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# Least Squares with a Quadratic Constraint

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**Summary.** We present the theory of the linear least squares problem with a quadratic constraint. New theorems characterizing properties of the solutions are given. A numerical application is discussed.

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## 1. Introduction

Let $\mathbf{A}$ be a $(m \times n)$ matrix, $\mathbf{C}$ a $(p \times n)$ matrix, $\mathbf{b}$ a $m$-vector, $\mathbf{d}$ a $p$-vector and $\alpha$ a positive number. Let $\|\cdot\|$ denote the Euclidean vector norm. We consider the problem of finding a $n$-vector $\mathbf{x}$ so that

$$\|\mathbf{A}\mathbf{x}-\mathbf{b}\| = \min$$

subject to (1.1)

$$\|\mathbf{C}\mathbf{x}-\mathbf{d}\| = \alpha.$$

Problems of this type arise in many applications e.g. when solving ill-posed problems by regularization [13] or when smoothing data [9]. In this paper we give a description of all possible solutions of (1.1). We also discuss the problem with the inequality constraint $\|\mathbf{C}\mathbf{x}-\mathbf{d}\| \leqq \alpha$, which turns out to be a special case of (1.1). For two special cases we show how to compute the solution using dual equations and finally we give an example where the theory is applied. The paper contains the main results of the Habilitationsschrift [3] of the author.

## 2. Some Assumptions

As suggested by a referee we first mention some conditions which guarantee that (1.1) has a solution.

*Assumption 1.* The set $F = \{\mathbf{x}\colon \|\mathbf{C}\mathbf{x}-\mathbf{d}\| = \alpha\}$ is not empty and especially $\alpha > \min\limits_{\mathbf{x}} \|\mathbf{C}\mathbf{x}-\mathbf{d}\|$.

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If $\alpha$ is too small then of course no solution may exist.

*Assumption 2.* rank $\begin{pmatrix}\mathbf{A}\\ \mathbf{C}\end{pmatrix}=n$.

If we do not assume this rank condition then the solution if it exists will not be unique since then we can add to it any element of the common nullspace-intersection of $\mathbf{A}$ and $\mathbf{C}$ without changing (1.1).

We note that if Assumptions 1 and 2 hold then there exists a global solution of (1.1). To prove this it suffices to show that if $\{\mathbf{x}_k\}$ is a sequence in $F$ with $\{\|\mathbf{A}\,\mathbf{x}_k-\mathbf{b}\|\}$ bounded then $\{\mathbf{x}_k\}$ is bounded. This is true since there is a $\mu$ such that

$$\left\|\begin{pmatrix}\mathbf{A}\\ \mathbf{C}\end{pmatrix}\mathbf{x}_k-\begin{pmatrix}\mathbf{b}\\ \mathbf{d}\end{pmatrix}\right\|\leqq\mu$$

holds and because of Assumption 2 it follows that $\{\mathbf{x}_k\}$ is bounded.

## 3. The Lagrange Function and the Normal Equations

Assumptions 1 and 2 guarantee that the solution of (1.1) is a stationary point of the *Lagrange function* $L$ (with Lagrange multiplier $\lambda$):

$$L(\mathbf{x},\lambda):=\|\mathbf{A}\,\mathbf{x}-\mathbf{b}\|^2+\lambda\{\|\mathbf{C}\,\mathbf{x}-\mathbf{d}\|^2-\alpha^2\}$$

and therefore a solution of $\dfrac{\partial L}{\partial \mathbf{x}}=\mathbf{0}$ and $\dfrac{\partial L}{\partial \lambda}=0$, which are the *normal equations:*

$$(\mathbf{A}^T\mathbf{A}+\lambda\mathbf{C}^T\mathbf{C})\,\mathbf{x}=\mathbf{A}^T\mathbf{b}+\lambda\mathbf{C}^T\mathbf{d}, \tag{3.1}$$

$$\|\mathbf{C}\,\mathbf{x}-\mathbf{d}\|^2=\alpha^2. \tag{3.2}$$

We emphasize that with Assumption 1 we exclude the case that the global solution of (1.1) also minimizes $\|\mathbf{C}\,\mathbf{x}-\mathbf{d}\|$ since this is only possible if $\alpha=\min\limits_{\mathbf{x}}\|\mathbf{C}\,\mathbf{x}-\mathbf{d}\|$ (No $\lambda$ exists in this case). Notice that Eq. (3.1) can also be written as

$$\operatorname{grad}\|\mathbf{A}\,\mathbf{x}-\mathbf{b}\|^2=-\lambda\operatorname{grad}\|\mathbf{C}\,\mathbf{x}-\mathbf{d}\|^2 \tag{3.3}$$

which is a necessary condition for the solution of (1.1) obtained by geometrical considerations. The normal Eqs. (3.1) and (3.2) may have several solutions and among them are the solutions of problem (1.1). The first question is therefore to decide which of the solutions of the normal equations will also solve problem (1.1). The following Theorem compares two solutions of the normal equations and will be useful to decide which of them makes $\|\mathbf{A}\,\mathbf{x}-\mathbf{b}\|$ smaller.

**Theorem 1.** *If* $(\mathbf{x}_1,\lambda_1)$ *and* $(\mathbf{x}_2,\lambda_2)$ *are solutions of the normal Eqs.* (3.1) *and* (3.2) *then*

$$\|\mathbf{A}\,\mathbf{x}_2-\mathbf{b}\|^2-\|\mathbf{A}\,\mathbf{x}_1-\mathbf{b}\|^2=\frac{\lambda_1-\lambda_2}{2}\|\mathbf{C}(\mathbf{x}_1-\mathbf{x}_2)\|^2. \tag{3.4}$$

*Proof.* Since $(\mathbf{x}_1, \lambda_1)$, $(\mathbf{x}_2, \lambda_2)$ are solutions of (3.1) we have

$$\mathbf{A}^T\mathbf{A}\mathbf{x}_1 - \mathbf{A}^T\mathbf{b} = -\lambda_1\mathbf{C}^T\mathbf{C}\mathbf{x}_1 + \lambda_1\mathbf{C}^T\mathbf{d}, \tag{3.5}$$

$$\mathbf{A}^T\mathbf{A}\mathbf{x}_2 - \mathbf{A}^T\mathbf{b} = -\lambda_2\mathbf{C}^T\mathbf{C}\mathbf{x}_2 + \lambda_2\mathbf{C}^T\mathbf{d}. \tag{3.6}$$

If we multiply Eq. (3.6) by $\mathbf{x}_2^T$ and Eq. (3.5) by $\mathbf{x}_1^T$ and subtract the resulting second equation from the first we obtain:

$$\begin{aligned}&\|\mathbf{A}\mathbf{x}_2\|^2 - \|\mathbf{A}\mathbf{x}_1\|^2 - \mathbf{b}^T\mathbf{A}(\mathbf{x}_2 - \mathbf{x}_1)\\ &\quad = \lambda_1(\|\mathbf{C}\mathbf{x}_1\|^2 - \mathbf{d}^T\mathbf{C}\mathbf{x}_1) - \lambda_2(\|\mathbf{C}\mathbf{x}_2\|^2 - \mathbf{d}^T\mathbf{C}\mathbf{x}_2).\end{aligned} \tag{3.7}$$

Similarly by multiplying (3.5) by $\mathbf{x}_2^T$ and subtracting Eq. (3.6) multiplied by $\mathbf{x}_1^T$ we get

$$-\mathbf{b}^T(\mathbf{A}\mathbf{x}_2 - \mathbf{x}_1) = \lambda_1(-\mathbf{x}_2^T\mathbf{C}^T\mathbf{C}\mathbf{x}_1 + \mathbf{d}^T\mathbf{C}\mathbf{x}_2) - \lambda_2(-\mathbf{x}_1^T\mathbf{C}^T\mathbf{C}\mathbf{x}_2 + \mathbf{d}^T\mathbf{C}\mathbf{x}_1). \tag{3.8}$$

Observe that

$$\|\mathbf{A}\mathbf{x}_2 - \mathbf{b}\|^2 - \|\mathbf{A}\mathbf{x}_1 - \mathbf{b}\|^2 = \|\mathbf{A}\mathbf{x}_2\|^2 - \|\mathbf{A}\mathbf{x}_1\|^2 - 2\mathbf{b}^T\mathbf{A}(\mathbf{x}_2 - \mathbf{x}_1).$$

Thus if we add (3.7)+(3.8) we get

$$\begin{aligned}&\|\mathbf{A}\mathbf{x}_2 - \mathbf{b}\|^2 - \|\mathbf{A}\mathbf{x}_1 - \mathbf{b}\|^2\\ &\quad = \lambda_1\{\|\mathbf{C}\mathbf{x}_1\|^2 - \mathbf{d}^T\mathbf{C}\mathbf{x}_1 - \mathbf{x}_1^T\mathbf{C}^T\mathbf{C}\mathbf{x}_2 + \mathbf{d}^T\mathbf{C}\mathbf{x}_2\}\\ &\qquad - \lambda_2\{\|\mathbf{C}\mathbf{x}_2\|^2 - \mathbf{d}^T\mathbf{C}\mathbf{x}_2 - \mathbf{x}_1^T\mathbf{C}^T\mathbf{C}\mathbf{x}_2 + \mathbf{d}^T\mathbf{C}\mathbf{x}_1\}.\end{aligned} \tag{3.9}$$

Now we have

$$\|\mathbf{C}\mathbf{x}_1 - \mathbf{d}\|^2 = \|\mathbf{C}\mathbf{x}_2 - \mathbf{d}\|^2 = \alpha^2$$

so that

$$\|\mathbf{C}\mathbf{x}_1\|^2 - 2\mathbf{d}^T\mathbf{C}\mathbf{x}_1 + \|\mathbf{d}\|^2 = \|\mathbf{C}\mathbf{x}_2\|^2 - 2\mathbf{d}^T\mathbf{C}\mathbf{x}_2 + \|\mathbf{d}\|^2$$

and

$$\|\mathbf{C}\mathbf{x}_1\|^2 - \mathbf{d}^T\mathbf{C}\mathbf{x}_1 + \mathbf{d}^T\mathbf{C}\mathbf{x}_2 = \|\mathbf{C}\mathbf{x}_2\|^2 - \mathbf{d}^T\mathbf{C}\mathbf{x}_2 + \mathbf{d}^T\mathbf{C}\mathbf{x}_1. \tag{3.10}$$

From (3.10) we conclude that the factors of $\lambda_1$ and $\lambda_2$ in (3.9) are the same. Therefore they also equal their arithmetic mean which is

$$\tfrac{1}{2}\{\|\mathbf{C}\mathbf{x}_1\|^2 - 2\mathbf{x}_1^T\mathbf{C}^T\mathbf{C}\mathbf{x}_2 + \|\mathbf{C}\mathbf{x}_2\|^2\} = \tfrac{1}{2}\|\mathbf{C}(\mathbf{x}_1 - \mathbf{x}_2)\|^2. \quad \square$$

We see from Theorem 1 that

$$\|\mathbf{A}\mathbf{x}_2 - \mathbf{b}\| > \|\mathbf{A}\mathbf{x}_1 - \mathbf{b}\| \qquad \text{when } \lambda_1 > \lambda_2$$

unless the right hand side of (3.4) is zero. If we can show that this right hand side is never zero then the solution of the original problem (1.1) is given as the solution of the normal equations with *largest* $\lambda$. The next theorem gives us a similar identity as Theorem 1.

**Theorem 2.** *If* $(\mathbf{x}_1, \lambda_1)$ *and* $(\mathbf{x}_2, \lambda_2)$ *are solutions of the normal Eqs.* (3.1) *and* (3.2) *then*

$$(\lambda_1+\lambda_2)\{\|\mathbf{A}\,\mathbf{x}_2-\mathbf{b}\|^2-\|\mathbf{A}\,\mathbf{x}_1-\mathbf{b}\|^2\}=(\lambda_2-\lambda_1)\|\,\mathbf{A}(\mathbf{x}_1-\mathbf{x}_2)\|^2. \tag{3.11}$$

*Proof.* From $(\mathbf{A}^T\mathbf{A}+\lambda\,\mathbf{C}^T\mathbf{C})\,\mathbf{x}=\mathbf{A}^T\mathbf{b}+\lambda\,\mathbf{C}^T\mathbf{d}$ we have

$$\lambda_1\,\mathbf{C}^T\mathbf{C}\,\mathbf{x}_1-\lambda_1\,\mathbf{C}^T\mathbf{d}=-\mathbf{A}^T\mathbf{A}\,\mathbf{x}_1+\mathbf{A}^T\mathbf{b} \tag{3.12}$$

$$\lambda_2\,\mathbf{C}^T\mathbf{C}\,\mathbf{x}_2-\lambda_2\,\mathbf{C}^T\mathbf{d}=-\mathbf{A}^T\mathbf{A}\,\mathbf{x}_2+\mathbf{A}^T\mathbf{b}. \tag{3.13}$$

By multiplying (3.13) by $\lambda_1\,\mathbf{x}_1^T$ and (3.12) by $\lambda_2\,\mathbf{x}_2^T$ and by subtracting the second resulting equation from the first we get:

$$\lambda_1\lambda_2\{(\mathbf{x}_2-\mathbf{x}_1)^T\mathbf{C}^T\mathbf{d}\}=(\lambda_2-\lambda_1)\,\mathbf{x}_1^T\mathbf{A}^T\mathbf{A}\,\mathbf{x}_2+(\lambda_1\,\mathbf{x}_1-\lambda_2\,\mathbf{x}_2)^T\mathbf{A}^T\mathbf{b}. \tag{3.14}$$

Similarly, by multiplying (3.13) by $\lambda_1\,\mathbf{x}_2^T$ and subtracting from it Eq. (3.12) multiplied by $\lambda_2\,\mathbf{x}_1^T$ we obtain:

$$\begin{aligned}&\lambda_1\lambda_2\{\|\mathbf{C}\,\mathbf{x}_2\|^2-\|\mathbf{C}\,\mathbf{x}_1\|^2+(\mathbf{x}_1-\mathbf{x}_2)\,\mathbf{C}^T\mathbf{d}\}\\&\quad=\lambda_2\,\|\mathbf{A}\,\mathbf{x}_1\|^2-\lambda_1\,\|\mathbf{A}\,\mathbf{x}_2\|^2+(\lambda_1\,\mathbf{x}_2-\lambda_2\,\mathbf{x}_1)^T\mathbf{A}^T\mathbf{b}.\end{aligned} \tag{3.15}$$

Observe that

$$\begin{aligned}0&=\|\mathbf{C}\,\mathbf{x}_2-\mathbf{d}\|^2-\|\mathbf{C}\,\mathbf{x}_1-\mathbf{d}\|^2\\&=\|\mathbf{C}\,\mathbf{x}_2\|^2-\|\mathbf{C}\,\mathbf{x}_1\|^2+2(\mathbf{x}_1-\mathbf{x}_2)^T\mathbf{C}^T\mathbf{d}.\end{aligned}$$

Thus if we subtract (3.14) from (3.15) we get

$$\begin{aligned}0=\;&\lambda_2\,\|\mathbf{A}\,\mathbf{x}_1\|^2-\lambda_1\,\|\mathbf{A}\,\mathbf{x}_2\|^2+(\lambda_1\,\mathbf{x}_2-\lambda_2\,\mathbf{x}_1-\lambda_1\,\mathbf{x}_1+\lambda_2\,\mathbf{x}_2)^T\mathbf{A}^T\mathbf{b}\\&+(\lambda_1-\lambda_2)\,\mathbf{x}_1^T\mathbf{A}^T\mathbf{A}\,\mathbf{x}_2,\end{aligned}$$

or by rearranging

$$\begin{aligned}&\lambda_1\{\|\mathbf{A}\,\mathbf{x}_2\|^2-\mathbf{x}_2^T\mathbf{A}^T\mathbf{b}+\mathbf{x}_1^T\mathbf{A}^T\mathbf{b}-\mathbf{x}_1^T\mathbf{A}^T\mathbf{A}\,\mathbf{x}_2\}\\&\quad=\lambda_2\{\|\mathbf{A}\,\mathbf{x}_1\|^2-\mathbf{x}_1^T\mathbf{A}^T\mathbf{b}+\mathbf{x}_2^T\mathbf{A}^T\mathbf{b}-\mathbf{x}_1^T\mathbf{A}^T\mathbf{A}\,\mathbf{x}_2\}.\end{aligned} \tag{3.16}$$

Now the bracket on the left hand side of (3.16) is

$$\begin{aligned}&\tfrac{1}{2}\,\|\mathbf{A}\,\mathbf{x}_2\|^2+\tfrac{1}{2}\{\|\mathbf{A}\,\mathbf{x}_2\|^2-2\,\mathbf{x}_1^T\mathbf{A}^T\mathbf{A}\,\mathbf{x}_2+\|\mathbf{A}\,\mathbf{x}_1\|^2\}\\&\quad-\tfrac{1}{2}\,\|\mathbf{A}\,\mathbf{x}_1\|^2+\mathbf{x}_1^T\mathbf{A}^T\mathbf{b}-\mathbf{x}_2^T\mathbf{A}^T\mathbf{b}+\tfrac{1}{2}\,\|\mathbf{b}\|^2-\tfrac{1}{2}\,\|\mathbf{b}\|^2\\&=\tfrac{1}{2}\{\|\mathbf{A}\,\mathbf{x}_2-\mathbf{b}\|^2-\|\mathbf{A}\,\mathbf{x}_1-\mathbf{b}\|^2+\|\mathbf{A}(\mathbf{x}_2-\mathbf{x}_1)\|^2\}.\end{aligned}$$

The right hand side of (3.16) simplifies analogously and by rearranging we obtain (3.11). □

We now investigate in which cases the right hand side of Eq. (3.4) may be zero. Let $(\mathbf{x}_1, \lambda_1)\neq(\mathbf{x}_2, \lambda_2)$ be two solutions of the normal equations and assume

$$\frac{\lambda_1-\lambda_2}{2}\,\|\mathbf{C}(\mathbf{x}_1-\mathbf{x}_2)\|^2=0. \tag{3.17}$$

This is only possible if

(i) $\lambda_1 = \lambda_2 =: \lambda$ but $\mathbf{x}_1 \neq \mathbf{x}_2$. In this case we have

$$(\mathbf{A}^T \mathbf{A} + \lambda \mathbf{C}^T \mathbf{C}) \mathbf{x}_1 = \mathbf{A}^T \mathbf{b} + \lambda \mathbf{C}^T \mathbf{d}$$
$$(\mathbf{A}^T \mathbf{A} + \lambda \mathbf{C}^T \mathbf{C}) \mathbf{x}_2 = \mathbf{A}^T \mathbf{b} + \lambda \mathbf{C}^T \mathbf{d}.$$

Subtracting the second equation from the first, we get

$$(\mathbf{A}^T \mathbf{A} + \lambda \mathbf{C}^T \mathbf{C})(\mathbf{x}_1 - \mathbf{x}_2) = \mathbf{0}. \tag{3.18}$$

Eq. (3.18) shows that in this case $\lambda = -\mu$ where $\mu$ is an eigenvalue of the generalised eigenvalue problem

$$\mathbf{A}^T \mathbf{A} \mathbf{x} = \mu \mathbf{C}^T \mathbf{C} \mathbf{x} \tag{3.19}$$

and

$$\mathbf{x}_1 = \mathbf{x}_2 + \mathbf{v}(\mu)$$

where $\mathbf{v}(\mu)$ is an eigenvector belonging to $\mu$. Thus if $\lambda_1 = \lambda_2 = -\mu$ then the two solutions $\mathbf{x}_1$ and $\mathbf{x}_2$ have the same value $\|\mathbf{A}\mathbf{x} - \mathbf{b}\|$.

(ii) $\lambda_1 \neq \lambda_2$ but $\|\mathbf{C}(\mathbf{x}_1 - \mathbf{x}_2)\|^2 = 0$. (3.20)

From Theorem 1, we then have $\|\mathbf{A}\mathbf{x}_2 - \mathbf{b}\|^2 - \|\mathbf{A}\mathbf{x}_1 - \mathbf{b}\|^2 = 0$. Therefore Theorem 2 gives

$$\|\mathbf{A}(\mathbf{x}_2 - \mathbf{x}_1)\|^2 = 0. \tag{3.21}$$

But (3.20) and (3.21) are equivalent to

$$\begin{pmatrix} \mathbf{A} \\ \mathbf{C} \end{pmatrix} (\mathbf{x}_2 - \mathbf{x}_1) = \mathbf{0}. \tag{3.22}$$

Because of Assumption 2 this means that $\mathbf{x}_1 = \mathbf{x}_2 =: \mathbf{x}'$. Using Eq. (3.3) we would have in this case

$$\operatorname{grad} \|\mathbf{A}\mathbf{x}' - \mathbf{b}\|^2 = \operatorname{grad} \|\mathbf{C}\mathbf{x}' - \mathbf{d}\|^2 = \mathbf{0}$$

and furthermore

$$\alpha = \|\mathbf{C}\mathbf{x}' - \mathbf{d}\| = \min_{\mathbf{x}} \|\mathbf{C}\mathbf{x} - \mathbf{d}\|$$

which is a contradiction to Assumption 1. This case is therefore not possible.

As a consequence we have:

**Lemma 1.** *Under Assumptions* 1 *and* 2 *let* $(\mathbf{x}_1, \lambda_1)$ *and* $(\mathbf{x}_2, \lambda_2)$ *be solutions of the normal equations. If* $\lambda_1 \neq \lambda_2$ *then*

$$\mathbf{C}\mathbf{x}_1 \neq \mathbf{C}\mathbf{x}_2 \quad \textit{and} \quad \mathbf{A}\mathbf{x}_1 \neq \mathbf{A}\mathbf{x}_2.$$

## 4. Characterization of the Solution

Combining Eqs. (3.4) with (3.11) we get

**Corollary 1.** *Let* $(\mathbf{x}_1, \lambda_1)$ *and* $(\mathbf{x}_2, \lambda_2)$ *be solutions of the normal equations and suppose Assumption* 1 *and* 2 *hold. Then*

$$-\frac{\lambda_1+\lambda_2}{2}\|\mathbf{C}(\mathbf{x}_1-\mathbf{x}_2)\|^2 = \|\mathbf{A}(\mathbf{x}_1-\mathbf{x}_2)\|^2. \tag{4.1}$$

Equation (4.1) has an important consequence: for any two solutions $(\mathbf{x}_1, \lambda_1)$, $(\mathbf{x}_2, \lambda_2)$ with $\lambda_1 \neq \lambda_2$ we must have $\lambda_1+\lambda_2<0$. This means that either both $\lambda_i$ are negative or if, say, $\lambda_1>0$ then $\lambda_2<-\lambda_1<0$. Therefore

**Corollary 2.** *The normal Eqs.* (3.1) *and* (3.2) *have at most one solution* $(\mathbf{x}, \tilde{\lambda})$ *with* $\tilde{\lambda}>0$. *For every other solution* $(\mathbf{x}, \lambda)$ *we have* $\lambda<-\tilde{\lambda}$.

*If the solution* $(\tilde{\mathbf{x}}, \tilde{\lambda})$ *exists* $\tilde{\mathbf{x}}$ *will solve the original problem* (1.1). *But if such a solution does not exist then a solution* $(\mathbf{x}', \lambda')$ *with* $\lambda' = \max_i \lambda_i \leqq 0$ *will solve* (1.1).

## 5. The Solutions of the Normal Equations

In this section we discuss the solutions $(\mathbf{x}, \lambda)$ of the normal equations:

$$(\mathbf{A}^T\mathbf{A}+\lambda\mathbf{C}^T\mathbf{C})\mathbf{x} = \mathbf{A}^T\mathbf{b}+\lambda\mathbf{C}^T\mathbf{d} \tag{5.1}$$

$$\|\mathbf{C}\mathbf{x}-\mathbf{d}\|^2 = \alpha^2. \tag{5.2}$$

If the matrix $\mathbf{A}^T\mathbf{A}+\lambda\mathbf{C}^T\mathbf{C}$ is nonsingular then we can define the *length function*

$$f(\lambda) := \|\mathbf{C}\mathbf{x}(\lambda)-\mathbf{d}\|^2 \tag{5.3}$$

where $\mathbf{x}(\lambda)$ is the solution of (5.1). If we now can determine $\lambda$ so that the *secular equation*

$$f(\lambda) = \alpha^2 \tag{5.4}$$

is satisfied then, $(\mathbf{x}, \lambda)$ is a solution of the normal equations. Using the *generalised singular value decomposition* which we henceforth denote as BSVD (cf. [14] for details of the computational aspects), we get:

$$\begin{aligned} &\mathbf{U}^T\mathbf{A}\mathbf{X} = \mathbf{D}_A = \operatorname{diag}(\alpha_1, \dots, \alpha_n), \quad \alpha_i \geqq 0 \\ &\mathbf{V}^T\mathbf{C}\mathbf{X} = \mathbf{D}_C = \operatorname{diag}(\gamma_1, \dots, \gamma_q), \quad \gamma_i \geqq 0, \quad q = \min(n,p) \\ &\text{with } \gamma_1 \geqq \dots \geqq \gamma_q, \end{aligned}$$

where $\mathbf{U}(m\times m)$ and $\mathbf{V}(p\times p)$ are orthogonal and $\mathbf{X}(n\times n)$ is nonsingular.

This decomposition only exists if $\mathbf{A}$ has at least as many rows as columns i.e. if $m \geqq n$. We can always assume this since we can add zero rows to $\mathbf{A}$ and zero elements to $\mathbf{b}$ without changing the solution. Note that if

$$\gamma_1 \geqq \gamma_2 \geqq \dots \geqq \gamma_r > \gamma_{r+1} = \dots = \gamma_q = 0$$

then

$$\mu_i = \alpha_i^2/\gamma_i^2, \quad i = 1, \dots, r \tag{5.5}$$

are the eigenvalues of the generalised eigenvalue problem

$$\mathbf{A}^T \mathbf{A}\, \mathbf{x} = \mu\, \mathbf{C}^T \mathbf{C}\, \mathbf{x}. \tag{5.6}$$

Defining $\mathbf{c} := \mathbf{U}^T \mathbf{b}$ and $\mathbf{e} := \mathbf{V}^T \mathbf{d}$ we obtain after a short calculation for the function $f$ the representation:

$$f(\lambda) = \sum_{i=1}^{r} \alpha_i^2 \left( \frac{\gamma_i c_i - \alpha_i e_i}{\alpha_i^2 + \lambda \gamma_i^2} \right)^2 + \sum_{i=r+1}^{p} e_i^2. \tag{5.7}$$

We see that $f$ is a rational function in $\lambda$ and its poles are a subset of $\{-\mu_i | i = 1, \dots, r\}$. If

$$\alpha^2 > \min_{\mathbf{x}} \|\mathbf{C}\mathbf{x} - \mathbf{d}\|^2 = \sum_{i=r+1}^{p} e_i^2 = \lim_{\lambda \to \infty} f(\lambda) \tag{5.8}$$

then the secular equation $f(\lambda) = \alpha^2$ does have solutions if $f$ has at least one pole. But the normal equations may also have solutions for some $\lambda = -\mu_i$. In this case the matrix of (5.1) is singular. If a solution to the normal equations should exist the linear system (5.1) must be consistent. This is e.g. true if $\mathbf{A}^T \mathbf{b} = \mathbf{C}^T \mathbf{d} = \mathbf{0}$ i.e. $f(\lambda) = \|\mathbf{d}\|^2 = \text{const}$. Then for $\lambda = -\mu_i$, $\mathbf{x}(\lambda)$ is an eigenvector to the eigenvalue $\mu_i$.

**Lemma 2.** *Let $\mu_i$ be an eigenvalue of* (5.6). *Then the linear system*

$$(\mathbf{A}^T \mathbf{A} - \mu_i \mathbf{C}^T \mathbf{C})\, \mathbf{x} = \mathbf{A}^T \mathbf{b} - \mu_i \mathbf{C}^T \mathbf{d} \tag{5.9}$$

*is consistent if and only if the length function $f$ does not have a pole for $\lambda = -\mu_i$.*

*Proof.* If $-\mu_i$ is not a pole of $f$ then $\lim_{\lambda \to -\mu_i} f(\lambda)$ exists or using the representation (5.7) we have

$$\alpha_j (c_j \gamma_j - \alpha_j e_j) = 0 \quad \text{for all } j \in J \tag{5.10}$$

where

$$J = \{ j | 1 \leqq j \leqq r \text{ and } \mu_i = \alpha_j^2/\gamma_j^2 \}. \tag{5.11}$$

Using the BSVD as above and putting $\mathbf{y} := \mathbf{X}^{-1} \mathbf{x}$ the system (5.9) becomes

$$\begin{aligned} (\alpha_k^2 + \lambda \gamma_k^2)\, y_k &= \alpha_k c_k + \lambda \gamma_k e_k, \quad k = 1, \dots, r \\ \alpha_k^2\, y_k &= \alpha_k c_k, \quad k = r+1, \dots, n. \end{aligned} \tag{5.12}$$

From Assumption 2 we have $\alpha_k \neq 0$ for $k = r+1, \dots, n$ cf. [14]. If now $\lambda = -\mu_i = -\alpha_i^2/\gamma_i^2$ then

$$(\alpha_j^2 - \mu_i \gamma_j^2) = 0 \quad \text{for all } j \in J$$

and consistency implies that also the right hand sides must be zero:

$$\begin{aligned} \alpha_j c_j - (\alpha_i^2/\gamma_i^2)\, \gamma_j e_j &= \alpha_j c_j - (\alpha_j^2/\gamma_j^2)\, \gamma_j e_j \\ &= \alpha_j (\gamma_j c_j - \alpha_j e_j)/\gamma_j = 0 \quad \text{for all } j \in J. \end{aligned} \tag{5.13}$$

Equation (5.13) is equivalent to (5.10) and we see from (5.7) that $f$ has no pole for $\lambda = -\mu_i$ i.e. $\lim_{\lambda \to -\mu_i} f(\lambda)$ exists. □

The following theorem describes all solutions of the normal equations:

**Theorem 3.** (i) *If there exists a* $\lambda$ *such that* $f(\lambda) = \alpha^2$ *and* $\det(\mathbf{A}^T\mathbf{A} + \lambda \mathbf{C}^T\mathbf{C}) \neq 0$ *then there exists a unique* $\mathbf{x}(\lambda)$ *such that* $(\mathbf{x}(\lambda), \lambda)$ *solves the normal equations.*

(ii) *If* $\lim_{\lambda \to -\mu_i} f(\lambda) \leqq \alpha^2$ *and* $\det(\mathbf{A}^T\mathbf{A} - \mu_i \mathbf{C}^T\mathbf{C}) = 0$ *then there exists a* $\mathbf{x}(-\mu_i)$ *so that* $(\mathbf{x}(-\mu_i), -\mu_i)$ *solves the normal equations, but* $\mathbf{x}(-\mu_i)$ *is only unique if* $\lim_{\lambda \to -\mu_i} f(\lambda) = \alpha^2$.

*Proof.* We have only to prove the second part. We assume that the transformed normal Eq. (5.12) are consistent for $\lambda = -\mu_i$. Then the solution $y$ is given by

$$y_k = \begin{cases} (\alpha_k c_k - \mu_i \gamma_k e_k)/(\alpha_k^2 - \mu_i \gamma_k^2), & k \notin J \\ \text{arbitrary}, \; k \in J \\ c_k/\alpha_k, & k = r+1, \ldots, n. \end{cases} \tag{5.14}$$

Furthermore

$$\tilde{y}_k := \lim_{\lambda \to -\mu_i} y_k(\lambda) = \begin{cases} (\alpha_k c_k - \mu_i \gamma_k e_k)/(\alpha_k^2 - \mu_i \gamma_k^2), & k \notin J \\ e_k/\gamma_k, & k \in J \\ c_k/\alpha_k, & k = r+1, \ldots, n. \end{cases} \tag{5.15}$$

Using the solution $y$ from (5.14) we have to satisfy the equation

$$\|\mathbf{D}_C \mathbf{y} - \mathbf{e}\|^2 = \alpha^2. \tag{5.16}$$

$$\|\mathbf{D}_C \mathbf{y} - \mathbf{e}\|^2 = \sum_{k \notin J} (\gamma_k y_k - e_k)^2 + \sum_{k \in J} (\gamma_k y_k - e_k)^2 + \sum_{k=r+1}^{n} e_k^2. \tag{5.17}$$

Obviously $\mathbf{y} = \tilde{\mathbf{y}}$ minimizes $\|\mathbf{D}_C \mathbf{y} - \mathbf{e}\|^2$. If

$$\lim_{\lambda \to -\mu_i} f(\lambda) = \|\mathbf{D}_C \tilde{\mathbf{y}} - \mathbf{e}\|^2 > \alpha^2$$

we cannot determine a solution $\mathbf{y}$ that satisfies (5.16). If $\lim_{\lambda \to -\mu_i} f(\lambda) = \alpha^2$ then the unique solution is $\mathbf{y} = \tilde{\mathbf{y}}$. Finally if $\lim_{\lambda \to -\mu_i} f(\lambda) < \alpha^2$ then we can choose $y_k$ $k \in J$ so that

$$\sum_{k \in J} (\gamma_k y_k - e_k)^2 = \alpha - \|\mathbf{D}_C \tilde{\mathbf{y}} - \mathbf{e}\|^2$$

and $\mathbf{y}(-\mu_i)$ is not unique. Having determined $\mathbf{y}$ we get $\mathbf{x}$ from the relationship $\mathbf{x} = \mathbf{X}\mathbf{y}$. □

## 6. Solving the Problem with Equality Constraint

We know that if $(\mathbf{x}, \lambda)$ is a solution of the normal equations then the Lagrange-multiplier $\lambda$ is either a solution of the secular equation or $\lambda = -\mu_i$ where $\mu_i$ is an eigenvalue of the generalized eigenvalue problem (cf. Theorem 3). From Corollary 2 it follows that the solution of (1.1) is the same as the solution $\mathbf{x}$ of the normal equations with largest $\lambda$. Therefore to solve

$$\|\mathbf{A}\,\mathbf{x}-\mathbf{b}\|^2=\min$$

subject to (6.1)

$$\|\mathbf{C}\,\mathbf{x}-\mathbf{d}\|^2=\alpha^2$$

we have to compute the *largest* solution $\lambda^*$ of the secular equation $f(\lambda)=\alpha^2$ and the smallest eigenvalue $\mu_r$ and a corresponding eigenvector $\mathbf{x}_r$ of the generalized eigenvalue problem

$$\mathbf{A}^T\mathbf{A}\,\mathbf{x}=\mu\,\mathbf{C}^T\mathbf{C}\,\mathbf{x}. \tag{6.2}$$

In two cases $\lambda^*$ may not exist:

(i) If $f(\lambda)=\text{const.}$ In this case the secular equation has no solution. The solutions of the normal equations are only given by

$$\lambda=-\mu_i \quad \text{and} \quad \mathbf{x}=\mathbf{x}'+\rho\,\mathbf{x}_i \tag{6.3}$$

where

$$\mathbf{x}_i \text{ is an eigenvector belonging to } \mu_i$$

and

$$\mathbf{x}'=\mathbf{x}(\lambda)=\text{const. is the constant solution of the system (5.1).}$$

The solution of (6.1) is then given for $\lambda=-\mu_r$ i.e. $\rho$ in (6.3) has to be chosen such that

$$\|\mathbf{C}(\mathbf{x}'+\rho\,\mathbf{x}_r)-d\|^2=\alpha^2. \tag{6.4}$$

As example for this case consider the special case where $\mathbf{A}^T\mathbf{b}=\mathbf{0}$ and $\mathbf{C}^T\mathbf{d}=\mathbf{0}$. Here we have $\mathbf{x}'=\mathbf{0}=\text{const.}$ and the solution of (6.1) is $\mathbf{x}=\rho\,\mathbf{x}_r$ with some $\rho$ that satisfies Eq. (6.4).

(ii) If $\lim_{\lambda\to\infty} f(\lambda)\geqq\alpha^2$. Since $\lim_{\lambda\to\infty} f(\lambda)=\min_{\mathbf{x}}\|\mathbf{C}\,\mathbf{x}-\mathbf{d}\|^2$ as we can see from Sect. 5, this case is excluded by Assumption 1. However if we have $\lim_{\lambda\to\infty} f(\lambda)=\alpha^2$ then problem (6.1) is equivalent to the problem

$$\|\mathbf{A}\,\mathbf{x}-\mathbf{b}\|^2=\min$$

subject to

$$\|\mathbf{C}\,\mathbf{x}-\mathbf{d}\|^2=\min,$$

and can be solved using the singular value decomposition.

If $\lambda^*$ exists then we have to distinguish two cases:

a) $\lambda^*>-\mu_r$: The solution of (6.1) is given by

$$\mathbf{x}^*=(\mathbf{A}^T\mathbf{A}+\lambda^*\,\mathbf{C}^T\mathbf{C})^{-1}(\mathbf{A}^T\mathbf{b}+\lambda^*\,\mathbf{C}^T\mathbf{d}).$$

b) $\lambda^*\leqq-\mu_r$: The solution has the form

$$\mathbf{x}(\rho)=\lim_{\lambda\to-\mu_r}\mathbf{x}(\lambda)+\rho\,\mathbf{x}_r$$

where $\rho$ has to be determined such that $\|\mathbf{C}\mathbf{x}(\rho)-\mathbf{d}\|^2=\alpha^2$. If $\rho \neq 0$ then the solution is not unique in this case.

Notice that for problem (6.1) $\lambda^*$ may be negative. This is not the case for the problem with inequality constraint. To distinguish between the two cases a) and b) one referee observed that in case a)

$$\mathbf{x}_r^T(\mathbf{A}^T\mathbf{b}-\mu_r\mathbf{C}^T\mathbf{d}) \neq 0$$

must hold which follows immediately if the linear system (5.9) with $i=r$ is inconsistent. Similarly in the case b) we must have consistency which means that

$$\mathbf{x}_r^T(\mathbf{A}^T\mathbf{b}-\mu_r\mathbf{C}^T\mathbf{d})=0.$$

However the last condition may not necessarily facilitate the decision in actual numerical computations.

The following examples show some of the possible cases:

*Example 1*

$$\alpha=6, \quad \mathbf{A}=\begin{pmatrix}1 & 0\\ 0 & 1\\ 1 & 1\end{pmatrix}, \quad \mathbf{b}=\begin{pmatrix}1\\ -1\\ 0\end{pmatrix},$$

$$\mathbf{C}=\begin{pmatrix}1 & 0\\ 0 & 2\end{pmatrix}, \quad \mathbf{d}=\begin{pmatrix}2\\ 0\end{pmatrix}.$$

The normal equations have the solutions:

$$\begin{aligned}
\lambda_1&=-2.979 & \mathbf{x}(\lambda_1)&=(5.76,\ 0.682)^T\\
\lambda_2&=-1.316 & \mathbf{x}(\lambda_2)&=(-1.96,\ -0.2.93)^T\\
\lambda_3&=-0.513 & \mathbf{x}(\lambda_3)&=(-0.936,\ 1.361)^T\\
\lambda_4&=-0.192 & \mathbf{x}(\lambda_4)&=(1.4357,\ -1.98)^T
\end{aligned}$$

The eigenvalues of $\mathbf{A}^T\mathbf{A}\mathbf{x}=\mu\mathbf{C}^T\mathbf{C}\mathbf{x}$ are

$$\mu_1=2.151, \qquad \mu_2=0.3486$$

Because $-\mu_2<\lambda_4$ the solution of (6.1) is given by $\mathbf{x}(\lambda_4)$.

*Example 2*

$$\alpha=200, \quad \mathbf{A}=\begin{pmatrix}10 & 10\\ 8 & 8\\ 1 & 0\end{pmatrix}, \quad \mathbf{b}=\begin{pmatrix}5\\ -5\\ 5\end{pmatrix},$$

$$\mathbf{C}=\mathbf{I}, \quad \mathbf{d}=\begin{pmatrix}9.9541053460\\ 0\end{pmatrix}.$$

Here $f$ has only one pole and the secular equation has the two solutions $\lambda_1$, $\lambda_2$:

$$\begin{aligned}
\lambda_1&=-340 & \mathbf{x}(\lambda_1)&=(151.6,\ 141.2)^T\\
\lambda_2&=-317 & \mathbf{x}(\lambda_2)&=(-131.7,\ -141.2)^T.
\end{aligned}$$

The eigenvalues are $\mu_1 = 328.5$ and $\mu_2 = 0.4992$. Since $\lambda^* := \lambda_2 < \mu_2$ the solution has the form

$$\mathbf{x}(\rho) = \lim_{\lambda \to -\mu_2} \mathbf{x}(\lambda) + \rho \mathbf{x}_2$$

where

$$\mathbf{x}_2 = (0.706, \ -0.708)^T \text{ is an eigenvector belonging to } \mu_2.$$

A short calculation yields

$$\lim_{\lambda \to -\mu_2} \mathbf{x}(\lambda) = (4.992, \ -4.947)^T.$$

We determine $\rho$ from $\|\mathbf{C}\mathbf{x}(\rho) - \mathbf{d}\|^2 = \alpha^2$ and get $\rho = \pm 199.88$, therefore we obtain the two solutions

$$\mathbf{x} = (-136.13, \ 136.60)^T \quad \text{and} \quad (146.11, \ -146.50)^T.$$

*Example 3*

$$\alpha = 6, \quad \mathbf{A} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix},$$

$$\mathbf{C} = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}, \quad \mathbf{d} = \begin{pmatrix} 1 \\ -2 \end{pmatrix}.$$

Here the first equation of the normal equations

$$(\mathbf{A}^T\mathbf{A} + \lambda \mathbf{C}^T\mathbf{C})\mathbf{x} = \mathbf{A}^T\mathbf{b} + \lambda \mathbf{C}^T\mathbf{d}$$

has the solution $\mathbf{x}(\lambda) = (1, -1)^T$ which does not depend on $\lambda$. Therefore $f(\lambda) = 0 = \text{const.}$ and $f(\lambda) = \alpha^2$ has no solution. However since $f(\lambda) < \alpha^2$ we know from Theorem 3 that the normal equations have solutions for $\lambda = -\mu_i$. The eigenvalues are the same as in Example 1. The eigenvector belonging to $\mu_2 = 0.3486$ is $\mathbf{x}_2 = (-0.518, \ 0.855)^T$ and the solution has the form

$$\mathbf{x} = (1, -1)^T + \rho \mathbf{x}_2$$

By determining $\rho$ from the constraint we get the solutions:

$$\mathbf{x} = (-0.739, \ 1.87)^T \quad \text{and} \quad (2.74, \ -3.87)^T.$$

## 7. The Problem with the Inequality Constraint

We consider the problem

$$\|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2 = \min$$

subject to (7.1)

$$\|\mathbf{C}\mathbf{x} - \mathbf{d}\|^2 \leqq \alpha^2.$$

Let $M = \{\mathbf{x} \mid \|\mathbf{A}\mathbf{x} - \mathbf{b}\| = \min\}$. If for some $\mathbf{x} \in M$ we have $\|\mathbf{C}\mathbf{x} - \mathbf{d}\| \leqq \alpha$ then this $\mathbf{x}$

is a solution. The vector $\mathbf{x}_0 \in M$ that minimizes $\|\mathbf{C}\mathbf{x}-\mathbf{d}\|$ is given by

$$\mathbf{x}_0 = \lim_{\lambda \to 0} (\mathbf{A}^T\mathbf{A} + \lambda \mathbf{C}^T\mathbf{C})^{-1}(\mathbf{A}^T\mathbf{b} + \lambda \mathbf{C}^T\mathbf{d}). \tag{7.2}$$

Observe that $\mathbf{x}_0$ is in general not $\mathbf{A}^+\mathbf{b}$ (see Sect. 5 (5.15) and (5.17)). Since the normal equations are consistent for $\lambda=0$, we can define the number

$$\begin{aligned} \alpha_{\max}^2 &= \|(\mathbf{I}-\mathbf{C}\mathbf{P}_A(\mathbf{C}\mathbf{P}_A)^+)(\mathbf{C}\mathbf{A}^+\mathbf{b}-\mathbf{d})\|^2 = \lim_{\lambda \to 0} f(\lambda) \\ \mathbf{P}_A &= \mathbf{I}-\mathbf{A}^+\mathbf{A}, \qquad \alpha_{\max} \geqq 0. \end{aligned} \tag{7.3}$$

If $\alpha \geqq \alpha_{\max}$ then the constraint is not active and a solution of (7.1) is $\mathbf{x}_0$ defined by (7.2) (If $\mathbf{A}^T\mathbf{A}$ is singular and $\alpha > \alpha_{\max}$ then the solution is not unique).

Similarly we can define $\alpha_{\min} \geqq 0$:

$$\alpha_{\min}^2 := \|(\mathbf{C}\mathbf{C}^+ - \mathbf{I})\mathbf{d}\|^2 = \lim_{\lambda \to \infty} f(\lambda). \tag{7.4}$$

Then (7.1) has no solution if $\alpha_{\min} > \alpha$ which contradicts Assumption 1. In general we will have $\alpha_{\min} < \alpha < \alpha_{\max}$. This means that we have to compute the unique positive solution $\lambda^*$ of the secular equation $f(\lambda) = \alpha^2$ and

$$\mathbf{x}^* = (\mathbf{A}^T\mathbf{A} + \lambda^* \mathbf{C}^T\mathbf{C})^{-1}(\mathbf{A}^T\mathbf{b} + \lambda^* \mathbf{C}^T\mathbf{d}) \tag{7.5}$$

solves (7.1).

The extremal case $\alpha = \alpha_{\max}$ corresponds to the problem

$$\|\mathbf{C}\mathbf{x}-\mathbf{d}\| = \min \quad \text{subject to} \quad \|\mathbf{A}\mathbf{x}-\mathbf{b}\| = \min. \tag{7.6}$$

The solution of (7.6) is given by (7.2) and may be computed using BSVD and (5.15).

Similarly the case $\alpha = \alpha_{\min}$ corresponds to the problem

$$\|\mathbf{A}\mathbf{x}-\mathbf{b}\| = \min \quad \text{subject to} \quad \|\mathbf{C}\mathbf{x}-\mathbf{d}\| = \min, \tag{7.7}$$

since then the set of $\mathbf{x}$ satisfying $\|\mathbf{C}\mathbf{x}-\mathbf{d}\| = \alpha_{\min}$ is given by $\operatorname{grad} \|\mathbf{C}\mathbf{x}-\mathbf{d}\|^2 = \mathbf{0}$.

Finally if $\alpha = \alpha_{\min} = 0$ the problem is reduced to a least squares problem with linear equality constraints

$$\|\mathbf{A}\mathbf{x}-\mathbf{b}\| = \min \quad \text{subject to} \quad \mathbf{C}\mathbf{x} = \mathbf{d}. \tag{7.8}$$

## 8. The Relaxed Least Squares Problem

We consider the special case $\mathbf{C} = \mathbf{I}$ and $\mathbf{d} = \mathbf{0}$:

$$\begin{gathered} \|\mathbf{A}\mathbf{x}-\mathbf{b}\| = \min \\ \text{subject to} \\ \|\mathbf{x}\| = \alpha. \end{gathered} \tag{8.1}$$

Assumption 2 is fulfilled and Assumption 1 too, if $\alpha > 0$. Problem (8.1) can be interpreted to find the minimum value of the quadratic form $\|\mathbf{A}\mathbf{x}-\mathbf{b}\|^2$ on the sphere $\|\mathbf{x}\|^2=\alpha^2$, which is a special case of finding the stationary values of a quadratic form on a sphere. This problem has first been analysed in Forsythe and Golub [2]. They proved that if $(\mathbf{x}_1,\lambda_1)$ and $(\mathbf{x}_2,\lambda_2)$ are solutions of the normal equations then

$$\lambda_1>\lambda_2 \Rightarrow \|\mathbf{A}\mathbf{x}_1-\mathbf{b}\|^2<\|\mathbf{A}\mathbf{x}_2-\mathbf{b}\|^2. \tag{8.2}$$

Kahan [5] gave an elementary proof for the theorem

$$\|\mathbf{A}\mathbf{x}_2-\mathbf{b}\|^2-\|\mathbf{A}\mathbf{x}_1-\mathbf{b}\|^2=\frac{\lambda_1-\lambda_2}{2}\|\mathbf{x}_2-\mathbf{x}_1\|^2 \tag{8.3}$$

which is Theorem 1 in this special case. Unfortunately Kahan did not publish his result. Spjøtvoll [12] independently showed later that

$$\|\mathbf{A}\mathbf{x}_2-\mathbf{b}\|^2-\|\mathbf{A}\mathbf{x}_1-\mathbf{b}\|^2=(\lambda_1-\lambda_2)(\alpha^2-\mathbf{x}_1^T\mathbf{x}_2)$$

but did not quite obtain Kahan's result (Notice that $\alpha^2=(\|\mathbf{x}_1\|^2+\|\mathbf{x}_2\|^2)/2$). The normal equations of (8.1) are

$$(\mathbf{A}^T\mathbf{A}+\lambda\mathbf{I})\mathbf{x}=\mathbf{A}^T\mathbf{b} \tag{8.4}$$

$$\|\mathbf{x}\|^2=\alpha^2. \tag{8.5}$$

If we let $\alpha\to 0$ then $\lambda\to\infty$ and $\|\mathbf{x}\|^2\to 0$. Therefore if we solve (8.4) with some positive $\lambda$ we get a shorter solution $\mathbf{x}$ as for $\lambda=0$. This technique is known as damped least squares [6] or relaxed least squares [10]. The idea is to estimate $\lambda$ to get a shorter solution without solving the secular equation [4]. This technique is also used in the Levenberg-Marquart algorithm; cf. [7] and [8]. The following theorem gives dual normal equations which may be numerically preferable for solving the problem.

**Theorem 4.** (i) *Let* $(\mathbf{x},\lambda)$ *be a solution of the primal normal equations* (8.4), (8.5) *with* $\lambda\neq 0$. *Then* $(\mathbf{z},\lambda)$ *with* $\mathbf{z}=(\mathbf{A}\mathbf{x}-\mathbf{b})/\lambda$ *is a solution of the dual normal equations:*

$$(\mathbf{A}\mathbf{A}^T+\lambda\mathbf{I})\mathbf{z}=-\mathbf{b} \tag{8.6}$$

$$\|\mathbf{A}^T\mathbf{z}\|^2=\alpha^2. \tag{8.7}$$

(ii) *Conversely let* $(\mathbf{z},\lambda)$ *be a solution of the dual normal Eqs.* (8.6), (8.7) *then* $\mathbf{x}=-\mathbf{A}^T\mathbf{z}$ *and* $\lambda$ *solve the primal normal equations.*

*Proof.*

(i) $$(\mathbf{A}\mathbf{A}^T+\lambda\mathbf{I})(\mathbf{A}\mathbf{x}-\mathbf{b})/\lambda=\frac{1}{\lambda}\mathbf{A}(\mathbf{A}^T\mathbf{A}+\lambda\mathbf{I})\mathbf{x}-\frac{1}{\lambda}\mathbf{A}\mathbf{A}^T\mathbf{b}-\mathbf{b}$$

$$=\frac{1}{\lambda}\mathbf{A}\mathbf{A}^T\mathbf{b}-\frac{1}{\lambda}\mathbf{A}\mathbf{A}^T\mathbf{b}-\mathbf{b}=-\mathbf{b}$$

and $\|\mathbf{A}^T\mathbf{z}\|^2=\|\mathbf{A}^T(\mathbf{A}\mathbf{x}-\mathbf{b})/\lambda\|^2=\|\mathbf{x}\|^2=\alpha^2$.

(ii) $(\mathbf{A}^T\mathbf{A}+\lambda\mathbf{I})(-\mathbf{A}^T\mathbf{z})=-\mathbf{A}^T(\mathbf{A}\mathbf{A}^T+\lambda\mathbf{I})\mathbf{z}=\mathbf{A}^T\mathbf{b}$
and $\|\mathbf{x}\|^2=\|-\mathbf{A}^T\mathbf{z}\|^2=\alpha^2$.

We finally remark that it is possible to reduce problem (1.1) to a problem (8.1) [1].

## 9. The Minimum Norm Solution

We consider another special case of problem (1.1) where $\mathbf{A}=\mathbf{I}$ and $\mathbf{b}=\mathbf{0}$:

$$\|\mathbf{x}\|=\min$$
subject to (9.1)
$$\|\mathbf{C}\mathbf{x}-\mathbf{d}\|=\alpha.$$

Assumption 1 is fulfilled and Assumption 2 means that $\mathbf{C}\neq\mathbf{0}$ and $\alpha>\|(\mathbf{C}\mathbf{C}^+-\mathbf{I})\mathbf{d}\|$. Problem (9.1) can be interpreted geometrically as determining a point $\mathbf{x}$ on the hyperellipsoid $\|\mathbf{C}\mathbf{x}-\mathbf{d}\|^2=\alpha^2$ which is nearest to the origin. The normal equations are

$$\begin{aligned}(\mathbf{I}+\lambda\mathbf{C}^T\mathbf{C})\mathbf{x}&=\lambda\mathbf{C}^T\mathbf{d}\\ \|\mathbf{C}\mathbf{x}-\mathbf{d}\|^2&=\alpha^2.\end{aligned}\tag{9.2}$$

Again we can formulate dual equations in this special case.

**Theorem 5.** (i) *Let* $(\mathbf{x},\lambda)$ *be a solution of the primal normal Eqs.* (9.2) *then* $(\mathbf{z},\lambda)$ *with* $\mathbf{z}=\mathbf{C}\mathbf{x}-\mathbf{d}$ *is a solution of the dual normal equations*

$$\begin{aligned}(\mathbf{I}+\lambda\mathbf{C}\mathbf{C}^T)\mathbf{z}&=-\mathbf{d}\\ \|\mathbf{z}\|^2&=\alpha^2.\end{aligned}\tag{9.3}$$

(ii) *Conversely let* $(\mathbf{z},\lambda)$ *be a solution of the dual normal Eqs.* (9.3) *then* $\mathbf{x}=-\lambda\mathbf{C}^T\mathbf{z}$ *is a solution of the primal normal Eqs.* (9.2).

*Proof.*
(i) $$\begin{aligned}(\mathbf{I}+\lambda\mathbf{C}\mathbf{C}^T)(\mathbf{C}\mathbf{x}-\mathbf{d})&=\mathbf{C}(\mathbf{I}+\lambda\mathbf{C}^T\mathbf{C})\mathbf{x}-\mathbf{d}-\lambda\mathbf{C}\mathbf{C}^T\mathbf{d}\\&=\mathbf{C}(\lambda\mathbf{C}^T\mathbf{d})-\mathbf{d}-\lambda\mathbf{C}\mathbf{C}^T\mathbf{d}=-\mathbf{d}\end{aligned}$$

and $\alpha^2=\|\mathbf{C}\mathbf{x}-\mathbf{d}\|^2=\|\mathbf{z}\|^2$.
(ii) $(\mathbf{I}+\mathbf{C}^T\mathbf{C})(-\lambda\mathbf{C}^T\mathbf{z})=-\lambda\mathbf{C}^T(\mathbf{I}+\lambda\mathbf{C}\mathbf{C}^T)\mathbf{z}=\lambda\mathbf{C}^T\mathbf{d}$
and $\|\mathbf{C}\mathbf{x}-\mathbf{d}\|^2=\|\mathbf{C}(-\lambda\mathbf{C}^T\mathbf{z})-\mathbf{d}\|^2=\|\mathbf{z}\|^2=\alpha^2$. □

## 10. Example

In [11] a method is proposed to smooth data. We present here a modified version of it. Let $\{d_i|i=1,\dots,n\}$ be given data of a smooth function and assume that the $d_i$ are perturbed by some measurements errors. We look for a new set of data $\{x_i|i=1,\dots,n\}$ that does not deviate too much from the given $d_i$ and which is smoother. If we assume that the $d_i$ are equidistant we might want to solve

$$\sum_{i=2}^{n-1}(x_{i+1}-2x_i+x_{i-1})^2=\min \tag{10.1}$$

subject to

$$\sum_{i=1}^{n}(x_i-d_i)^2\leqq n\delta^2. \tag{10.2}$$

Here $\delta$ is a given measure for the mean deviation we want to allow the new data $x_i$ to differ from the $d_i$:

$$\delta\simeq\left[\left\{\sum_{i=1}^{n}(x_i-d_i)^2\right\}\bigg/n\right]^{1/2}.$$

The larger we choose $\delta$ the more smooth the $x_i$ will be. Introducing the vectors $\mathbf{d}$ and $\mathbf{x}$ and the $(n-2)\times n$ matrix

$$\mathbf{A}=\begin{pmatrix}1 & -2 & 1 & & & 0\\ & 1 & -2 & 1 & & \\ & & \cdots & & & \\ 0 & & & 1 & -2 & 1\end{pmatrix}$$

we have to solve the problem

$$\|\mathbf{Ax}\|=\min$$

subject to (10.3)

$$\|\mathbf{x}-\mathbf{d}\|\leqq\alpha, \qquad \text{with } \alpha=\sqrt{n}\,\delta.$$

The normal equation for this problem are

$$(\mathbf{A}^T\mathbf{A}+\lambda\mathbf{I})\mathbf{x}=\lambda\mathbf{d}, \tag{10.4}$$

$$\|\mathbf{x}-\mathbf{d}\|^2=\alpha^2. \tag{10.5}$$

Instead of solving (10.4) and (10.5) it is proposed in [11] to estimate a "smoothing parameter" $\gamma>0$ and to solve

$$(\mathbf{I}+\gamma\mathbf{A}^T\mathbf{A})\mathbf{x}=\mathbf{d} \tag{10.6}$$

which is Eq. (10.4) for $\gamma=1/\lambda$. The condition number of the matrix in (10.6) is $1+16\gamma$ (Notice that $\mathbf{A}^T\mathbf{A}$ is singular). Choosing a large $\gamma$ (or small $\lambda$) however may be meaningful; for $\gamma\to\infty$ the new values $x_i$ lie on a straight line: the linear regression of the data $d_i$.

If we make the change of variables $\mathbf{w}:=\mathbf{x}-\mathbf{d}$ and $\mathbf{b}:=-\mathbf{Ad}$ our problem becomes

$$\|\mathbf{Aw}-\mathbf{b}\|=\min$$

subject to (10.7)

$$\|\mathbf{w}\|\leqq\alpha.$$

The normal equations of (10.7) are

$$\begin{aligned}(\mathbf{A}^T\mathbf{A}+\lambda\mathbf{I})\mathbf{w}&=\mathbf{A}^T\mathbf{b}\\ \|\mathbf{w}\|^2&=\alpha^2.\end{aligned} \tag{10.8}$$

If we use the dual equations

$$\begin{aligned}(\mathbf{A}\mathbf{A}^T+\lambda\mathbf{I})\mathbf{z}&=-\mathbf{b}=\mathbf{A}\mathbf{d}\\ \|\mathbf{A}^T\mathbf{z}\|^2&=\alpha^2\end{aligned} \tag{10.9}$$

with $\mathbf{w}=-\mathbf{A}^T\mathbf{z}$ i.e. $\mathbf{x}=\mathbf{d}-\mathbf{A}^T\mathbf{z}$

we observe that $\lambda\to 0$ causes no problems any more since $\mathbf{A}\mathbf{A}^T$ is not singular.

## 11. Final Remarks

It is discussed in [1] and in [3] how to solve the normal equations numerically. That is for $\lambda>0$ it is preferable to solve

$$(\mathbf{A}^T\mathbf{A}+\lambda\mathbf{C}^T\mathbf{C})\mathbf{x}=\mathbf{A}^T\mathbf{b}+\lambda\mathbf{C}^T\mathbf{d}$$

as the least squares problem

$$\begin{pmatrix}\mathbf{A}\\ \sqrt{\lambda}\mathbf{C}\end{pmatrix}\mathbf{x}\approx\begin{pmatrix}\mathbf{b}\\ \sqrt{\lambda}\mathbf{d}\end{pmatrix}$$

using orthogonal transformations. It is also shown how to compute the derivatives of the length function $f$ which may be necessary to solve the secular equation.

Theorems 1 and 2 may be generalised for a general quadratic form $F(\mathbf{x})=\mathbf{x}^T\mathbf{A}\mathbf{x}+\mathbf{b}^T\mathbf{x}+\gamma$ where $\mathbf{A}$ is a square matrix. The reader is referred to [3].

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