ALGORITHMS FOR LAYING POINTS OPTIMALLY ON A PLANE AND A CIRCLE.

R. A. Sharipov

Abstract. Two averaging algorithms are considered which are intended for choosing an optimal plane and an optimal circle approximating a group of points in three-dimensional Euclidean space.

1. Introduction.

Assume that in the three-dimensional Euclidean space $\mathbb{E}$ we have a group of points visually resembling a circle (see Fig. 1.1). The problem is to find the best plane and the best circle approximating this group of points. Any plane in $\mathbb{E}$ is given by the equation

$$(\mathbf{r},\mathbf{n})=D, \tag{1.1}$$

where $\mathbf{n}$ is the normal vector of the plane and D is some constant. The vector $\mathbf{r}$ in (1.1) is the radius-vector of a point on that plane, while $(\mathbf{r},\mathbf{n})$ is the scalar product of the vectors $\mathbf{r}$ and $\mathbf{n}$.

Once a plane (1.1) is fixed and $\mathbf{r}$ is the radius-vector of some point on it, a circle on this plane is given by the equation

$$|\mathbf{r}-\mathbf{R}|=\rho. \tag{1.2}$$

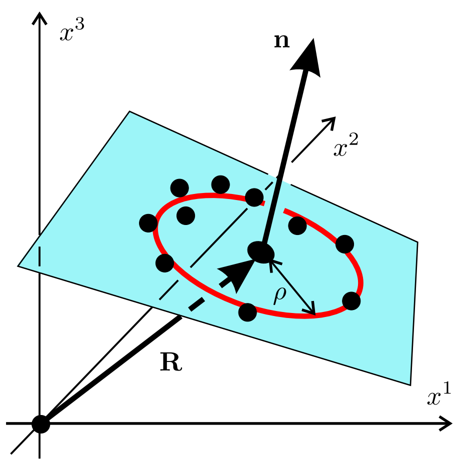

Fig. 1.1

Here ρ is the radius of the circle (1.2) and $\mathbf{R}$ is the radius-vector of its center. Having a group of points $\mathbf{r}[1], \dots, \mathbf{r}[N]$ in $\mathbb{E}$, our goal is to design an algorithm for calculating the parameters $\mathbf{n}$, D, $\mathbf{R}$, and ρ in (1.1) and (1.2) thus defining a plane and a circle being optimal approximations of our points in some definite sense.

2. Defining an optimal plane.

Assume that $\mathbf{n}$ is a unit vector, i. e $|\mathbf{n}|=1$, and assume that we have some plane defined by the equation (1.1). Then the distance from the point $\mathbf{r}[i]$ to this plane

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is given by the following well-known formula:

$$d[i]=\frac{|(\mathbf{r}[i],\mathbf{n})-D|}{|\mathbf{n}|}=|(\mathbf{r}[i],\mathbf{n})-D|. \tag{2.1}$$

If we denote by d the root of mean square of the quantities (2.1), then we have

$$d^{\,2}=\frac{1}{N}\sum_{i=1}^{N}d[i]^2=\frac{1}{N}\sum_{i=1}^{N}|(\mathbf{r}[i],\mathbf{n})-D|^2. \tag{2.2}$$

Definition 2.1. A plane given by the formula (1.1) with $|\mathbf{n}|=1$ is called an *optimal root mean square plane* if the quantity (2.2) takes its minimal value.

It is easy to see that $d^{\,2}$ in (2.2) is a function of two parameters: $\mathbf{n}$ and D. It is a quadratic function of the parameter D. Indeed, we have

$$d^{\,2}=D^2-\frac{2}{N}\sum_{i=1}^{N}(\mathbf{r}[i],\mathbf{n})\,D+\frac{1}{N}\sum_{i=1}^{N}(\mathbf{r}[i],\mathbf{n})^2. \tag{2.3}$$

The quadratic polynomial in the right hand side of (2.3) takes its minimal value if

$$D=\frac{1}{N}\sum_{i=1}^{N}(\mathbf{r}[i],\mathbf{n}). \tag{2.4}$$

Substituting (2.4) back into the formula (2.3), we obtain

$$d^{\,2}=\frac{1}{N}\sum_{i=1}^{N}(\mathbf{r}[i],\mathbf{n})^2-\left(\frac{1}{N}\sum_{i=1}^{N}(\mathbf{r}[i],\mathbf{n})\right)^2. \tag{2.5}$$

In the next steps we use some mechanical analogies. If we place unit masses $m[i]=1$ at the points $\mathbf{r}[1],\,\ldots\,,\mathbf{r}[N]$, then the vector

$$\mathbf{r}_{\text{cm}}=\frac{1}{N}\sum_{i=1}^{N}\mathbf{r}[i] \tag{2.6}$$

is the radius-vector of the center of mass. In terms of this radius vector the formula (2.6) for D is written as follows:

$$D=(\mathbf{r}_{\text{cm}},\mathbf{n}). \tag{2.7}$$

Now remember that the inertia tensor for a system of point masses $m[i]=1$ is defined as a quadratic form given by the formula:

$$I(\mathbf{n},\mathbf{n})=\sum_{i=1}^{N}|\mathbf{r}[i]|^2\,|\mathbf{n}|^2-\sum_{i=1}^{N}(\mathbf{r}[i],\mathbf{n})^2 \tag{2.8}$$

(see [1] for more details). We shall take the inertia tensor relative to the center of mass. Therefore, we substitute $\mathbf{r}[i]-\mathbf{r}_{\rm cm}$ for $\mathbf{r}[i]$ into the formula (2.8). As a result we get the following expression for $I(\mathbf{n},\mathbf{n})$:

$$I(\mathbf{n},\mathbf{n})=\sum_{i=1}^{N}|\mathbf{r}[i]-\mathbf{r}_{\rm cm}|^2\,|\mathbf{n}|^2-\sum_{i=1}^{N}(\mathbf{r}[i]-\mathbf{r}_{\rm cm},\mathbf{n})^2. \tag{2.9}$$

Each quadratic form in a three-dimensional Euclidean space has 3 scalar invariants. One of them is trace the invariant. In the case of the quadratic form (2.9), the trace invariant is given by the following formula:

$$\operatorname{tr}(I)=2\sum_{i=1}^{N}|\mathbf{r}[i]-\mathbf{r}_{\rm cm}|^2. \tag{2.10}$$

Combining (2.9) and (2.10), we write

$$I(\mathbf{n},\mathbf{n})=\frac{\operatorname{tr}(I)}{2}\,|\mathbf{n}|^2-\sum_{i=1}^{N}(\mathbf{r}[i]-\mathbf{r}_{\rm cm},\mathbf{n})^2. \tag{2.11}$$

Taking into account the formula (2.6), we transform (2.11) as follows:

$$I(\mathbf{n},\mathbf{n})=\frac{\operatorname{tr}(I)}{2}\,|\mathbf{n}|^2-\sum_{i=1}^{N}(\mathbf{r}[i],\mathbf{n})^2+N\,(\mathbf{r}_{\rm cm},\mathbf{n})^2. \tag{2.12}$$

Comparing (2.12) with (2.5) and again taking into account (2.6), we get

$$d^{\,2}=\frac{\operatorname{tr}(I)}{2\,N}\,|\mathbf{n}|^2-\frac{I(\mathbf{n},\mathbf{n})}{N}. \tag{2.13}$$

The formula (2.13) means that $d^{\,2}$ is a quadratic form similar to the inertia tensor. We call it the *non-flatness form* and denote $Q(\mathbf{n},\mathbf{n})$:

$$\begin{gathered}Q(\mathbf{n},\mathbf{n})=\frac{\operatorname{tr}(I)}{2\,N}\,|\mathbf{n}|^2-\frac{I(\mathbf{n},\mathbf{n})}{N}=\\=\frac{1}{N}\sum_{i=1}^{N}(\mathbf{r}[i],\mathbf{n})^2-\left(\frac{1}{N}\sum_{i=1}^{N}(\mathbf{r}[i],\mathbf{n})\right)^2.\end{gathered} \tag{2.14}$$

Like the inertia form (2.9), the non-flatness form (2.14) is positive, i. e.

$$Q(\mathbf{n},\mathbf{n})\geqslant 0\quad\text{for}\quad\mathbf{n}\neq 0.$$

If the inertia tensor is brought to its primary axes, i. e. if it is diagonalized in some orthonormal basis, then the form (2.14) diagonalizes in the same basis.

Theorem 2.1. *A plane is an optimal root mean square plane for a group of points if and only if it passes through the center of mass of these points and if its normal vector* $\mathbf{n}$ *is directed along a primary axis of the non-flatness form* Q *of these points corresponding to its minimal eigenvalue.*

The proof is derived immediately from the definition 2.1 due to the formula (2.7) and the formula $d^2 = Q(\mathbf{n}, \mathbf{n})$.

Theorem 2.2. *An optimal root mean square plane for a group of points is unique if and only if the minimal eigenvalue λ_{min} of their non-flatness form Q is distinct from two other eigenvalues, i. e. $\lambda_{\text{min}} = \lambda_1 < \lambda_2$ and $\lambda_{\text{min}} = \lambda_1 < \lambda_3$.*

3. Defining an optimal circle.

Having found an optimal root mean square plane for the points $\mathbf{r}[1], \ldots, \mathbf{r}[N]$, we can replace them by their projections onto this plane:

$$\mathbf{r}[i] \mapsto \mathbf{r}[i] - ((\mathbf{r}[i], \mathbf{n}) - D)\,\mathbf{n}. \tag{3.1}$$

Our next goal is to find an optimal circle approximating a group of points lying on some plane (1.1). Let $\mathbf{r}[1], \ldots, \mathbf{r}[N]$ be their radius-vectors. The deflection of the point $\mathbf{r}[i]$ from the circle (1.2) is characterized by the following quantity:

$$d[i] = \left| |\mathbf{r}[i] - \mathbf{R}|^2 - \rho^2 \right|. \tag{3.2}$$

Like in the case of (2.1), we denote by d the root mean square of the quantities (3.2). Then we get the following formula:

$$d^2 = \frac{1}{N}\sum_{i=1}^{N} d[i]^2 = \frac{1}{N}\sum_{i=1}^{N} (|\mathbf{r}[i] - \mathbf{R}|^2 - \rho^2)^2. \tag{3.3}$$

The quantity d^2 in (3.3) is a function of two parameters: $\mathbf{R}$ and ρ^2. With respect to ρ^2 it is a quadratic polynomial. Indeed, we have

$$d^2 = (\rho^2)^2 - \frac{2\,\rho^2}{N}\sum_{i=1}^{N} |\mathbf{r}[i] - \mathbf{R}|^2 + \frac{1}{N}\sum_{i=1}^{N} |\mathbf{r}[i] - \mathbf{R}|^4. \tag{3.4}$$

Being a quadratic polynomial of ρ^2, the quantity d^2 takes its minimal value for

$$\rho^2 = \frac{1}{N}\sum_{i=1}^{N} |\mathbf{r}[i] - \mathbf{R}|^2. \tag{3.5}$$

Substituting (3.5) back into the formula (3.4), we derive

$$d^2 = \frac{1}{N}\sum_{i=1}^{N} |\mathbf{r}[i] - \mathbf{R}|^4 - \left(\frac{1}{N}\sum_{i=1}^{N} |\mathbf{r}[i] - \mathbf{R}|^2\right)^2. \tag{3.6}$$

Upon expanding the expression in the right hand side of the formula (3.6) we need to perform some simple, but rather huge calculations. As result we get

$$d^2 = \frac{1}{N}\sum_{i=1}^{N} |\mathbf{r}[i]|^4 - \left(\frac{1}{N}\sum_{i=1}^{N} |\mathbf{r}[i]|^2\right)^2 - \frac{4}{N}\sum_{i=1}^{N} |\mathbf{r}[i]|^2\,(\mathbf{r}[i], \mathbf{R}) +$$

$$+ 4\left(\frac{1}{N}\sum_{i=1}^{N}|\mathbf{r}[i]|^2\right)\left(\frac{1}{N}\sum_{i=1}^{N}(\mathbf{r}[i],\mathbf{R})\right) + \frac{4}{N}\sum_{i=1}^{N}(\mathbf{r}[i],\mathbf{R})^2 - 4\left(\frac{1}{N}\sum_{i=1}^{N}(\mathbf{r}[i],\mathbf{R})\right)^2.$$

We see that the above expression is not higher than quadratic with respect to $\mathbf{R}$. The fourth order terms and the cubic terms are canceled. Note also that the quadratic part of the above expression is determined by the form Q considered in previous section. For this reason we write d^2 as

$$d^2 = 4\,Q(\mathbf{R},\mathbf{R}) - 4\,(\mathbf{L},\mathbf{R}) + M. \tag{3.7}$$

The vector $\mathbf{L}$ and the scalar M in (3.7) are given by the following formulas:

$$\mathbf{L} = \frac{1}{N}\sum_{i=1}^{N}|\mathbf{r}[i]|^2\,(\mathbf{r}[i] - \mathbf{r}_{\text{cm}}), \tag{3.8}$$

$$M = \frac{1}{N}\sum_{i=1}^{N}|\mathbf{r}[i]|^4 - \left(\frac{1}{N}\sum_{i=1}^{N}|\mathbf{r}[i]|^2\right)^2. \tag{3.9}$$

The quantity d^2 takes its minimal value if and only if $\mathbf{R}$ satisfies the equation

$$2\mathbf{Q}(\mathbf{R}) = \mathbf{L}, \tag{3.10}$$

where $\mathbf{Q}$ is the symmetric linear operator associated with the form Q through the standard Euclidean scalar product. The equality

$$(\mathbf{Q}(\mathbf{X}),\mathbf{Y}) = Q(\mathbf{X},\mathbf{Y}),$$

which should be fulfilled for arbitrary two vectors $\mathbf{X}$ and $\mathbf{Y}$, is a formal definition of the operator $\mathbf{Q}$ (see [2] for more details).

In general case the operator $\mathbf{Q}$ is non-degenerate. Hence, $\mathbf{R}$ does exist and uniquely fixed by the equation (3.10). However, if the points $\mathbf{r}[1], \ldots, \mathbf{r}[N]$ are laid onto the plane (1.1) by means of the projection procedure (3.1), then the operator $\mathbf{Q}$ is degenerate. Moreover, one can prove the following theorem.

Theorem 3.1. *The non-flatness form Q and its associated operator $\mathbf{Q}$ are degenerate if and only if the points $\mathbf{r}[1], \ldots, \mathbf{r}[N]$ lie on some plane.*

In this flat case provided by the theorem 3.1 one should move the origin to that plane where the points $\mathbf{r}[1], \ldots, \mathbf{r}[N]$ lie and treat their radius-vectors as two-dimensional vectors. Then, using (2.14), (3.8), and (3.9), one should rebuild the two-dimensional versions of the non-flatness form Q, its associated operator $\mathbf{Q}$ and the parameters $\mathbf{L}$ and M. If again the two-dimensional non-flatness form is degenerate, this case is described by the following theorem.

Theorem 3.2. *The two-dimensional non-flatness form Q and its associated operator $\mathbf{Q}$ are degenerate if and only if all of the points $\mathbf{r}[1], \ldots, \mathbf{r}[N]$ lie on some straight line.*

In this very special case we say that straight line approximation for the points $\mathbf{r}[1], \ldots, \mathbf{r}[N]$ is more preferable than the circular approximation. Note that the same decision can be made in some cases even if the points $\mathbf{r}[1], \ldots, \mathbf{r}[N]$ do not lie on one straight line exactly. If two eigenvalues of the three-dimensional non-flatness form Q are sufficiently small, i.e. if they both are much smaller than the third eigenvalue of this form, then we can say that

$$\lambda_{\text{min}} \approx \lambda_1, \qquad\qquad \lambda_{\text{min}} \approx \lambda_2.$$

Taking two eigenvectors $\mathbf{n}_1$ and $\mathbf{n}_2$ of the form Q corresponding to the eigenvalues λ_1 and λ_2, we define two planes

$$(\mathbf{r}, \mathbf{n}_1) = D_1, \qquad\qquad (\mathbf{r}, \mathbf{n}_2) = D_2. \tag{3.11}$$

The constants D_1 and D_2 in (3.11) are given by the formula (2.7). The intersection of two planes (3.11) yields a straight line being the optimal straight line approximation for the points $\mathbf{r}[1], \ldots, \mathbf{r}[N]$ in this case.

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References

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5 Rabochaya street, 450003 Ufa, Russia
Cell Phone: +7-(917)-476-93-48
E-mail address: r-sharipov@mail.ru
R_Sharipov@ic.bashedu.ru

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