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

1. Introduction

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

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

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 some additional discussion of this topic, see the recent paper by Nievergelt [4] and the references therein. An analysis of this problem, and more general TLS problems, is also given by Golub and Van Loan [3] and by Van Huffel and Vanderwalle [12].

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 $x_1 = x_2 = \cdots = x_n$ (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 $(\tilde{x}_k, \tilde{y}_k)$ passes through the origin [4, §4.259].

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's denote these centered points as the complex numbers

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

and let

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

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) $\alpha = \tan$ 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 $\tilde{z}_k$ 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 z_k points is unaffected by this rotation, and the perpendicular distances from the w_k points 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 (7) is unknown, we can determine some of its basic properties by applying the normal equations (2) to the points (x_k, y_k):

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

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

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

and

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

The first condition (9) says that the sum of the perpendicular errors d_k is zero. The

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,

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

via a formula that does not involve τ.

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

$$\begin{aligned} \rho &= \sum (e^{-i\tau}\tilde{z}_k)^2 && (12)\\ &= \sum \left[\mathrm{Re}(e^{-i\tau}\tilde{z}_k) + i\,\mathrm{Im}(e^{-i\tau}\tilde{z}_k)\right]^2 && (13)\\ &= \sum \mathrm{Re}^2(e^{-i\tau}\tilde{z}_k) - \sum \mathrm{Im}^2(e^{-i\tau}\tilde{z}_k) + 2i\left\{\sum \mathrm{Re}(e^{-i\tau}\tilde{z}_k)\,\mathrm{Im}(e^{-i\tau}\tilde{z}_k)\right\}. && (14) \end{aligned}$$

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

$$s = \sum \tilde{z}_k^2 \tag{15}$$

and simplify the term

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

to get the exponential form

$$s = \rho e^{2i\tau}. \tag{17}$$

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

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

and, for the angle in the exponential form, determine that

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

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 [5] and [3, Chapter 13, Section 4]. If τ is defined, we then have the TLS slope $\alpha = \tan(\tau)$. The point-slope form

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

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 s in (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

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

and, from (12)–(14),

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

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

$$2 \sum \mathrm{Im}^2(e^{-i\tau}\tilde{z}_k), \tag{27}$$

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,

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

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

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

so that

$$\tilde{z}_k = z_k - \bar{z}. \tag{30}$$

The error for the total least squares fit is

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

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

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

Moreover, by arranging the formula (31) as

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

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

$$\left|\sum \tilde{z}_k^2\right| \le \sum |\tilde{z}_k^2| = \sum |\tilde{z}_k|^2 \tag{34}$$

as a special case. Thus, (33) establishes an important relation between the TLS error to $\tilde{z}_k$ and the triangle inequality for $\tilde{z}_k^2$. 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 points $\tilde{x}_k^2$, (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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