A Few Methods for Fitting Circles to Data

Dale Umbach, Kerry N. Jones

Abstract—**Five methods are discussed to fit circles to data. Two of the methods are shown to be highly sensitive to measurement error. The other three are shown to be quite stable in this regard. Of the stable methods, two have the advantage of having closed form solutions. A positive aspect of all of these models is that they are coordinate free in the sense that the same estimating circles are produced no matter where the axes of the coordinate system are located nor how they are oriented. A natural extension to fitting spheres to points in 3-space is also given.**

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I. Introduction

The problem of fitting a circle to a collection of points in the plane is a fairly new one. In particular, it is an important problem in metrology and microwave measurement. While certainly not the earliest reference to a problem of this type, Kåsa, in [4], describes a circle fitting procedure. In [2], Cox and Jones expand on this idea to fit circles based on a more general error structure.

In general, suppose that we have a collection of $n \geq 3$ points in 2-space labeled (x_1, y_1), $(x_2, y_2), \ldots, (x_n, y_n)$. Our basic problem is to find a circle that best represents the data in some sense. With our circle described by $(x-a)^2 + (y-b)^2 = r^2$, we need to determine values for the center (a, b) and the radius r for the best fitting circle.

A reasonable measure of the fit of the circle $(x-a)^2 + (y-b)^2 = r^2$ to the points (x_1, y_1), $(x_2, y_2), \ldots, (x_n, y_n)$ is given by summing the squares of the distances from the points to the circle. This measure is given by

$$SS(a,b,r) = \sum_{i=1}^{n} \left(r - \sqrt{(x_i - a)^2 + (y_i - b)^2} \right)^2$$

[1] discusses numerical algorithms for the minimization SS over a, b, and r. Gander, Golub, and Strebel in [3] also discuss this problem. In [4], Kåsa also presents an alternative method that we will discuss in Section 2.4. [1] gives a slight generalization of the Kåsa method.

II. The Various Methods

For notational convenience, we make the following conventions:

$$\begin{aligned} X_{ij} &= x_i - x_j \\ \tilde{X}_{ijk} &= X_{ij} X_{jk} X_{ki} \\ X_{ij}^{(2)} &= x_i^2 - x_j^2 \\ Y_{ij} &= y_j - y_j \\ \tilde{Y}_{ijk} &= Y_{ij} Y_{jk} Y_{ki} \\ Y_{ij}^{(2)} &= y_i^2 - y_j^2 \end{aligned}$$

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A. Full Least Squares Method

An obvious approach is to choose a, b, and r to minimize SS. Differentiation of SS yields

$$\begin{aligned} \frac{\partial SS}{\partial r} &= -2 \sum_{i=1}^{n} \sqrt{(x_i - a)^2 + (y_i - b)^2} \\ &\quad +2nr \end{aligned} \tag{II.1}$$

$$\begin{aligned} \frac{\partial SS}{\partial a} &= 2r \sum_{i=1}^{n} \frac{x_i - a}{\sqrt{(x_i - a)^2 + (y_i - b)^2}} \\ &\quad -2n\overline{x} + 2na \end{aligned}$$

$$\begin{aligned} \frac{\partial SS}{\partial b} &= 2r \sum_{i=1}^{n} \frac{y_i - b}{\sqrt{(x_i - a)^2 + (y_i - b)^2}} \\ &\quad -2n\overline{y} + 2nb. \end{aligned}$$

Simultaneously equating these partials to zero does not produce closed form solutions for a, b, and r. However, many software programs will numerically carry out this process quite efficiently. We shall refer to this method as the Full Least Squares method (FLS) with resulting values of a, b, and r labeled as a_F, b_F, and r_F. The calculation of the FLS estimates has been discussed in [1] and [3], among others.

B. Average of Intersections Method

We note that solving (II.1) = 0 for r produces

$$r = \sum_{i=1}^{n} \sqrt{(x_i - a)^2 + (y_i - b)^2}/n. \tag{II.2}$$

This suggests that if one obtains values of a and b by some other method, a good value for r can be obtained using (II.2).

To obtain a value for (a, b), the center of the circle, we note that for a circle the perpendicular bisectors of all chords intersect at the center. There are $\binom{n}{3}$ triplets of points that could each be considered as endpoints of chords along the circle. Each of these triplets would thus produce an estimate for the center. Thus, one could average all $\binom{n}{3}$

of these estimates to obtain a value for the center. Using these values in (II.2) then produces a value for the radius. We shall refer to this method as the Average of Intersections Method (AI) with resulting values of a, b, and r labeled as a_A, b_A, and r_A.

A positive aspect of this method is that it yields closed form solutions. In particular, with

$$\begin{aligned} w_{ijk} &= x_i Y_{jk} + x_j Y_{ki} + x_k Y_{ij} \quad \text{(II.3)} \\ \tilde{w}_{ijk} &= x_i^2 Y_{jk} + x_j^2 Y_{ki} + x_k^2 Y_{ij} \\ z_{ijk} &= y_i X_{jk} + y_j X_{ki} + y_k X_{ij} \quad \text{(II.4)} \\ \tilde{z}_{ijk} &= y_i^2 X_{jk} + y_j^2 X_{ki} + y_k^2 X_{ij}, \end{aligned}$$

we have

$$\begin{aligned} a_A &= \frac{1}{2\binom{n}{3}} \sum_{i=1}^{n-2} \sum_{j=i+1}^{n-1} \sum_{k=j+1}^{n} \frac{\tilde{w}_{ijk} - \tilde{Y}_{ijk}}{w_{ijk}} \\ b_A &= \frac{1}{2\binom{n}{3}} \sum_{i=1}^{n-2} \sum_{j=i+1}^{n-1} \sum_{k=j+1}^{n} \frac{\tilde{z}_{ijk} - \tilde{X}_{ijk}}{z_{ijk}} \\ r_A &= \sum_{i=1}^{n} \sqrt{(x_i - a_I)^2 + (y_i - b_I)^2}/n \end{aligned}$$

An obvious drawback to this method is that it fails if any three of the points are collinear. This is obvious from the construction, but it also follows from the fact that if (x_i, y_i), (x_j, y_j), and (x_k, y_k) are collinear then $w_{ijk} = 0$ and $z_{ijk} = 0$ in (II.3) and (II.4). The method is also very unstable in that small changes in relatively close points can drastically change some of the approximating centers, thus producing very different circles.

This method is similar to fitting a circle to each of the triplets of points, thus getting $\binom{n}{3}$ estimates of the coordinates of the center and the radius, and then averaging these results for each of the three parameters. It differs in the calculation of the radius. AI averages the distance from each of the n points to the same center (a_I, b_I).

C. Reduced Least Squares Method

This leads to consideration of different estimates of the center (a, b). Again, if all of the data points lie on a circle then the perpendicular bisectors of the line segments connecting them will intersect at the same point, namely (a, b). Thus it seems reasonable to locate the center of the circle at the point where the sum of the distances from (a, b) to each of the perpendicular bisectors is minimum. Thus, we seek to minimize

$$SSR(a,b) = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \frac{\left(aX_{ji} + bY_{ji} - 0.5(Y_{ji}^{(2)} + X_{ji}^{(2)})\right)^2}{X_{ji}^2 + Y_{ji}^2} \quad \text{(II.5)}$$

As in the Full Least Squares method, equating the partial derivatives of SSR to zero does not produce closed form solutions for a and b. Again, however, numerical solutions are not difficult. Let us label the resulting values for a and b as a_R and b_R. Using these solutions in (II.2) yields the radius of the fitted circle, r_R. We shall refer to this method as the Reduced Least Squares method (RLS).

As will be discussed in Section 3, this method of estimation is not very stable. In particular, the $X_{ji}^2 + Y_{ji}^2$ in the denominator of (II.5) becomes problematic when two data points are very close together.

D. Modified Least Squares Methods

To downweight pairs of points that are close together, we will consider minimization of

$$SSM(a,b) = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \left(aX_{ji} + bY_{ji} - 0.5(X_{ij}^{(2)} + Y_{ij}^{(2)})\right)^2 \quad \text{(II.6)}$$

Differentiation of SSM yields

$$\begin{aligned} \frac{\partial SSM}{\partial a} &= 2b \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} X_{ji} Y_{ji} - \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} X_{ji} Y_{ji}^{(2)} \\ &\quad + 2a \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} X_{ji}^2 - \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} X_{ji} X_{ji}^{(2)} \\ \frac{\partial SSM}{\partial b} &= 2a \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} Y_{ji} X_{ji} - \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} Y_{ji} X_{ji}^{(2)} \\ &\quad + 2b \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} Y_{ji}^2 - \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} Y_{ji} Y_{ji}^{(2)} \end{aligned}$$

We note that for any vectors (α_i) and (β_i),

$$\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} (\alpha_j - \alpha_i)(\beta_j - \beta_i) = n \sum_{i=1}^{n} \alpha_i \beta_i - \left(\sum_{i=1}^{n} \alpha_i\right) \left(\sum_{i=1}^{n} \beta_i\right) \quad \text{(II.7)}$$

Noting that (II.7) is $n(n-1)S_{\alpha\beta}$, where $S_{\alpha\beta}$ is the usual covariance, we see that equating these partial derivatives to zero produces a pair of linear equations whose solution can be expressed as

$$\begin{aligned} a_M &= \frac{DC - BE}{AC - B^2} \quad \text{(II.8)} \\ b_M &= \frac{AE - BD}{AC - B^2}, \quad \text{(II.9)} \end{aligned}$$

where

$$\begin{aligned} A &= n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2 = n(n-1)S_x^2 \quad \text{(II.10)} \\ B &= n \sum_{i=1}^{n} x_i y_i - \left(\sum_{i=1}^{n} x_i\right) \left(\sum_{i=1}^{n} y_i\right) \end{aligned}$$

$$= n(n-1)S_{xy} \quad \text{(II.11)}$$

$$C = n\sum_{i=1}^{n} y_i^2 - \left(\sum_{i=1}^{n} y_i\right)^2 = n(n-1)S_y^2 \quad \text{(II.12)}$$

$$\begin{aligned} D &= 0.5\left\{n\sum_{i=1}^{n} x_i y_i^2 - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i^2\right)\right. \\ &\quad \left. +n\sum_{i=1}^{n} x_i^3 - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} x_i^2\right)\right\} \\ &= 0.5n(n-1)(S_{xy^2} + S_{xx^2}) \quad \text{(II.13)} \end{aligned}$$

$$\begin{aligned} E &= 0.5\left\{n\sum_{i=1}^{n} y_i x_i^2 - \left(\sum_{i=1}^{n} y_i\right)\left(\sum_{i=1}^{n} x_i^2\right)\right. \\ &\quad \left. +n\sum_{i=1}^{n} y_i^3 - \left(\sum_{i=1}^{n} y_i\right)\left(\sum_{i=1}^{n} y_i^2\right)\right\} \\ &= 0.5n(n-1)(S_{yx^2} + S_{yy^2}) \quad \text{(II.14)} \end{aligned}$$

Again, we find the radius using (II.2) as

$$r_M = \sum_{i=1}^{n} \sqrt{(x_i - a_M)^2 + (y_i - b_M)^2}/n \quad \text{(II.15)}$$

We shall refer to this as the Modified Least Squares method (MLS).

A different approach was presented in [4]. There, Kåsa proposes choosing a, b, and r to minimize

$$SSK(a,b,r) = \sum_{i=1}^{n} \left(r^2 - (x_i - a)^2 - (y_i - b)^2\right)^2$$

He indicates that solution for a and b can be obtained by solving linear equations, but does not describe the result of the process much further. It can be shown that the minimization of SSK produces the same center for the fitted circle as the MLS method. The minimizing value of r, say r_K, is slightly different from r_M. It turns out that

$$r_K = \sqrt{\sum_{i=1}^{n} \left((x_i - a_M)^2 + (y_i - b_M)^2\right)/n}$$

By Jensen's inequality, we see that r_K, being the square root of the average of squares, is at least as large as r_M, being the corresponding average.

III. Comparison of the Methods

We first note that if the n data points all truly lie on a circle with center (a^*, b^*) and radius r^*, then all five methods will produce this circle. For FLS, this follows since the nonnegative function SS is 0 at (a^*, b^*, r^*). For AI, this follows from the observation that the intersections of all of the perpendicular bisectors occur at the same point (a^*, b^*), and hence each of the n values in (II.2) that are to be averaged is r^*, and hence $r_A = r^*$. For RLS and MLS, we note that the terms in SSM in (II.6) are all 0 at (a^*, b^*) as then are the terms in SSR as well. Again, the radii of the RLS and MLS methods are r^* for the same reason as given for AI. Since the values to be averaged for r_M are all identical, we also have $r_K = r_M = r^*$.

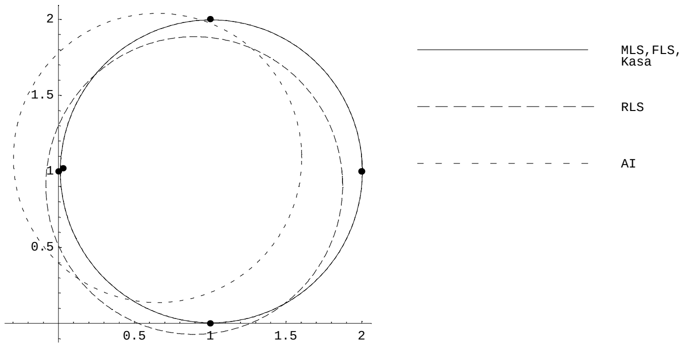

Fig. 1. Fits of FLS, AI, RLS, MLS, and Kåsa circles to five data points.

If any three points are collinear, then AI fails because the perpendicular bisectors for this triple are parallel, thus producing no intersection point. Thus averaging over the intersection points of all triples fails. The other four methods produce unique results in this situation, unless, of course, all of the data points are collinear.

If all of the points are collinear, then all five methods fail. FLS fails because the larger the radius of the circle, with appropriate change in the center, the closer the fit to the data. For MLS and Kåsa, we note that if all of the data points are collinear, then $S_{xy}^2 = S_x^2 S_y^2$, and hence the denominators of a_M and b_M in (II.8) and (II.9) are 0 using (II.10), (II.11), and (II.12). RLS fails because for this case there will be an infinite collection of points that minimize the distance from the point (a, b) to the parallel lines that form the perpendicular bisectors.

To give an indication of how sensitive the methods are to measurement error, we consider fits to a few collections of data.

All five methods fit the circle $(x-1)^2+(y-1)^2 = 1$ to the following collection of five points, (0,1), (2,1), (1,0), (1,2), and $(0.015, 1 + \sqrt{0.029775})$. Suppose that the last data point, however, was incorrectly recorded as (0.03,1.02), a point only 0.15329 units away. The results of the fits to these five points are displayed in Figure 1. As is evident from the figure, we see that the AI circle was drastically affected. The fit is not close at all to the circle of radius 1 centered at (1,1). Not quite as drastically affected, but seriously affected, nonetheless, is the RLS circle. In contrast, the FLS, Kåsa, and MLS circles are not perspectively different from the circle of radius 1 centered at (1,1). This strongly suggests that the FLS, Kåsa, and MLS methods are robust against measurement error.

Figure 2 contains FLS, MLS, and Kåsa fits to the following seven data points, (0,1), (2,1), (2,1.5), (1.5,0), (0.5,0.7), (0.5,2), and (1.5,2.2). These three circles are fairly similar, but not identical. Each seems to describe the data points well. It is open to interpretation as to which circle best fits the seven points.

These fits point favorably to using the MLS and Kåsa

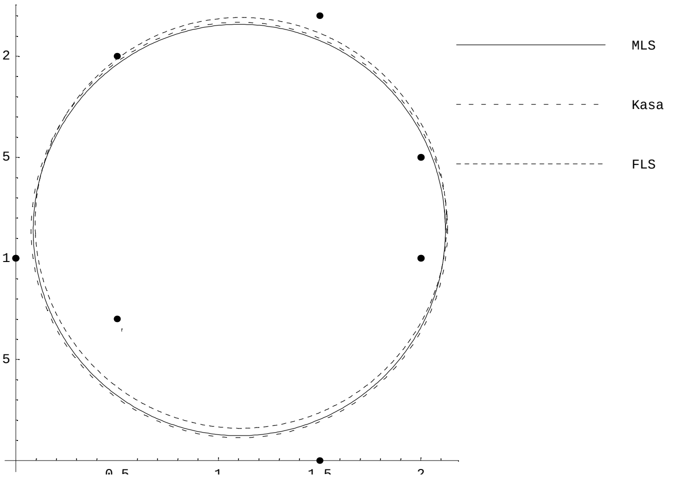

Fig. 2. Fits of FLS, MLS, and Kåsa circles to seven data points.

methods to fit circles. The robustness of the methods and the existence of closed form solutions are very appealing properties. Recall that these circles are concentric, with the Kåsa circle outside the MLS circle. Thus, outliers inside the circles would make the Kåsa fit seem superior. Whereas, outliers outside the circles would make the MLS fit seem superior.

IV. Fitting Spheres in 3-space

These methods are not difficult to generalize to fitting spheres to points in 3-space. So, suppose that we have a collection of $n \geq 4$ points in 3-space labeled (x_1, y_1, z_1), $(x_2, y_2, z_2), \ldots, (x_n, y_n, z_n)$. The basic problem is to find a sphere that best represents the data in some sense. With our sphere described by $(x-a)^2 + (y-b)^2 + (z-c)^2 = r^2$, we need to determine values for the center (a, b, c) and the radius r for the best fitting circle.

Based on the comparative results in Section 3, we will only consider extensions of the FLS, MLS, and Kåsa methods. For FLS, we seek to minimize

$$SS^*(a,b,r) = \sum_{i=1}^{n} \left(r - \sqrt{(x_i-a)^2 + (y_i-b)^2 + (z_i-c)^2} \right)^2$$

As in the 2 dimensional case, one must resort to numerical solutions.

The derivation of the MLS estimate proceeds in a similar manner in 3-space. The plane passing through the midpoint of any chord of a sphere which is perpendicular to that chord will pass through the center of the sphere. Thus we seek the point (a, b, c) which minimizes the sum of the squares of the distances from (a, b, c) to each of the $\binom{n}{2}$ planes formed by pairs of points. This leads to minimization of $SSR^*(a, b, c) =$

$$\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \frac{\left(\begin{array}{c} X_{ji}a + Y_{ji}b + Z_{ji}c \\ -0.5(X_{ji}^{(2)} + Y_{ji}^{(2)} + Z_{ji}^{(2)}) \end{array} \right)^2}{X_{ji}^2 + Y_{ji}^2 + Z_{ji}^2}$$

Minimization of SSR^* requires a numerical solution. This solution also suffers in that it is very sensitive to changes in data points that are close together.

Thus, as in the 2 dimensional case, we consider the modification produced by instead minimizing $SSM^*(a,b,c) =$

$$\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \left(\begin{array}{c} aX_{ji} + bY_{ji} + cZ_{ji} \\ -0.5(X_{ji}^{(2)} + Y_{ji}^{(2)} + Z_{ji}^{(2)}) \end{array} \right)^2$$

Analogous to the 2 dimensional case, we obtain closed form solutions, (a_M, b_M, c_M), to the minimization problem.

Defining the mean squares as in (II.10) through (II.14), we obtain

$$a_M = \frac{\left\{ \begin{array}{c} (S_{xx^2} + S_{xy^2} + S_{xz^2})(S_y^2 S_z^2 - S_{yz}^2) \\ +(S_{yx^2} + S_{yy^2} + S_{yz^2})(S_{xz}S_{yz} - S_{xy}S_z^2) \\ +(S_{zx^2} + S_{zy^2} + S_{zz^2})(S_{xy}S_{yz} - S_{xz}S_y^2) \end{array} \right\}}{2\left\{ \begin{array}{c} S_x^2 S_y^2 S_z^2 + 2S_{xy}S_{yz}S_{xz} \\ -S_x^2 S_{yz}^2 - S_y^2 S_{xz}^2 - S_z^2 S_{xy}^2 \end{array} \right\}}$$

$$b_M = \frac{\left\{ \begin{array}{c} (S_{xx^2} + S_{xy^2} + S_{xz^2})(S_{xz}S_{yz} - S_{xy}S_z^2) \\ +(S_{yx^2} + S_{yy^2} + S_{yz^2})(S_x^2 S_z^2 - S_{xz}^2) \\ +(S_{zx^2} + S_{zy^2} + S_{zz^2})(S_{xy}S_{xz} - S_{yz}S_x^2) \end{array} \right\}}{2\left\{ \begin{array}{c} S_x^2 S_y^2 S_z^2 + 2S_{xy}S_{yz}S_{xz} \\ -S_x^2 S_{yz}^2 - S_y^2 S_{xz}^2 - S_z^2 S_{xy}^2 \end{array} \right\}}$$

$$c_M = \frac{\left\{ \begin{array}{c} (S_{xx^2} + S_{xy^2} + S_{xz^2})(S_{xy}S_{yz} - S_{xy}S_y^2) \\ +(S_{yx^2} + S_{yy^2} + S_{yz^2})(S_{xz}S_{xy} - S_{yz}S_x^2) \\ +(S_{zx^2} + S_{zy^2} + S_{zz^2})(S_x^2 S_y^2 - S_{xy}^2) \end{array} \right\}}{2\left\{ \begin{array}{c} S_x^2 S_y^2 S_z^2 + 2S_{xy}S_{yz}S_{xz} \\ -S_x^2 S_{yz}^2 - S_y^2 S_{xz}^2 - S_z^2 S_{xy}^2 \end{array} \right\}}$$

Analogous to (II.15), we find

$$r_M = \sum_{i=1}^{n} \sqrt{(x_i - a_M)^2 + (y_i - b_M)^2 + (z_i - c_M)^2}/n$$

For this problem, it is not difficult to show that the fit of [4] has the center described by a_M, b_M, and c_M. The radius for the fitted circle is

$$r_K = \sqrt{\sum_{i=1}^{n} \left((x_i - a_M)^2 + (y_i - b_M)^2 + (z_i - c_M)^2 \right)/n}$$

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