Total Least Squares

—— in Three-Dimensional Space

Distance between point (x_i, y_i, z_i) and plane $ax + by + cz + d = 0$ ($a^2+b^2+c^2=1$):

$$|\mathrm{a}x_i + \mathrm{b}y_i + \mathrm{c}z_i + d|$$

Let

$$E = \sum_{i=1}^{n} (ax_i + by_i + cz_i + d)^2$$

$$\frac{\partial E}{\partial d} = \sum_{i=1}^{n} 2(ax_i + by_i + cz_i + d) = 0$$

$$-d = \frac{a}{n}\sum_{i=1}^{n} x_i + \frac{b}{n}\sum_{i=1}^{n} y_i + \frac{c}{n}\sum_{i=1}^{n} z_i = a\bar{x} + b\bar{y} + c\bar{z}$$

then

$$E = \sum_{i=1}^{n} \left(a(x_i - \bar{x}) + b(y_i - \bar{y}) + c(z_i - \bar{z})\right)^2 = \left\| \begin{bmatrix} x_1 - \bar{x} & y_1 - \bar{y} & z_1 - \bar{z} \\ \vdots & \vdots & \vdots \\ x_n - \bar{x} & y_n - \bar{y} & z_n - \bar{z} \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} \right\|^2$$

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$$U = \begin{bmatrix} x_1 - \bar{x} & y_1 - \bar{y} & z_1 - \bar{z} \\ \vdots & \vdots & \vdots \\ x_n - \bar{x} & y_n - \bar{y} & z_n - \bar{z} \end{bmatrix} \quad \text{and} \quad N = \begin{bmatrix} a \\ b \\ c \end{bmatrix}$$

then

$$E = (UN)^T(UN)$$

$$\frac{dE}{dN} = 2(U^T U)N = 0$$

Solution to $(U^T U)N = 0$, subject to $||N||^2 = 1$: eigenvector of $U^T U$ associated with the smallest eigenvalue (least squares solution to homogeneous linear system $UN = 0$)