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

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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 $E$ 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 $E$ is given by the equation

$$(r, n) = D, \quad (1.1)$$

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

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

$$|r - R| = \rho. \quad (1.2)$$

Here $\rho$ is the radius of the circle (1.2) and $R$ is the radius-vector of its center. Having a group of points $r[1], \ldots, r[N]$ in $E$, our goal is to design an algorithm for calculating the parameters $n$, $D$, $R$, and $\rho$ 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 $n$ is a unit vector, i.e. $|n| = 1$, and assume that we have some plane defined by the equation (1.1). Then the distance from the point $r[i]$ to this plane

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is given by the following well-known formula:

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

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

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

**Definition 2.1.** A plane given by the formula (1.1) with $|n| = 1$ 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: $n$ and $D$. It is a quadratic function of the parameter $D$. Indeed, we have

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

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

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

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

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

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

$$r_{cm} = \frac{1}{N} \sum_{i=1}^{N} r[i]$$ \hfill (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:

$$D = (r_{cm}, n).$$ \hfill (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:

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

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

\[
I(n, n) = \sum_{i=1}^{N} |r[i] - r_{cm}|^2 |n|^2 - \sum_{i=1}^{N} (r[i] - r_{cm}, n)^2.
\] (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:

\[
\text{tr}(I) = 2 \sum_{i=1}^{N} |r[i] - r_{cm}|^2.
\] (2.10)

Combining (2.9) and (2.10), we write

\[
I(n, n) = \frac{\text{tr}(I)}{2} |n|^2 - \sum_{i=1}^{N} (r[i] - r_{cm}, n)^2.
\] (2.11)

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

\[
I(n, n) = \frac{\text{tr}(I)}{2} |n|^2 - \sum_{i=1}^{N} (r[i], n)^2 + N (r_{cm}, n)^2.
\] (2.12)

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

\[
d^2 = \frac{\text{tr}(I)}{2N} |n|^2 - \frac{I(n, n)}{N}.
\] (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 \( Q(n, n) \):

\[
Q(n, n) = \frac{\text{tr}(I)}{2N} |n|^2 - \frac{I(n, n)}{N} = \frac{1}{N} \sum_{i=1}^{N} (r[i], n)^2 - \left( \frac{1}{N} \sum_{i=1}^{N} (r[i], n) \right)^2.
\] (2.14)

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

\[
Q(n, n) \geq 0 \quad \text{for} \quad n \neq 0.
\]

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 \( n \) 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 \( \lambda_{\min} \) of their non-flatness form \( Q \) is distinct from two other eigenvalues, i.e. \( \lambda_{\min} = \lambda_1 < \lambda_2 \) and \( \lambda_{\min} = \lambda_1 < \lambda_3 \).

3. DEFINING AN OPTIMAL CIRCLE.

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

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

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

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

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:

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

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

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

Being a quadratic polynomial of \( \rho^2 \), the quantity \( d^2 \) takes its minimal value for

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

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

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

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

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

We see that the above expression is not higher than quadratic with respect to \( R \). 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

\[ d^2 = 4Q(R, R) - 4(L, R) + M. \quad (3.7) \]

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

\[ L = \frac{1}{N} \sum_{i=1}^{N} |r[i]|^2 (r[i] - r_{cm}), \quad \text{(3.8)} \]

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

The quantity \( d^2 \) takes its minimal value if and only if \( R \) satisfies the equation

\[ 2Q(R) = L, \quad \text{(3.10)} \]

where \( Q \) is the symmetric linear operator associated with the form \( Q \) through the standard Euclidean scalar product. The equality

\[ (Q(X), Y) = Q(X, Y), \]

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

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

**Theorem 3.1.** The non-flatness form \( Q \) and its associated operator \( Q \) are degenerate if and only if the points \( r[1], \ldots, r[N] \) 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 \( r[1], \ldots, r[N] \) 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 \( Q \) and the parameters \( L \) 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 \( Q \) are degenerate if and only if all of the points \( r[1], \ldots, r[N] \) lie on some straight line.

In this very special case we say that straight line approximation for the points \( r[1], \ldots, r[N] \) is more preferable than the circular approximation. Note that the same decision can be made in some cases even if the points \( r[1], \ldots, r[N] \) 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

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

Taking two eigenvectors $n_1$ and $n_2$ of the form $Q$ corresponding to the eigenvalues $\lambda_1$ and $\lambda_2$, we define two planes

$$(r, n_1) = D_1, \quad (r, n_2) = D_2.$$  \hspace{1cm} (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 $r[1], \ldots, r[N]$ in this case.

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References

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