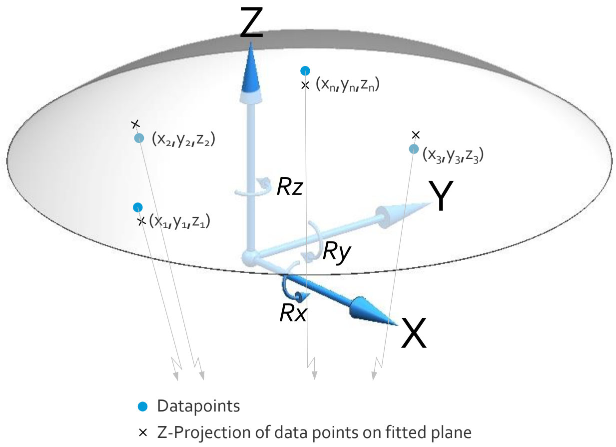
FIT SPHERE THROUGH POINTS

Introduction

Method to derive a best fit of a sphere through a number (≥ 4) of XYZ data points, where the summed square errors of the data points in relation to the fit-sphere are in the direction perpendicular to the surface.



Equation of a sphere

$z(x,y) = \sqrt{(R^2 - (x - x_c)^2 - (y - y_c)^2)} + z_c$

(x_c, y_c, z_c) is the location of the center of the sphere, and R is the radius of the sphere.

Data points

$$\begin{bmatrix} x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ x_3 & y_3 & z_3 \\ x_3 & y_4 & z_4 \\ & \vdots & \\ x_n & y_n & z_n \end{bmatrix}$$

Center location and radius of fitted sphere

$$\mathrm{A} = 2 \cdot \begin{bmatrix} \sum_{i=1}^{i=n} \frac{x_i \cdot (x_i - \bar{x})}{n} & \sum_{i=1}^{i=n} \frac{x_i \cdot (y_i - \bar{y})}{n} & \sum_{i=1}^{i=n} \frac{x_i \cdot (z_i - \bar{z})}{n} \\ \sum_{i=1}^{i=n} \frac{y_i \cdot (x_i - \bar{x})}{n} & \sum_{i=1}^{i=n} \frac{y_i \cdot (y_i - \bar{y})}{n} & \sum_{i=1}^{i=n} \frac{y_i \cdot (z_i - \bar{z})}{n} \\ \sum_{i=1}^{i=n} \frac{z_i \cdot (x_i - \bar{x})}{n} & \sum_{i=1}^{i=n} \frac{z_i \cdot (y_i - \bar{y})}{n} & \sum_{i=1}^{i=n} \frac{z_i \cdot (z_i - \bar{z})}{n} \end{bmatrix}$$

$$\mathrm{B} = \begin{bmatrix} \sum_{i=1}^{n} \frac{(x_i^2 + y_i^2 + z_i^2) \cdot (x_i - \bar{x})}{n} \\ \sum_{i=1}^{n} \frac{(x_i^2 + y_i^2 + z_i^2) \cdot (y_i - \bar{y})}{n} \\ \sum_{i=1}^{n} \frac{(x_i^2 + y_i^2 + z_i^2) \cdot (z_i - \bar{z})}{n} \end{bmatrix}$$

$$\bar{\mathrm{x}} = \frac{1}{\mathrm{n}} \sum_{\mathrm{i}=1}^{\mathrm{i}=\mathrm{n}} \mathrm{x_i}, \quad \bar{\mathrm{y}} = \frac{1}{\mathrm{n}} \sum_{\mathrm{i}=1}^{\mathrm{i}=\mathrm{n}} \mathrm{y_i}, \quad \bar{\mathrm{z}} = \frac{1}{\mathrm{n}} \sum_{\mathrm{i}=1}^{\mathrm{i}=\mathrm{n}} \mathrm{z_i}$$

$$\begin{bmatrix} x_c \\ y_c \\ z_c \end{bmatrix} = (A^T \cdot A)^{-1} \cdot A^T \cdot B$$

$$R = \sqrt{\frac{\sum_{i=1}^{i=n} ((x_i - x_c)^2 + (y_i - y_c)^2 + (z_i - z_c)^2)}{n}}$$

Fit quality – Coefficient of determination = R²

$$R^2 = 1 - \frac{\sum_{i=1}^{i=n} \left(z_i - z(x_i, y_i)\right)^2}{\sum_{i=1}^{i=n} \left(z_i - \frac{1}{n} \sum_{i=1}^{n} z_i\right)^2}$$

A value of R^2 which is close to 1 indicates a good fit quality.