Optimal Plane Fitting

Given a set of n points $\mathbf{x}_i$, for $i = 1, \ldots, n$, consider a plane P that best fits to these data points:

$$P : \langle \mathbf{x} - \mathbf{c}, \mathbf{n} \rangle = 0,$$

where $\mathbf{c}$ is a point on the plane and $\mathbf{n}$ is a plane normal. We may assume

$$\langle \mathbf{n}, \mathbf{n} \rangle = 1. \tag{1}$$

An optimal plane that best fits to the given data points $\mathbf{x}_i$ can be found as a solution to the following constrained optimization problem:

$$\text{Minimize } \sum_{i=1}^{n} \langle \mathbf{x}_i - \mathbf{c}, \mathbf{n} \rangle^2 ,$$

$$\text{subject to } \langle \mathbf{n}, \mathbf{n} \rangle = 1.$$

Since there is no constaint on the point $\mathbf{c}$, an optimal solution satisfies

$$\sum_{i=1}^{n} -2 \langle \mathbf{x}_i - \mathbf{c}, \mathbf{n} \rangle \mathbf{n} = \mathbf{0}, \quad \text{or} \quad \left\langle n\mathbf{c} - \sum_{i=1}^{n} \mathbf{x}_i, \mathbf{n} \right\rangle \mathbf{n} = \mathbf{0},$$

The center of gravity of $\mathbf{x}_i$'s:

$$\mathbf{c} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}_i$$

satisfies the above equation.

Now, let's consider an optimal solution for the unit normal vector $\mathbf{n}$. Using the Lagrange multiplier applied to the constraint $\langle \mathbf{n}, \mathbf{n} \rangle = 1$, we have the following relation:

$$\sum_{i=1}^{n} 2 \langle \mathbf{x}_i - \mathbf{c}, \mathbf{n} \rangle (\mathbf{x}_i - \mathbf{c}) - \lambda 2\mathbf{n} = \mathbf{0}.$$

Considering all vectors as column vectors, we have

$$\sum_{i=1}^{n} (\mathbf{x}_i - \mathbf{c})^T \mathbf{n} (\mathbf{x}_i - \mathbf{c}) = \lambda \mathbf{n},$$

and equivalently,

$$\sum_{i=1}^{n} (\mathbf{x}_i - \mathbf{c})(\mathbf{x}_i - \mathbf{c})^T \mathbf{n} = \lambda \mathbf{n}.$$

Now let a 3×3 matrix A to be defined as

$$A = \sum_{i=1}^{n} (\mathbf{x}_i - \mathbf{c})(\mathbf{x}_i - \mathbf{c})^T,$$

then we have

$$A\mathbf{n} = \lambda \mathbf{n}.$$

Thus $\mathbf{n}$ is an eigenvector of the matrix A. We select the eigenvector $\mathbf{n}$ with the smallest eigenvalue.

Optimal Line Fitting

Given a set of n points $\mathbf{x}_i$, for $i = 1, \ldots, n$, consider two orthogonal planes P_1 and P_2, the intersection line of which best fits to the data points:

$$P_1 : \langle \mathbf{x} - \mathbf{c}, \mathbf{n}_1 \rangle = 0,$$
$$P_2 : \langle \mathbf{x} - \mathbf{c}, \mathbf{n}_2 \rangle = 0,$$

where $\mathbf{c}$ is a point on the intersection line, and $\mathbf{n}_i$ is a plane normal to the plane P_i, $(i = 1, 2)$. We may assume that the plane normals $\mathbf{n}_i$ satisfy

$$\langle \mathbf{n}_1, \mathbf{n}_1 \rangle = 1, \ \langle \mathbf{n}_2, \mathbf{n}_2 \rangle = 1, \ \langle \mathbf{n}_1, \mathbf{n}_2 \rangle = 0.$$

An optimal line that best fits to the given data points $\mathbf{x}_i$ can be found as a solution to the following constrained optimization problem:

$$\text{Minimize } \sum_{i=1}^{n} \left(\langle \mathbf{x}_i - \mathbf{c}, \mathbf{n}_1 \rangle^2 + \langle \mathbf{x}_i - \mathbf{c}, \mathbf{n}_2 \rangle^2 \right)$$

$$\text{subject to } \langle \mathbf{n}_1, \mathbf{n}_1 \rangle = 1, \ \langle \mathbf{n}_2, \mathbf{n}_2 \rangle = 1, \ \langle \mathbf{n}_1, \mathbf{n}_2 \rangle = 0.$$

The optimal location of the point $\mathbf{c}$ is similarly given as

$$\mathbf{c} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}_i.$$

Using the Lagrange multipliers, we have

$$\sum_{i=1}^{n} (\mathbf{x}_i - \mathbf{c})(\mathbf{x}_i - \mathbf{c})^T \mathbf{n}_1 = A\mathbf{n}_1 = \lambda_1 \mathbf{n}_1 + \mu_1 \mathbf{n}_2,$$

$$\sum_{i=1}^{n} (\mathbf{x}_i - \mathbf{c})(\mathbf{x}_i - \mathbf{c})^T \mathbf{n}_2 = A\mathbf{n}_2 = \lambda_2 \mathbf{n}_2 + \mu_2 \mathbf{n}_1.$$

By setting $\mu_1 = \mu_2 = 0$, we have

$$A\mathbf{n}_1 = \lambda_1 \mathbf{n}_1, \quad A\mathbf{n}_2 = \lambda_2 \mathbf{n}_2.$$

Thus $\mathbf{n}_1$ and $\mathbf{n}_2$ are eigenvectors of the matrix A. We select the eigenvectors $\mathbf{n}_i$ that correspond to the two smaller eigenvalues of A.