1. Introduction.

This (tutorial) paper grew out of the need to motivate the usual formulation of a “Total Least Squares problem” and to explain the way it is solved using the “Singular Value Decomposition”. Although it is an important generalization of (ordinary) least squares and not more difficult to understand, it is hardly treated in numerical textbooks up to now. In the well-known book of Golub & Van Loan [2] and in [4], the problem is formulated as follows:

\[\begin{align*}
\text{Given a matrix } A \in \mathbb{R}^{m \times n} \text{ with } m > n \text{ and a vector } b \in \mathbb{R}^m, \\
\text{find residuals } E \in \mathbb{R}^{m \times n} \text{ and } r \in \mathbb{R}^m \text{ that minimize} \\
\quad \text{the Frobenius norm } \| (E \mid r) \|_F \text{ subject to the condition } b + r \in \text{Im}(A + E). \\
\end{align*}\]

(1.1)

It is proposed as a more natural way to approximate the data if both \( A \) and \( b \) are contaminated by “errors”. In our opinion, it is not made clear sufficiently well, why this indeed is a natural generalization of the standard least squares problem and why it makes sense to study it. On the other hand, the classroom note of Y. Nievergelt [3] gives a very nice introduction, but it tells only half of the story in that it considers (multiple) regression only.

In this note, we shall give a unified view of ordinary and total least squares problems and their solution. As the geometry underlying the problem setting greatly contributes to the understanding of the solution, we shall introduce least squares problems and their generalization via interpretations in both column space and (the dual) row space and we shall use both approaches to clarify the solution. After a study of the least squares approximation for simple regression in section 3, we introduce the notion of approximation in the sense of “Total Least Squares (TLS)” for this problem in section 4. In the next section we consider ordinary and total least squares approximations for multiple regression problems and in section 6 we study the solution of a general overdetermined system of equations in TLS-sense. In a final section we consider generalizations with multiple right-hand sides and with “frozen” columns. We remark that a TLS-approximation needs not exist in general; however, the line (or hyperplane) of best approximation in TLS-sense for a regression problem does exist always.

As numerical algorithms such as the QR-factorization and the Singular Value Decomposition (SVD) are relatively well-known and nicely implemented in a package like MATLAB, we shall not consider numerical algorithms to compute the solutions effectively.

2. Primal vs. dual approach.

To make clear how both column- and row-space arguments can be used to derive the solution of a least squares problem, we consider least squares in one dimension:

\[
\text{Given } m \text{ points } \{x_i \mid i = 1, \ldots, m\}, \text{ find } z \in \mathbb{R} \text{ that minimizes the quadratic functional} \\
f(z) := \sum_{i=1}^{m} (x_i - z)^2.
\]

(2.1)

The function \( z \mapsto f(z) \) is a parabola. When we shift its center to the average \( \bar{x} := \frac{1}{m} \sum_{i=1}^{m} x_i \),

\[
f(z) = \sum_{i=1}^{m} (x_i - z)^2 = \sum_{i=1}^{m} \left\{ (x_i - \bar{x})^2 + 2(x_i - \bar{x})(\bar{x} - z) + (\bar{x} - z)^2 \right\},
\]

(2.2)
we see that the sum of double products vanishes. Hence, the average $\overline{x}$ is the unique minimizer.

In the dual approach we consider the data as one point in $x \in \mathbb{R}^m$. The functional $f(z)$ then measures the square of the Euclidean distance to the point $ze$,

$$f(z) = \|x - ze\|^2_2,$$

where $x := \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{pmatrix}$ and $e := \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$.

![Fig. 1. Vector $x$, its orthogonal projection on span$\{e\}$ and the residual vector $x - ze$ in the dual approach.](image)

From fig. 1, which shows the plane in $\mathbb{R}^m$ spanned by $x$ and $e$, we find the orthogonal projection of $x$ on span$\{e\}$ as minimizer,

$$\overline{x} = \frac{x^T e}{e^T e} = \frac{1}{m} \sum_{i=1}^{m} x_i.$$

We see that both the primal and the dual approach provide the solution in different ways. In the primal approach we use the fact that linear terms vanish by a shift towards the average. In the dual approach we use an orthogonality argument.

3. Simple regression. In the plane $\mathbb{R}^2$ we are given $m$ data points (abscissae and ordinates)

$$\{(x_i, y_i) \in \mathbb{R}^2 \mid i = 1, \ldots, m\}$$

that should satisfy the linear (affine) relation $y(x) = a + bx$; find the parameters $a$ and $b$ that provide a “best fit”, minimizing the sum of squares of the residuals

$$f(a, b) := \sum_{i=1}^{m} (y_i - a - bx_i)^2.$$  

(3.2)

We can interpret this as searching the line $\ell := \{(x, y) \in \mathbb{R}^2 \mid y = a + bx\}$ “nearest” to the datapoints, minimizing vertical distances and making the tacit assumption that model errors in the data-model $y = a + bx$ are confined to the observed $y$-coordinates, as depicted in fig. 2.

Analogously to (2.2) using the centroid $\overline{y} := (\overline{x}, \overline{y})^T = (\frac{1}{m} \sum_{i=1}^{m} x_i, \frac{1}{m} \sum_{i=1}^{m} y_i)^T$ we rewrite $f$ and find as before, that the double products vanish,

$$f(a, b) := \sum_{i=1}^{m} (y_i - a - bx_i)^2 = \sum_{i=1}^{m} \left( y_i - \overline{y} + b (x_i - \overline{x}) \right)^2 + m (\overline{y} - a - b \overline{x})^2 \geq \sum_{i=1}^{m} \left( y_i - \overline{y} + b (x_i - \overline{x}) \right)^2, \quad \forall a, b,$$

(3.3)
with equality if \( \bar{y} = a + b \bar{x} \). This implies that the centroid is located on the line: \( \bar{z} \in \ell \). Eliminating \( a \) it remains to minimize a function of \( b \) alone, which is a parabola. Hence the minimizer of (3.2) is

\[
b = \frac{\sum_{i=1}^{m} (\bar{x} - x_i)(\bar{y} - y_i)}{\sum_{i=1}^{m} (x_i - \bar{x})^2} \quad \text{and} \quad a = \bar{y} - b\bar{x}.
\]

(3.4)

In the dual approach in \( \mathbb{R}^m \) we interpret \( x_i \) and \( y_i \) as components of vectors \( x \) and \( y \in \mathbb{R}^m \),

\[
x := \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{pmatrix} \quad \text{and} \quad y := \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix} \quad \text{and} \quad e := \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \quad \text{and} \quad A := (e \mid x) \in \mathbb{R}^{m \times 2}.
\]

(3.5)

In this setting the functional \( f \) measures the square of the distance from \( y \) to a linear combination of \( e \) and \( x \),

\[
f(a, b) = \| y - a e - b x \|^2 = \| y - A \begin{pmatrix} a \\ b \end{pmatrix} \|^2.
\]

(3.6)

As in (2.4) it is minimized by the orthogonal projection of \( y \) on the span of \( x \) and \( e \)

\[
f \text{ minimal } \iff y - A \begin{pmatrix} a \\ b \end{pmatrix} \perp \text{Im}(A).
\]

(3.7)

If the rank of \( A \) is maximal, the solution can be computed, see [2], from the Normal Equations or better by an Orthogonal Factorization

\[
A^T A \begin{pmatrix} a \\ b \end{pmatrix} = A^T y \quad \text{or better} \quad A = QR \quad \text{and} \quad R \begin{pmatrix} a \\ b \end{pmatrix} = Q^T y.
\]

(3.8)

Otherwise we can use the Singular Value Decomposition

\[
A = U \Sigma V^T \quad \text{and} \quad \begin{pmatrix} a \\ b \end{pmatrix} = V \Sigma^+ U^T y.
\]

(3.9)

4. Total Least Squares for simple regression. In (3.2) and fig. 2 we considered the problem of locating a line nearest to a collection of points, where the distance is measured along the \( y \)-axis. It looks “more natural” to use the (shorter) true Euclidean distance instead, as drawn in fig. 3, which yields the line of Total Least Squares.

So we consider the Total Least Squares problem of finding the line \( \ell \) that minimizes the sum of squares of true distances:

\[
f(\ell) := \sum_{i=1}^{m} \text{dist}(x_i, y_i, \ell)^2
\]

(4.1)
Instead of asking for a line \( y = ax + b \), we use the more symmetric form

\[
\ell = \{ (x, y) \in \mathbb{R}^2 \mid a + r_1 x + r_2 y = 0 \} = w + r^\perp, \quad \text{with} \quad \|r\|^2 = r_1^2 + r_2^2 = 1, \tag{4.2}
\]

where \( w \) is an arbitrary point on the line \( \ell \), i.e. \( a + r_1 w_1 + r_2 w_2 = 0 \). With this parametrization of \( \ell \) we accept the possibility, that \( r_2 \) may become zero, and hence, that the line cannot be recast in the form \( y = \alpha + \beta x \). In the description \( \ell = w + r^\perp \), where \( r \) is of unit length, the distance from a point \( z \) to \( \ell \) is given by, see fig. 4,

\[
dist(z, \ell) = |r^T (z - w)| \quad \text{where} \quad \ell = w + r^\perp = \{ z \in \mathbb{R}^2 \mid r^T (z - w) = 0 \} \quad \text{and} \quad \|r\| = 1. \tag{4.3}
\]

Hence the TLS problem is to find \( r \) and \( w \) that minimize the functional

\[
I(r, w) := \sum_{i=1}^{m} (r^T(z_i - w))^2 = \sum_{i=1}^{m} (r_1 (x_i - w_1) + r_2 (y_i - w_2))^2 \tag{4.4}
\]

where

\[
z_i = \begin{pmatrix} x_i \\ y_i \end{pmatrix} \quad \text{and} \quad r = \begin{pmatrix} r_1 \\ r_2 \end{pmatrix}, \quad \|r\|^2 = r_1^2 + r_2^2 = 1.
\]
Making the shift to the centroid, as in (3.3) and (2.2), we find again, that the sum of double products vanishes,

\[ I(r, w) = \sum_{i=1}^{m} (r^{T}(z_i - w))^2 \]

\[ = \sum_{i=1}^{m} (r^{T}(z_i - \bar{z}))^2 + \sum_{i=1}^{m} 2r^{T}(z_i - \bar{z})r^{T}(\bar{z} - w) + m(r^{T}(\bar{z} - w))^2 \]

\[ = I(r, \bar{z}) + m(r^{T}(\bar{z} - w))^2 \geq I(r, \bar{z}). \quad (4.5) \]

Clearly, the centroid \( \bar{z} := (\bar{x}, \bar{y})^{T} \) minimizes the functional \( w \mapsto I(r, w) \) for every \( r \in \mathbb{R}^2 \). This implies, that the minimizing line \( \ell = \bar{z} + r^{\perp} \) passes through the centroid (as did the line of simple regression) and that we are left with the reduced minimization problem:

Find the vector \( r \) with \( \|r\|_2 = 1 \) minimizing

\[ I(r, \bar{z}) = \sum_{i=1}^{m} \left( r_1(x_i - \bar{x}) + r_2(y_i - \bar{y}) \right)^2 = \|Br\|_2^2 = r^{T}B^{T}Br, \quad (4.6) \]

where \( B \in \mathbb{R}^{m \times 2} \) is the matrix

\[ B := (x - \bar{x} \ e \ y - \bar{y} \ e) = \begin{pmatrix} x_1 - \bar{x} & y_1 - \bar{y} \\ x_2 - \bar{x} & y_2 - \bar{y} \\ \vdots & \vdots \\ x_m - \bar{x} & y_m - \bar{y} \end{pmatrix}. \quad (4.7) \]

The problem of minimizing \( \|Br\|_2^2 \) subject to \( \|r\|_2 = 1 \) is solved by the Singular Value Decomposition of \( B \),

\[ B = U \Sigma V^{T} \quad \text{with} \quad \Sigma = \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix} \quad \text{and} \quad \sigma_1 \geq \sigma_2. \]

The solution vector \( r \) of (4.6) is the right singular vector of \( B \) corresponding to the smaller singular value of \( B \). So we conclude:

a. The solution always exists and is given by the line through the centroid orthogonal to the subdominant singular vector of \( B \).

b. As \( r_2 \) can be zero, the solution needs not be expressible in the form \( y = \alpha + \beta x \).

c. The solution is unique iff \( \sigma_1 \neq \sigma_2 \).

d. The shift (4.5) to the centroid \( z \in \ell \) is the key in finding the solution, as shown in (4.4).

In the dual formulation we consider the vectors \( x, y \) and \( e \) as in (3.5) and we describe the line \( \ell \) as in (1.2) by \( \ell : = \{(\xi, \eta) \mid a + r_1 \xi + r_2 \eta = 0\} \). For \( i = 1 \cdots m \) we denote by \( (f_i, g_i) \) the point on \( \ell \) nearest to \( (x_i, y_i) \), see fig. 4.

![Fig. 5](image)
and by \( (\overline{f}, \overline{g}) := \frac{1}{m} \sum_{i=1}^{m} (x_i, y_i) \) we denote their average. We define the vectors of first and second components \( f, g \in \mathbb{R}^m \),
\[
    f := (f_1, f_2, \cdots, f_m)^T \quad \text{and} \quad g := (g_1, g_2, \cdots, g_m)^T.
\]
These vectors clearly satisfy the relation \( a\, e + r_1\, f + r_2\, g = 0 \). So we can rephrase the minimization problem \((4.3)\) as the quest for vectors \( f \) and \( g \) that minimize the sum of squares of distances
\[
    I(a, r) := \sum_{i=1}^{m} (x_i - f_i)^2 + \sum_{i=1}^{m} (y_i - g_i)^2 = \|x - f\|^2 + \|y - g\|^2
\]
subject to \( a\, e + r_1\, f + r_2\, g = 0 \), \( r_1^2 + r_2^2 = 1 \).
Decomposing the vectors in their components in \( \text{span}(e) \) and in the orthogonal complement \( e^\perp \) we obtain
\[
    I(a, r) = \|x - f - (\overline{x} - \overline{f}) e\|^2 + \|y - g - (\overline{y} - \overline{g}) e\|^2 + m(\overline{x} - \overline{f})^2 + m(\overline{y} - \overline{g})^2.
\]
(4.8)
The contributions from the parts in \( \text{span}(e) \) are minimized by the choice \( \overline{f} = \overline{x} \) and \( \overline{g} = \overline{y} \) and the subsidiary condition implies \( a + r_1 \overline{x} + r_2 \overline{y} = 0 \) for that choice. Choosing \( \tilde{f} := f - \overline{x} e \) and \( \tilde{g} := g - \overline{y} e \) we are left with the problem to minimize in \( e^\perp \) the functional:
\[
    \|x - \overline{x} e - \tilde{f}\|^2 + \|y - \overline{y} e - \tilde{g}\|^2 \quad \text{subject to} \quad r_1\, \tilde{f} + r_2\, \tilde{g} = 0.
\]
(4.10)
It is not necessary to impose the condition \( \tilde{f}, \tilde{g} \in e^\perp \), since it is automatically satisfied by the minimizer, because \( x - \overline{x} e \) and \( x - \overline{x} e \) satisfy this condition. In matrix notation with \( B := (x - \overline{x} e \mid y - \overline{y} e) \) and \( E := (\tilde{f} \mid \tilde{g}) \) this minimization problem takes the form
\[
    \text{minimize} \quad \|B - E\|^2_F \quad \text{subject to} \quad \text{rank}(E) = 1.
\]
(4.11)
From the Singular Value Decomposition of \( B \),
\[
    B = \sigma_1 \, u_1 \, v_1^T + \sigma_2 \, u_2 \, v_2^T \quad \text{we find} \quad E = \sigma_1 \, u_1 \, v_1^T, \quad \text{provided} \quad \sigma_1 > \sigma_2.
\]
Hence the total least squares solution is (as before) given by,
\[
    E \, v_2 = 0 \quad \text{implying} \quad r = v_2.
\]
There is a difference in flavour between both approaches. Whereas the primal formulation \((4.8)\) directly produces the minimizing vector, the dual approach \((4.11)\) takes a roundabout. The latter provides a minimizing matrix \( E \); the parameters of the line are found only afterwards as the coefficients in the linear combination of the columns of \( E \) that equals zero.

5. **Multiple regression.** The extension of ordinary and total least squares to multiple regression is almost straightforward. As most ideas in 2D-regression easily carry over, we can be brief about it. We are given the cloud of \( m \) datapoints in \( \mathbb{R}^n \) (each point consisting of an “abscissa” in \( \mathbb{R}^{n-1} \) and an ordinate in \( \mathbb{R} \)),
\[
    \{ z_i := (x_{i1}^{(i)}, \cdots, x_{i(n-1)}^{(i)}, y_i)^T \in \mathbb{R}^n \mid i = 1, \cdots, m \},
\]
(5.1)
that should satisfy the linear (affine) model \( y(x_1, \cdots, x_{n-1}) = c_0 + c_1 x_1 + c_2 x_2 + \cdots + c_{n-1} x_{n-1} \). In ordinary least squares the parameters are determined by minimizing the functional \( J \),
\[
    J(c) := \sum_{i=1}^{m} (y_i - c_0 - c_1 x_{i1}^{(i)} - \cdots - c_{n-1} x_{i(n-1)}^{(i)})^2, \quad c := (c_0, \cdots, c_{n-1})^T.
\]
(5.2)
and we can interpret this as the search for the best fitting hyperplane in \( \mathbb{R}^n \),
\[
    \{(x_1, \cdots, x_{n-1}, y)^T \in \mathbb{R}^n \mid y = c_0 + c_1 x_1 + c_2 x_2 + \cdots + c_{n-1} x_{n-1} \}.
\]
(5.3)
As in (4.3), the double products vanish by a shift of the center to the centroid, implying

\[ J(c) \geq \sum_{i=1}^{m} \left( y_i - \overline{y} - c_1(x_1^{(i)} - \overline{x}_1) - \cdots - c_{n-1}(x_{n-1}^{(i)} - \overline{x}_{n-1}) \right)^2 \]

with equality if \( \overline{y} = c_0 + c_1 \overline{x}_1 + \cdots + c_{n-1} \overline{x}_{n-1} \). Hence, the centroid is in the hyperplane. However, more than one unknown parameter is left and the easy argument of (4.3) cannot be applied directly. On the other hand, the dual approach (in “column space”) (5.3) is straightforward and provides the solution easily. Defining vectors \( x_k \) and \( y \in \mathbb{R}^n \) and the matrix \( A \in \mathbb{R}^{m \times n} \),

\[
x_k := \begin{pmatrix} x_k^{(1)} \\ x_k^{(2)} \\ \vdots \\ x_k^{(m)} \end{pmatrix}, \quad y := \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix}, \quad \text{and} \quad A := (e \mid x_1 \mid \cdots \mid x_{n-1}) = \begin{pmatrix} 1 & x_1^{(1)} & \cdots & x_{n-1}^{(1)} \\ 1 & x_1^{(2)} & \cdots & x_{n-1}^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(m)} & \cdots & x_{n-1}^{(m)} \end{pmatrix}
\]

the functional (5.2) takes the form:

\[ J(c) = \|y - c_0e - \cdots - c_{n-1}x_{n-1}\|^2 = \|y - Ac\|^2. \]  

(5.4)

As in (4.4) and (4.7) it is minimized by the orthogonal projection of \( y \) on the span of \( x_1 \cdots x_{n-1} \) and \( e \), i.e. on \( \text{Im}(A) \),

\[ f \text{ minimal } \iff y - Ac \perp \text{Im}(A). \]  

(5.5)

As before, if the rank of \( A \) is maximal, the solution can be computed from the Normal Equations or better by an Orthogonal Factorization, see (4).

\[ A^TAc = A^Ty \quad \text{or better} \quad A = QR \quad \text{and} \quad Rc = Q^Ty. \]  

(5.6)

Otherwise we can use the Singular Value Decomposition

\[ A = U\Sigma V^T \quad \text{and} \quad c = V\Sigma^1U^Ty. \]  

(5.7)

The total least squares approximation minimizes the sum of squares of true distances. We do not attribute a special position to the \( y \)-coordinate and describe the hyperplane in \( \mathbb{R}^n \), as in (4.2), by \( w + r^\perp \). The functional to minimize is:

\[ I(r, w) := \sum_{i=1}^{m} (r^T(z_i - w))^2 = \sum_{i=1}^{m} (r^T(z_i - \overline{z}))^2 + m(r^T(\overline{z} - w))^2 \]  

(5.8)

subject to \( \|r\| = 1 \). Since the double products in the second right-hand side cancel, the centroid (again) is in the hyperplane and it minimizes (5.8) for all \( r \). We are left with the reduced minimization problem, to find \( r \) with \( \|r\|_2 = 1 \) minimizing

\[ I(r, \overline{z}) = \|Br\|_2^2, \quad \text{with} \quad B := \begin{pmatrix} x_1^{(1)} - \overline{x}_1 & \cdots & x_{n-1}^{(1)} - \overline{x}_{n-1} & y_1 - \overline{y} \\ x_1^{(2)} - \overline{x}_1 & \cdots & x_{n-1}^{(2)} - \overline{x}_{n-1} & y_2 - \overline{y} \\ \vdots & \ddots & \vdots & \vdots \\ x_1^{(m)} - \overline{x}_1 & \cdots & x_{n-1}^{(m)} - \overline{x}_{n-1} & y_m - \overline{y} \end{pmatrix}. \]  

(5.9)

The solution vector \( r \) is the right singular vector of \( B \) corresponding to the smallest singular value of \( B \). We conclude:

a. A solution always exists; it is given by the hyperplane through the centroid and orthogonal to the right singular vector belonging to the smallest singular value of matrix \( B \). It is not expressible in the form (5.3) if \( r_n = 0 \).

b. The solution is unique, if \( \sigma_{n-1} > \sigma_n \).
c. The shift of \((5.8)\) to the centroid \(z \in \ell\) is the key in finding the solution.

**In the dual approach** we again consider the hyperplane \((5.3)\), but now the \(y\)-coordinate has no special position in the defining equation,

\[
\{(x_1, \ldots, x_{n-1}, y) \in \mathbb{R}^n \mid c_0 + c_1 x_1 + c_2 x_2 + \cdots + c_{n-1} x_{n-1} + c_n y = 0 \}; \tag{5.10}
\]

instead of \(c_n = -1\) we require \(\sum_{k=1}^n c_k^2 = 1\). We choose (for each \(i\)) the point \((f_k^{(1)}, f_k^{(2)}, \ldots, f_k^{(m)})^T\) on this hyperplane nearest to the datapoint \(z_i\), \((i = 1 \ldots m)\). The first, second, etc. coordinates of these points form in \(\mathbb{R}^m\) the vectors \(f_k (k = 1 \cdots n-1)\) and \(g\),

\[
f_k = (f_k^{(1)}, f_k^{(2)}, \ldots, f_k^{(m)})^T \quad \text{and} \quad g = (g_1, g_2, \ldots, g_m)^T,
\]

which clearly satisfy the relation \(c_0 e + c_1 f_1 + \cdots + c_{n-1} f_{n-1} + c_n g = 0\). The minimization of the sum of squares of distances from the datapoints \(z_i\) to the hyperplane can now be reformulated as the problem of finding vectors \(f_k (k = 1 \cdots n-1)\) and \(g\) in \(\mathbb{R}^m\) that minimize the functional

\[
\| y - g \|_2^2 + \sum_{k=1}^{n-1} \| x_k - f_k \|_2^2 \quad \text{subject to} \quad c_0 e + c_1 f_1 + \cdots + c_{n-1} f_{n-1} + c_n g = 0, \tag{5.11}
\]

where \(\sum_{k=1}^n c_k^2 = 1\). As in \((4.9)-(4.10)\) we may restrict this minimization problem to \(e^\bot\) and eliminate the unknown \(c_0 = -c_n y_n - \sum_{k=1}^{n-1} c_k \pi_k\), by orthogonalization w.r.t. \(e\); essentially this amounts to the same as the shift to the centroid in the primal approach in \(\mathbb{R}^n\). So we find the restricted problem of finding vectors \(f_k (k = 1 \cdots n-1)\) and \(g\) that minimize

\[
\| y - \pi e - g \|_2^2 + \sum_{k=1}^{n-1} \| x_k - \pi_k e - f_k \|_2^2 \quad \text{subject to} \quad c_1 f_1 + \cdots + c_{n-1} f_{n-1} + c_n g = 0.
\]

Without imposing it, the minimizing vectors are orthogonal to \(e\) automatically, as in \((5.10)\). Defining the matrices \(B\) and \(E\),

\[
B := (x_1 - \pi_1 e \mid \cdots \mid x_{n-1} - \pi_{n-1} e \mid y - \pi e) \quad \text{and} \quad E := (f_1 \mid \cdots \mid f_{n-1} \mid g)
\]

we can reformulate the problem as:

\[
\minimize \| B - E \|_F^2 \quad \text{subject to} \quad \text{rank}(E) = n - 1. \tag{5.12}
\]

In this form it is easily solved by the SVD. If \(B = \sum_{i=1}^n \sigma_i u_i v_i^T\), then \(E = \sum_{i=1}^{n-1} \sigma_i u_i v_i^T\) is a minimizer of \((5.12)\), which is unique, if \(\sigma_{n-1} > \sigma_n\). The coefficients \(c_1, \cdots, c_n\) determining the hyperplane are the coordinates of the right singular vector \(v_n\) as before:

\[
E v_n = 0, \quad \implies \begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix} = v_n.
\]

6. **General Least Squares.** For a given matrix \(A \in \mathbb{R}^{m \times n}\) with \(m > n\) and right-hand side \(b \in \mathbb{R}^m\) we consider the problem to find the minimizer \(c \in \mathbb{R}^n\) of the functional

\[
J(c) := \| A c - b \|_2^2 \quad \text{with} \quad c := \begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix}.
\tag{6.1}
\]
The TLS-approximation minimizes the sum of squares of the distances between the (given) points $w \in \mathbb{R}^m$. The solution to the TLS problem for the overdetermined system of equations $Ax = b$ is orthogonal to $\text{Im}(A)$ and it may be computed by normal equations, QR-factorization or SVD.

What is interesting for the TLS generalization is the interpretation of (6.3) in row space. We have introduced the TLS approximation in the sections 4 and 5 as the one that minimizes the sum of squares of the true distances of $m$ points to a hyperplane, whereas ordinary least squares measures the distances along the $y$-axis. We can interpret (6.3) in this sense. The rows of the extended matrix $(A | -b)$ define a cloud of $m$ points in $\mathbb{R}^{n+1}$,

$$
z_k := (a_{k,1}, \ldots, a_{k,n}, -b_k)^T \in \mathbb{R}^{n+1}, \quad \text{such that} \quad (z_1 | \cdots | z_m) = (A | -b)^T,
$$

(6.2)

to which we try to fit a linear function $b(x_1 \cdots x_n) = c_1 x_1 + \cdots + c_n x_n$. In other words, we look for an $n$-dimensional subspace $\hat{c}^\perp$ in $\mathbb{R}^{n+1}$ (and not a hyperplane in $\mathbb{R}^n$ as in the regression problem), that is nearest to the datapoints (6.2), minimizing

$$
J(c) = \| (A | -b) \left( \begin{array}{c} c \\ 1 \end{array} \right) \|_F^2 = \sum_{k=1}^m (z_k^T \hat{c})^2 \quad \text{where} \quad \hat{c} := \left( \begin{array}{c} c \\ 1 \end{array} \right) \in \mathbb{R}^{n+1}.
$$

(6.3)

In this sum of squares the quantity $z_k^T \hat{c}$ measures the distance from $z_k$ to $\hat{c}^\perp$ along the $n+1$-st coordinate axis.

The **Total Least Squares** approximation for the cloud of points (6.2) minimizes the sum of squares of **true** distances to the subspace $\hat{c}^\perp$. As the true distance from $z_k$ to the subspace is given by $z_k^T c / c^T c$, see (4.3), the TLS-approximation minimizes the functional:

$$
I(c) := \sum_{k=1}^m \frac{(z_k^T \hat{c})^2}{c^T c} = \frac{\| (A | -b) \hat{c} \|_F^2}{c^T c} \quad \text{where} \quad \hat{c} := \left( \begin{array}{c} c \\ 1 \end{array} \right).
$$

(6.4)

The functional $r \mapsto \| (A | -b) r \|_F^2$ subject to $\|r\| = 1$ is minimal, if $r$ is the right singular vector corresponding to the smallest singular value of the matrix $(A | -b)$. Renormalizing the last component to $-1$, if possible, provides the solution to the TLS problem for the overdetermined system of equations $Ax = b$. If the $n+1$-st component of this right singular vector is zero, no solution exists to the TLS-problem. The solution is unique if $\sigma_n > \sigma_{n+1}$.

**Interpretation of TLS in Column Space:** To each point $z_k$ $(k = 1 \cdots m)$ in the cloud (6.2)

$$
z_k = \left( \begin{array}{c} a_{k,1} \\ \vdots \\ a_{k,n} \\ -b_k \end{array} \right)
$$

corresponds its best approximation $w_k := \left( \begin{array}{c} f_{k,1} \\ \vdots \\ f_{k,n} \\ -g_k \end{array} \right) \in \hat{c}^\perp.
$$

(6.5)

The TLS-approximation minimizes the sum of squares of the distances between the (given) points $z_k$ and the points $w_k$ in the subspace $\hat{c}^\perp$. We can write this sum of squares as the Frobenius norm of a matrix, if we consider the components $f_{k,i}$ as the elements of a matrix $F \in \mathbb{R}^{m \times n}$, and the components $g_k$ as the components of a vector $g \in \mathbb{R}^m$. Hence, TLS minimizes

$$
\sum_{k=1}^m \|z_k - w_k\|^2 = \|A - F\|^2_F + \|b - g\|^2 = \|(A | -b) - (F | -g)\|^2_F.
$$

(6.6)
Since the rows of the matrix $E := (F | -g) \in \mathbb{R}^{m \times (n+1)}$ are orthogonal to $\hat{c}$, the rank of $E$ is $n$ at most. In other words, TLS minimizes

$$
\| (A| - b) - E \|_F^2 \quad \text{subject to} \quad E \in \mathbb{R}^{m \times (n+1)} \quad \text{and} \quad \operatorname{rank}(E) \leq n.
$$

We may interpret this as the quest for the solution of the solvable linear system $Fc = g$ “nearest” to the (unsolvable) system $Ax = b$, where “solvable” means: $g \in \operatorname{Im}(F)$.

The minimization problem (6.7) is solved by the SVD. If $\begin{pmatrix} A | - b \end{pmatrix} = \sum_{i=1}^{n+1} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$, then $E = \sum_{i=1}^{n} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$ and the required solution of the TLS-problem is the null-vector $v_{n+1}$ of $E$, i.e. the right singular vector $v_{n+1}$ of $\begin{pmatrix} A | - b \end{pmatrix}$ corresponding to the smallest singular value $\sigma_{n+1}$, provided the $n+1$-st component is non-zero. As stated at the end of section 4, the formulation (6.7) takes a roundabout in comparison to the equivalent formulation (6.4) in that it asks for a minimizing system of equations, instead of the solution $\hat{c}$ itself.

We conclude, that in general a best approximation of the over determined system $Ax = b$ in TLS-sense may not exist, because we are not satisfied with the subspace as in a problem of regression; we want the equation for the subspace $b = c_1 x_1 + \cdots + c_n x_n$ to be explicit w.r.t. $b$. Furthermore, the solution is not necessarily unique. We shall illustrate this by two examples.

**Example 1:** Consider the cloud of 4 points in $\mathbb{R}^2$:

$$(1, 1), \ (-1, 1), \ (1, -1), \ and \ (-1, -1)$$

The LS-approximation is the horizontal line $\{(x, y) \mid y = 0\}$. The TLS-approximation makes the SVD of the matrix $B$,

$$B := \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ -1 & 1 \\ -1 & -1 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \sqrt{2} \\ 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 2 & 0 \\ 0 & 2 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

As both singular values are equal, there is no unicity; every line through the origin provides a solution, as shown in fig. 6. The sum of squares of distances from the points to a line with slope $\tan \phi$ is independent of the slope.

**Example 2:** Solve the following problem in LS-sense and TLS-sense:

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

The normal equations for the LS-approximation are:

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \implies x = 1 \text{ and } y \text{ undetermined.}$$
The SVD for TLS-problem is:

\[ B = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \]  

The smallest singular value is 0. However, the 3rd component of the corresponding right singular vector \((0, 1, 0)^T\) is 0 as well, such that no TLS-solution exists!

7. Generalizations: (a) Multiple RHS. In ordinary least squares there is no difference between the treatment of one and multiple right-hand sides (RHS). In Total Least Squares the column space of the matrix is bent towards the RHS. If there are given several RHS’s, we can treat each of them separately and compute the SVD of an extended matrix for each RHS. In a different approach we can try to bend the matrix to all RHS’s collectively. So we consider the problem: given \(A \in \mathbb{R}^{m \times n} (m \geq n + p)\) and \(B \in \mathbb{R}^{m \times p}\) find \(X \in \mathbb{R}^{n \times p}\) that solves the overdetermined system of equations \(AX = B\) in TLS-sense. By analogy to (6.6) we have to find the solution \(X\) of a solvable matrix equation \(FX = G\) (i.e. \(\text{Im}(G) \subset \text{Im}(F)\)) nearest to \(AX = B\); we have to minimize

\[ \|A - F\|_F^2 + \|B - G\|_F^2 \quad \text{subject to} \quad F \in \mathbb{R}^{m \times n}, \ G \in \mathbb{R}^{m \times p} \text{ and } F X = G. \quad (7.1) \]

Otherwise stated, find an approximation \(E = (F \mid G) \in \mathbb{R}^{m \times (n + p)}\) to \((A \mid B)\), such that

\[ \| (A \mid B) - E \|_F^2 \quad \text{is minimal subject to} \quad \text{rank}(E) = n. \quad (7.2) \]

The solution of (7.2) is constructed by making the SVD of \((A \mid B)\):

\[ (A \mid B) = U \Sigma V^T = \begin{pmatrix} (m \times n) \\ U_1 \end{pmatrix} \begin{pmatrix} (n \times n) \\ 0 \\ \Sigma_1 \end{pmatrix} \begin{pmatrix} (n \times n) \\ V_{1,1} \end{pmatrix} + \begin{pmatrix} (m \times p) \\ U_2 \end{pmatrix} \begin{pmatrix} (p \times n) \\ \Sigma_2 \end{pmatrix} \begin{pmatrix} (p \times n) \\ V_{2,1} \end{pmatrix} \begin{pmatrix} (p \times p) \\ V_{2,2} \end{pmatrix} \]  

\[ (7.3) \]

Theorem. If we assume:

a. \(\text{rank}(V_{2,2}) = p\),
b. \(\Sigma = \text{diag}(\sigma_1, \cdots, \sigma_n, 0, \cdots, 0)\) with \(\sigma_j \geq \sigma_{j+1}\) and \(\sigma_n \neq 0\),

then the TLS problem (7.2) has the unique solution \(X = -V_{1,2} V_{2,2}^{-1}\).

Proof: From (7.3) and the assumption \(\sigma_n > \sigma_{n+1}\) it follows, that the best rank \(n\) approximation\(^1\) of \((A \mid B)\) in the Frobenius norm is given by \(E\),

\[ E := (U_1 \mid U_2) \begin{pmatrix} \Sigma_1 \\ 0 \end{pmatrix} \begin{pmatrix} V_{1,1} \\ V_{2,1} \end{pmatrix}^T = U_1 \Sigma_1 \begin{pmatrix} V_{1,1}^T \mid V_{1,2}^T \end{pmatrix} = (F \mid G), \quad (7.4) \]

where \(F := U_1 \Sigma_1 V_{1,1}^T\) and \(G := U_1 \Sigma_1 V_{1,2}^T\). The orthogonality of the columns of \(V\) implies

\[ \begin{pmatrix} V_{1,1} \\ V_{2,1} \end{pmatrix}^T \begin{pmatrix} V_{1,2} \\ V_{2,2} \end{pmatrix} = (0) \quad \text{and hence} \quad E \begin{pmatrix} V_{1,2} \\ V_{2,2} \end{pmatrix} = F V_{1,2} + G V_{2,2} = (0). \]

Under the assumption \(\text{rank}(V_{2,2}) = p\) we may conclude, that \(X := -V_{1,2} V_{2,2}^{-1}\) solves the approximate equation \(FX = G\).

(b) Fixed columns: In section\(^2\) we have introduced the simple (bivariate) regression problem and we have shown that it is solved in LS-sense by the LS-solution of the overdetermined system of equations \(A(\theta)^T = (e \mid x)(\theta)^T = y\)

\(^1\) see theorem 2.5.2
This is solved as eq. (7.2) by the SVD of \( (CR) \). We choose \( A \) it has to be minimized subject to the equations \( R \). We can rewrite the functional as partitioning the matrices in parts consisting of the topmost \( \), because the Frobenius norm is orthogonally invariant, the functional (7.6) is equal to guided by the idea of (4.8), where we orthogonalized w.r.t. the frozen column, we find the solution: a. Orthogonalize columns of \( A_2 \) and \( B \) w.r.t. columns of \( A_1 \). b. Solve TLS-problem in the orthogonal complement \( \text{Im}(A_1)^+ \). Proof: If \( A_1 \) is of full column rank \( \text{rank}(A_1) = j \), we make the QR-factorization

\[
A_1 = U \begin{pmatrix} R_1 \\ 0 \end{pmatrix} \quad \text{with} \quad U \in \mathbb{R}^{m \times m} \text{ orthogonal and } R_1 \in \mathbb{R}^{j \times j}.
\]

Because the Frobenius norm is orthogonally invariant, the functional (7.6) is equal to

\[
\| U^T A_2 - U^T C \|_F^2 + \| U^T B - U^T D \|_F^2.
\]

Partitioning the matrices in parts consisting of the topmost \( j \) rows and the remaining \( m - j \) rows respectively,

\[
\begin{pmatrix} A_{12} \\ A_{22} \end{pmatrix} := U^T A_2, \quad \begin{pmatrix} B_1 \\ B_2 \end{pmatrix} := U^T B, \quad \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} := U^T C, \quad \begin{pmatrix} D_1 \\ D_2 \end{pmatrix} := U^T D,
\]

we can rewrite the functional as

\[
\| A_{12} - C_1 \|_F^2 + \| B_1 - D_1 \|_F^2 + \| A_{22} - C_2 \|_F^2 + \| B_2 - D_2 \|_F^2.
\]

It has to be minimized subject to the equations \( R_1 X_1 + C_1 X_2 = D_1 \) and \( C_2 X_2 = D_2 \). If \( X_2 \) is known, and if we choose \( A_{12} = C_1 \) and \( B_1 = D_1 \), the first two terms in (7.10) vanish and \( X_1 \) can be solved from the equation \( R_1 X_1 + C_1 X_2 = D_1 \). Hence it suffices to minimize

\[
\| A_{22} - C_2 \|_F^2 + \| B_2 - D_2 \|_F^2 \quad \text{subject to} \quad C_2 X_2 = D_2.
\]

This is solved as eq. (7.2) by the SVD of \( (C_2 \mid D_2) \).
If $A$ is not of full column rank ($\text{rank}(A_1) = r < j$), we use the SVD of $A_1$:

$$A_1 = U \begin{pmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} V_1^T \\ V_2^T \end{pmatrix}$$

with $U \in \mathbb{R}^{m \times m}$, $\Sigma_1 \in \mathbb{R}^{r \times r}$, $V_1 \in \mathbb{R}^{j \times r}$, $V_2 \in \mathbb{R}^{j \times (j-r)}$.

With the same partitioning as in (7.9), but now with the $r$ topmost rows in the upper parts and the remaining $m-r$ rows in the lower parts, we arrive at the minimization of (7.10) subject to the conditions

$$\Sigma_1 V_1^T X_1 + C_1 X_2 = D_1 \quad \text{and} \quad C_2 X_2 = D_2.$$  \hfill (7.12)

Choosing $A_{12} = C_1$ and $B_1 = D_1$ and solving $X_2$ from (7.11) we can solve $V_1^T X_1$ from (7.12). This makes the first two terms in (7.10) zero, such that the problem again is reduced to the form (7.2). As in standard LS-problems in which the matrix is not of full column rank, the part $X_1$ is not uniquely defined; we may add to it any linear combination of the columns of $V_2$.

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