A resourceful least-squares Taylor-based torus fitting algorithm

Alejandro Garnung Menéndez

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Uncentered torus fitting

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

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

Recall the centered torus equation;:

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

Its uncentered version is:

$$\left(c - \sqrt{(x - x_0)^2 + (y - y_0)^2}\right)^2 + (z - z_0)^2 - a^2 = 0. \tag{3}$$

Expanding and rearranging the terms:

$$c^2 + (x - x_0)^2 + (y - y_0)^2 - 2c \boxed{\sqrt{(x - x_0)^2 + (y - y_0)^2}} + (z - z_0)^2 - a^2 = 0. \tag{4}$$

The proposed workaround, due to the nonlinearity of the equation, is to linearize the term highlighted in the box.

Remark:

Taylor series: The Taylor series decomposition of a function at a point x_0, y_0 is given by:

$$f(x_0, y_0) = f(x_0^{(0)}, y_0^{(0)}) + \sum_{n=1}^{\infty} \left[\frac{1}{n!} \frac{\partial^n f}{\partial x_0^n} \Big|_{(x_0^{(0)}, y_0^{(0)})} \cdot (x_0 - x_0^{(0)})^n + \frac{1}{n!} \frac{\partial^n f}{\partial y_0^n} \Big|_{(x_0^{(0)}, y_0^{(0)})} \cdot (y_0 - y_0^{(0)})^n \right] + \cdots$$

The first-order approximation keeps only the first-order derivative terms:

$$f(x_0, y_0) \approx f(x_0^{(0)}, y_0^{(0)}) + \frac{\partial f}{\partial x_0} \Big|_{(x_0^{(0)}, y_0^{(0)})} \cdot (x_0 - x_0^{(0)}) + \frac{\partial f}{\partial y_0} \Big|_{(x_0^{(0)}, y_0^{(0)})} \cdot (y_0 - y_0^{(0)})$$

Let $(x_0^{(0)}, y_0^{(0)})$ be the "initial point" or "operating point". The Taylor decomposition of the two-dimensional function $f(x_0, y_0)$ can be written as:

$$f(x_0, y_0) \approx f(x_0^{(0)}, y_0^{(0)}) + \frac{\partial f}{\partial x_0} \Big|_{(x_0^{(0)}, y_0^{(0)})} \cdot (x_0 - x_0^{(0)}) + \frac{\partial f}{\partial y_0} \Big|_{(x_0^{(0)}, y_0^{(0)})} \cdot (y_0 - y_0^{(0)})$$

Let us define $f(x_0, y_0) = \sqrt{(x - x_0)^2 + (y - y_0)^2}$. Its fist-order Taylor approximation is:

$$f(x_0, y_0) \approx \sqrt{(x - x_0^{(0)})^2 + (y - y_0^{(0)})^2} - \frac{(x - x_0^{(0)})(x_0 - x_0^{(0)}) + (y - y_0^{(0)})(y_0 - y_0^{(0)})}{\sqrt{(x - x_0^{(0)})^2 + (y - y_0^{(0)})^2}}. \tag{5}$$

Let this linearization be $f_L(x_0, y_0)$, so that $f(x_0, y_0) \approx f_L(x_0, y_0)$ locally. Now, Equation (4) rewrites as:

$$c^2 + (x - x_0)^2 + (y - y_0)^2 - 2cf_L + (z - z_0)^2 - a^2 = 0. \tag{6}$$

We hypothesize that a reasonable choice for the operating point $(x_0^{(0)}, y_0^{(0)})$ is the centroid of the data (constant):

$$x_0^{(0)} \approx \frac{1}{m} \sum_{i=1}^{m} x_i, \quad y_0^{(0)} \approx \frac{1}{m} \sum_{i=1}^{m} y_i.$$

Another alternative would be selecting the origin, in which case the equilibrium equation, describing a system where the function $f(x_0, y_0)$ approximates a specific value at a given operating point, would be:

$$f_0 \equiv f(x_0^{(0)}, y_0^{(0)}) = f(0,0) = \sqrt{x^2 + y^2}. \tag{7}$$

Let us define:

$$L_i = \sqrt{(x - x_0^{(0)})^2 + (y - y_0^{(0)})^2} \quad \text{(constant for } i\text{, as } x \equiv x_i, y \equiv y_i\text{)}, \tag{8}$$

$$f_L = L_i - \frac{(x - x_0^{(0)})(x_0 - x_0^{(0)}) + (y - y_0^{(0)})(y_0 - y_0^{(0)})}{L_i}, \tag{9}$$

$$x^2 + y^2 + z^2 = p_i. \tag{10}$$

We will attempt to reformulate Equation (6):

$$\begin{aligned} c^2 + x^2 + x_0^2 - 2xx_0 + y^2 + y_0^2 - 2cL_i + \frac{2c}{L_i}\Big[(x - x_0^{(0)})(x_0 - x_0^{(0)}) \\ +(y - y_0^{(0)})(y_0 - y_0^{(0)})\Big] + z^2 + z_0^2 - 2zz_0 - a^2 = 0. \end{aligned} \tag{11}$$

Let:

$$\alpha = c^2 - a^2, \quad \beta = x_0^2 + y_0^2 + z_0^2, \quad \gamma_i = 2xx_0 + 2yy_0 + 2zz_0.$$

Then, the equation can be rewritten as:

$$\begin{aligned} \alpha + p_i + \beta - \gamma_i - 2cL_i\frac{2c}{L_i}[(x - x_0^{(0)})(x_0 - x_0^{(0)}) \\ +(y - y_0^{(0)})(y_0 - y_0^{(0)})] = 0. \end{aligned} \tag{12}$$

Expanding:

$$\begin{aligned} \alpha + p_i + \beta - \gamma_i - 2cL_i + \frac{2c}{L_i}\Big[((x_0^{(0)})^2 + (y_0^{(0)})^2 - xx_0^{(0)} - yy_0^{(0)}) \\ +(xx_0^{(0)} + yy_0^{(0)}) - (x_0^{(0)}x_0^{(0)} + y_0^{(0)}y_0^{(0)})\Big] \end{aligned} \tag{13}$$

Let $\chi = (x_0^{(0)})^2 + (y_0^{(0)})^2 - xx_0^{(0)} - yy_0^{(0)}$ (constant for i), then:

$$\begin{aligned} \alpha + p_i + \beta - \gamma_i - 2cL_i + \frac{2}{L_i}\cdot\chi\cdot c + \frac{2c}{L_i}\cdot(xx_0^{(0)} + yy_0^{(0)}) \\ -\frac{2c}{L_i}\cdot(x_0x_0^{(0)} + y_0y_0^{(0)}) = 0 \end{aligned} \tag{14}$$

$$\begin{aligned} \alpha + p_i + \beta - 2xx_0 - 2yy_0 - 2zz_0 + \left(\frac{2\chi}{L_i} - 2L_i\right)\cdot c \\ + \left(\frac{2x - 2x_0^{(0)}}{L_i}\right)\cdot cx_0 + \left(\frac{2y - 2y_0^{(0)}}{L_i}\right)\cdot cy_0 = 0 \end{aligned} \tag{15}$$

$$\alpha + p_i + \beta - 2xx_0 - 2yy_0 - 2zz_0 + 2\left(\frac{\chi - L_i^2}{L_i}\right) \cdot c$$
$$+2\left(\frac{x - x_0^{(0)}}{L_i}\right) \cdot cx_0 + 2\left(\frac{y - y_0^{(0)}}{L_i}\right) \cdot cy_0 = 0 \tag{16}$$

Finally, let $\delta = cx_0$, $\epsilon = xy_0$.

Now, our unknowns are α, β, x_0, y_0, z_0, c, δ, and ϵ. There may be some redundancy, and a better separation of variables could be made, but for now, we will continue in this way. We can write our (now linear) equation in closed form:

$$\boxed{\alpha} + \boxed{\beta} + (-2x)\boxed{x_0} + (-2y)\boxed{y_0} + (-2z)\boxed{z_0} + \left(2\frac{(\chi - L_i^2)}{L_i}\right)\boxed{c}$$
$$+\left(2\frac{(x - x_0^{(0)})}{L_i}\right)\boxed{\delta} + \left(2\frac{(y - y_0^{(0)})}{L_i}\right)\boxed{\epsilon} = \boxed{p_i} \tag{17}$$

This leads us to the following system of linear equations for each sample i:

$$\begin{bmatrix} 1 & 1 & -2x_i & -2y_i & -2z_i & \frac{2(\chi - L_i^2)}{L_i} & \frac{2(x_i - x_0^{(0)})}{L_i} & \frac{2(y_i - y_0^{(0)})}{L_i} \end{bmatrix} \cdot \begin{bmatrix} \alpha \\ \beta \\ x_0 \\ y_0 \\ z_0 \\ c \\ \delta \\ \epsilon \end{bmatrix} = \begin{bmatrix} p_i \end{bmatrix} \tag{18}$$

After resolving the equations, the parameters of our torus can be derived by disentangling the artificial (redundant) parameters created, imposing positivity of a by the torus definition (3):

$$\alpha = c^2 - a^2 \quad \Longleftrightarrow \quad a = +\sqrt{\frac{c^2}{\alpha}} \tag{19}$$

$$\delta = cx_0 \quad \Longleftrightarrow \quad c = \frac{\delta}{x_0} \tag{20}$$

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:

$$
\begin{bmatrix}
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
1 & 1 & -2x_1 & -2y_1 & -2z_1 & \frac{2(\chi - L_1^2)}{L_1} & \frac{2(x_1 - x_0^{(0)})}{L_1} & \frac{2(y_1 - y_0^{(0)})}{L_1} \\
1 & 1 & -2x_2 & -2y_2 & -2z_2 & \frac{2(\chi - L_2^2)}{L_2} & \frac{2(x_2 - x_0^{(0)})}{L_2} & \frac{2(y_2 - y_0^{(0)})}{L_2} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
1 & 1 & -2x_8 & -2y_8 & -2z_8 & \frac{2(\chi - L_8^2)}{L_8} & \frac{2(x_8 - x_0^{(0)})}{L_8} & \frac{2(y_8 - y_0^{(0)})}{L_8} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots
\end{bmatrix}
\cdot
\begin{bmatrix}
\alpha \\ \beta \\ x_0 \\ y_0 \\ z_0 \\ c \\ \delta \\ \epsilon
\end{bmatrix}
=
\begin{bmatrix}
\vdots \\ p_1 \\ p_2 \\ \vdots \\ p_8 \\ \vdots
\end{bmatrix}
\tag{21}
$$

This approach has the advantage of being completely linear, which allows us to use efficient methods such as SVD or A^+. A disadvantage is that we need 8 points, whereas it could be done with just 4 points in a nonlinear approach, but this would be nothing more than a local approximation, potentially affected by poorly conditioned input data.