Least-squares Fit to Circles and Spheres

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I. Least-squares formula

If a set of simultaneous, linear equations can be formulated as

$$\mathbb{A}\mathbf{x} = \mathbf{y}, \tag{1}$$

and if all the columns of $\mathbb{A}$ are linearly independent, then there exists only one least-squares solution $\hat{\mathbf{x}}$, as defined by equation (2)) (see Ref. [1]).

$$\hat{\mathbf{x}} = \left(\mathbb{A}^T\mathbb{A}\right)^{-1}\mathbb{A}^T\mathbf{y}. \tag{2}$$

II. General equation for a circle

The general equation for a circle is

$$(x - x_0)^2 + (y - y_0)^2 = r^2, \tag{3}$$

where the center of the circle is defined at (x_0, y_0), and r is its radius. Expansion of (3) yields

$$x^2 - 2xx_0 + x_0^2 + y^2 - 2yy_0 + y_0^2 = r^2. \tag{4}$$

By rearranging (4) so that

$$-2xx_0 - 2yy_0 + x_0^2 + y_0^2 - r^2 = -\left(x^2 + y^2\right), \tag{5}$$

the generalized equation for a circle can be rearranged into the form of the matrix-vector equation (1).

The variables to be solved (x_0, y_0, and r) must be packed into the vector $\mathbf{x}$. Define

$$\mathbf{x} = \begin{bmatrix} x_0 \\ y_0 \\ x_o^2 + y_0^2 - r^2 \end{bmatrix}_{3\times 1}, \tag{6}$$

and rearrange equation (5) so that

$$\begin{bmatrix} -2x & -2y & +1 \end{bmatrix} \begin{bmatrix} x_0 \\ y_0 \\ x_o^2 + y_0^2 - r^2 \end{bmatrix} = \left[-\left(x^2 + y^2\right)\right]. \tag{7}$$

For a set of n measurements, the remaining matrices to completely define (3) in the form of (1) are

$$\mathbb{A} = \begin{bmatrix} -2x_1 & -2y_1 & +1 \\ -2x_2 & -2y_2 & +1 \\ -2x_3 & -2y_3 & +1 \\ \vdots & \vdots & \vdots \\ -2x_n & -2y_n & +1 \end{bmatrix}_{n\times 3} \tag{8}$$

and

$$\mathbf{y} = \begin{bmatrix} -\left(x_1^2 + y_1^2\right) \\ -\left(x_2^2 + y_2^2\right) \\ -\left(x_3^2 + y_3^2\right) \\ \vdots \\ -\left(x_n^2 + y_n^2\right) \end{bmatrix}_{n\times 1} \tag{9}$$

For distinct values of x_i and y_i, the columns of $\mathbb{A}$ are all linearly independent, satisfying the condition for (2).

III. General equation of a sphere

The procedure is similar for a sphere. The general equation of a sphere is

$$(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2 = r^2 \tag{10}$$

where the center of the sphere is defined at (x_0, y_0, z_0) and r is its radius. Expansion yields

$$x^2 - 2xx_0 + x_0^2 + y^2 - 2yy_0 + y_0^2 + z^2 - 2zz_0 + z_0^2 = r^2, \tag{11}$$

and rearranging yields

$$-2xx_0 - 2yy_0 - 2zz_0 + x_0^2 + y_0^2 + z_0^2 - r^2 = -\left(x^2 + y^2 + z^2\right), \tag{12}$$

and the matrix-vector equation is now

$$\begin{bmatrix} -2x & -2y & -2z & +1 \end{bmatrix} \begin{bmatrix} x_0 \\ y_0 \\ z_0 \\ x_o^2 + y_0^2 + z_0^2 - r^2 \end{bmatrix} = \left[-\left(x^2 + y^2 + z^2\right) \right] \tag{13}$$

The matrices defining the least-squares solution are, therefore,

$$\mathbb{A} = \begin{bmatrix} -2x_1 & -2y_1 & -2z_1 & +1 \\ -2x_2 & -2y_2 & -2z_2 & +1 \\ -2x_3 & -2y_3 & -2z_3 & +1 \\ \vdots & \vdots & \vdots & \\ -2x_n & -2y_n & -2z_n & +1 \end{bmatrix}_{n \times 4} \tag{14}$$

$$\mathbf{x} = \begin{bmatrix} x_0 \\ y_0 \\ z_0 \\ x_o^2 + y_0^2 + z_0^2 - r^2 \end{bmatrix}_{4 \times 1} \tag{15}$$

and

$$\mathbf{y} = \begin{bmatrix} -\left(x_1^2 + y_1^2 + z_1^2\right) \\ -\left(x_2^2 + y_2^2 + z_2^2\right) \\ -\left(x_3^2 + y_3^2 + z_3^2\right) \\ \vdots \\ -\left(x_n^2 + y_n^2 + z_n^2\right) \end{bmatrix}_{n \times 1} \tag{16}$$

For distinct values of x_i, y_i, and z_i the columns of $\mathbb{A}$ are all linearly independent, satisfying the condition for (2).

IV. Weighted Least-squares

Suppose each measurement is to be weighted. Define a weighting matrix as

$$\mathbb{W} = \begin{bmatrix} w_1 & 0 & \dots & 0 \\ 0 & w_2 & \dots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & & \dots & w_n \end{bmatrix}_{n \times n} \tag{17}$$

where each w_i is applied to the i^{th} measurement y_i.

The normal equation for the weighted-least squares solution is now (see Ref. [2])

$$(\mathbb{W}\mathbb{A})^T \, \mathbb{W}\mathbb{A}\mathbf{x} = (\mathbb{W}\mathbb{A})^T \, \mathbb{W}\mathbf{y}, \tag{18}$$

and if the columns of $\mathbb{W}\mathbb{A}$ are linearly independent, then there exists only one least-squares solution for $\mathbf{x}$

References

[1] D. C. Lay, *Linear Algebra and Its Applications, 3rd Edition*, **Addison Wesley**, Chapter 6.5, 2003.
[2] D. C. Lay, *Linear Algebra and Its Applications, 3rd Edition*, **Addison Wesley**, Chapter 6.8, 2003.