Best Fit: The least squares Method

Mechanical parts are manufactured to meet stated specifications. A surface must be level, a drilled hole circular, and a ball bearing spherical. But, exactly how level, how circular, and how spherical are the manufactured parts? In practice, we need to answer this question: does an object meet the tolerances required by its specifications? The answer to this question often is obtained by measuring the part using a coordinate measuring machine (CMM). A small number of measurements are made, which are then analyzed to determine an associated fitted reference object (circle or sphere or straight line). If the reference object meets the stated tolerance, the part is said to meet the specifications.

Example: Straight line $y(x) = P_1 + P_2x$ with P_1 and P_2 two parameters

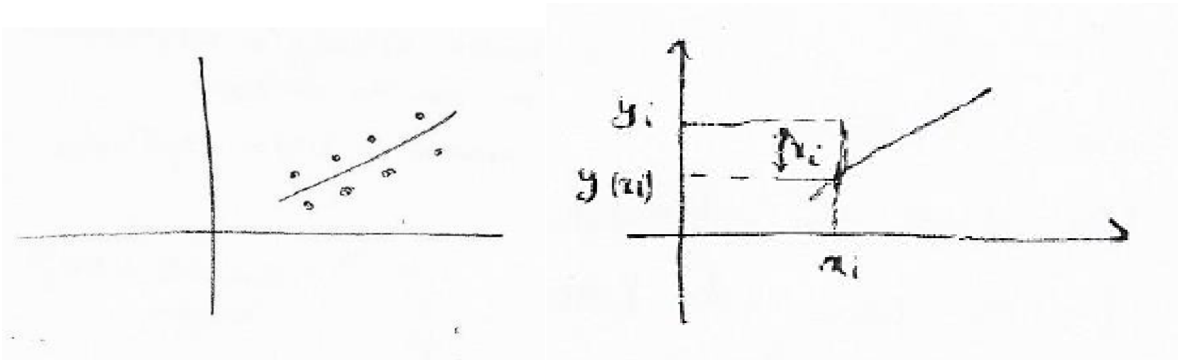
m measurements $(x_1; y_1)$ ... $(x_m; y_m)$

$$y_1 = y(x_1) + r_1 = P_1 + P_2x_1 + r_1$$

$$y_i = y(x_i) + r_i = P_1 + P_2x_i + r_i$$

$$y_m = y(x_m) + r_m = P_1 + P_2x_m + r_m$$

Where y_i: measured values; $y(x_i)$ estimated values and r_i: residual or the difference between measured and estimated values



Best Fit with least squares method

The least squares method finds its optimum when the sum of square residuals is minimum.

$$S = \sum_{i=1}^{m} r_i^2 = r_1^2 + r_i^2 + ..r_m^2 = \sum_{i=1}^{m} [y_i - y(x_i)]^2 = \sum_{i=1}^{m} [y_i - P_1 - P_2x_i]^2$$

Let $Y = \begin{bmatrix} y_1 \\ \vdots \\ y_i \\ \vdots \\ y_m \end{bmatrix}_{m,1}$ and $A = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_m \end{bmatrix}_{m,2}$ $P = \begin{bmatrix} P_1 \\ P_2 \end{bmatrix}_{2,1}$ $r = \begin{bmatrix} r_1 \\ \vdots \\ r_i \\ \vdots \\ r_m \end{bmatrix}_{m,1}$ $r^T = [r_1 \dots r_i \dots r_m]_{1,m}$

$$Y = AP + r \text{ matrix form}$$

$$S = r^T r = (Y - AP)^T (Y - AP) = \sum_{i=1}^{m} r_i^2 = f(P_1, P_2)$$

The minimum of the sum squares is found by setting gradient equal to 0

$$\overrightarrow{grad} S = \vec{0} = \begin{pmatrix} \frac{\partial f}{\partial P_1} \\ \frac{\partial f}{\partial P_2} \end{pmatrix}$$

$$\frac{\partial f}{\partial P_1} = -2 \sum_{i=1}^{m} [y_i - P_1 - P_2 x_i] = 0$$

$$\frac{\partial f}{\partial P_2} = -2 \sum_{i=1}^{m} x_i [y_i - P_1 - P_2 x_i] = 0$$

$$\sum_{i=1}^{m} y_i = \sum_{i=1}^{m} P_1 + P_2 \sum_{i=1}^{m} x_i$$

$$\sum_{i=1}^{m} x_i y_i = P_1 \sum_{i=1}^{m} x_i + P_2 \sum_{i=1}^{m} x_i^2$$

$$\begin{cases} mP_1 + \left(\sum_{i=1}^{m} x_i\right) P_2 = \sum_{i=1}^{m} y_i \\ \left(\sum_{i=1}^{m} x_i\right) P_1 + \left(\sum_{i=1}^{m} x_i^2\right) P_2 = \sum_{i=1}^{m} x_i y_i \end{cases}$$

$$\begin{bmatrix} m & \sum_{i=1}^{m} x_i \\ \sum_{i=1}^{m} x_i & \sum_{i=1}^{m} x_i^2 \end{bmatrix} \begin{bmatrix} P_1 \\ P_2 \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{m} y_i \\ \sum_{i=1}^{m} x_i y_i \end{bmatrix}$$

$A^T A P = A^T Y$ the equation to be solved.

$P = (A^T A)^{-1} A^T Y$

General method

We want to estimate n unknowns basing on m measurements where $n < m$. In the case of linear measurements, the unknowns should satisfy an overdetermined system of linear equations. In general, such system has no solution. Assuming measurements errors, we obtain the following system of linear equations:

$$Y_1 = X_{11}P_1 + X_{12}P_2 + \cdots + X_{1n}P_n + r_1$$

$$\vdots$$

$$Y_m = X_{m1}P_1 + X_{m2}P_2 + \cdots + X_{mn}P_n + r_m$$

We have

$$Y_i = X_{i1}P_1 + X_{i2}P_2 + \cdots + X_{in}P_n + r_i$$

Where X_{ij} is the i^{th} measurement of the j^{th} variable. X_{ij} and Y_i are known measurements and P_i are unknown parameters.

$1 \leq i \leq m$ and $1 \leq j \leq n$

$$Y = \begin{bmatrix} y_1 \\ \vdots \\ y_i \\ \vdots \\ y_m \end{bmatrix}_{m,1} = \begin{bmatrix} X_{11} & \dots & X_{1n} \\ \vdots & \vdots & \vdots \\ X_{m1} & \dots & X_{mn} \end{bmatrix}_{m,n} \begin{bmatrix} P_1 \\ \vdots \\ P_i \\ \vdots \\ P_n \end{bmatrix}_{n,1} + \begin{bmatrix} r_1 \\ \vdots \\ r_i \\ \vdots \\ r_m \end{bmatrix}_{m,1}$$

$Y = AP + r$ matrix form

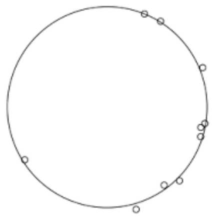
We use the same procedure: the optimum solution is the vector $\hat{P}$ verifying the following equation:

$A^T AP = A^T Y$ the equation to be solved.

$P = (A^T A)^{-1} A^T Y$

Circle that best fits n points $(x_i; y_i)$

Equation of the circle: $(x-a)^2 + (y-b)^2 = R^2$



Unknown parameters (a, b) and R optimum solution $(\hat{a}, \hat{b})$ and $\hat{R}$

Linearization of the equation: $x^2 - 2ax + a^2 + y^2 - 2by + b^2 = R^2$

$$x^2 + y^2 = 2ax + 2by + R^2 - a^2 - b^2$$

Change variable $z_i = x_i^2 + y_i^2$; $c = R^2 - a^2 - b^2$; $A = 2a$ and $B = 2b$

$$z_i = Ax_i + By_i + C$$

$$Z = MP + r$$

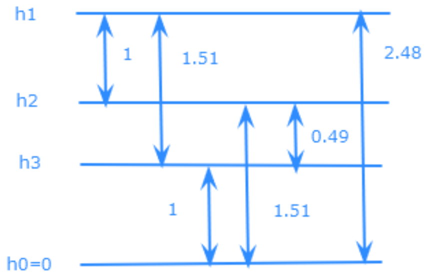
$$Z = \begin{bmatrix} z_1 \\ \vdots \\ z_m \end{bmatrix}_{m,1} \; ; \; M = \begin{bmatrix} x_1 & y_1 & 1 \\ \vdots & \vdots & \vdots \\ x_m & y_m & 1 \end{bmatrix}_{m,3} \; ; P = \begin{bmatrix} A \\ B \\ C \end{bmatrix}_{3,1} \text{ and } r = \begin{bmatrix} r_1 \\ \vdots \\ r_m \end{bmatrix}_{m,1}$$

Equation to be solved: $M^T M \hat{P} = M^T Z$ with $\hat{P} = \begin{bmatrix} \hat{A} \\ \hat{B} \\ \hat{C} \end{bmatrix}$

$\hat{a} = \frac{\hat{A}}{2}$; $\hat{b} = \frac{\hat{B}}{2}$ and $\hat{R} = \sqrt{\hat{c} + \hat{a}^2 + \hat{b}^2}$

Ex1

We want to estimate the altitudes: h_1, h_2 and h_3 of a field ($3\, levels$) by making direct measurements and by measuring the differences between the $3\, levels$. Estimate h_1, h_2 and h_3 by using the least square method.



$h_0 = 0$

$2.48 = h_1 + r_1$

$1.51 = h_2 + r_2$

$0.49 = h_2 - h_3 + r_3$

$1 = h_3 + r_4$

$1.51 = h_1 - h_3 + r_5$

$1 = h_1 - h_2 + r_6$

$$Y = \begin{bmatrix} 2.48 \\ 1.51 \\ 0.49 \\ 1 \\ 1.51 \\ 1 \end{bmatrix}; A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \\ 1 & 0 & -1 \\ 1 & -1 & 0 \end{bmatrix}; \; P = \begin{bmatrix} h_1 \\ h_2 \\ h_3 \end{bmatrix} \text{ and } r = \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \\ r_5 \\ r_6 \end{bmatrix}$$

$A^T A \hat{P} = A^T Y$ the equation to be solved.

$$A^T A = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & -1 \\ 0 & 0 & -1 & 1 & -1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \\ 1 & 0 & -1 \\ 1 & -1 & 0 \end{bmatrix} = \begin{bmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{bmatrix}$$

$$A^T Y = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & -1 \\ 0 & 0 & -1 & 1 & -1 & 0 \end{bmatrix} \begin{bmatrix} 2.48 \\ 1.51 \\ 0.49 \\ 1 \\ 1.51 \\ 1 \end{bmatrix} = \begin{bmatrix} 4.99 \\ 1 \\ -1 \end{bmatrix}$$

$$\begin{bmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{bmatrix} \begin{bmatrix} \widehat{h_1} \\ \widehat{h_2} \\ \widehat{h_3} \end{bmatrix} = \begin{bmatrix} 4.99 \\ 1 \\ -1 \end{bmatrix}$$

$\widehat{h_1} = 2.495$; $\widehat{h_2} = 1.4975$ and $\widehat{h_3} = 0.997$

Ex2

Find the equation of the circle that best fits the 5 points: $(0;0)$; $(0;5)$; $(1;6)$; $(2;7)$; $(8;7)$

$$\begin{bmatrix} 0^2+0^2 \\ 0^2+5^2 \\ 1^2+6^2 \\ 2^2+7^2 \\ 8^2+7^2 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 5 & 1 \\ 1 & 6 & 1 \\ 2 & 7 & 1 \\ 8 & 7 & 1 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \end{bmatrix} + \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \\ r_5 \end{bmatrix}$$

$$Z = MP + r$$

$$M = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 5 & 1 \\ 1 & 6 & 1 \\ 2 & 7 & 1 \\ 8 & 7 & 1 \end{bmatrix}; \quad P = \begin{bmatrix} A \\ B \\ C \end{bmatrix} \quad Z = \begin{bmatrix} 0 \\ 25 \\ 37 \\ 53 \\ 113 \end{bmatrix}; \quad r = \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \\ r_5 \end{bmatrix}$$

Equation to be solved: $M^T M \hat{P} = M^T Z$ with $\hat{P} = \begin{bmatrix} \hat{A} \\ \hat{B} \\ \hat{C} \end{bmatrix}$

$\hat{a} = \frac{\hat{A}}{2}$; $\hat{b} = \frac{\hat{B}}{2}$ and $\hat{R} = \sqrt{\hat{c} + \hat{a}^2 + \hat{b}^2}$

$$M^T M = \begin{bmatrix} 0 & 0 & 1 & 2 & 8 \\ 0 & 5 & 6 & 7 & 7 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 5 & 1 \\ 1 & 6 & 1 \\ 2 & 7 & 1 \\ 8 & 7 & 1 \end{bmatrix} = \begin{bmatrix} 69 & 76 & 11 \\ 76 & 159 & 25 \\ 11 & 25 & 5 \end{bmatrix}$$

$$M^T Z = \begin{bmatrix} 0 & 0 & 1 & 2 & 8 \\ 0 & 5 & 6 & 7 & 7 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 25 \\ 37 \\ 53 \\ 113 \end{bmatrix} = \begin{bmatrix} 1047 \\ 1509 \\ 228 \end{bmatrix}$$

$$\begin{bmatrix} 69 & 76 & 11 \\ 76 & 159 & 25 \\ 11 & 25 & 5 \end{bmatrix} \begin{bmatrix} \hat{A} \\ \hat{B} \\ \hat{C} \end{bmatrix} = \begin{bmatrix} 1047 \\ 1509 \\ 228 \end{bmatrix}$$

$\hat{A} = 9.975$; $\hat{B} = 4.692$; $\hat{C} = 0.195$

$\hat{a} = 4.987$; $\hat{b} = 2.346$ and $\hat{R} = 5.53$

Ex3

Find the equation of the parabola that best fits the 4 points: $(0;6)$; $(1;0)$; $(2;0)$; $\left(\frac{1}{2};1\right)$

Equation of the parabola: $y = ax^2 + bx + c$

$y_i = aX_i + bx_i + c$ with $X_i = x_i^2$

$$Y = AP + r$$

$$Y = \begin{bmatrix} 6 \\ 0 \\ 0 \\ 1 \end{bmatrix} ; A = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 1 & 1 \\ 4 & 2 & 1 \\ \frac{1}{4} & \frac{1}{2} & 1 \end{bmatrix} ; P = \begin{bmatrix} a \\ b \\ c \end{bmatrix} ; \; r = \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \\ r_5 \end{bmatrix}$$

$A^T A\hat{P} = A^T Y$ the equation to be solved.

$$A^T A = \begin{bmatrix} 0 & 1 & 4 & \frac{1}{4} \\ 0 & 1 & 2 & \frac{1}{2} \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 1 & 1 & 1 \\ 4 & 2 & 1 \\ \frac{1}{4} & \frac{1}{2} & 1 \end{bmatrix} = \begin{bmatrix} 17.0625 & 9.125 & 5.25 \\ 9.125 & 5.25 & 3.5 \\ 5.25 & 3.5 & 4 \end{bmatrix}$$

$$A^T Y = \begin{bmatrix} 0 & 1 & 4 & \frac{1}{4} \\ 0 & 1 & 2 & \frac{1}{2} \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 6 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \frac{1}{4} \\ \frac{1}{2} \\ 7 \end{bmatrix}$$

$$\begin{bmatrix} 17.0625 & 9.125 & 5.25 \\ 9.125 & 5.25 & 3.5 \\ 5.25 & 3.5 & 4 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} \frac{1}{4} \\ \frac{1}{2} \\ 7 \end{bmatrix}$$

$a = \frac{38}{11}$; $b = -\frac{107}{11}$; $c = \frac{63}{11}$