A brief introduction to geometric fitting algorithms

Alejandro Garnung Menéndez

21 January 2025

Contents

Geometric fitting algorithms **1**
Circle fitting 1
Centered torus 4

Geometric fitting algorithms

Suppose we have a set of 3D points denoted as:

$$\{\mathbf{x}_i\}_{i=1}^{m} = \{\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_m\}, \quad \text{where} \quad \mathbf{x}_i \in \mathbb{R}^3. \tag{1}$$

We can approach the problem of fitting geometric entities in two ways:

1. Through definition. One approach is to solve a (typically) overdetermined linear system derived from the equations of the geometric entities themselves and stacking as many data points as we have.

2. Another approach is to make the equations of these entities contingent on the observed data, minimizing the error between the observed points and the theoretical points defined by each parameter of the entity within the parameter space where the optimization is performed. With this, we will find the parameters of the entity that best fit under the defined error criterion.

3D Circle fitting

In a Cartesian coordinate system in three-dimensional Euclidean space, the equation of a sphere with radius r and center $O(a, b, c)$ is given by:

$$(x-a)^2 + (y-b)^2 + (z-c)^2 - r^2 = 0. \tag{2}$$

Our main objective is to rearrange this equation to separate the independent variables/unknowns from the coefficient/data terms. Expanding the equation of the sphere:

$$x^2 + a^2 - 2xa + y^2 + b^2 - 2yb + z^2 + c^2 - 2zc = r^2. \tag{3}$$

Reorganizing terms, we get:

$$(x^2 + y^2 + z^2) + (2x \cdot a + 2y \cdot b + 2z \cdot c) + (a^2 + b^2 + c^2 - r^2) = 0. \tag{4}$$

Let $\alpha = a^2 + b^2 + c^2 - r^2$. The equation becomes:

$$(2x \cdot a + 2y \cdot b + 2z \cdot c) + \alpha = (x^2 + y^2 + z^2). \tag{5}$$

In matrix form, this can be expressed as:

$$\begin{bmatrix} 2x & 2y & 2z & 1 \end{bmatrix}_{1\times 4} \cdot \begin{bmatrix} a \\ b \\ c \\ \alpha \end{bmatrix}_{4\times 1} = \begin{bmatrix} x^2 + y^2 + z^2 \end{bmatrix}_{1\times 1}, \tag{6}$$

which is highly recognizable as a system of the form $A\mathbf{x} = \mathbf{b}$ (our best friend).

It is very convenient that we can express a geometric entity in a system of linear equations in closed form. This system can be solved for our data using methods such as Gaussian elimination, matrix decomposition (e.g., LU, QR, SVD or Moore-Penrose pseudoinverse A^+).

Nevertheless, we can derive a solution from another perspective.

Let us have a point cloud $\mathcal{P}$, defined as:

$$\mathcal{P} = \{(x_i, y_i, z_i)\}_{i=1}^{m}, \quad m > 4. \tag{7}$$

Using a least-squares approach, we can define the loss function $E(\cdot)$, which measures the accumulated squared error between the distances of the points to the center and an ideal distance r:

$$\begin{aligned} E(a, b, c, r) &= \frac{1}{2} \sum_{i=1}^{m} \left(\sqrt{(x_i - a)^2 + (y_i - b)^2 + (z_i - c)^2} - r \right)^2 \\ &= \frac{1}{2} \sum_{i=1}^{m} (L_i - r)^2 . \end{aligned} \tag{8}$$

We see that the points of $\mathcal{P}$ are our data, and the variables a, b, c, r are our unknowns. We aim to find the sphere that best fits the data in a least-squares sense (hence the squared difference in the expression we defined for $E(\cdot)$), where this function reaches a minimum. Since $E(\cdot)$ is a convex quadratic function, its minimum is determined by the optimality condition. To find this minimum, we calculate the derivatives of $E(a, b, c, r)$ with respect to its variables and set them to zero.

For the variable r:

$$\frac{\partial E}{\partial r} = -\cancel{2}\frac{1}{\cancel{2}}\sum_{i=1}^{m}(L_i - r) = -\sum_{i=1}^{m}(L_i - r) = r\sum_{i=1}^{m}1 - \sum_{i=1}^{m}L_i = r\cdot m - \sum_{i=1}^{m}L_i. \tag{9}$$

$$\frac{\partial E}{\partial r} = 0 \implies \boxed{r = \frac{1}{m}\sum_{i=1}^{m}L_i}. \tag{10}$$

For the variable a:

$$\frac{\partial E}{\partial a} = \sum_{i=1}^{m}(L_i - r)\frac{\partial L_i}{\partial a}. \tag{11}$$

Knowing that

$$\frac{\partial L_i}{\partial a} = -\frac{x_i - a}{L_i}, \tag{12}$$

we have:

$$\begin{aligned}
\frac{\partial E}{\partial a} &= \sum_{i=1}^{m}(L_i - r)\left(-\frac{x_i - a}{L_i}\right) \\
&= \sum_{i=1}^{m}\left((x_i - a) - r\frac{x_i - a}{L_i}\right) \\
&= \sum_{i=1}^{m}(x_i - a) - \sum_{i=1}^{m}r\frac{x_i - a}{L_i} \\
&= (m - \sum_{i=1}^{m}\frac{r}{L_i})(x_i - a).
\end{aligned} \tag{13}$$

$$\frac{\partial E}{\partial a} = 0 \implies \sum_{i=1}^{m}(x_i - a) = \sum_{i=1}^{m}\left(r\frac{x_i - a}{L_i}\right). \tag{14}$$

$$\sum_{i=1}^{m}x_i - \sum_{i=1}^{m}a = \sum_{i=1}^{m}\frac{r(x_i - a)}{L_i}. \tag{15}$$

$$\sum_{i=1}^{m}x_i - a\sum_{i=1}^{m}1 = r\sum_{i=1}^{m}\frac{x_i}{L_i} - r\sum_{i=1}^{m}\frac{a}{L_i}. \tag{16}$$

$$\sum_{i=1}^{m}x_i - r\sum_{i=1}^{m}\frac{x_i}{L_i} = a\left(m + r\sum_{i=1}^{m}\frac{1}{L_i}\right). \tag{17}$$

$$\boxed{a = \frac{\sum_{i=1}^{m}x_i - r\sum_{i=1}^{m}\frac{x_i}{L_i}}{m + r\sum_{i=1}^{m}\frac{1}{L_i}}}. \tag{18}$$

Analogously, for the variables b and c, we have:

$$\boxed{b = \frac{\sum_{i=1}^{m} y_i - r \sum_{i=1}^{m} \frac{y_i}{L_i}}{m + r \sum_{i=1}^{m} \frac{1}{L_i}}}. \tag{19}$$

$$\boxed{c = \frac{\sum_{i=1}^{m} z_i - r \sum_{i=1}^{m} \frac{z_i}{L_i}}{m + r \sum_{i=1}^{m} \frac{1}{L_i}}}. \tag{20}$$

These are the parameters of the sphere that best fit our data in the least-squares sense.

Centered torus

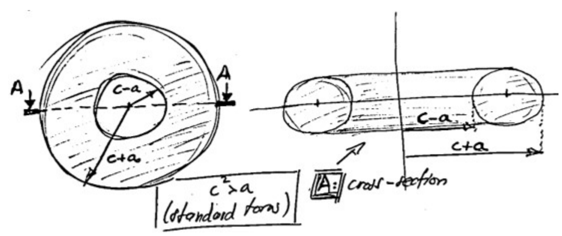

Figure 1: A centered torus with radii specified by c and a.

In a Cartesian coordinate system in three-dimensional Euclidean space, the equation of a symmetric torus azimuthally on the z -axis, with radius c from the center of the hole to the center of the torus tube, and radius of the tube a, is given by:

$$\left(c - \sqrt{x^2 + y^2}\right)^2 + z^2 - a^2 = 0. \tag{21}$$

Expanding and rearranging the terms:

$$c^2 + \left(x^2 + y^2\right) - 2c\sqrt{x^2 + y^2} + z^2 - a^2 = 0. \tag{22}$$

Simplifying further:

$$c^2 - 2c\sqrt{x^2 + y^2} - a^2 = -\left(x^2 + y^2 + z^2\right). \tag{23}$$

Let $\alpha = c^2 - a^2$. Substituting α into the equation:

$$\alpha - 2c\sqrt{x^2 + y^2} = -\left(x^2 + y^2 + z^2\right). \tag{24}$$

Finally, this can be rewritten in matrix form, which can be efficiently solved:

$$\begin{bmatrix} 1 & -2\sqrt{x^2 + y^2} \end{bmatrix} \cdot \begin{bmatrix} \alpha \\ c \end{bmatrix} = \begin{bmatrix} -\left(x^2 + y^2 + z^2\right) \end{bmatrix}. \tag{25}$$

In the end, we typically end up with an overdetermined system that needs to be solved from the data points $\mathcal{P} = \{(x_i, y_i, z_i)\}_{i=1}^{m}$ with which we have at our disposal. Let $r_i = \sqrt{x_i^2 + y_i^2}$ and $d_i = x_i^2 + y_i^2 + z_i^2$, we end with:

$$\begin{bmatrix} \vdots & \vdots \\ 1 & -2r_1 \\ 1 & -2r_2 \\ 1 & -2r_3 \\ 1 & -2r_4 \\ \vdots & \vdots \end{bmatrix} \cdot \begin{bmatrix} \alpha \\ c \end{bmatrix} = \begin{bmatrix} \vdots \\ -d_1 \\ -d_2 \\ -d_3 \\ -d_4 \\ \vdots \end{bmatrix}, \tag{26}$$

and it is suitable to be solved by any of the methods mentioned for systems of the type $A\mathbf{x} = \mathbf{b}$