CIRCLE FITTING BY LINEAR AND NONLINEAR LEAST SQUARES[1]

by

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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 generalisation to n–dimensions) is easily formulated as a nonlinear total least squares problem which may be solved using a Gauss-Newton minimisation 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 test 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.

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1. Introduction

The problem of determining the circle of best fit, in a total least squares sense, to a set of data points, $\mathbf{a}_j \in \mathbf{R}^n, j = 1, 2, \ldots, m$, is a special case, ($n = 2$), of the following (nonlinear) total least squares problem (TLS).

Determine values of $\mathbf{x} \in \mathbf{R}^n$ and $r \in \mathbf{R}^+$ which solve the problem

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

where $F_j(\mathbf{x}, r)$ is the distance of the point $\mathbf{a}_j$ from the fitted "circle,"

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

Here, $\mathbf{x}$ denotes the centre of the "circle" and r its radius and the terminology "total least squares" is used to emphasise that it is the sum of squares of the Euclidean distances between the points $\mathbf{a}_j$ and the corresponding *nearest* points on the fitted circle that is minimised rather than the vertical distances that are used in the more familiar "method of least squares."

Writing $S(\mathbf{x}, r) = \sum F_j^2(\mathbf{x}, r)$ a necessary condition for a solution to problem (1) is $\frac{\partial S}{\partial r} = 0$, which provides the equation

$$r(\mathbf{x}) = \frac{1}{m} \sum_{j=1}^{m} \|\mathbf{x} - \mathbf{a}_j\|_2. \tag{3}$$

Writing $V(\mathbf{x}) = S(\mathbf{x}, r(\mathbf{x}))$ and substituting for $r(\mathbf{x})$ in (1) then leads to the problem

$$\begin{aligned} \min_{\mathbf{x} \in \mathbf{R}^n} V(\mathbf{x}) &= \sum_{j=1}^{m} \left(\|\mathbf{x} - \mathbf{a}_j\|_2 - \frac{1}{m} \sum_{i=1}^{m} \|\mathbf{x} - \mathbf{a}_i\|_2 \right)^2, \qquad (4) \\ &= \sum_{j=1}^{m} \|\mathbf{x} - \mathbf{a}_j\|_2^2 - \frac{1}{m} \left(\sum_{j=1}^{m} \|\mathbf{x} - \mathbf{a}_j\|_2 \right)^2, \end{aligned}$$

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

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

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).

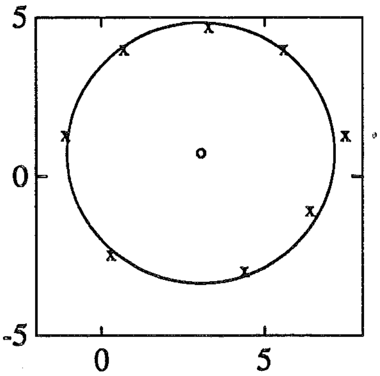

Figure 1. Gruntz[1] data.
TLS fit on 8 points, 4 iterations.
$\mathbf{x}=(3.04324, 0.74568)$; $r=4.10586$.

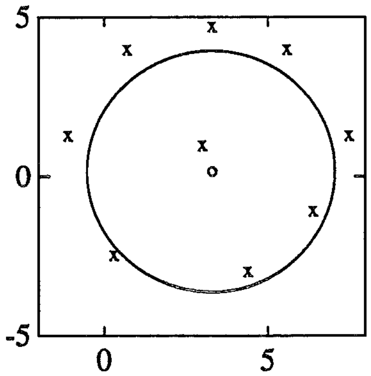

Figure 2. Adding an outlier.
TLS fit on 9 points, 49 iterations.
$\mathbf{x}=(3.26566, 0.16583)$; $r=3.79302$.

Gruntz[1] has considered problem (1) and has made available a MATLAB[1] 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 successful when the sums of squares function is "small" at the solution or when the nonlinearities are "mild" (see, for example, Fletcher[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 $F_j(\mathbf{x}, r)$ is not differentiable with respect to $\mathbf{x}$ at $\mathbf{x} = \mathbf{a}_j, j = 1, 2, \ldots, m$. Although this is, perhaps, only likely to cause difficulties on problems where "outliers" occur close to the centre of the fitted circle, the result, when it does occur, is significant. As an illustration, consider the data of Gruntz[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 centre and radius were $\mathbf{x} = (3.04324, 0.74568), r = 4.10586$. The fitted circle is displayed in figure 1 (centre denoted 'o' data points denoted 'x') and it is certainly a pleasing fit. However, the addition of one more data point $(3, 1)$ close to the previously fitted centre has a significant effect on the fitting procedure ($\mathbf{x} = (3.26566, 0.16583), r = 3.79302$). Although the radius is affected

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

only slightly, the centre has shifted to such an extent that the fitted circle is no longer visually pleasing, as can be seen in figure 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. A Linear Least Squares Problem

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

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

where $f_j(\mathbf{x},r)$ is the "residual",

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

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

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

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

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

Then letting $\mathbf{b}_j = \begin{bmatrix} \mathbf{a}_j \\ 1 \end{bmatrix}$, $j=1,2,\ldots,m$, the problem (6) becomes

$$\min_{\mathbf{y}\in\mathbf{R}^{n+1}} \sum_{j=1}^{m} \{\mathbf{a}_j^T\mathbf{a}_j - \mathbf{b}_j^T\mathbf{y}\}^2, \tag{10}$$

or more compactly,

$$\min_{\mathbf{y}} \|\mathbf{B}\mathbf{y}-\mathbf{d}\|_2^2,$$

where $\mathbf{B}^T = [\mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_m]$ is the matrix whose columns are the vectors $\mathbf{b}_j, j=1,2,\ldots,m$, and $\mathbf{d}$ is the vector with components $d_j = \|\mathbf{a}_j\|_2^2$, $j=1,2,\ldots,m$. Thus, problem (10) is a simple linear least squares (LLS) problem which is easily solved. The optimal values of the original variables $\mathbf{x}, r$ can then be recovered from the formulae

$$x_i = \tfrac{1}{2} y_i,\ i = 1, 2, \ldots, n, \qquad r = \sqrt{y_{n+1} + \mathbf{x}^T \mathbf{x}}. \tag{11}$$

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

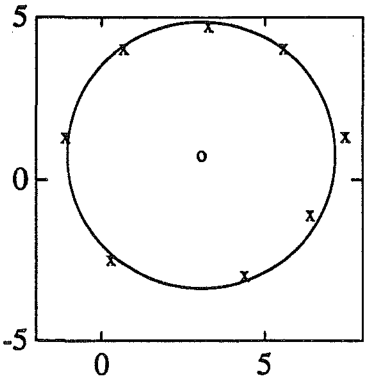

Figure 3. Gruntz[1] data.
LLS fit on 8 points.
$\mathbf{x}=(3.06030, 0.74361)$; $r=4.10914$.

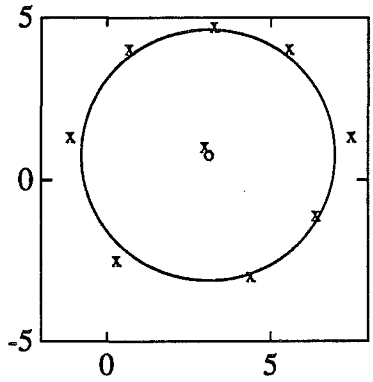

Figure 4. Adding an outlier.
LLS fit on 9 points.
$\mathbf{x}=(3.10253, 0.75467)$; $r=3.87132$.

The circle in figure 3 differs only slightly from that of figure 1 but that in figure 4 gives a much more visually pleasing fit than that of the "total least squares" fit of figure 2; the presence of the outlier has had much less effect on the fitted circle for the linear least squares formulation. Comparing the sums of squares function $S(\mathbf{x}, r)$ for the TLS solution and LLS solution of figures 1 and 3 shows that the LLS solution is quite close to optimality in the TLS sense. Specifically, $S(\mathbf{x}_1, r_1) = 0.295948$ and $S(\mathbf{x}_3, r_3) = 0.297115$, where $(\mathbf{x}_i, r_i)$ denotes the solution depicted in figure i. The solution in figure 4, however, is far from optimal in the TLS sense as can be seen from the values, $S(\mathbf{x}_2, r_2) = 11.475855$, $S(\mathbf{x}_4, r_4) = 13.378989$.

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 figures 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

$$|f_j(\mathbf{x}, r)| = |r - \|\mathbf{x} - \mathbf{a}_j\|_2| \times |r + \|\mathbf{x} - \mathbf{a}_j\|_2|,$$

where the first factor is expression (2) representing the distance of the point $\mathbf{a}_j$ to the nearest point on the circle. The second factor is, of course, the distance from the point $\mathbf{a}_j$ to the furthest point on the circle. Thus problem (6) has the geometrical interpretation of minimising 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.

A related problem was posed by J.J. Sylvester in a one sentence article [3] published in the first volume of the Quarterly Journal of Pure & 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 minimisation problem

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

subject to the quadratic inequality constraints

$$\|\mathbf{x} - \mathbf{a}_j\|_2^2 \le r^2, \quad j = 1, 2, \ldots, m. \tag{13}$$

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

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

subject to the linear inequality constraints

$$\mathbf{B}\mathbf{y} \geq \mathbf{d}, \tag{15}$$

where the matrix $\mathbf{B}$ and vector $\mathbf{d}$ 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[4]. Techniques for solving it efficiently can be found in [5].

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Appendix

A MATLAB program (function) for solving the "best fit" circle problem using a linear least squares approach is included here.

```
% FITCIRCL Solves the n-dimensional 'circle' fitting problem
%          using a linear least squares method:
%
%                 [x,r] = fitcircl(A)
%
%          returns the coordinates of the centre, x, and
%          radius, r, of the best linear least squares
%          n-dimensional 'circle' to the set of m vectors
%          represented by the columns of the n × m
%          matrix A.
%
function [x,r] = fitcircl(A)
[n,m] = size(A);
y = [A', ones(m,1)]\sum(A.*A)';
x = .5*y(1:n);
r = sqrt(y(n+1) + x'*x);
```

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