A NOTE ON THE TOTAL LEAST SQUARES FIT TO COPLANAR POINTS *

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Abstract. The Total Least Squares (TLS) fit to the points (x_k, y_k), $k = 1, \cdots, n$, minimizes the sum of the squares of the *perpendicular* distances from the points to the line. This sum is the TLS error, and minimizing its magnitude is appropriate if x_k and y_k are uncertain. A priori formulas for the TLS fit and TLS error to coplanar points were originally derived by Pearson in [*Phil. Mag.*, 2 (1901), pp. 559-572], and they are expressed in terms of the mean, standard deviation and correlation coefficient for the data. In this note, these TLS formulas are derived in a more elementary fashion. The TLS fit is obtained via the ordinary least squares problem and the algebraic properties of complex numbers. The TLS error is formulated in terms of the triangle inequality for complex numbers.

Key words. regression, total least squares, triangle inequality

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1. Introduction.

Given the set of points (x_k, y_k), $k = 1, \cdots, n$, it is often desirable to find the straight line

$$y = \alpha x + \beta \tag{1.1}$$

that minimizes the sum of the squares of the *perpendicular* distances from the points to the line. Properly speaking, the above is a total least squares (TLS) problem. The desired line is the TLS fit to the points (x_k, y_k), and the TLS error is the sum to be minimized. Such a fitting is appropriate if x_k and y_k are subject to error. For additional background on this topic, see the original paper by Pearson [6] or the recent paper by Nievergelt [5]. A comprehensive analysis of this problem, and more general TLS problems, is also given by Golub and Van Loan in [2] and by Van Huffel and Vanderwalle in [3]. Finally, we remark that algorithms for the TLS-fitting of lines, rectangles and squares to coplanar points are given by Gander and Hřebíček in [1, Chap. 6.2].

2. Main results.

In the least squares (LS) problem, we are interested in finding the straight line $y = ax + b$ that minimizes the sum of the squares of the vertical distances from the points (x_k, y_k) to the line. It is well known that the solution to the LS problem can be obtained by solving the following system of "normal equations":

$$\begin{bmatrix} n & \sum x_k \\ \sum x_k & \sum x_k^2 \end{bmatrix} \begin{bmatrix} b \\ a \end{bmatrix} = \begin{bmatrix} \sum y_k \\ \sum x_k y_k \end{bmatrix}. \tag{2.1}$$

The solution is unique, unless $x_1 = \cdots = x_n$ (i.e., the points are vertically aligned).

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We can learn a great deal about the TLS problem by first transforming it into a LS problem and then applying the normal equations (2.1). A few observations are needed before pursuing this approach. In particular, for the mean values

$$\bar{x} = \frac{\sum x_k}{n} \quad \text{and} \quad \bar{y} = \frac{\sum y_k}{n},$$

let

$$\tilde{x}_k = x_k - \bar{x} \quad \text{and} \quad \tilde{y}_k = y_k - \bar{y}$$

so that the TLS fit to the points $(\tilde{x}_k, \tilde{y}_k)$ passes through the origin [5, p. 259]. The TLS slope α and TLS error are unaffected by this translation. We now proceed to work in terms of $(\tilde{x}_k, \tilde{y}_k)$ to determine the slope and angle at which the TLS fit crosses the origin. For notational convenience, let us denote these centered points as the complex numbers

$$\tilde{z}_k = \tilde{x}_k + i\,\tilde{y}_k,$$

and let

$$0 \le \tau < \pi$$

denote the angle (in the counterclockwise direction) that the TLS fit makes with the positive real axis. Thus, we have the trivial relations that slope $\alpha = \tan(\tau)$ and $\tau = \tan^{-1}(\alpha)$. The analysis that follows is simpler if we work in terms of the TLS angle τ.

2.1. Total Least Squares Fit. In principle, we can transform the TLS problem into a LS problem by rotating the points $\tilde{z}_k$ by $-\tau$ so that the TLS fit to the points

$$w_k = e^{-i\tau}\tilde{z}_k \tag{2.2}$$

lies along the real axis. The TLS error to the points $\tilde{z}_k$ is unaffected by this rotation, and the perpendicular distances from the points w_k to the TLS fit lie strictly in the vertical direction. In this way, we establish the real axis as the solution to a TLS and LS problem.

Although the τ in (2.2) is unknown, we can determine some of its basic properties by applying the normal equations (2.1) to the points w_k; namely,

$$\begin{bmatrix} n & \sum \mathrm{Re}(w_k) \\ \sum \mathrm{Re}(w_k) & \sum \mathrm{Re}^2(w_k) \end{bmatrix} \begin{bmatrix} b \\ a \end{bmatrix} = \begin{bmatrix} \sum \mathrm{Im}(w_k) \\ \sum \mathrm{Re}(w_k)\,\mathrm{Im}(w_k) \end{bmatrix}. \tag{2.3}$$

Equation (2.3) has the solution $a = 0$, $b = 0$ since the real axis is the LS fit to the points (2.2). Based on this unique LS solution, the right-hand side of (2.3) must also be zero. The second component

$$\sum \mathrm{Re}(e^{-i\tau}\tilde{z}_k)\,\mathrm{Im}(e^{-i\tau}\tilde{z}_k) = 0 \tag{2.4}$$

is especially valuable because the summation of cross terms suggests a strategy for explicitly determining τ. (We disregard the first component because

$$\sum \operatorname{Im}(e^{-i\tau}\tilde{z}_k) = 0 \tag{2.5}$$

for any value of τ.) Later, we show that we can obtain the total least squares error,

$$\text{TLS error} \equiv \sum |d_k|^2 = \sum \operatorname{Im}^2(e^{-i\tau}\tilde{z}_k), \tag{2.6}$$

via a formula that does not involve computing the total least squares fit.

To deduce the TLS angle τ, we introduce the term

$$\rho = \sum (e^{-i\tau}\tilde{z}_k)^2 \tag{2.7}$$

and display its real and imaginary parts via

$$\sum (e^{-i\tau}\tilde{z}_k)^2 = \sum \left[\operatorname{Re}(e^{-i\tau}\tilde{z}_k) + i\operatorname{Im}(e^{-i\tau}\tilde{z}_k)\right]^2 \tag{2.8}$$

$$= \sum \operatorname{Re}^2(e^{-i\tau}\tilde{z}_k) - \sum \operatorname{Im}^2(e^{-i\tau}\tilde{z}_k) + 2i\left\{\sum \operatorname{Re}(e^{-i\tau}\tilde{z}_k)\operatorname{Im}(e^{-i\tau}\tilde{z}_k)\right\}. \tag{2.9}$$

Notice that the summation of cross terms, in curly brackets, is zero due to condition (2.4). Thus, another important property of the unknown τ is that ρ in (2.7) is always a real number.

To proceed further, we now compute the complex number

$$s = \sum \tilde{z}_k^2 \tag{2.10}$$

and simplify the term

$$\rho = \sum (e^{-i\tau}\tilde{z}_k)^2 = e^{-2i\tau}\sum \tilde{z}_k^2 = e^{-2i\tau}s$$

to get the exponential form

$$s = \rho e^{2i\tau}. \tag{2.11}$$

We can establish ρ as a positive real number by denoting $0 \le 2\tau < 2\pi$ as the angle (in the counterclockwise direction) that s makes with the positive real axis. By working with the complex form of s, we can exhibit the real and imaginary parts via

$$s = \sum \tilde{z}_k^2 = \sum (\tilde{x}_k + i\,\tilde{y}_k)^2 = \sum \tilde{x}_k^2 - \sum \tilde{y}_k^2 + 2i\sum \tilde{x}_k\tilde{y}_k$$

and, for the TLS angle τ in (2.11), determine that

$$\tan(2\tau) = \frac{\operatorname{Im}(s)}{\operatorname{Re}(s)} = \frac{2\sum \tilde{x}_k\tilde{y}_k}{\sum \tilde{x}_k^2 - \sum \tilde{y}_k^2}. \tag{2.12}$$

In general, there are two values of τ that satisfy (2.12); these two values will differ by $\pi/2$. The TLS angle is the one that also satisfies (2.4). Other approaches to deriving (2.12) are described in [4, Chap. 13], [6, p. 566]. If $\tan(\tau)$ is defined, we then have the TLS slope $\alpha = \tan(\tau)$. The point-slope form

$$y - \bar{y} = \alpha(x - \bar{x})$$

can be used to obtain the β term of the TLS fit (1.1).

2.2. Total Least Squares Error. An a priori formula for the TLS error comes from

$$\sum |e^{-i\tau}\tilde{z}_k|^2 = \sum |\tilde{z}_k|^2 \tag{2.13}$$

and the following lemma.

LEMMA 2.1. *For the total least squares angle τ to the points $\tilde{z}_k$,*

$$\sum (e^{-i\tau}\tilde{z}_k)^2 = \left|\sum \tilde{z}_k^2\right|. \tag{2.14}$$

Proof. From (2.7), we have

$$\sum (e^{-i\tau}\tilde{z}_k)^2 = \rho.$$

From the exponential form of s in (2.11), we know that ρ equals the magnitude of s. Thus, we finish with

$$\rho = |s| = \left|\sum \tilde{z}_k^2\right|.$$

□

For the TLS angle τ, we can also show that

$$\sum |e^{-i\tau}\tilde{z}_k|^2 = \sum \mathrm{Re}^2(e^{-i\tau}\tilde{z}_k) + \sum \mathrm{Im}^2(e^{-i\tau}\tilde{z}_k) \tag{2.15}$$

and, from (2.7)–(2.9),

$$\sum (e^{-i\tau}\tilde{z}_k)^2 = \sum \mathrm{Re}^2(e^{-i\tau}\tilde{z}_k) - \sum \mathrm{Im}^2(e^{-i\tau}\tilde{z}_k). \tag{2.16}$$

At this stage, notice that (2.15) and (2.16) differ by

$$2 \sum \mathrm{Im}^2(e^{-i\tau}\tilde{z}_k),$$

which is precisely twice the TLS error for the problem; see (2.6). Moreover, (2.13) and (2.14) show that this difference is a readily computable quantity; namely,

$$2\ (\text{TLS error}) = \sum |\tilde{z}_k|^2 - \left|\sum \tilde{z}_k^2\right|. \tag{2.17}$$

THEOREM 2.2. *Given the points (x_k, y_k), $k = 1, \cdots, n$, let*

$$z_k = x_k + i\,y_k \quad \text{and} \quad \bar{z} = \frac{1}{n}\sum z_k$$

so that

$$\tilde{z}_k = z_k - \bar{z}.$$

The error for the total least squares fit is

$$\sum |d_k|^2 = \frac{1}{2}\left(\sum |\tilde{z}_k|^2 - \left|\sum \tilde{z}_k^2\right|\right), \tag{2.18}$$

where $|d_k|$ *is the perpendicular distance from* (x_k, y_k) *to the fit.*

Proof. The theorem follows from (2.17). □

The TLS error formula in (2.18) is a concise version of Pearson's formula [6, p. 566], which is also given in Appendix A. Moreover, by arranging (2.18) as

$$\left|\sum \tilde{z}_k^2\right| + 2\sum |d_k|^2 = \sum |\tilde{z}_k|^2, \tag{2.19}$$

we can drop the term $2\sum |d_k|^2$ and thereby obtain the triangle inequality

$$\left|\sum \tilde{z}_k^2\right| \le \sum |\tilde{z}_k^2| = \sum |\tilde{z}_k|^2 \tag{2.20}$$

as a special case. Thus, Theorem 2.2 establishes an important relationship between the TLS error to z_k and the triangle inequality for the complex numbers $\tilde{z}_k^2$. In particular, we find that the error in the TLS fit equals half the "error" in the triangle inequality applied to the square of the centered points, $\tilde{z}_k^2$; see (2.18).

Unfortunately, this new derivation for the TLS fit and TLS error does not generalize to higher dimensions. Algorithms for fitting a hyperplane to higher-dimensional data are described in [1, Chap. 6.3], [5], for example.

Appendix A. Pearson's formulas for the total least squares problem. In [6], formulas for the TLS fit and TLS error to coplanar points are expressed in terms of the mean

$$\bar{x} = \frac{\sum x_k}{n}, \quad \bar{y} = \frac{\sum y_k}{n},$$

standard deviation

$$\sigma_x = \frac{\sum x_k^2}{n} - \bar{x}^2, \quad \sigma_y = \frac{\sum y_k^2}{n} - \bar{y}^2,$$

and correlation coefficient

$$r_{xy} = \frac{\sum x_k y_k - n\bar{x}\bar{y}}{n\sigma_x\sigma_y}$$

for the data. In particular, Pearson shows that the TLS angle τ satisfies

$$\tan(2\tau) = \frac{2r_{xy}\sigma_x\sigma_y}{\sigma_x^2 - \sigma_y^2}$$

and that

$$\frac{\sum |d_k|^2}{n} \equiv (\text{Mean sq. residual})^2 = \frac{1}{2}(\sigma_{\mathrm{x}}^2 + \sigma_{\mathrm{y}}^2) - \frac{1}{2}\sqrt{(\sigma_{\mathrm{x}}^2 - \sigma_{\mathrm{y}}^2)^2 + 4\mathrm{r}_{\mathrm{xy}}^2\sigma_{\mathrm{x}}^2\sigma_{\mathrm{y}}^2}.$$

The above formulas simplify to those given in (2.12) and (2.18), which we obtained via the ordinary least squares problem, the triangle inequality, and some elementary properties of complex numbers.

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