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**A NOTE ON THE TOTAL LEAST SQUARES PROBLEM
FOR COPLANAR POINTS**

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Abstract

The Total Least Squares (TLS) fit to the points $k = 1, \dots, n$, minimizes the sum of the squares of the *perpendicular* distances from the points to the line. This sum is the TLS error, and minimizing it is appropriate if x and y are uncertain. A priori formulas for the TLS fit and TLS error to coplanar points were originally derived by Fisher in [*Phil. Mag.*, 2 (1901), pp. 559-572], and they are expressed in terms of the mean, standard deviation and correlation coefficient of the data. In this note, these TLS formulas are derived in a more elementary way. 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.

1. Introduction

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

$$y = \alpha x + \beta \tag{1}$$

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 the data are subject to error. For some additional discussion of this topic, see the recent paper by Nivergelt [4] and the references therein. An analysis of this problem and more general TLS problems, is also given by Golub and Van Loan [1] and by Van Huffel and Vanderwalle in [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”:

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

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

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). A few observations are needed before pursuing this approach. In particular, for the mean values

$$\bar{x} = \frac{1}{n} \sum x_k \quad \text{and} \quad \bar{y} = \frac{1}{n} \sum y_k, \tag{3}$$

let

$$\tilde{x}_k = x_k - \bar{x} \quad \text{and} \quad \tilde{y}_k = y_k - \bar{y} \tag{4}$$

so that the TLS fit to the points (x_k, y_k) passes through the origin [4, 259].

The TLS slope α and TLS error are unaffected by this translation. We now proceed to work in terms $(\tilde{x}_k, \tilde{y}_k)$ to determine the slope and angle at which the TLS fit crosses the origin. For notational convenience, let's denote these centered points as the complex numbers

$$\tilde{z}_k = \tilde{x}_k + i \tilde{y}_k, \tag{5}$$

and let

$$0 \leq \tau < \pi \tag{6}$$

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 τ .

In principle, we can transform the TLS problem into a LS problem by rotating the points s_k by $-\tau$ so that the TLS fit to the points

$$w_k = e^{-i\tau} \tilde{z}_k \tag{7}$$

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

Although the τ in (7) is unknown, we can determine some of its basic properties by applying the normal equations (2) to the points w_k

$$\begin{bmatrix} n & \sum \operatorname{Re}(w_k) \\ \sum \operatorname{Re}(w_k) & \sum \operatorname{Re}^2(w_k) \end{bmatrix} \begin{bmatrix} b \\ a \end{bmatrix} = \begin{bmatrix} \sum \operatorname{Im}(w_k) \\ \sum \operatorname{Re}(w_k) \operatorname{Im}(w_k) \end{bmatrix}. \tag{8}$$

Equation (8) has the solution $a=0, b=0$ since the real axis is the LS fit to the points (7). Based on this unique LS solution, the right-hand side of (8) must also be zero, and we find that the unknown τ satisfies

$$\sum \operatorname{Im}(e^{-i\tau} \tilde{z}_k) = 0 \tag{9}$$

and

$$\sum \operatorname{Re}(e^{-i\tau} \tilde{z}_k) \operatorname{Im}(e^{-i\tau} \tilde{z}_k) = 0. \tag{10}$$

The first condition (9) says that the sum of the perpendicular error

second condition (10) is also valuable since the summation of cross terms suggests a strategy for explicitly determining τ . Later, we show that we can obtain the total least squares error,

$$\text{TLS error} \equiv \sum |d_k|^2 = \sum \text{Im}^2(e^{-i\tau\tilde{z}_k}), \quad (11)$$

via a formula that does not involve τ .

To deduce the TLS angle τ , we begin by expanding the term

$$\rho = \sum (e^{-i\tau\tilde{z}_k})^2 \quad (12)$$

$$= \sum [\text{Re}(e^{-i\tau\tilde{z}_k}) + i\text{Im}(e^{-i\tau\tilde{z}_k})]^2 \quad (13)$$

$$= \sum \text{Re}^2(e^{-i\tau\tilde{z}_k}) - \sum \text{Im}^2(e^{-i\tau\tilde{z}_k}) + 2i \left\{ \sum \text{Re}(e^{-i\tau\tilde{z}_k}) \text{Im}(e^{-i\tau\tilde{z}_k}) \right\}. \quad (14)$$

Notice that the summation of cross terms, in curly brackets, is zero due to condition (10). Thus, the third important property of the unknown τ is that ρ is a real number.

To proceed further, we now compute the complex number

$$s = \sum \tilde{z}_k^2 \quad (15)$$

and simplify the term

$$\rho = \sum (e^{-i\tau\tilde{z}_k})^2 = e^{-2i\tau} \sum \tilde{z}_k^2 = e^{-2i\tau} s \quad (16)$$

to get the exponential form

$$s = \rho e^{2i\tau}. \quad (17)$$

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

$$s = \sum \tilde{z}_k^2 = \sum (\tilde{x}_k + i\tilde{y}_k)^2 = \sum \tilde{x}_k^2 - \sum \tilde{y}_k^2 + 2i \sum \tilde{x}_k\tilde{y}_k \quad (18)$$

and, for the angle in the exponential form determine that

$$\tan(2\tau) = \frac{\text{Im}(s)}{\text{Re}(s)} = \frac{2\sum \tilde{x}_k\tilde{y}_k}{\sum \tilde{x}_k^2 - \sum \tilde{y}_k^2}. \quad (19)$$

In general, there are two values of τ that satisfy (19); these two values will differ by $\pi/2$. The TLS angle is the one that also satisfies (9). Other approaches to deriving (19) appear in [3 Chapter 13, Section 4]. If it is defined, we then have the TLS slope $\alpha = \tan(\tau)$. The point-slope form

$$y - y_0 = \alpha(x - x_0) \tag{20}$$

can be used to obtain the β term of the TLS fit (1).

An a priori formula for the TLS error comes from

$$\sum |e^{-i\tau\tilde{z}_k}|^2 = \sum |\tilde{z}_k|^2 \tag{21}$$

and the following lemma.

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

$$\sum (e^{-i\tau\tilde{z}_k})^2 = \left| \sum \tilde{z}_k^2 \right|. \tag{22}$$

Proof: From (12), we have

$$\sum (e^{-i\tau\tilde{z}_k})^2 = \rho. \tag{23}$$

From the exponential form of \sin (17), we know that ρ equals the magnitude of s . Thus, we finish with

$$\rho = |s| = \left| \sum \tilde{z}_k^2 \right|. \tag{24}$$

■

For the TLS angle τ , we can also show that

$$\sum |e^{-i\tau\tilde{z}_k}|^2 = \sum \text{Re}^2(e^{-i\tau\tilde{z}_k}) + \sum \text{Im}^2(e^{-i\tau\tilde{z}_k}) \tag{25}$$

and, from (12)-(14),

$$\sum (e^{-i\tau\tilde{z}_k})^2 = \sum \text{Re}^2(e^{-i\tau\tilde{z}_k}) - \sum \text{Im}^2(e^{-i\tau\tilde{z}_k}). \tag{26}$$

At this stage, notice that (25) and (26) differ by

$$2 \sum \text{Im}^2(e^{-i\tau} z_k), \quad (27)$$

which is precisely twice the TLS error for the problem see (11). Moreover, (21) and (22) show that this difference is a readily computable quantity; namely,

$$2 \text{ (TLS error)} = \sum |\tilde{z}_k|^2 - \left| \sum \tilde{z}_k^2 \right|. \quad (28)$$

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

$$z_k = x_k + i y_k \quad \text{and} \quad \bar{z} = \frac{1}{n} \sum z_k \quad (29)$$

so that

$$\tilde{z}_k = z_k - \bar{z}. \quad (30)$$

The error for the total least squares fit is

$$\sum |d_k|^2 = \frac{1}{2} \left(\sum |\tilde{z}_k|^2 - \left| \sum \tilde{z}_k^2 \right| \right), \quad (31)$$

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

Proof: The theorem follows from (28). ■

The TLS error formula in (31) is a concise version of Pearson's formula [5 pg. 566]. For comparison, note that the latter result reduces to

$$\sum |d_k|^2 = \frac{1}{2} \left(\sum \tilde{x}_k^2 + \sum \tilde{y}_k^2 - \left[\left(\sum \tilde{x}_k^2 - \sum \tilde{y}_k^2 \right)^2 + 4 \left(\sum \tilde{x}_k \tilde{y}_k \right)^2 \right]^{1/2} \right). \quad (32)$$

Moreover, by arranging the formula (31) as

$$\left| \sum \tilde{z}_k^2 \right| + 2 \sum |d_k|^2 = \sum |\tilde{z}_k|^2, \quad (33)$$

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

$$\left| \sum \tilde{z}_k^2 \right| \leq \sum |\tilde{z}_k|^2 = \sum |\tilde{z}_k|^2 \quad (34)$$

as a special case. Thus, (33) establishes an important relation between the TLS error $\sum |d_k|^2$ and the triangle inequality. In particular, we find that the error

in the TLS fit equals half the “error” in the triangle inequality for the square of the centered point \tilde{z} , (see Theorem 2.2).

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].

Acknowledgments

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3. References

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