A resourceful least-squares Taylor-based torus fitting algorithm

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

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

Recall the centered torus equation;:

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

Its uncentered version is:

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

Expanding and rearranging the terms:

$$c^{2} + (x - x_{0})^{2} + (y - y_{0})^{2} - 2c \left[\sqrt{(x - x_{0})^{2} + (y - y_{0})^{2}} \right] + (z - z_{0})^{2} - a^{2} = 0.$$
 (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:

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

$$c^{2} + (x - x_{0})^{2} + (y - y_{0})^{2} - 2cf_{L} + (z - z_{0})^{2} - a^{2} = 0.$$
 (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:

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

Let us define:

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

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

$$x^2 + y^2 + z^2 = p_i. (10)$$

We will attempt to reformulate Equation (6):

$$c^{2} + x^{2} + x_{0}^{2} - 2xx_{0} + y^{2} + y_{0}^{2} - 2cL_{i} + \frac{2c}{L_{i}} \left[(x - x_{0}^{(0)})(x_{0} - x_{0}^{(0)}) + (y - y_{0}^{(0)})(y_{0} - y_{0}^{(0)}) \right] + z^{2} + z_{0}^{2} - 2zz_{0} - a^{2} = 0.$$

$$(11)$$

Let:

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

Then, the equation can be rewritten as:

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

Expanding:

$$\alpha + p_i + \beta - \gamma_i - 2cL_i + \frac{2c}{L_i} \left[((x_0^{(0)})^2 + (y_0^{(0)})^2 - xx_0^{(0)} - yy_0^{(0)}) + (xx_0^{(0)} + yy_0^{(0)}) - (x_0^{(0)}x_0^{(0)} + y_0^{(0)}y_0^{(0)}) \right]$$
(13)

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

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

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

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

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

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

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

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):

$$\alpha = c^2 - a^2 \iff a = +\sqrt{\frac{c^2}{\alpha}}$$
 (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:

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

$$(21)$$

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.