A tutorial on the total least squares method for fitting a straight line and a plane

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A tutorial on the total least squares method for fitting a straight line and a plane

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Abstract—**The classic least squares regression fits a line to data where errors may occur only in the dependent variable, while the independent variable is assumed to have no errors. The total least squares regression fits a line where errors may occur in both variables. This tutorial provides an introduction to the method of total least squares supplementing a first course in statistics or linear algebra.**

I. INTRODUCTION

Detecting geometric features (lines, circles, surfaces, etc.) from data points is a fundamental task in several fields of science and engineering; for instance, metrology, computer vision, mobile robotics, etc.

Let $Z = \{z_1, \dots, z_n\}$ be a set of n measurements or points where each point $z_i = \langle x_i, y_i \rangle$ is represented by its rectangular coordinates. A linear relation between x and y is usually written as

$$y = ax + b \tag{1}$$

where a is the slope of the straight line and b is the y-axis intersection. In the classic Least Squares (LS) the abscissa data $(x_i, i = 1, \dots, n)$ are assumed to be known exactly while the uncertainties of the ordinate data (y_i) are used as weights for fitting the line $\langle a, b \rangle$, given by (1), to the set of measurements Z.

The solution to fit a line using the least squares regression, appears with complete derivations in textbooks at many levels: calculus, linear algebra, numerical analysis, probability, statistics, and others.

However, measured data are never free of uncertainty. This means, in order to determine a best fit to a line, a method is required which takes the uncertainties of the x_i and y_i data into account [3]. The Total Least Squares regression (TLS) was introduced by Golub and Van Loan [2] to deal with both uncertainties. Despite its usefulness and its simplicity, TLS has not yet appeared in numerical analysis, statistics or linear algebra texts.

Introducing students to TLS is the purpose of this tutorial, and it may complement the usual courses in numerical analysis, statistics or linear algebra, or serve as a transition from such courses to a more advanced and specialized course. Additional references to TLS are the introductory paper by Yves Nievergelt [5]; an overview of the TLS methods, by Ivan Markovsky and Sabine Van Huffel [4]; or the book by Sabine Van Huffel and Joos Vandewalle, about the TLS problem [7].

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II. PRELIMINARIES

A. Normal form of a line

There is a disadvantage of using equation (1) to represent a line: vertical lines can not be represented, because $a \to \infty$. To avoid this problem, a line in the plane is represented by its normal form,

$$\ell = \langle r, \phi \rangle \tag{2}$$

where r and ϕ are the length and the angle of inclination of the normal, respectively. As shown in Figure 1, the normal is the shortest segment between the line and the origin of a given coordinate frame. Using this form, points $z = \langle x, y \rangle$ that are on the line $\ell = \langle r, \phi \rangle$ satisfy

$$r = \mathrm{x} \cos\phi + y \sin\phi \tag{3}$$

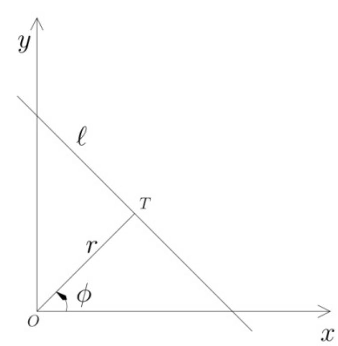

Fig. 1. Line parameters in the normal form. The shortest distance from the origin to the line ℓ is $r = \overline{OT}$.

The relation between the normal form $\langle r, \phi \rangle$ to the representation $\langle a, b \rangle$ given by eq. (1) can be obtained dividing eq. (3) by $\sin\phi$ (while $\phi \neq 0$, avoiding vertical lines) and reordering terms:

$$\begin{aligned} y &= -\frac{\cos\phi}{\sin\phi} x + \frac{r}{\sin\phi} \\ y &= -\frac{1}{\tan\phi} x + \frac{r}{\sin\phi} \end{aligned} \tag{4}$$

From this last equation, the parameters of the line $\langle a, b\rangle$ are given by:

$$a = -\frac{1}{tan\phi}, \qquad b = \frac{r}{\sin\phi} \tag{5}$$

B. *Orthogonal distance from a point to a line*

The shortest distance from a given point $z_i = \langle x_i, y_i\rangle$ to a line $\ell = \langle r, \phi\rangle$, denoted by $d_\perp(z_i, \ell)$, is easily computed as follows.

A line ℓ_i through the point z_i, parallel to line ℓ, is given by:

$$r_i = x_i \cos\phi + y_i \sin\phi$$

The separation between this new line l_i with parameters $\langle r_i, \phi\rangle$ and the line ℓ with parameters $\langle r, \phi\rangle$ is the difference $d_i = r_i - r$, because both lines have the same ϕ (see Figure 2). So the desired distance, called orthogonal distance, is

$$d_\perp(z_i, \ell) = x_i \cos\phi + y_i \sin\phi - r \tag{6}$$

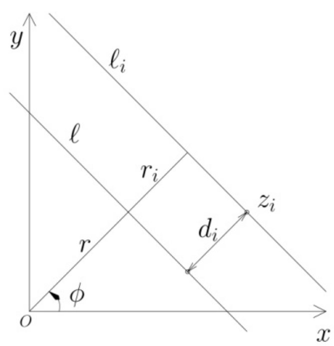

Fig. 2. Orthogonal distance d_i from point z_i to line ℓ.

III. THE TOTAL LEAST SQUARES REGRESSION

A. *The problem definition*

In the literature, the problem of fitting a straight line to data with errors in both coordinates was first formulated by Pearson as early as in 1901 [3]. Deming in 1943 [1] suggests to minimize the sum

$$\chi^2(\ell, z_1, \ldots, z_n) = \sum_{i=1}^{n}\left[\frac{(x_k - X_k)^2}{u_{x,k}^2} + \frac{(y_k - Y_k)^2}{u_{y,k}^2}\right] \tag{7}$$

where (x_k, y_k) are the points coordinates with corresponding uncertainties $(u_{x,k}, u_{y,k})$ and (X_k, Y_k) denote its corresponding point of the straight line ℓ. The best line minimizes χ^2. In the case $u_{x,k} = u_{y,k} = \sigma, k = 1, \ldots, n$, the problem is reduced to the so-called total least-squares problem and minimizing (7) is equivalent to minimizing the orthogonal distance of the measured points (x_k, y_k) to the fitting line. Therefore, this is also often referred to as orthogonal regression [3]. In this case, the best line minimizes

$$\chi^2(\ell; Z) = \sum_{i=1}^{n}\frac{d_\perp^2(z_i, \ell)}{\sigma^2} \tag{8}$$

B. *Finding the best line*

Replacing eq. (6) into (8), the best line ℓ minimizes

$$\chi^2(\ell; Z) = \frac{1}{\sigma^2}\sum_{i=1}^{n}(x_i \cos\phi + y_i \sin\phi - r)^2 \tag{9}$$

A condition for a minimum is that the partial derivatives of χ^2 with respect to the parameters of the line (r and ϕ) vanish: $\frac{\partial\chi^2}{\partial r} = \frac{\partial\chi^2}{\partial\phi}$=0.

Lets do $\frac{\partial\chi^2}{\partial r} = 0$ first

$$\frac{\partial(\frac{1}{\sigma^2}\sum_{i=1}^{n}(x_i\cos\phi + x_i\sin\phi - r)^2)}{\partial r} = 0$$

$$\frac{-2}{\sigma^2}\sum_{i=1}^{n}(x_i\cos\phi + y_i\sin\phi - r) = 0$$

$$\cos\phi\sum_{i=1}^{n}(x_i) + \sin\phi\sum_{i=1}^{n}(y_i) - \sum_{i=1}^{n}(r) = 0$$

$$\cos\phi\sum_{i=1}^{n}(x_i) + \sin\phi\sum_{i=1}^{n}(y_i) - nr = 0$$

$$\cos\phi\left[\frac{1}{n}\sum_{i=1}^{n}(x_i)\right] + \sin\phi\left[\frac{1}{n}\sum_{i=1}^{n}(y_i)\right] - r = 0 \tag{10}$$

Expressions in square brackets are the well known means of x and y, defined as follows

$$\bar{x} = \tfrac{1}{n}\textstyle\sum_{i=1}^{n} x_i, \qquad \bar{y} = \tfrac{1}{n}\textstyle\sum_{i=1}^{n} y_i \tag{11}$$

Equation (10) reduces to

$$\begin{gathered}\cos\phi\,\bar{x} + \sin\phi\bar{y} - r = 0\\ r = \bar{x}\cos\phi + \bar{y}\sin\phi\end{gathered} \tag{12}$$

Comparing equations (3) and (12), we get an important result:

> The centroid of points given by $\langle\bar{x}, \bar{y}\rangle$ is a point of the line ℓ with parameters $\langle r, \phi\rangle$ which minimizes eq. (9).

Replacing eq. (12) into (9), $\chi^2(\ell; Z)$ can be expressed as

$$\chi^2(\ell; Z) = \frac{1}{\sigma^2}\sum_{i=1}^{n}[(x_i - \bar{x})\cos\phi + (y_i - \bar{y})\sin\phi]^2 \tag{13}$$

In eq. (13) the only unknown parameter is ϕ. So, lets do $\frac{\partial\chi^2}{\partial\phi} = 0$, in order to find the right ϕ.

$$\frac{\partial(\frac{1}{\sigma^2}\sum_{i=1}^{n}[(x_i - \bar{x})\cos\phi + (y_i - \bar{y})\sin\phi]^2)}{\partial\phi} = 0$$

$$\frac{1}{\sigma^2}\sum_{i=1}^{n} 2\,[(x_i - \bar{x})\cos\phi + (y_i - \bar{y})\sin\phi] \times$$
$$[-(x_i - \bar{x})\sin\phi + (y_i - \bar{y})\cos\phi] = 0$$

$$\sum_{i=1}^{n} -(x_i - \bar{x})^2\, 2\cos\phi\sin\phi + 2(x_i - \bar{x})(y_i - \bar{y})\cos^2\phi$$

$$-2(x_i-\bar{x})(y_i-\bar{y})\sin^2\phi+(y_i-\bar{y})^2 2\cos\phi\sin\phi=0$$

$$\sum_{i=1}^{n} 2\cos\phi\sin\phi\,[(y_i-\bar{y})^2-(x_i-\bar{x})^2]+ 2(x_i-\bar{x})(y_i-\bar{y})(\cos^2\phi-\sin^2\phi)=0 \quad (14)$$

Using the following trigonometric identities

$$\sin 2\phi = 2\cos\phi\sin\phi\,,\quad \cos 2\phi=\cos^2\phi-\sin^2\phi \quad (15)$$

Equation (14) reduces to

$$\sum_{i=1}^{n}\sin 2\phi[(y_i-\bar{y})^2-(x_i-\bar{x})^2]+ 2(x_i-\bar{x})(y_i-\bar{y})\cos 2\phi=0$$

$$\sin 2\phi\sum_{i=1}^{n}[(y_i-\bar{y})^2-(x_i-\bar{x})^2]+ 2\cos 2\phi\sum_{i=1}^{n}[(x_i-\bar{x})(y_i-\bar{y})=0$$

$$\tan 2\phi=\frac{\sin 2\phi}{\cos 2\phi}=\frac{-2\sum_{i=1}^{n}[(x_i-\bar{x})(y_i-\bar{y})]}{\sum_{i=1}^{n}[(y_i-\bar{y})^2-(x_i-\bar{x})^2]}$$

$$\phi=\frac{1}{2}\arctan\left(\frac{-2\sum_{i=1}^{n}[(x_i-\bar{x})(y_i-\bar{y})]}{\sum_{i=1}^{n}[(y_i-\bar{y})^2-(x_i-\bar{x})^2]}\right) \quad (16)$$

Equations (16) and (12) get the desired line parameters $\langle r,\phi\rangle$. In practice, equation (16) uses the four quadrant arc tangent (atan2). $atan2(y,x)$ computes $\arctan(y/x)$ but uses the signs of both x and y to determine the quadrant in which the resulting angle lies. For example $atan2(-2,-2)=-135°$, whereas $atan2(2,2)=45°$, a distinction which would be lost with a single-argument arc tangent function. Another practical consideration must be done when eq. (12) gives an $r<0$. In that case, the line $\langle r',\phi'\rangle$, where $r'=-r$ and $\phi'=\phi+\pi$, represents the same line $\langle r,\phi\rangle$, but in this representation $r'>0$.

C. Example

Consider the data given in Table I. We want to determine the line of total least squares for these points.

TABLE I
AN EXAMPLE WITH 7 POINTS.

point	z_1	z_2	z_3	z_4	z_5	z_6	z_7
x	3	4	5	6	7	8	9
y	7	7	11	11	15	16	19

To calculate the line parameters, we use equations (11), (16) and (12),

$$n=7$$

$$\bar{x}=\frac{3+4+\cdots+8+9}{7}=6$$

$$\bar{y}=\frac{7+7+\cdots+16+19}{7}=12.286$$

$$\phi=\frac{1}{2}\arctan\left(\frac{-116}{97.429}\right)=-0.4361$$

$$r=0.24889$$

Figure 3 shows the line as well as the points and their orthogonal distances. For reference, Figure 4 shows the line obtained using the classical Least Square Method. In the same Figure the vertical distances from points to the line are shown.

D. Matrix form to obtain the angle ϕ

Equation 13 can be rewritten in the matrix form

$$\chi^2(\ell;Z)=\frac{1}{\sigma^2}\|\mathbf{Mp}\|^2 \quad (17)$$

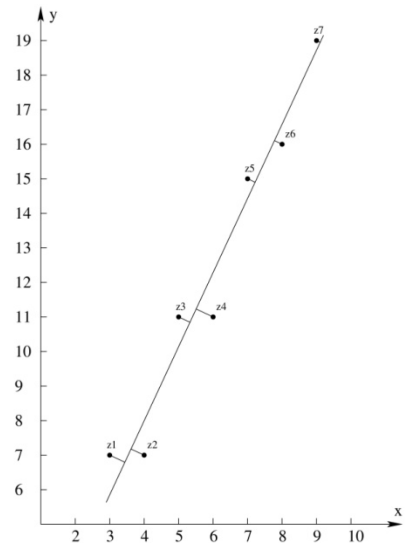

Fig. 3. Line fitting minimizing orthogonal distances from points to line (TLS).

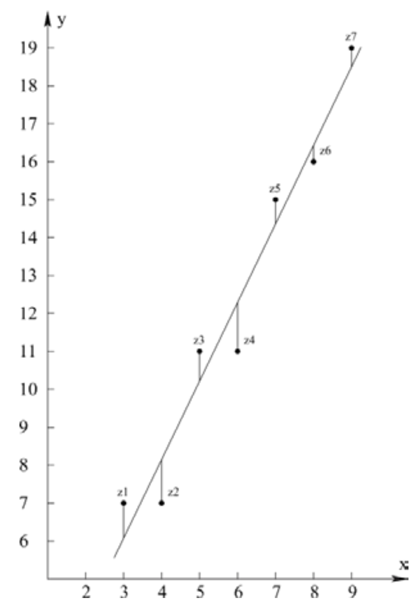

Fig. 4. Line fitting minimizing vertical distances from points to line (LS).

where $\mathbf{M}$ is a matrix of dimension $n\times 2$, $\mathbf{p}$ is a vector,

$$\mathbf{M} = \begin{bmatrix} x_1 - \bar{x} & y_1 - \bar{y} \\ x_2 - \bar{x} & y_2 - \bar{y} \\ \vdots & \vdots \\ x_n - \bar{x} & y_n - \bar{y} \end{bmatrix} \quad , \quad \mathbf{p} = \begin{bmatrix} \cos\phi \\ \sin\phi \end{bmatrix} \tag{18}$$

and $\|\mathbf{v}\|$ denotes the Euclidean norm of vector $\mathbf{v}$ with coordinates $[v_1 v_2 \dots v_k]^t$, defined as

$$\|\mathbf{v}\| = \sqrt{v_1^2 + v_2^2 + \cdots + v_k^2} \tag{19}$$

Now the goal is to find a vector $\mathbf{p}$ which minimizes eq. (17). In other words, a vector $\mathbf{t}$ which minimizes the norm of the linear map: $\mathbf{Mp}$. Note that $\mathbf{t}$ is a unit vector, because $\|\mathbf{p}\| = \sqrt{\cos^2\phi + \sin^2\phi} = 1$.

To achieve this goal, the Euclidean norm also can be expressed using de inner product of the vector and itself,

$$\|\mathbf{v}\| = \sqrt{\mathbf{v}^t\mathbf{v}} \tag{20}$$

where $\mathbf{v}^t$ denotes the transpose of vector $\mathbf{v}$. Using the inner product to compute the norm, eq. (17) can be written as

$$\chi^2(\ell;Z) = \frac{1}{\sigma^2}(\mathbf{Mp})^t(\mathbf{Mp}) \tag{21}$$

From this expression, using the properties of the transpose and the associative law for the matrix product, we get a quadratic form

$$\chi^2(\ell;Z) = \frac{1}{\sigma^2}(\mathbf{p}^t\mathbf{M}^t)(\mathbf{Mp})$$
$$\chi^2(\ell;Z) = \frac{1}{\sigma^2}\mathbf{p}^t(\mathbf{M}^t\mathbf{M})\mathbf{p}$$
$$\chi^2(\ell;Z) = \frac{1}{\sigma^2}\mathbf{p}^t\mathbf{A}\mathbf{p} \tag{22}$$

Let see the form of the matrix $\mathbf{A} = \mathbf{M}^t\mathbf{M}$, of dimension 2×2,

$$\mathbf{A} = \begin{bmatrix} \sum_{i=1}^{n}(x_i - \bar{x})^2 & \sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y}) \\ \sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y}) & \sum_{i=1}^{n}(y_i - \bar{y})^2 \end{bmatrix} \tag{23}$$

Because matrix $\mathbf{A}$ has real elements, is symmetric ($\boldsymbol{A}^t = \boldsymbol{A}$) and is positive semidefinite ($\mathbf{v}^t A \mathbf{v} \geq 0$ for $\mathbf{v} \neq 0$), matrix $\mathbf{A}$ has two real eigenvalues: $\lambda_1 \geq 0$, $\lambda_2 \geq 0$; and two orthonormal eigenvectors (unit vectors with inner product equal to zero).

Let $\mathbf{u_1} = [u_{1,1} \ u_{2,1}]^t$ and $\mathbf{u_2} = [u_{1,2} \ u_{2,2}]^t$ be the coordinates of eigenvectors $\mathbf{u_1}$ and $\mathbf{u_2}$. Eigenvalues and eigenvectors are related by

$$\mathbf{Au_1} = \lambda_1\mathbf{u_1} = [\lambda u_{1,1} \ \lambda u_{2,1}]^t \tag{24}$$
$$\mathbf{Au_2} = \lambda_1\mathbf{u_2} = [\lambda u_{1,2} \ \lambda u_{2,2}]^t \tag{25}$$

Equations (24) and (25) can be joined into a single relation

$$\mathbf{A}\begin{bmatrix} u_{1,1} & u_{1,2} \\ u_{2,1} & u_{2,2} \end{bmatrix} = \begin{bmatrix} \lambda_1 u_{1,1} & \lambda_2 u_{1,2} \\ \lambda_1 u_{2,1} & \lambda_2 u_{2,2} \end{bmatrix}$$
$$\mathbf{A}\begin{bmatrix} u_{1,1} & u_{1,2} \\ u_{2,1} & u_{2,2} \end{bmatrix} = \begin{bmatrix} u_{1,1} & u_{1,2} \\ u_{2,1} & u_{2,2} \end{bmatrix}\begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}$$

Let $\mathbf{U}$ be a matrix which first column is $\mathbf{u_1}$ and second column is $\mathbf{u_2}$; and let $\mathbf{D}$ be a diagonal matrix with elements λ_1 and λ_2. Using these matrices we can write last equation in a simpler form

$$\mathbf{AU} = \mathbf{UD} \tag{26}$$

The orthonormal matrix $\mathbf{U}$ has an interesting property: its inverse is its transpose ($\mathbf{UU}^{-1} = \mathbf{UU}^t = \mathbf{I}$, where $\mathbf{I}$ is the identity matrix). Using this property and equation (26), the matrix $\mathbf{A}$ can be expressed in terms of $\mathbf{U}$ and $\mathbf{D}$,

$$\mathbf{A} = \mathbf{UDU}^t \tag{27}$$

Replacing the matrix $\mathbf{A}$, given by the equation (27), into equation (22),

$$\chi^2(\ell;Z) = \frac{1}{\sigma^2}\mathbf{p}^t(\mathbf{UDU}^T)\mathbf{p}$$
$$\chi^2(\ell;Z) = \frac{1}{\sigma^2}(\mathbf{U}^t\mathbf{p})^t\mathbf{D}(\mathbf{U}^t\mathbf{p})$$
$$\chi^2(\ell;Z) = \frac{1}{\sigma^2}[\mathbf{u_1}^t\mathbf{p} \quad \mathbf{u}_2^t\mathbf{p}]\begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}\begin{bmatrix} \mathbf{u}_1^t\mathbf{p} \\ \mathbf{u}_2^t\mathbf{p} \end{bmatrix}$$
$$\chi^2(\ell;Z) = \frac{1}{\sigma^2}\{\lambda_1(\mathbf{u}_1^t\mathbf{p})^2 + \lambda_2(\mathbf{u}_2^t\mathbf{p})^2\} \tag{28}$$

To see the maximum and minimum value of λ^2, suppose that $\lambda_1 < \lambda_2$. Taking into account that the inner product of two vectors with coordinates $\mathbf{v_1}$ and $\mathbf{v_2}$ is defined as

$$\mathbf{v}_1^{\mathbf{t}}\mathbf{v_2} = \|\mathbf{v_1}\|\|\mathbf{v_2}\|\cos\gamma \tag{29}$$

where γ is the angle between both vectors. Given that $\mathbf{u_1}, \mathbf{u_2}$ and $\mathbf{p}$ are the coordinates of unit vectors and $\mathbf{u_1}$ and $\mathbf{u_2}$ are orthogonal vectors, we have

$$\mathbf{u}_1^t\mathbf{p} = \cos\alpha \tag{30}$$
$$\mathbf{u}_2^t\mathbf{p} = \cos(\alpha \pm \pi/2) = \pm\sin\alpha \tag{31}$$

where α is the angle between vector $\mathbf{u_1}$ and $\mathbf{t}$. Replacing these results into equation (28),

$$\chi^2(\ell;Z) = \frac{1}{\sigma^2}\{\lambda_1\cos^2\alpha + \lambda_2\sin^2\alpha\}$$
$$\chi^2(\ell;Z) = \frac{1}{\sigma^2}\{\lambda_1\cos^2\alpha + \lambda_2(1 - \cos^2\alpha)\} \tag{32}$$

Let $s = \cos^2\alpha$, where s is a value in the range [0,1], and $s = 1$ when vector $\mathbf{p}$ is identical to vector $\mathbf{u_1}$ ($\alpha = 0$). Using this new variable s in Equation (32), we have finally

$$\chi^2(\ell;Z) = \frac{1}{\sigma^2}\{\lambda_1 s + \lambda_2(1 - s)\}$$
$$\chi^2(\ell;Z) = \frac{1}{\sigma^2}\{(\lambda_1 - \lambda_2)s + \lambda_2\} \tag{33}$$

The expression $(\lambda_1 - \lambda_2)s + \lambda_2$ corresponding to a line $\langle a, b\rangle$ with a negative slope $a = \lambda_1 - \lambda_2$ (because $\lambda_1 < \lambda_2$) and y-axis intersection $b = \lambda_2$. The maximum value of $\chi^2(\ell, Z)$ is $\frac{1}{\sigma^2}\lambda_2$ when $s = 0$, and the minimum value is $\frac{1}{\sigma^2}\lambda_1$ when $s = 1$. Therefore,

> Vector $\mathbf{t} = \mathbf{u_1}$, the eigenvector associated to the minimum eigenvalue λ_1 of matrix $\mathbf{M}^t\mathbf{M}$, minimizes $\chi^2(\ell, Z)$.

From $\mathbf{u_1} = [u_{1,1}, u_{2,1}]^t$ and $\mathbf{p} = [\cos\phi \sin\phi]^t$ we get the desired angle ϕ,

$$\phi = \arctan(u_{2,1}/u_{1,1}) \tag{34}$$

Using the four quadrant arc tangent (atan2) to compute ϕ (eq. (34)), we can get the parameter r of the line using eq. (12),

$$r = \bar{x}u_{1,1} + \bar{y}u_{2,1} \tag{35}$$

Using equation (3) and previous results, we can see an interesting property of vector $\mathbf{u_1}$,

$$\begin{gathered} r = x\cos\phi + y\sin\phi \\ \bar{x}u_{1,1} + \bar{y}u_{2,1} = xu_{1,1} + yu_{2,1} \\ 0 = (x-\bar{x})u_{1,1} + (y-\bar{y})u_{2,1} \\ \mathbf{0} = (\mathbf{z}^t - \mathbf{C}^t)\mathbf{u_1} \end{gathered} \tag{36}$$

where $\mathbf{z} = [x\ y]^t$, and $\mathbf{C} = [\bar{x}\ \bar{y}]^t$ is the centroid of points. Note that vector with coordinates $\mathbf{z}^t - \mathbf{C}^t$ must be orthogonal to vector $\mathbf{u_1}$, in order to satisfy equation (36).

E. Example (cont.)

Continuing the example from Section III-C, we can compute the matrix $\mathbf{A}$,

$$\mathbf{A} = \begin{bmatrix} 28.000 & 58.000 \\ 58.000 & 125.429 \end{bmatrix} \tag{37}$$

and its eigenvalues and eigenvectors (using the function svd of the octave program):

$$\lambda_1 = 0.97076, \quad \lambda_2 = 152.45781 \tag{38}$$

$$\mathbf{u_1} = [-0.90641\ \ 0.42241]^t \quad \mathbf{u_2} = [-0.90641\ \ 0.42241]^t \tag{39}$$

From eigenvector $\mathbf{u_1}$, we can compute ϕ using equation (34),

$$\phi = \arctan\left(\frac{0.42241}{-0.90641}\right) = 2.7055 \tag{40}$$

Using eq. (12) with this value for ϕ, we get a negative value for r. In this case $\phi' = \phi + \pi$, and we get the same result for r as in section III-C.

IV. THE LINE SEGMENT

Sometimes it is useful to know the line segment associated to the set of points Z, instead of only the infinite line expressed by the parameters $\langle r, \phi\rangle$. This section addresses this problem.

First we move the origin of coordinates to the centroid of points $\mathbf{C} = [\bar{x}\ \ \bar{y}]^t$. For each point $\mathbf{z_i} = [x_i\ y_i]^t \in Z$, the translated point $\mathbf{z_i}'$ is defined by

$$\mathbf{z}_\mathbf{i}' = \mathbf{z_i} - \mathbf{C} \tag{41}$$

Then we rotate points using a rotation matrix $\mathbf{R}(\theta)$

$$\mathbf{R}(\theta) = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \tag{42}$$

The matrix $\mathbf{R}(\theta)$ rotates points in the xy-Cartesian plane counter-clockwise through an angle θ about the origin of the Cartesian coordinate system. To perform the rotation using a rotation matrix $\mathbf{R}$, the position of each point must be represented by a column vector $\mathbf{z}$, containing the coordinates of the point. A rotated vector is obtained by using the matrix multiplication $\mathbf{Rz}$.

If we rotate all points $\mathbf{z}_i'$ an angle $-\phi$, the rotated points $\mathbf{z}_i''$ follows a vertical line,

$$\mathbf{z}_i'' = \mathbf{R}(-\phi)\mathbf{z}_i' \tag{43}$$

Let y''_{max} and y''_{min} be the maximum and minimum values respectively of all coordinates y''_i, in $\mathbf{z}''_\mathbf{i} = [x''_i\ \ y''_i]^t$, $i = 1, \dots, n$. The points $\mathbf{e}''_\mathbf{1} = [0\ \ y''_{max}]$ and $\mathbf{e}''_\mathbf{2} = [0\ \ y''_{min}]$ are the ending points of the desired line segment, corresponding to the highest and the lowest point. The final steps are to undo the rotation and translation made,

$$\mathbf{e}'_\mathbf{1} = \mathbf{R}(\phi)\boldsymbol{e}''_\mathbf{1} \quad , \quad \mathbf{e}'_\mathbf{2} = \mathbf{R}(\phi)\boldsymbol{e}''_\mathbf{2} \tag{44}$$

$$\mathbf{e_1} = \mathbf{e}'_\mathbf{1} + \mathbf{C} \quad , \quad \mathbf{e_2} = \mathbf{e}'_\mathbf{2} + \mathbf{C} \tag{45}$$

The line segment is the line between points $\mathbf{e_1}$ and $\mathbf{e_2}$.

As an example, Figure 5 shows five line segments computed from a set of points given by measurements of an Infrared sensor of a small mobile robot, using the Line Tracking algorithm [6] (with TLS). The robot rotates 360° taking measurements.

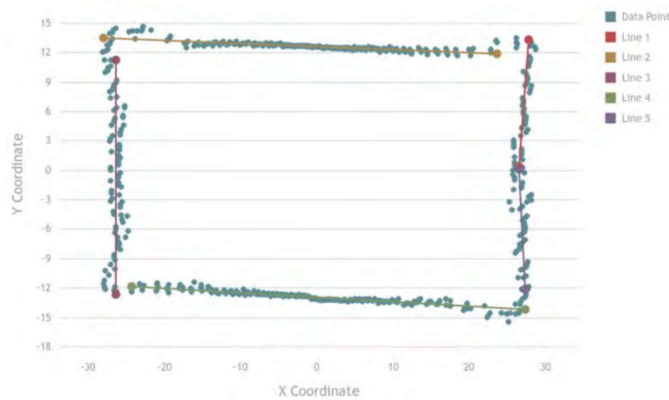

Fig. 5. Finding the best lines of a set of points given by an IR sensor of a small mobile robot.

V. SOME EXTENSIONS

A. Weighted total least squares

In section III-A we consider the same uncertainty σ for all points. If we consider an uncertainty σ_i for point z_i $i = 1, \dots, n$, the best line minimizes

$$\chi^2(\ell; Z) = \sum_{i=1}^{n} \frac{d_\perp^2(z_i, \ell)}{\sigma_i^2} \tag{46}$$

Following a procedure similar to section III-B, we can get the solution

$$r = \bar{x}\cos\phi + \bar{y}\sin\phi \tag{47}$$

$$\phi = \frac{1}{2} arctan \frac{-2\sum_{i=1}^{n} w_i(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n} w_i[(y_i - \bar{y})^2 - (x_i - \bar{x})^2]} \tag{48}$$

where

$$\bar{x} = \left(\sum_{i=1}^{n} w_i x_i\right) \Big/ \left(\sum_{i=1}^{n} w_i\right) \tag{49}$$

$$\bar{y} = \left(\sum_{i=1}^{n} w_i y_i\right) \Big/ \left(\sum_{i=1}^{n} w_i\right) \tag{50}$$

are the weighted means; with individual weights $w_i = 1/\sigma_i^2$ for each measurement. This approach is known as weighted least squares.

B. Fitting a set of points to a plane

The method to find the best line in the total least squares sense, can be extended easily to find the best plane of a set of points in three dimensions.

A plane π is represented by four parameters $\pi = \langle r, \alpha, \beta, \gamma \rangle$, where r, α, β and γ are the length of the normal, and the angle between the normal and the x-axis, y-axis and z-axis respectively. The normal is the shortest line segment between the plane π and the origin.

A point $z = \langle x, y, z \rangle$ that is on the plane π satisfy

$$r = x \cos\alpha + y \cos\beta + z \cos\gamma \tag{51}$$

The orthogonal distance from a point z_i to plane π is given by

$$d_\perp(z_i, \pi) = x_i \cos\alpha + y_i \cos\beta + z_i \cos\gamma - r \tag{52}$$

In this case, the best line minimize

$$\chi^2(\pi; Z) = \sum_{i=1}^{n} \frac{d_\perp^2(z_i, \pi)}{\sigma^2} \tag{53}$$

Doing $\frac{\partial \chi^2}{\partial r} = 0$, as before, we get a similar result: the centroid of points given by $\langle \bar{x}, \bar{y}, \bar{z} \rangle$ is a point of the plane π which minimizes eq. (53),

$$r = \bar{x} \cos\alpha + \bar{y} \cos\beta + \bar{z} \cos\gamma \tag{54}$$

where

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i \;, \quad \bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i \;, \quad \bar{z} = \frac{1}{n}\sum_{i=1}^{n} z_i \tag{55}$$

To find the angles α, β and γ we use a similar procedure to the matrix formulation. Replacing equations (52) and (54) into (53),

$$\chi^2(\pi; Z) = \frac{1}{\sigma^2} \|\mathbf{Mp}\|^2 \tag{56}$$

where $\mathbf{M}$ is a matrix of dimension $n \times 3$, $\mathbf{p}$ is a vector,

$$\mathbf{M} = \begin{bmatrix} x_1 - \bar{x} & y_1 - \bar{y} & z_1 - \bar{z} \\ x_2 - \bar{x} & y_2 - \bar{y} & z_2 - \bar{z} \\ \vdots & \vdots & \vdots \\ x_n - \bar{x} & y_n - \bar{y} & z_n - \bar{z} \end{bmatrix} \;, \quad p = \begin{bmatrix} \cos\alpha \\ \cos\beta \\ \cos\gamma \end{bmatrix} \tag{57}$$

Note that $\mathbf{p}$ is a unit vector, because $\|\mathbf{p}\| = \sqrt{\cos^2\alpha + \cos^2\beta + \cos^2\gamma} = 1$.

The best plane is given by $\mathbf{p} = \mathbf{u_1} = [u_{1,1}\ u_{2,1}\ u_{3,1}]^t$, the eigenvector associated to the smallest eigenvalue λ_1 of matrix $\mathbf{M}^t\mathbf{M}$. From $\mathbf{p} = \mathbf{u_1}$ we can obtain r, using equation (54),

$$r = \bar{x}u_{1,1} + \bar{y}u_{2,1} + \bar{z}u_{3,1} \tag{58}$$

Therefore the plane can be expressed by

$$r = xu_{1,1} + yu_{2,1} + zu_{3,1} \tag{59}$$

$$\mathbf{0} = (\mathbf{z}^t - \mathbf{C}^t)\mathbf{u_1} \tag{60}$$

where $z = [x\ y\ z]^t$, and $\mathbf{C} = [\bar{x}\ \bar{y}\ \bar{z}]^{\boldsymbol{t}}$ is the centroid of points.

VI. CONCLUSION

This article presents a tutorial about the method of Total Least Squares to fit a line, developing a closed formula for calculating the line parameters; and also the matrix formulation, which can be easily extended to the case of fitting a Cartesian plane to points in three dimensions.

It is written in a simple form which should be easy to understand, even for students with a basic knowledge of calculus and linear algebra. Also, the closed formulation is useful for low computational resources, such as microcontrollers for small mobile robots.

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VIII. BIOGRAPHIES

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