TECHNICAL NOTE

Least-Square Fitting with Spheres

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Communicated by H. J. Oberle

Abstract. Fitting circles and spheres to given data in $\mathbb{R}^2$ or $\mathbb{R}^3$ is at least relevant in computational metrology (Ref. 1) and reflectrometry (Ref. 2). A new descent algorithm, developed for circles in Ref. 3, is generalized to spheres. Numerical examples are given.

Key Words. Least-square fitting, spheres.

1. Model

Let given data points $(x_r, y_r, z_r)$, $r = 1, \ldots, s \geq 3$, in the three-dimensional Euclidean space. Let $(A, B, C)$ be the unknown center, and let $R$ be the unknown radius of a sphere

$$(x - A)^2 + (y - B)^2 + (z - C)^2 = R^2$$

(1)

to be fitted to the data. The most natural fitting principle consists of minimizing the sum of squared distances from the given data points to points on the sphere given by the intersection of a straight line through a data point and the center.

One formulation of this objective function is

$$S(A, B, C, R) = \sum_{r=1}^{s} \sqrt{(x_r - A)^2 + (y_r - B)^2 + (z_r - C)^2 - R^2}. \quad (2)$$

Another one is obtained using the parametric representation of a sphere, i.e.,

$$x = A + R \cos u \sin v, \quad (3a)$$
$$y = B + R \sin u \sin v, \quad (3b)$$
$$z = C + R \cos v, \quad (3c)$$

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with $0 \leq u \leq \pi$, $0 \leq v < 2\pi$. With unknown parameter values $(u_r, v_r)$, $r = 1, \ldots, s$, corresponding to the intersection points above, the objective function becomes

$$\tilde{S}(A, B, C, R, u_1, \ldots, u_s, v_1, \ldots, v_s)$$

$$= \sum_{r=1}^{s} (x_r - A - R \cos u_r \sin v_r)^2$$

$$+ (y_r - B - R \sin u_r \sin v_r)^2 + (z_r - C - R \cos v_r)^2.$$  \hfill (4)

At first glance, (4) looks far more complicated than (2), but it will turn out that (4) is easier to deal with when considering the necessary conditions for a minimum.

For $S$, the equations

$$\frac{\partial S}{\partial A} = \frac{\partial S}{\partial B} = \frac{\partial S}{\partial C} = \frac{\partial S}{\partial R} = 0$$

contain $A, B, C$ nonlinearly; for $\tilde{S}$, the relations

$$\frac{\partial \tilde{S}}{\partial A} = \frac{\partial \tilde{S}}{\partial B} = \frac{\partial \tilde{S}}{\partial C} = \frac{\partial \tilde{S}}{\partial R} = 0$$

yield the $4 \times 4$ linear system of equations

$$\begin{bmatrix}
s & 0 & 0 & \sum_{r=1}^{s} \cos u_r \sin v_r \\
0 & s & 0 & \sum_{r=1}^{s} \sin u_r \sin v_r \\
0 & 0 & s & \sum_{r=1}^{s} \cos v_r \\
\sum_{r=1}^{s} \cos u_r \sin v_r & \sum_{r=1}^{s} \sin u_r \sin v_r & \sum_{r=1}^{s} \cos v_r & s
\end{bmatrix}
\begin{bmatrix}
e_1 \\
e_2 \\
e_3 \\
e_4
\end{bmatrix}
= \begin{bmatrix}
e_1 \\
e_2 \\
e_3 \\
e_4
\end{bmatrix},$$

\hfill (7)

where

$$e_1 = \sum_{r=1}^{s} x_r, \quad e_2 = \sum_{r=1}^{s} y_r, \quad e_3 = \sum_{r=1}^{s} z_r,$$

$$e_4 = \sum_{r=1}^{s} (x_r \cos u_r \sin v_r + y_r \sin u_r \sin v_r + z_r \cos v_r).$$

\hfill (8a)

\hfill (8b)