use the same technique that led to (4.15) to determine \hat{x} as explained in the above section on multiple singular values.

We can be more explicit about the uniqueness of solutions. Assume A has multiple singular values at σ_n and let U_n denote the matrix with singular vectors that spans the left singular subspace of A associated with these singular values:

1. When $\|U_n^T b\| \neq 0$, the solution \hat{x} is unique and it corresponds to a root $\hat{\alpha} < \sigma_n^2$ as shown above.
2. When $\|U_n^T b\| = 0$, then either an $\hat{\alpha}_1 < \sigma_n^2$ exists and the solution \hat{x} is unique. Otherwise, $\hat{\alpha} = \sigma_n^2$ and multiple solutions \hat{x} exist.

5. Restricted perturbations. We have so far considered the case in which all the columns of the A matrix are subject to perturbations. It may happen in practice, however, that only selected columns are uncertain, while the remaining columns are known precisely. This situation can be handled by the approach of this paper as we now clarify.

Given $A \in \mathbf{R}^{m \times n}$, we partition it into block columns,

$$A = \begin{bmatrix} A_1 & A_2 \end{bmatrix},$$

and assume, without loss of generality, that only the columns of A_2 are subject to perturbations while the columns of A_1 are known exactly. We then pose the following problem.

Given $A \in \mathbf{R}^{m \times n}$, with $m \geq n$ and A full rank, $b \in \mathbf{R}^m$, and a nonnegative real number η_2 , determine \hat{x} such that

$$(5.1) \quad \min_{\hat{x}} \min \left\{ \left\| \begin{bmatrix} A_1 & A_2 + \delta A_2 \end{bmatrix} \hat{x} - b \right\|_2 : \|\delta A_2\|_2 \leq \eta_2 \right\}.$$

If we partition \hat{x} accordingly with A_1 and A_2 , say,

$$\hat{x} = \begin{bmatrix} \hat{x}_1 \\ \hat{x}_2 \end{bmatrix},$$

then we can write

$$\left\| \begin{bmatrix} A_1 & A_2 + \delta A_2 \end{bmatrix} \hat{x} - b \right\|_2 = \|(A_2 + \delta A_2)\hat{x}_2 - (b - A_1\hat{x}_1)\|_2.$$

Assuming, for any vector (\hat{x}_1, \hat{x}_2) , the fundamental condition

$$\eta_2 \|\hat{x}_2\|_2 < \|A_2 \hat{x}_2 - (b - A_1 \hat{x}_1)\|_2 = \|Ax - b\|_2,$$

we can follow the argument at the beginning of section 3 to conclude that the minimum over δA_2 is achievable and is equal to

$$\|A_2 \hat{x}_2 - (b - A_1 \hat{x}_1)\|_2 - \eta_2 \|\hat{x}_2\|_2.$$

In this way, statement (5.1) reduces to the minimization problem

$$(5.2) \quad \min_{\hat{x}_1, \hat{x}_2} \left(\left\| \begin{bmatrix} A_1 & A_2 \end{bmatrix} \begin{bmatrix} \hat{x}_1 \\ \hat{x}_2 \end{bmatrix} - b \right\|_2 - \eta_2 \|\hat{x}_2\|_2 \right).$$

This statement can be further reduced to the problem treated in Theorem 4.2 as follows. Introduce the QR decomposition of A , say

$$A = QR = Q \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \\ 0 & 0 \end{bmatrix},$$

where we have partitioned R accordingly with the sizes of A_1 and A_2 . Define

$$\begin{bmatrix} \bar{b}_{1A} \\ \bar{b}_{2A} \\ \bar{b}_2 \end{bmatrix} = Q^T b.$$

Then (5.2) is equivalent to

$$(5.3) \quad \min_{\hat{x}_1, \hat{x}_2} \left(\left\| \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \hat{x}_1 \\ \hat{x}_2 \end{bmatrix} - \begin{bmatrix} \bar{b}_{1A} \\ \bar{b}_{2A} \\ \bar{b}_2 \end{bmatrix} \right\|_2 - \eta_2 \|\hat{x}_2\|_2 \right),$$

which can be further rewritten as

$$(5.4) \quad \min_{\hat{x}_1, \hat{x}_2} \left(\left\| \begin{bmatrix} R_{11} \hat{x}_1 + R_{12} \hat{x}_2 - \bar{b}_{1A} \\ R_{22} \hat{x}_2 - \bar{b}_{2A} \\ \bar{b}_2 \end{bmatrix} \right\|_2 - \eta_2 \|\hat{x}_2\|_2 \right).$$

This shows that once the optimal \hat{x}_2 has been determined, the optimal choice for \hat{x}_1 is necessarily the one that annihilates the entry $R_{11} \hat{x}_1 + R_{12} \hat{x}_2 - \bar{b}_{1A}$. That is,

$$(5.5) \quad \hat{x}_1 = R_{11}^{-1} [\bar{b}_{1A} - R_{12} \hat{x}_2].$$

The optimal \hat{x}_2 is the solution of

$$(5.6) \quad \min_{\hat{x}_2} \left(\left\| \begin{bmatrix} R_{22} \\ 0 \end{bmatrix} \hat{x}_2 - \begin{bmatrix} \bar{b}_{2A} \\ \bar{b}_2 \end{bmatrix} \right\|_2 - \eta_2 \|\hat{x}_2\|_2 \right).$$

This optimization is of the same form as the problem stated earlier in (3.4) with \hat{x} replaced by \hat{x}_2 , η replaced by η_2 , A replaced by $\begin{bmatrix} R_{22} \\ 0 \end{bmatrix}$, and b replaced by $\begin{bmatrix} \bar{b}_{2A} \\ \bar{b}_2 \end{bmatrix}$.

Therefore, the optimal \hat{x}_2 can be obtained by applying the result of Theorem 4.2. Once \hat{x}_2 has been determined, the corresponding \hat{x}_1 follows from (5.5).

6. Conclusion. In this paper we have proposed and solved a new optimization problem for parameter estimation in the presence of data uncertainties. The problem incorporates a priori bounds on the size of the perturbations. It has a “closed” form solution that is obtained by solving an “indefinite” regularized least-squares problem with a regression parameter that is determined from the positive root of a secular equation.

Several extensions are possible. For example, weighted versions with uncertainties in the weight matrices are useful in several applications, as well as cases with multiplicative uncertainties and applications to filtering theory. Some of these cases, in addition to more discussion on estimation and control problems with bounded uncertainties, can be found in [11, 12, 13, 14].

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