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TECHNICAL NOTE

Circle Fitting by Linear and Nonlinear Least Squares[1]

I. D. COOPE[2]

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Abstract. The problem of determining the circle of best fit to a set of points in the plane (or the obvious generalization to n-dimensions) is easily formulated as a nonlinear total least-squares problem which may be solved using a Gauss–Newton minimization algorithm. This straightforward approach is shown to be inefficient and extremely sensitive to the presence of outliers. An alternative formulation allows the problem to be reduced to a linear least squares problem which is trivially solved. The recommended approach is shown to have the added advantage of being much less sensitive to outliers than the nonlinear least squares approach.

Key Words. Curve fitting, circle fitting, total least squares, nonlinear least squares.

1. Introduction

The problem of determining the circle of best fit, in a total least squares sense, to a set of data points $a_j \in \mathbb{R}^n$, $j = 1, 2, \ldots, m$, is a special case ($n = 2$) of the following (nonlinear) total least-squares problem (TLS): Determine values of $x \in \mathbb{R}^n$ and $r \in \mathbb{R}^+$ which solve the problem

$$\min_{x,r} \sum_{j=1}^{m} \{F_j(x, r)\}^2, \tag{1}$$

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[2]Senior Lecturer, Department of Mathematics, University of Canterbury, Christchurch, New Zealand.

where $F_j(x, r)$ is the distance of the point a_j from the fitted circle,

$$F_j(x, r) = |r - \|x - a_j\|_2|. \tag{2}$$

Here, x denotes the center of the circle and r its radius, and the terminology total least squares is used to emphasize that it is the sum of squares of the Euclidean distances between the points a_j and the corresponding nearest points on the fitted circle that is minimized, rather than the vertical distances that are used in the more familiar method of least squares.

Writing

$$S(x, r) = \sum F_j^2(x, r),$$

a necessary condition for a solution to problem (1) is $\partial S/\partial r = 0$, which provides the equation

$$r(x) = (1/m) \sum_{j=1}^{m} \|x - a_j\|_2. \tag{3}$$

Writing

$$V(x) = S(x, r(x))$$

and substituting for $r(x)$ in (1) then leads to the problem

$$\begin{aligned} \min_{x \in \mathbb{R}^n} V(x) &= \sum_{j=1}^{m} \left[\|x - a_j\|_2 - (1/m) \sum_{\substack{j=1 \\ i=1}}^{m} \|x - a_i\|_2 \right]^2 \\ &= \sum_{j=1}^{m} \|x - a_j\|_2^2 - (1/m) \left[\sum_{j=1}^{m} \|x - a_j\|_2 \right]^2, \end{aligned} \tag{4}$$

which is a minimum variance problem. The gradient vector $\nabla V(x)$ is then given by the expression

$$\nabla V(x) = 2 \left[\sum_{j=1}^{m} (x - a_j) - r(x) \sum_{j=1}^{m} \frac{x - a_j}{\|x - a_j\|_2} \right]. \tag{5}$$

Although problem (4) is a little simpler than the equivalent problem (1), it is still a nonlinear problem and there is little to be gained from this reformulation apart from a reduction in dimensionality from $n+1$ variables to n (which is, of course, still worthwhile).

Gruntz (Ref. 1) has considered problem (1) and has made available a MATLAB[3] program for computing a solution by the Gauss–Newton method for the case $n = 2$. It is well known that the Gauss–Newton method is most

[3] MATLAB is a registered trade mark of the MathWorks Inc.

successful when the sums of squares function is small at the solution or when the nonlinearities are mild [see, for example, Fletcher (Ref. 2)]. Therefore, the presence of outliers can seriously impede efficiency for the Gauss–Newton method, and frequently quasi-Newton methods are used instead on large residual problems. However, difficulties may still be anticipated for large residual problems even if quasi-Newton methods are used, since $F_j(x, r)$ is not differentiable with respect to x at $x = a_j$, $j = 1, 2, \ldots, m$. Although this is, perhaps, only likely to cause difficulties on problems where outliers occur close to the center of the fitted circle, the result, when it does occur, is significant. As an illustration, consider the data of Gruntz (Ref. 1), which comprises the 8 points

$$(0.7, 4.0),\ (3.3, 4.7),\ (5.6, 4.0),\ (7.5, 1.3),$$
$$(6.4, -1.1),\ (4.4, -3.0),\ (0.3, -2.5),\ (-1.1, 1.3).$$

Gruntz's procedure was used to calculate the best fit, and the computed values for the center and radius were

$$x = (3.04324, 0.74568), \qquad r = 4.10586.$$

The fitted circle is displayed in Fig. 1 (center denoted $\circ$, data points denoted $\times$) and it is certainly a pleasing fit. However, the addition of one more data point (3, 1) close to the previously fitted center has a significant effect on the fitting procedure,

$$x = (3.26566, 0.16583), \qquad r = 3.79302.$$

Although the radius is affected only slightly, the center has shifted to such an extent that the fitted circle is no longer visually pleasing, as can be seen

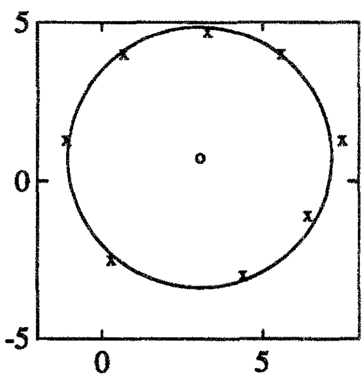

Fig. 1. Gruntz data (Ref. 1). TLS fit on 8 points, 4 iterations; $x = (3.04324, 0.74568)$, $r = 4.10586$.

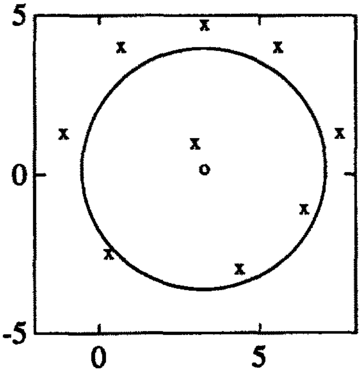

Fig. 2. Adding an outlier. TLS fit on 9 points, 49 iterations; $x=(3.26566, 0.16583)$, $r=3.79302$.

in Fig. 2. Moreover, the number of iterations required to achieve similar accuracy has also increased significantly from 4 in the first case to 49 in the second. It is worth noting that a quasi-Newton method applied to problem (4) required 4 iterations and 6 iterations, respectively!

2. Linear Least Squares Problem

An alternative to the nonlinear total least squares problem (1) is the problem

$$\min_{x,r} \sum_{j=1}^{m} \{f_j(x, r)\}^2, \tag{6}$$

where $f_j(x, r)$ is the residual,

$$f_j(x, r) = \|x - a_j\|_2^2 - r^2. \tag{7}$$

At first sight, this problem is also a nonlinear least squares problem; however, writing $f_j(x, r)$ in the form

$$f_j(x, r) = x^T x - 2x^T a_j + a_j^T a_j - r^2, \tag{8}$$

where the superscript T denotes transpose, allows the nonlinearity to be removed by making the following simple (nonlinear) transformation of variables:

$$y_i = 2x_i, \quad i = 1, 2, \ldots, n, \qquad y_{n+1} = r^2 - x^T x. \tag{9}$$

Then letting

$$b_j=\begin{bmatrix} a_j \\ 1 \end{bmatrix}, \qquad j=1,2,\ldots,m,$$

the problem (6) becomes

$$\min_{y\in\mathbb{R}^{n+1}} \sum_{j=1}^{m} \{a_j^T a_j - b_j^T y\}^2, \tag{10}$$

or more compactly,

$$\min_y \|By-d\|_2^2,$$

where $B^T=[b_1, b_2, \ldots, b_m]$ is the matrix whose columns are the vectors b_j, $j=1,2,\ldots,m$, and d is the vector with components $d_j=\|a_j\|_2^2$, $j=1,2,\ldots,m$. Thus, problem (10) is a simple linear least squares (LLS) problem which is easily solved. The optimal values of the original variables x, r can then be recovered from the formulas

$$x_i=(1/2)y_i, \quad i=1,2,\ldots,n, \qquad r=\sqrt{y_{n+1}+x^Tx}. \tag{11}$$

Applying this technique to the data and extended data of Gruntz defined in Section 1 resulted in the fitted circles displayed in Figs. 3 and 4.

The circle in Fig. 3 differs only slightly from that of Fig. 1, but that in Fig. 4 gives a much more visually pleasing fit than that of the total least squares fit of Fig. 2; the presence of the outlier has had much less effect on the fitted circle for the linear least squares formulation. Comparing the sums

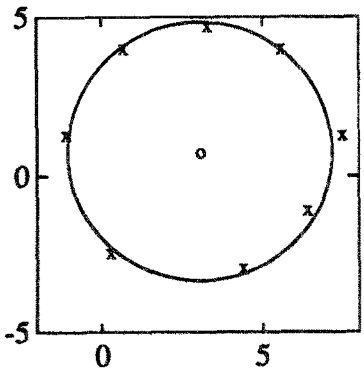

Fig. 3. Gruntz data (Ref. 1). LLS fit on 8 points; $x=(3.06030, 0.74361)$, $r=4.10914$.

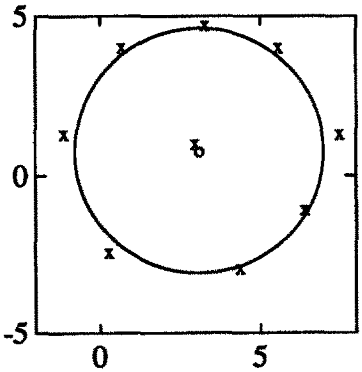

Fig. 4. Adding an outlier. LLS fit on 9 points; $x=(3.10253, 0.75467)$, $r=3.87132$.

of squares function $S(x, r)$ for the TLS solution and LLS solution of Figs. 1 and 3 shows that the LLS solution is quite close to optimality in the TLS sense. Specifically,

$$S(x_1, r_1)=0.295948, \qquad S(x_3, r_3)=0.297115,$$

where (x_i, r_i) denotes the solution depicted in Fig. i. The solution in Fig. 4, however, is far from optimal in the TLS sense, as can be seen from the values

$$S(x_2, r_2)=11.475855, \qquad S(x_4, r_4)=13.378989.$$

3. Discussion

The linear least squares formulation of the circle fitting problem (10) has been shown to be preferable to the total least squares formulation (1), or the equivalent problem (4), from the viewpoint of ease of calculation. It also seems preferable in terms of robustness in the presence of outliers, as the examples of this paper have illustrated. Both formulations are exact, in principle, if the data exactly matches a circle, but the linear least squares approach is usually an order of magnitude faster. However, if users insist on finding the total least squares fit, then an initial approximation is still required and the linear least squares approach is recommended for providing a good starting point. This was the approach taken in this paper for solving the nonlinear total least squares fits displayed in Figs. 1 and 2. Note that, in spite of being given reasonable initial approximations, the Gauss–Newton procedure required many iterations to achieve the quoted accuracy in the latter case.

It is interesting to ask if the recommended formulation (6) has any geometrical significance. The modulus of the residual (7) can be factored as

$$|f_j(x, r)| = |r - \|x - a_j\|_2| \times |r + \|x - a_j\|_2|,$$

where the first factor is expression (2) representing the distance of the point a_j to the nearest point on the circle. The second factor is, of course, the distance from the point a_j to the furthest point on the circle. Thus problem (6) has the geometrical interpretation of minimizing the sums of squares of the products of these two distances. A simple MATLAB function for computing the best linear least squares fit for the n-dimensional circle fitting problem is given in the Appendix of Ref. 3.

A related problem was posed by Sylvester in a one-sentence article (Ref. 4) published in the first volume of the Quarterly Journal of Pure and Applied Mathematics in 1857: "It is required to find the least circle which shall contain a given set of points in the plane." Although this problem is quite different from the circle fitting problem considered in this paper, it is related because the nonlinear transformation (9) reduces it to a problem in linear algebra. Specifically, Sylvester's problem in n-dimensions is the nonlinearly constrained minimization problem

$$\min_{x,r} r^2, \tag{12}$$

subject to the quadratic inequality constraints

$$\|x - a_j\|_2^2 \leq r^2, \qquad j = 1, 2, \ldots, m. \tag{13}$$

Applying the transformation (9) reduces (12), (13) to the convex quadratic programming problem

$$\min_{y \in \mathbb{R}^{n+1}} \left\{ y_{n+1} + (1/4) \sum_{j=1}^{n} y_j^2 \right\}, \tag{14}$$

subject to the linear inequality constraints

$$By \geq d, \tag{15}$$

where the matrix B and vector d are as defined in Section 2. A discussion of Sylvester's problem (12)–(13) including the alternative formulation (14)–(15) and its dual, is given by Kuhn (Ref. 5). Techniques for solving it efficiently can be found in Ref. 6.

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