Least Squares Fit of a Plane to a Set of 3D Points

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The equation of a plane in three dimensions with coordinates x, y, z is

$$Ax + By + Cz + D = 0 \tag{1a}$$

The vector

$$\hat{\mathbf{R}} = \begin{bmatrix} A \\ B \\ C \end{bmatrix} \tag{2a}$$

has length

$$R = \left|\hat{\mathbf{R}}\right| = \sqrt{A^2 + B^2 + C^2} \tag{2b}$$

Vector (2a) is perpendicular to the plane (1a).

For the set of N points

$$x_i\,,\ y_i\,,\ z_i\,;\ \ i = 1, \dots, N \tag{3}$$

the perpendicular distance of each point to the plane (1a) is

$$d_i = \frac{1}{R}(Ax_i + By_i + Cz_i + D) \tag{4}$$

This distance (4) can be positive or negative depending on which side of the plain the point resides. One measure E of how close the set of points (3) cluster about the plane is given by the average of all the point's squared distances (4)

$$E = \frac{1}{R^2 N}\sum_{i=1}^{N}(Ax_i + By_i + Cz_i + D)^2 \tag{5a}$$

The extremal of E for a variation of the constant D in (1a) is

$$\frac{dE}{dD} = 0 = \frac{2}{R^2 N}\left(A\sum_{i=1}^{N} x_i + B\sum_{i=1}^{N} y_i + C\sum_{i=1}^{N} z_i + ND\right) \tag{6}$$

The center of mass of the points (3) is

$$\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i\,,\ \bar{y} = \frac{1}{N}\sum_{i=1}^{N} y_i\,,\ \bar{z} = \frac{1}{N}\sum_{i=1}^{N} z_i \tag{7}$$

Inserting (7) into (6) yields

$$D = -(A\bar{x} + B\bar{y} + C\bar{z}) \tag{8a}$$

The constant D will be determined by (8a) after $A, B,$ and C are found.

The plane's equation (1a) becomes

$$A(x-\bar{x})+B(y-\bar{y})+C(z-\bar{z})=0 \tag{1b}$$

Transform coordinates to u, v, w so that the new origin is at the center of mass of the points.

$$u=x-\ \bar{x}\ ,\ v=y-\ \bar{y}\ ,\ w=z-\bar{z} \tag{9}$$

Equation (1b) becomes

$$Au+Bv+Cw=0 \tag{1c}$$

The plane (1c) now passes through the origin of coordinates. Equation (5a) becomes

$$E=\frac{1}{R^2N}\sum_{i=1}^{N}(Au_i+Bv_i+Cw_i)^2 \tag{5b}$$

In (5b) R is also a function of A. The **extremal** value of (5b) for the variation of A is

$$\frac{dE}{dA}=\ 0=\frac{\partial E}{\partial R}\frac{\partial R}{\partial A}+\frac{\partial E}{\partial A}=\ \frac{2}{R^2}\left(-AE+A\frac{1}{N}\sum_{i=1}^{N}{u_i}^2+B\frac{1}{N}\sum_{i=1}^{N}u_iv_i+C\frac{1}{N}\sum_{i=1}^{N}u_iw_i\right) \tag{10}$$

Introduce the notation

$$S_{uu}=\frac{1}{N}\sum_{i=1}^{N}{u_i}^2,\ S_{vv}=\frac{1}{N}\sum_{i=1}^{N}{v_i}^2\ ,\ S_{ww}=\ \frac{1}{N}\sum_{i=1}^{N}{w_i}^2 \tag{11a}$$

and

$$S_{uv}=S_{vu}=\ \frac{1}{N}\sum_{i=1}^{N}u_iv_i\ ,\ S_{vw}=S_{wv}=\frac{1}{N}\sum_{i=1}^{N}v_iw_i\ ,\ S_{wu}=S_{uw}=\frac{1}{N}\sum_{i=1}^{N}w_iu_i \tag{11b}$$

Equation (10) reduces to

$$S_{uu}A+S_{uv}B+S_{uw}C=EA \tag{12a}$$

Similarly, setting $\frac{dE}{dB}=\ 0$ and $\frac{dE}{dC}=\ 0$ yields

$$S_{vu}A+S_{vv}B+S_{vw}C=EB \tag{12b}$$

$$S_{wu}A+S_{wv}B+S_{ww}C=EC \tag{12c}$$

Casting equations (12a,b,c) into matrix form with

$$\boldsymbol{M}=\begin{bmatrix}S_{uu} & S_{uv} & S_{uw}\\ S_{vu} & S_{vv} & S_{vw}\\ S_{wu} & S_{wv} & S_{ww}\end{bmatrix} \tag{13}$$

yields

$$\mathbf{M}\widehat{\mathbf{R}}=E\widehat{\mathbf{R}} \tag{14}$$

The vector $\widehat{\mathbf{R}}$ is given by (2a). Equation (14) is a matrix eigen problem of a real symmetric matrix (13) having eigen vectors

$$\widehat{\mathbf{R_k}} = \begin{bmatrix} A_k \\ B_k \\ C_k \end{bmatrix}; \;\; k = 1,2,3 \tag{2c}$$

that correspond to eigen values

$$E_k; \; k = 1,2,3 \tag{5c}$$

The eigen values (5c) are real and by (5a) not negative. They are the roots of the cubic equation.

$$det \begin{bmatrix} S_{uu} - E & S_{uv} & S_{uw} \\ S_{vu} & S_{vv} - E & S_{vw} \\ S_{wu} & S_{wv} & S_{ww} - E \end{bmatrix} = 0 \tag{15}$$

The plane's constant value D is determined by (8a)

$$D_k = -(A_k\bar{x} + B_k\bar{y} + C_k\bar{z}); \;\; k = 1,2,3 \tag{8b}$$

The eigen values (5c) represent the minimum, in-between, and maximum average square distance of the set of points from the three eigen plains

$$A_k x + B_k y + C_k z + D_k = 0; \;\; k = 1,2,3 \tag{1d}$$

Since matrix (13) is symmetric, the eigen vectors (2c) and hence, the three eigen planes (1d) are mutually perpendicular to one another. The eigen vector (2c), corresponding the plane (1d), that best fits the set of points has the smallest eigen value (5c). The worst fit has the largest.

When all the points (3) lie in a common plane, the matrix (13) is singular meaning that (5a) will be zero since the average squared deviation or smallest eigen value is zero. The plane can still be determined by employing three simultaneous equations formed by inserting three non collinear points $x_i, y_i, z_i; i = 1,2,3$ from the set (3) into (1a). Then, fix one of the unknowns $A, B, C,$ or D to a constant. Finally, solve for the remaining three unknowns in terms of that fixed value.