Best Fit Circles made Easy

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A problem with Best Fit Circles is that the equations, resulting from a Least Squares procedure, are *non-linear* most of the time. In this paper, alternative procedures are proposed, which - by design - always result in *linear* equations to be solved.

HdB's Method

The common, very well known equation for a circle is:

$$(x-a)^2 + (y-b)^2 = R^2$$

With a special choice for midpoint (a, b) and radius R , this becomes:

$$(x - \frac{1}{2}p)^2 + (y - \frac{1}{2}q)^2 = \left[\sqrt{(p/2)^2 + (q/2)^2}\right]^2$$

$$\Longrightarrow \quad x^2 - p.x + (p/2)^2 + y^2 - q.y + (q/2)^2 = (p/2)^2 + (q/2)^2$$

$$\Longrightarrow \quad x(x-p) + y(y-q) = 0$$

A tremendous advantage of the last equation is that it is *linear* in the parameters (p, q) . The midpoint of this circle is at $(p/2, q/2)$, its radius is $\sqrt{(p/2)^2 + (q/2)^2}$ and both the points $(0, 0)$ and (p, q) are on the perimeter of the circle.
Now suppose we have a bunch of points (x_i, y_i) in the plane, that is: a two-dimensional *points cloud*. We seek a circle that is a Best Fit to this points cloud. In a Least Squares sense:

$$\sum_i w_i \left[x_i(x_i - p) + y_i(y_i - q)\right]^2 = \text{minimum}(p, q)$$

In order to find the minimum, we shall differentiate to p and q and put the result to zero:

$$\frac{\partial}{\partial p}\text{minimum}(p, q) = -2 \times \sum_i w_i x_i \left[x_i(x_i - p) + y_i(y_i - q)\right] = 0$$

$$\frac{\partial}{\partial q}\text{minimum}(p, q) = -2 \times \sum_i w_i y_i \left[x_i(x_i - p) + y_i(y_i - q)\right] = 0$$

Body work out:

$$\left(\sum_i w_i x_i^2\right) p + \left(\sum_i w_i x_i y_i\right) q = \left(\sum_i w_i x_i^3\right) + \left(\sum_i w_i x_i y_i^2\right)$$

$$\left(\sum_i w_i x_i y_i\right) p + \left(\sum_i w_i y_i^2\right) q = \left(\sum_i w_i x_i^2 y_i\right) + \left(\sum_i w_i y_i^3\right)$$

In matrix format:

$$\begin{bmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{xy} & \sigma_{yy} \end{bmatrix} \begin{bmatrix} p \\ q \end{bmatrix} = \begin{bmatrix} \sigma_{xxx} + \sigma_{xyy} \\ \sigma_{xxy} + \sigma_{yyy} \end{bmatrix}$$

Where the σ's are summations are over all points in the cloud, with respect to an origin $(0,0)$ which can be freely chosen.

$$\sigma_{ab} = \frac{\sum_i w_i a_i b_i}{\sum_i w_i} \quad \text{and} \quad \sigma_{abc} = \frac{\sum_i w_i a_i b_i c_i}{\sum_i w_i}$$

The Jacobian matrix (second order derivative) of this problem is the matrix at the left hand side, which is positive definite. The extremum obtained by the Least Squares procedure therfore is a genuine minimum. Now we can solve very easily for p and q:

$$\begin{bmatrix} p \\ q \end{bmatrix} = \begin{bmatrix} \sigma_{yy} & -\sigma_{xy} \\ -\sigma_{xy} & \sigma_{xx} \end{bmatrix} /\text{Det} \begin{bmatrix} \sigma_{xxx} + \sigma_{xyy} \\ \sigma_{xxy} + \sigma_{yyy} \end{bmatrix}$$

Where $\text{Det} = \sigma_{xx}\sigma_{yy} - \sigma_{xy}^2$ must be greater than zero.

Method by RI

Another formulation of the problem was provided by Robert Israel ('sci.math'). Again, the common, very well known equation for a circle is:

$$(x-a)^2 + (y-b)^2 = R^2$$

With a special choice for the radius, $R^2 = C + a^2 + b^2$, this becomes:

$$(x-a)^2 + (y-b)^2 = C + a^2 + b^2 \quad \Longrightarrow \quad x(x-2a) + y(y-2b) = C$$

And the Least Squares principle is:

$$\sum_i w_i \left[x_i(x_i - 2a) + y_i(y_i - 2b) - C\right]^2 = \text{minimum}(a, b, C)$$

In order to find the minimum, we shall differentiate to (a, b, C) and put the result to zero:

$$\frac{\partial}{\partial a}\text{minimum}(a, b, C) = \sum_i w_i x_i \left[x_i(x_i - 2a) + y_i(y_i - 2b) - C\right] = 0$$

$$\frac{\partial}{\partial b}\text{minimum}(a, b, C) = \sum_i w_i y_i \left[x_i(x_i - 2a) + y_i(y_i - 2b) - C\right] = 0$$

$$\frac{\partial}{\partial C}\text{minimum}(a,b,C) = \sum_i w_i\left[x_i(x_i-2a)+y_i(y_i-2b)-C\right] = 0$$

Body work out as above. Casted in matrix format:

$$\begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \mu_x \\ \sigma_{xy} & \sigma_{yy} & \mu_y \\ \mu_x & \mu_y & 1 \end{bmatrix} \begin{bmatrix} 2a \\ 2b \\ C \end{bmatrix} = \begin{bmatrix} \sigma_{xxx}+\sigma_{xyy} \\ \sigma_{xxy}+\sigma_{yyy} \\ \sigma_{xx}+\sigma_{yy} \end{bmatrix}$$

Where the σ's are summations are over all points in the cloud, with respect to an origin $(0,0)$ which can be freely chosen, so far.

$$\mu_p = \frac{\sum_i w_i p_i}{\sum_i w_i} \quad \text{and} \quad \sigma_{pq} = \frac{\sum_i w_i p_i q_i}{\sum_i w_i} \quad \text{and} \quad \sigma_{pqr} = \frac{\sum_i w_i p_i q_i r_i}{\sum_i w_i}$$

Now it is *highly* advantageous to choose the origin in a special way, namely exactly at the midpoint (μ_x,μ_y) of the whole points cloud. Then $\mu_x = 0$ and $\mu_y = 0$ and the linear equations system becomes:

$$\begin{bmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ \sigma_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2a \\ 2b \\ C \end{bmatrix} = \begin{bmatrix} \sigma_{xxx}+\sigma_{xyy} \\ \sigma_{xxy}+\sigma_{yyy} \\ \sigma_{xx}+\sigma_{yy} \end{bmatrix}$$

Consequently, it is partitioned in two separate pieces:

$$\begin{bmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{xy} & \sigma_{yy} \end{bmatrix} \begin{bmatrix} 2a \\ 2b \end{bmatrix} = \begin{bmatrix} \sigma_{xxx}+\sigma_{xyy} \\ \sigma_{xxy}+\sigma_{yyy} \end{bmatrix}$$

And:

$$C = \sigma_{xx}+\sigma_{yy}$$

Now we can solve very easily for a and b :

$$2\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \sigma_{yy} & -\sigma_{xy} \\ -\sigma_{xy} & \sigma_{xx} \end{bmatrix} /\text{Det} \begin{bmatrix} \sigma_{xxx}+\sigma_{xyy} \\ \sigma_{xxy}+\sigma_{yyy} \end{bmatrix}$$

Where Det $= \sigma_{xx}\sigma_{yy} - \sigma_{xy}^2$ must be greater than zero. At last, the radius of the circle is calculated with:

$$R = \sqrt{C+a^2+b^2} = \sqrt{(\sigma_{xx}+a^2)+(\sigma_{yy}+b^2)}$$

It is noted that the expression $(C+a^2+b^2)$ can never become negative. The coordinates (a,b) must be translated back to screen coordinates $(a+\mu_x, b+\mu_y)$, in order to be able to actually draw the RI Best Fit Circle. No doubt that the radius is quite independent of such a transformation.

Disclaimers

Anything free comes without referee :-(
My English may be better than your Dutch.