# Total linear least squares and the algebraic Riccati equation 

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#### Abstract

It is shown that the solution to a total linear least squares problem satisfies a quadratic matrix equation, which turns into an algebraic Riccati equation when the matrix of unknowns is square. If there is an additional symmetry constraint on the solution, the optimal solution is given by the anti-stabilizing solution of this Riccati equation.


Keywords: Least squares; singular value decomposition; quadratic matrix equation; Riccati equation; control theory.

## 1. Introduction

In the control community, it is common believe that behind every least squares problem, there is an algebraic Riccati equation. This belief is confirmed here for the solution of the Total Linear Least Squares problem (TLLS). We show that the solutions (which are rectangular matrices in general) satisfy a quadratic matrix equation. In the case that the matrix of unknowns is square, this quadratic matrix equation becomes an algebraic Riccati equation. With an additional symmetry constraint on the solution, the TLLS solution is given by the anti-stabilizing solution of a 'symmetrized' algebraic Riccati equation.

This paper is organized as follows:
First, in Section 2, we develop a classical Lagrangean approach to the general TLLS problem, in which we derive its well known solution via the singular value decomposition (SVD). In Section 3, we show that the TLLS solutions satisfy a certain quadratic matrix equation. A brief survey of the solution of such quadratic matrix equations via the invariant subspaces of a certain matrix is included in an appendix. In Section 4, we first discuss linear least squares problems with a symmetry constraint. Next we show that symmetry constrained TLLS solutions are given by the anti-stabilizing solution of an algebraic Riccati equation.

## 2. Total least squares and SVD

Consider the following TLLS problem [6]:
Let $A \in \mathbb{R}^{p \times a}, B \in \mathbb{R}^{p \times r}$ be given. Find the matrices $P, Q, X$ and $Y$ such that

$$
\|(A B)-(P Q)\|_{\mathrm{F}}^{2}
$$

[^0]is minimized, subject to the constraints
\[

\left($$
\begin{array}{ll}
P & Q
\end{array}
$$\right)\binom{X}{Y}=0, \quad Y=-I_{r} .
\]

The motivation behind this problem is the following: Suppose we want to obtain $r$ linear relations (which are linearly independent) that 'explain' the columns of the matrix $B$ as a function of those of $A$. Obviously, in order for such linear relations to exist, the concatenated matrix ( $A B$ ) must be rank deficient. Its null space must be $r$-dimensional. If this is not the case, we can approximate both the matrices $A$ and $B$, by two matrices $P$ and $Q$, such that the concatenated matrix ( $P Q$ ) is rank deficient, which is imposed by the first constraint, and the corresponding null space is $r$-dimensional, which is ensured by the second constraint. The least squares solution to $\min _{X}\|A X-B\|_{\mathrm{F}}^{2}$, which is given via the pseudo-inverse of $A$ as $X=A^{\dagger} B$ is another possible approach to find linear relations. If the equation $A X=B$ is not consistent (because the column space of $A$ and $B$ do for instance not intersect), the solution to the least squares problem satisfies $\left(A^{t} A\right) X=A^{t} B$, which is a consistent equation and hence can be solved exactly. As a matter of fact, the exact equation that is solved can be rewritten as $A X=A A^{\dagger} B$, where now the right hand side is a matrix for which the column space is the orthogonal projection of the column space of $B$ onto that of $A$. Hence the geometrical interpretation that only the right hand side $B$ is modified. In many applications however, where both the data in $A$ and in $B$ are inexact, there is as much reason to modify the matrix $A$ as there is to modify $B$, in order to find a linear model. Whence the motivation behind TLLS.

The so-called Lagrangean associated with this optimization problem, is

$$
\begin{aligned}
\mathscr{L}(P, Q, X, Y)= & \operatorname{trace}\left(A^{\mathrm{t}} A+B^{\mathrm{t}} B-2 A^{\mathrm{t}} P+P^{\mathrm{t}} P+Q^{\mathrm{t}} Q-2 B^{\mathrm{t}} Q\right) \\
& +\sum_{i=1}^{p} \sum_{j=1}^{r} l_{i j}(P X+Q Y)_{i j}+\sum_{i=1}^{r} \sum_{j=1}^{r} \lambda_{i j}\left(y_{i j}+\delta_{i j}\right)
\end{aligned}
$$

where $l_{i j}, \lambda_{i j}$ are Lagrange multipliers associated with the constraints and $\delta_{i j}$ is the Kronecker delta. Let $L \in \mathbb{R}^{p \times r}$ and $\Lambda \in \mathbb{R}^{r \times r}$ be matrices with Lagrange multipliers. Then setting to zero all possible derivatives of the Lagrangean results in

$$
\begin{align*}
& \frac{\partial \mathscr{L}}{\partial P}=0 \Rightarrow P-A+L X^{\mathrm{t}}=0,  \tag{1}\\
& \frac{\partial \mathscr{L}}{\partial Q}=0 \Rightarrow Q-B+L Y^{\mathrm{t}}=0,  \tag{2}\\
& \frac{\partial \mathscr{L}}{\partial X}=0 \Rightarrow P^{\mathrm{t}} L=0,  \tag{3}\\
& \frac{\partial \mathscr{L}}{\partial Y}=0 \Rightarrow Q^{\mathrm{t}} L+\Lambda=0,  \tag{4}\\
& \frac{\partial \mathscr{L}}{\partial \Lambda}=0 \Rightarrow Y=-I_{r},  \tag{5}\\
& \frac{\partial \mathscr{L}}{\partial L}=0 \Rightarrow P X+Q Y=0 . \tag{6}
\end{align*}
$$

Of course, we can immediately eliminate $Y=-I_{\mathrm{r}} .{ }^{1}$ It follows from (6) that $P X=Q$. Use this in (4) to find that $X^{\mathrm{t}} P^{\mathrm{t}} L+\Lambda=0$, but from (3) it then follows directly that $\Lambda=0$. We also find from (1) that $P=A-L X^{\mathrm{t}}$, which means that the matrix $P$ is obtained by subtracting a certain matrix from the given
matrix $A$. For instance, if $r=1$, this is a rank one modification. Using $Q=P X$ and (2) and (3), we find also

$$
\begin{equation*}
P^{\mathrm{t}} P X=P^{\mathrm{t}} B \tag{7}
\end{equation*}
$$

Observe that this expression provides the least squares solution $X$ to $\|B-P X\|_{\mathrm{F}}^{2}$, if $P$ would be known.
In addition, from (1) and (2), we find

$$
\begin{equation*}
P=\left(A+B X^{\mathrm{t}}\right)\left(I_{q}+X X^{\mathrm{t}}\right)^{-1} \tag{8}
\end{equation*}
$$

which gives $P$ as a function of $X$ only. Note that the factor on the right is always invertible. By premultiplying (1) and (2) with $L^{1}$ and using (3) we find

$$
L^{\mathrm{t}} A=L^{\mathrm{t}} L X^{\mathrm{t}}, \quad L^{\prime} B=-L^{\mathrm{t}} L
$$

which can be rewritten as

$$
\binom{A^{\mathrm{t}}}{B^{\mathrm{t}}} L=\binom{X}{-I_{r}} L^{\mathrm{t}} L .
$$

Similarly, we find

$$
\left(\begin{array}{ll}
A & B
\end{array}\right)\binom{X}{-I_{r}}=L\left(I+X^{t} X\right)
$$

From these two expressions, it is easy to show that the columns of $L$ must generate a left singular subspace and those of $\left(X^{\mathrm{t}}-I_{r}\right)^{\mathrm{t}}$, the corresponding right singular subspace of the matrix $(A B)$. Also note that

$$
\left\|\left(\begin{array}{ll}
A & B
\end{array}\right)-\left(\begin{array}{ll}
P & Q
\end{array}\right)\right\|_{\mathrm{F}}^{2}=\left\|L\left(\begin{array}{ll}
X^{\mathrm{t}} & -I_{r}
\end{array}\right)\right\|_{F}^{2}
$$

which implies that we need to take the singular subspaces corresponding to the $r$ smallest singular values. Hence, we have essentially proved the following well known result:

Theorem 1 (Generic TLLS). A solution to the total least squares problem

$$
\min _{P, X}\|A-P\|_{\mathrm{F}}^{2}+\|B-P X\|_{\mathrm{F}}^{2}
$$

where $A \in \mathbb{R}^{p \times q}$ and $B \in \mathbb{R}^{p \times r}$ are given with $p \geq r$, can be obtained from the SVD of ( $A B$ ):

$$
\left(\begin{array}{ll}
A & B
\end{array}\right)=\left(\begin{array}{ll}
U_{1} & U_{2}
\end{array}\right)\left(\begin{array}{cc}
\Sigma_{1} & 0 \\
0 & \Sigma_{2}
\end{array}\right)\left(\begin{array}{ll}
V_{11}^{\mathrm{t}} & V_{21}^{\mathrm{t}} \\
V_{12}^{\mathrm{t}} & V_{22}^{\mathrm{t}}
\end{array}\right)
$$

where $U_{1} \in \mathbb{R}^{p \times q}, U_{2} \in \mathbb{R}^{p \times r}, \Sigma_{1} \in \mathbb{R}^{q \times q}, \Sigma_{2} \in \mathbb{R}^{r \times r}, V_{11} \in \mathbb{R}^{q \times q}, V_{12} \in \mathbb{R}^{q \times r}, V_{21} \in \mathbb{R}^{r \times q}, V_{22} \in \mathbb{R}^{r \times r}$, as

$$
X=-V_{12} V_{22}^{-1}, \quad P=U_{1} \Sigma_{1} V_{11}^{\mathrm{t}}
$$

The epitheton 'generic' refers to the fact that in some rare non-generic cases, the matrix $V_{22}$ might be non-invertible. In that case, one can either chose a different constraint on the matrices $X$ and $Y$ that generate the null space (e.g. a quadratic one for which the problem does not occur) or else obtain the solution to this non-generic TLLS problem with the techniques described in [9].

[^1]
## 3. TLLS solutions and quadratic matrix equations

Let us now derive the following result:
Theorem 2. All matrices $X \in \mathbb{R}^{q \times r}$ satisfying the set of Lagrangean equations (1)-(6) also satisfy the quadratic matrix equation

$$
\begin{equation*}
X B^{\mathrm{t}} A X+A^{\mathrm{t}} A X-X B^{\mathrm{t}} B-A^{\mathrm{t}} B=0 . \tag{9}
\end{equation*}
$$

Proof. Insert (8) in (7) to find

$$
\left(I_{q}+X X^{\mathrm{t}}\right)^{-1}\left(A^{\mathrm{t}}+X B^{\mathrm{t}}\right)\left(A+B X^{\mathrm{t}}\right)\left(I_{q}+X X^{\mathrm{t}}\right)^{-1} X-\left(I_{q}+X X^{\mathrm{t}}\right)^{-1}\left(A^{\mathrm{t}}+X B^{\mathrm{t}}\right) B=0
$$

Noting that $\left(I_{q}+X X^{\mathrm{t}}\right)^{-1} X=X\left(I_{r}+X^{\mathrm{t}} X\right)^{-1}$ we find

$$
\left(A^{\mathrm{t}}+X B^{\mathrm{t}}\right)\left(A+B X^{\mathrm{t}}\right) X-\left(A^{\mathrm{t}}+X B^{\mathrm{t}}\right) B\left(I_{r}+X^{\mathrm{t}} X\right)=0
$$

which is precisely (9).
Actually, quite a bit is known about quadratic matrix equations of the type (9) where the solution $X$ is a rectangular matrix. We refer to the appendix for some details. From these general results on quadratic matrix equations, we can now see that there is a relation between the solutions of equation (9) and the invariant subspaces of the matrix

$$
T=\left(\begin{array}{cc}
-B^{\mathrm{t}} B & B^{\mathrm{t}} A  \tag{10}\\
A^{\mathrm{t}} B & -A^{\mathrm{t}} A
\end{array}\right)=-\binom{B^{\mathrm{t}}}{-A^{\mathrm{t}}}\left(\begin{array}{ll}
B & -A
\end{array}\right) .
$$

Note that this matrix is symmetric negative definite, so all of its eigenvalues are real negative. An invariant subspace will be described as

$$
\left(\begin{array}{cc}
-B^{\mathrm{t} B} & B^{\prime} A  \tag{11}\\
A^{\mathrm{t}} B & -A^{\mathrm{A}} A
\end{array}\right)\binom{U}{V}=\binom{U}{V} \Lambda .
$$

A solution to the quadratic matrix equation (9) is now given by $X=V U^{-1}$ for invertible $U$.
The relation with the SVD solution of Theorem 1 can be clarified in a trivial manner as follows:

$$
-\binom{B^{\mathrm{t}}}{-A^{\mathrm{t}}}\left(\begin{array}{ll}
B & -A
\end{array}\right)\binom{U}{V}=\binom{U}{V} \Lambda \Leftrightarrow\binom{A^{\mathrm{t}}}{B^{\mathrm{t}}}\left(\begin{array}{ll}
A & B
\end{array}\right)\binom{-V}{U}=\binom{-V}{U}(-\Lambda) .
$$

So, invariant subspaces of $T$ (10) can be derived from invariant right singular subspaces of the matrix ( $A B$ ).

We can also re-evaluate the object function as follows:

$$
\begin{aligned}
\|A-P\|_{F}^{2}+\|B-P X\|_{F}^{2} & =\operatorname{trace}\left(A^{\mathrm{t}} A+B^{\mathrm{t}} B\right)+\operatorname{trace}\left(P^{\mathrm{t}} P-2 A^{\mathrm{t}} P+X^{\mathrm{t}} P^{\mathrm{t}} P X-2 B^{\mathrm{t}} P X\right) \\
& =\operatorname{trace}\left(A^{\mathrm{t}} A+B^{\mathrm{t}} B\right)+\operatorname{trace}\left(-2\left(A^{\mathrm{t}}+X B^{\mathrm{t}}\right) P+P^{\mathrm{t}} P\left(I+X X^{\mathrm{t}}\right)\right) \\
& =\operatorname{trace}\left(A^{\mathrm{t}} A+B^{\mathrm{t}} B\right)-\operatorname{trace}\left(\left(A^{\mathrm{t}}+X B^{\mathrm{t}}\right)\left(A+B X^{\mathrm{t}}\right)\left(I+X X^{\mathrm{t}}\right)^{-1}\right) .
\end{aligned}
$$

Now from (9), it follows that

$$
\operatorname{trace}\left(X B^{\mathrm{t}} B X^{\mathrm{t}}+A^{\mathrm{t}} B X^{\mathrm{t}}\right)\left(I+X X^{\mathrm{t}}\right)^{-1}=\operatorname{trace}\left(X B^{\mathrm{t}} A X X^{\mathrm{t}}+A^{\mathrm{t}} A X X^{\mathrm{t}}\right)\left(I+X X^{\mathrm{t}}\right)^{-1}
$$

so that

$$
\|A-P\|_{F}^{2}+\|B-P X\|_{F}^{2}=\operatorname{trace}\left(A^{\mathrm{t}} A+B^{\mathrm{t}} B\right)-\operatorname{trace}\left(A^{\mathrm{t}} A+A^{\mathrm{t}} B X\right)=\operatorname{trace}\left(B^{\mathrm{t}} B-B^{\mathrm{t}} A X\right) .
$$

Now consider the eigenvalue problem (11) associated with the quadratic equation (9), then we find from (28) that

$$
\begin{equation*}
\operatorname{trace}\left(B^{\mathrm{t}} B-B^{\mathrm{t}} A X\right)=-\operatorname{trace}(\Lambda) \tag{12}
\end{equation*}
$$

so that we need to pick those $r$ eigenvalues of $T$ in (10) that have least absolute value (recall all eigenvalues are negative).

As far as we are aware, expression (12) provides a new interpretation of the TLLS problem.
Yet another expression for the object function, which relates more to the SVD result of Theorem 1, can be obtained by using $I_{q}-\left(I_{q}+X X^{t}\right)^{-1}=X\left(I_{r}+X^{t} X\right)^{-1} X^{t}$ as follows:

$$
\left.\begin{array}{rl}
\|A-P\|_{\mathrm{F}}^{2}+\|B-P X\|_{\mathrm{F}}^{2}= & \left\|A-\left(A+B X^{\mathrm{t}}\right)\left(I+X X^{\mathrm{t}}\right)^{-1}\right\|_{\mathrm{F}}^{2}+\left\|B-\left(A+B X^{\mathrm{t}}\right)\left(I+X X^{\mathrm{t}}\right)^{-1} X\right\|_{\mathrm{F}}^{2} \\
= & \left\|A X\left(I+X^{\mathrm{t}} X\right)^{-1} X^{\mathrm{t}}-B\left(I+X^{\mathrm{t} X}\right)^{-1} X^{\mathrm{t}}\right\|_{\mathrm{F}}^{2} \\
& +\left\|B\left(I+X^{\mathrm{t}} X\right)^{-1}-A X\left(I+X^{\mathrm{t}} X\right)^{-1}\right\|_{\mathrm{F}}^{2} \\
= & \left\|(A X-B)\left(I+X^{\mathrm{t}} X\right)^{-1} X^{\mathrm{t}}\right\|_{\mathrm{F}}^{2}+\left\|(A X-B)\left(I+X^{\mathrm{t}} X\right)^{-1}\right\|_{\mathrm{F}}^{2} \\
= & \operatorname{trace}\left(I+X^{\mathrm{t}} X\right)^{-1}\left(X^{\mathrm{t}} A^{\mathrm{t}}-B^{\mathrm{t}}\right)(A X-B) \\
= & \operatorname{trace}\left(I_{r}+X^{\mathrm{t}} X\right)^{-1 / 2}\left(X^{\mathrm{t}}\right. \\
-I_{r}
\end{array}\right)\binom{A^{\mathrm{t}}}{B^{\mathrm{t}}}\left(\begin{array}{ll}
A & B)\binom{X}{-I_{r}}\left(I_{r}+X^{\mathrm{t}} X\right)^{-1 / 2}
\end{array}\right.
$$

## 4. Total linear least squares with a symmetry constraint

Let us first consider the following least squares problem with a symmetry constraint:
Given two matrices $A, B \in \mathbb{R}^{p \times q}$, find $X \in \mathbb{R}^{q \times q}$ so that $\|A X-B\|_{\mathrm{F}}^{2}$ is minimized, subject to the symmetry constraint: $X=X^{\mathrm{t}}$.

The Lagrangean for this optimization problem is:

$$
\mathscr{L}(X, L)=\operatorname{trace}\left(B^{\mathrm{t}} B+X A^{\mathrm{t}} A X-2 B^{\mathrm{t}} A X\right)+\sum_{i=1}^{q} \sum_{j=1}^{q} l_{i j}\left(x_{i j}-x_{j i}\right)
$$

where $l_{i j}$ are the Lagrange multipliers associated with the symmetry constraint. Setting to zero all derivatives results in

$$
\begin{aligned}
& \frac{\partial \mathscr{L}}{\partial X}=0 \Rightarrow A^{\mathrm{t}} A X-A^{\mathrm{t}} B+L-L^{\mathrm{t}}=0 \\
& \frac{\partial \mathscr{L}}{\partial L}=0 \Rightarrow X=X^{\mathrm{t}}
\end{aligned}
$$

If $A$ is of full column rank (which is assumed from now on), we have

$$
\begin{equation*}
X=\left(A^{\mathrm{t}} A\right)^{-1} A^{\mathrm{t}} B+\left(A^{\mathrm{t}} A\right)^{-1}\left(L^{\mathrm{t}}-L\right) \tag{13}
\end{equation*}
$$

Observe that the first term would be the unconstrained least squares solution. Next we define $Z=L^{t}-L$ and note that

$$
\begin{equation*}
Z^{\mathrm{t}}=-Z \tag{14}
\end{equation*}
$$

We find that $X$ is symmetric if $Z$ satisfies $\left(A^{\mathrm{t}} A\right)^{-1}\left(A^{\mathrm{t}} B+Z\right)=\left(Z^{\mathrm{t}}+B^{\mathrm{t}} A\right)\left(A^{\mathrm{t}} A\right)^{-1}$ which can be rewritten using (14) as the Lyapunov equation

$$
\begin{equation*}
Z\left(A^{\mathrm{t}} A\right)+\left(A^{\mathrm{t}} A\right) Z=\left(A^{\mathrm{t}} A\right)\left(B^{\mathrm{t}} A\right)-\left(A^{\mathrm{t}} B\right)\left(A^{\mathrm{t}} A\right) . \tag{15}
\end{equation*}
$$

It is well known that a linear equation of this form has a unique solution. Now from (13) we find that $Z=\left(A^{t} A\right) X-A^{t} B$ so that (15) can be rewritten as

$$
\begin{equation*}
X\left(A^{\mathrm{t}} A\right)+\left(A^{\mathrm{t}} A\right) X=A^{\mathrm{t}} B+B^{\mathrm{t}} A . \tag{16}
\end{equation*}
$$

The conclusion is that a least squares problem with a symmetry constraint can be solved via the Lyapunov equation (16).

The symmetry constrained total linear least squares problem is the following:
Let $A, B \in \mathbb{R}^{p \times q}$ be given. Find $X \in \mathbb{R}^{q \times q}$ so that $\|A-P\|_{\mathrm{F}}^{2}+\|B-P X\|_{\mathrm{F}}^{2}$ is minimized, subject to the symmetry constraint $X=X^{\mathrm{t}}$.

We will prove the following result:
Theorem 3 (Symmetry constrained TLLS). The solution to the symmetry constrained TLLS problem is given by the anti-stabilizing solution to the algebraic Riccati equation

$$
X\left(A^{\mathrm{t}} B+B^{\mathrm{t}} A\right) X+\left(A^{\mathrm{t}} A-B^{\mathrm{t}} B\right) X+X\left(A^{\mathrm{t}} A-B^{\mathrm{t}} B\right)-\left(A^{\mathrm{t}} B+B^{\mathrm{t}} A\right)=0
$$

i.e., the symmetric solution $X$ such that all eigenvalues of $\left(A^{t} A-B^{t} B\right)+\left(A^{t} B+B^{t} A\right) X$ have positive real part.

The remainder of this section is devoted to a derivation of this result.
The Lagrangean for this optimization problem is

$$
\mathscr{L}(P, X, L)=\operatorname{trace}\left(A^{\mathrm{t}} A+P^{\mathrm{t}} P-2 A^{\mathrm{t}} P+B^{\mathrm{t}} B-2 B^{\mathrm{t}} P X+X P^{\mathrm{t}} P X\right)+\sum_{i=1}^{q} \sum_{j=1}^{q} l_{i j}\left(x_{i j}-x_{j i}\right)
$$

which results in the equations

$$
\begin{aligned}
& \frac{\partial \mathscr{L}}{\partial P}=0 \Rightarrow P-A-B X^{\mathrm{t}}+P X X^{\mathrm{t}}=0, \\
& \frac{\partial \mathscr{L}}{\partial X}=0 \Rightarrow-P^{\mathrm{t}} B+P^{\mathrm{t}} P X+L-L^{\mathrm{t}}=0, \\
& \frac{\partial \mathscr{L}}{\partial L}=0 \Rightarrow X=X^{\mathrm{t}} .
\end{aligned}
$$

An expression for $P$ follows immediately as

$$
\begin{equation*}
P=(A+B X)\left(I+X^{2}\right)^{-1} \tag{17}
\end{equation*}
$$

Note also, that with $Z=L^{\mathrm{t}}-L$, we find

$$
\begin{equation*}
\left(P^{\mathrm{t}} P\right) X=P^{\mathrm{t}} B+Z \tag{18}
\end{equation*}
$$

which is the symmetry constrained least squares solution to $\|B-P X\|_{\mathrm{F}}^{2}$ is $P$ were known. Substituting (17) into (18), we find

$$
\left(I+X^{2}\right)^{-1}\left(A^{\mathrm{t}}+X B^{\mathrm{t}}\right)(A+B X)\left(I+X^{2}\right)^{-1} X=\left(I+X^{2}\right)^{-1}\left(A^{\mathrm{t}}+X B^{\mathrm{t}}\right) B+Z
$$

which can be rewritten as

$$
\left(A^{\mathrm{t}}+X B^{\mathrm{t}}\right)(A+B X) X-\left(A^{\mathrm{t}}+X B^{\mathrm{t}}\right) B\left(I+X^{2}\right)=\left(I+X^{2}\right) Z\left(I+X^{2}\right)
$$

or as

$$
\begin{equation*}
X B^{\mathrm{t}} A X+A^{\mathrm{t}} A X-X B^{\mathrm{t}} B-A^{\mathrm{t}} B=\left(I+X^{2}\right) Z\left(I+X^{2}\right) \tag{19}
\end{equation*}
$$

Comparing this quadratic equation to the general one (9), we see that, due to the symmetry constraint, the left hand side does not vanish identically. However, we can get rid of the right hand side by exploiting the anti-symmetry (14) of $Z$. Hereto take the transpose of (19) and use (14) to find

$$
\begin{equation*}
X A^{\mathrm{t}} B X+X A^{\mathrm{t}} A-B^{\mathrm{t}} B X-B^{\mathrm{t}} A=-\left(I+X^{2}\right) Z\left(I+X^{2}\right) \tag{20}
\end{equation*}
$$

Next, adding (19) and (20) results in

$$
\begin{equation*}
X\left(A^{\mathrm{t}} B+B^{\mathrm{t}} A\right) X+\left(A^{\mathrm{t}} A-B^{\mathrm{t}} B\right) X+X\left(A^{\mathrm{t}} A-B^{\mathrm{t}} B\right)-\left(A^{\mathrm{t}} B+B^{\mathrm{t}} A\right)=0 \tag{21}
\end{equation*}
$$

which is an algebraic Riccati equation. The matrix $T$ associated to this quadratic equation is

$$
T=\left(\begin{array}{cc}
A^{\mathrm{t}} A-B^{\mathrm{t}} B & A^{\mathrm{t}} B+B^{\mathrm{t}} A  \tag{22}\\
A^{\mathrm{t}} B+B^{\mathrm{t}} A & B^{\mathrm{t}} B-A^{\mathrm{t}} A
\end{array}\right)
$$

Observe that $T$ is symmetric. Let us demonstrate that it has $q$ positive and $q$ negative eigenvalues. Let $\Lambda$ contain $q$ of the eigenvalues. Then, using the notations $M=A^{\mathrm{t}} A-B^{\mathrm{t}} B$ and $N=A^{\mathrm{t}} B+B^{\mathrm{t}} A$, we find

$$
\left(\begin{array}{cc}
M & N  \tag{23}\\
N & -M
\end{array}\right)\binom{U}{V}=\binom{U}{V} \Lambda \Leftrightarrow\left(\begin{array}{cc}
M & N \\
N & -M
\end{array}\right)\binom{V}{-U}=\binom{V}{-U}(-\Lambda) .
$$

Hence there are $q$ positive and $q$ negative eigenvalues. Let the complete eigenvalue decomposition of $T$ be given as

$$
\left(\begin{array}{cc}
M & N \\
N & -M
\end{array}\right)\left(\begin{array}{cc}
U & V \\
V & -U
\end{array}\right)=\left(\begin{array}{cc}
U & V \\
V & -U
\end{array}\right)\left(\begin{array}{cc}
\Lambda & 0 \\
0 & -\Lambda
\end{array}\right)
$$

where $\Lambda \in \mathbb{R}^{q \times q}$ is a real diagonal matrix with $q$ eigenvalues of $T$. Let us now investigate whether there exist symmetric solutions $X=V U^{-1}$, and if so, how many. If $X=V U^{-1}$ is a symmetric solution, then obviously $U^{\mathrm{t}} V-V^{\mathrm{t}} U=0$. Since the matrix of eigenvectors is orthogonal, we find that there are certainly symmetric solutions. Next let $S \in \mathbb{R}^{2 q \times q}$ be a selector matrix, which selects $q$ columns of the matrix to which it is applied. Then, a corresponding solution $X$ which would be derived from selecting $q$ columns of the matrix of eigenvectors, would be symmetric if

$$
S^{\mathrm{t}}\binom{U^{\mathrm{t}}}{V^{\mathrm{t}}}\left(\begin{array}{ll}
V & -U
\end{array}\right) S-S^{\mathrm{t}}\binom{V^{\mathrm{t}}}{-U^{\mathrm{t}}}\left(\begin{array}{ll}
U & V
\end{array}\right) S=0 \quad \text { or } \quad S^{\mathrm{t}}\left(\begin{array}{cc}
0 & -I \\
I & 0
\end{array}\right) S=0
$$

Hence, all symmetric solutions can be obtained by picking out all possible $q \times q$ zero matrices from the $2 q \times 2 q$ matrix $\left(\begin{array}{cc}0 \\ \hline\end{array}-\frac{I}{0}\right.$ ). It can be shown that there are precisely $2^{n}$ possible selector matrices. So we have shown that there are at most $2^{n}$ symmetric solutions. There might be less if some of the selected matrices $U$ are not invertible.

Using the Riccati equation (21), it is straightforward to show (in a manner similar to the approach followed in section 3) that $\|A-P\|_{\mathrm{F}}^{2}+\|B-P X\|_{\mathrm{F}}^{2}=\operatorname{trace}\left(B^{\mathrm{t}} B-B^{\mathrm{t}} A X\right)$. The minimizing solution $X$ will however also maximize trace $\left(A^{\mathrm{t}} A-B^{\mathrm{t}} B+A^{\mathrm{t}} B X+B^{\mathrm{t}} A X\right.$ ). But we know from (28) (see appendix) that $\operatorname{trace}\left(A^{\mathrm{t}} A-B^{\mathrm{t}} B+\left(A^{\mathrm{t}} B+B^{\mathrm{t}} A\right) X\right)=\operatorname{trace}(\Lambda)$ if the matrix $(I X)^{\mathrm{t}}$ generates an invariant subspace of the matrix $T$ (22) with $X=X^{\text {t }}$. Hence, all we need to do is to find such an invariant subspace associated with the $q$ largest eigenvalues of $T$, which are the positive ones. In control theory, the corresponding solution is called the anti-stabilizing solution. The corresponding solution $X$ is called the anti-stabilizing one because the matrix $\left[\left(A^{t} A-B^{t} B\right)+\left(A^{\mathrm{t}} B+B^{\mathrm{t}} A\right) X\right]$ has all its eigenvalues in the right half complex plane.

## 5. Conclusions

In this paper, we have first developed a solution to the total least squares problem, using a classical optimization approach via Lagrange multipliers. It was shown that the solution also satisfies a quadratic
matrix equation. In the case that the matrix of unknowns becomes square, this quadratic equation turns into an algebraic Riccati equation. If in addition, there is a symmetry constraint on the solution, we can show that we need to take the anti-stabilizing solution.

In the context of dynamical systems such as $[1,2,3,7,8]$, related results have been obtained. The precise connection with our presented here, remains to be investigated.

## Appendix: Quadratic matrix equations

There is a close connection between invariant subspaces of certain matrices and the solutions to quadratic matrix equations. Hereto, consider the matrix

$$
T=\left(\begin{array}{cc}
F & G  \tag{24}\\
H & J
\end{array}\right)
$$

where $F \in \mathbb{R}^{m \times m}, G \in \mathbb{R}^{m \times n}, H \in \mathbb{R}^{n \times m}$ and $J \in \mathbb{R}^{n \times n}$. Consider now an invariant subspace associated with $m$ of its eigenvalues

$$
\left(\begin{array}{cc}
F & G \\
H & J
\end{array}\right)\binom{U}{V}=\binom{U}{V} \Lambda
$$

where $U \in \mathbb{C}^{m \times m}$ and $V \in \mathbb{C}^{n \times m}$. Then $F U+G V=U \Lambda$ and $H U+J V=V \Lambda$. If $U$ is invertible, we find $V U^{-1} F+V U^{-1} G V U^{-1}-H-J V U^{-1}=0$ which is a quadratic equation in $X=V U^{-1}$ :

$$
\begin{equation*}
X G X+X F-J X-H=0 \tag{25}
\end{equation*}
$$

As a matter of fact, this argument can be turned into a rigorous proof [5, p.545]. First, for any matrix $X \in \mathbb{C}^{n \times m}$, we define the graph of $X$ as the set of vectors

$$
\mathscr{G}(X)=\left\{\left.\binom{x}{X x} \right\rvert\, x \in \mathbb{C}^{m}\right\}
$$

Then:
Theorem 4. For any matrix $X \in \mathbb{C}^{n \times m}$, the subspace $\mathscr{E}(X)$ is invariant for $T$ (24) if and only if $X$ satisfies $X G X+X F-J X-H=0$.

Apparently, real solutions $X$ to (25) (if there are any) can also be generated from these invariant subspaces. A solution $X$ to (25) is called isolated if there exists a neighbourhood of $X$ that does not contain other solutions. With respect to real solutions, it can be shown [5, p.556]:

Theorem 5. $X_{0}$ is an isolated solution to $X G X+X F-J X-H=0$ if and only if every common eigenvalue of $F+G X_{0}$ and $J-X_{0} G$ has geometric multiplicity one as an eigenvalue of the matrix $T$ (24).

There appears to be a close connection between the robustness of solutions $X$ with respect to perturbations on the matrices $F, G, H$ and $J$ and the isolatedness of the solution. In fact, only isolated solutions are robust [5, p.551].

Note that, if $X$ is a solution to the quadratic matrix equation (25), then

$$
\left(\begin{array}{cc}
I & 0  \tag{26}\\
-X & I
\end{array}\right)\left(\begin{array}{cc}
F & G \\
H & J
\end{array}\right)\left(\begin{array}{cc}
I & 0 \\
X & I
\end{array}\right)=\left(\begin{array}{cc}
F+G X & G \\
0 & J-X G
\end{array}\right)
$$

which is a similarity transformation. Hence, the union of the sets of eigenvalues of $F+G X$ and $J-X G$ is the set of eigenvalues of $T$. Moreover, from

$$
\left(\begin{array}{cc}
F & G  \tag{27}\\
H & J
\end{array}\right)\binom{I}{X}=\binom{I}{X}\left(U \Lambda U^{-1}\right)
$$

and using the similarity transformation as in (26) we find

$$
\left(\begin{array}{cc}
F+G X & G \\
0 & J-X G
\end{array}\right)\binom{I}{0}=\binom{I}{0}\left(U \Lambda U^{-1}\right)
$$

which implies the eigenvalue decomposition

$$
(F+G X) U=U \Lambda
$$

We will also need the following result which is an immediate consequence of (27):
Lemma 1. Let $X=V U^{-1}$ be a solution to $X G X+X F-J X-H=0$ derived from the invariant subspace ( $(\underset{V}{U})$ belonging to the eigenvalue $\Lambda$. Then

$$
\begin{equation*}
\operatorname{trace}(F+G X)=\operatorname{trace}(\Lambda) \tag{28}
\end{equation*}
$$

If the condition for isolatedness of solutions is satisfied, the relation with the eigenvalue problem of the matrix $T$ can be exploited to show that there is only a finite number of solutions to the quadratic matrix equation (25), which is at most $C_{m}^{m+n}=(m+n)!/(m!n!)$ since this is the number of different $m$-dimensional invariant subspaces.

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[^1]:    ${ }^{1}$ The reason to keep this constraint explicitly in the derivation, is to include the Lagrange multipliers $\Lambda$ and show that they must be zero. The fact that the Lagrange multipliers, associated to this constraint on the matrices that describe the null space, are all zero, can be generalized to other constraints. For instance, if we would use a quadratic constraint of the form $X^{\mathrm{t}} X+Y^{\mathrm{t}} Y=I_{r}$ instead of the linear one, the set of Lagrangean equations becomes 〈1〉P-A+LX $=0,\langle 2\rangle Q-B+L Y^{t}=0,\langle 3\rangle$ $P^{\mathrm{t}} L+X \Lambda=0,\langle 4\rangle Q^{\mathrm{t}} L+Y \Lambda=0,\langle 5\rangle P X+Q Y=0,\langle 6\rangle X^{\mathrm{t}} X+Y^{\mathrm{t}} Y=I$. It is easy to show again that $\Lambda=0$.

