ON LINEAR REGRESSION IN THREE-DIMENSIONAL EUCLIDEAN SPACE.

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ABSTRACT. The three-dimensional linear regression problem is a problem of finding a spacial straight line best fitting a group of points in three-dimensional Euclidean space. This problem is considered in the present paper and a solution to it is given in a coordinate-free form.

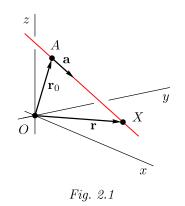
1. INTRODUCTION.

The linear regression problem in two-dimensional case (i. e. on a plane) typically arises when approximating experimental data with a linear function (see [1]). Its solution using least squares method was first published by Legendre in 1805 (see [2]). In an unpublished form the least squares method is attributed to Carl Friedrich Gauss 1795. His work was published only in 1809 (see [3]).

There are various fitting problems in three-dimensional Euclidean space (see plane, circle and ellipse fitting problems in [4] and [5], see ellipsoid fitting problem in [6] and [7]). The linear regression problem in three-dimensional case is the problem of best fitting some straight line to a group of points in three-dimensional Euclidean space. A solution of this problem is given by Jean Jacquelin in [8]. His method is substantially based on direct calculations using coordinates. Our goal in the present paper is to give a coordinate-free solution to the problem.

2. PARAMETRIC AND NON-PARAMETRIC VECTORIAL EQUATIONS OF A STRAIGHT LINE.

Let's consider the straight line AX in Fig 2.1. The point A is a fixed point of this line, its radius-vector is \mathbf{r}_0 . The point X is a variable point, its radius-vector



is **r**. These two radius-vectors are related to each other by means of the equation

$$\mathbf{r} = \mathbf{r}_0 + \mathbf{a} t, \qquad (2.1)$$

where **a** is some non-zero vector on the line and t is a scalar parameter. The equality (2.1) is called the *vectorial parametric* equation of the line in the space (see [9]).

The choice of the point A on the line is not unique. Therefore the equation (2.1) has some extent of ambiguity. In order to avoid this ambiguity non-parametric

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equations are used. Let's multiply both sides of the equality (2.1) by the vector **a** using the vector product¹ operation. As a result we get

$$[\mathbf{r}, \mathbf{a}] = [\mathbf{r}_0, \mathbf{a}]. \tag{2.2}$$

The product of two constant vectors in the right hand side of (2.2) is a constant vector. If we denote it through **b**, we get the equality

$$[\mathbf{r}, \mathbf{a}] = \mathbf{b}, \text{ where } \mathbf{b} \perp \mathbf{a}.$$
 (2.3)

The equality (2.3) is known as the non-parametric vectorial equation of the line in the space (see [9]). Note that the vector $\mathbf{b} = [\mathbf{r}_0, \mathbf{a}]$ has no ambiguity arising from the uncertainty in choosing the initial point A on the line. Indeed, it is easy to see that \mathbf{b} is invariant with respect to the transformation $\mathbf{r}_0 \to \mathbf{r}_0 + \mathbf{a} t$.

3. The statement of the problem.

Let X_1, \ldots, X_n be a group of points in the space given by their radius-vectors $\mathbf{r}_1, \ldots, \mathbf{r}_n$. The linear regression problem consists in finding a line given by the equation (2.2) such that the root mean square of the distances d_1, \ldots, d_n from the points X_1, \ldots, X_n to the line (2.2) takes its minimal value:

$$\bar{d}^2 = \frac{1}{n} \sum_{i=1}^n d_i^2.$$
(3.1)

4. The solution of the problem.

The distance from the point X_i to the line (2.1) is given by the formula

$$d_i = \frac{|[\mathbf{r}_i - \mathbf{r}_0, \mathbf{a}]|}{|\mathbf{a}|}.$$
(4.1)

Without loss of generality we can assume that

$$|\mathbf{a}| = 1. \tag{4.2}$$

Then, taking into account $\mathbf{b} = [\mathbf{r}_0, \mathbf{a}]$ and (4.2), from (4.1) we derive

$$d_i = |[\mathbf{r}_i, \mathbf{a}] - \mathbf{b}|. \tag{4.3}$$

Now we substitute (4.3) into (3.1). As a result we obtain

$$\bar{d}^2 = |\mathbf{b}|^2 - \frac{2}{n} \sum_{i=1}^n ([\mathbf{r}_i, \mathbf{a}], \mathbf{b}) + \frac{1}{n} \sum_{i=1}^n |[\mathbf{r}_i, \mathbf{a}]|^2.$$
(4.4)

The formula (4.4) is an analog of the formula (2.3) in [4]. The round brackets in (4.4) denote the scalar product² operation.

Definition 4.1. A line given by the equation (2.3) with $|\mathbf{a}| = 1$ is called an *optimal* root mean square line if the quantity (4.4) takes its minimal value.

¹ It is also called the cross product, i.e. $[\mathbf{x}, \mathbf{y}] = \mathbf{x} \times \mathbf{y}$.

² It is also called the dot product, i.e. $(\mathbf{x}, \mathbf{y}) = \mathbf{x} \cdot \mathbf{y}$.

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The right hand side of (4.4) is a quadratic polynomial with respect to the components of the vector **b**. It takes its minimal value if **b** is given by the formula

$$\mathbf{b} = \frac{1}{n} \sum_{i=1}^{n} [\mathbf{r}_i, \mathbf{a}]. \tag{4.5}$$

Substituting (4.5) back into (4.3), we derive

$$\bar{d}^2 = \frac{1}{n} \sum_{i=1}^n |[\mathbf{r}_i, \mathbf{a}]|^2 - \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n ([\mathbf{r}_i, \mathbf{a}], [\mathbf{r}_j, \mathbf{a}]).$$
(4.6)

The formula (4.6) is an analog of the formula (2.5) in [4]. Its right hand side is a quadratic form wit respect to the vector **a**. We denote it through $Q(\mathbf{a}, \mathbf{a})$:

$$Q(\mathbf{a}, \mathbf{a}) = \frac{1}{n} \sum_{i=1}^{n} |[\mathbf{r}_i, \mathbf{a}]|^2 - \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} ([\mathbf{r}_i, \mathbf{a}], [\mathbf{r}_j, \mathbf{a}])$$
(4.7)

and call the *non-linearity form* for a group of points in three-dimensional Euclidean space. Like the non-flatness form (2.14) in [4], the non-linearity form (4.7) is positive in the sense of the following inequality:

$$Q(\mathbf{a}, \mathbf{a}) \ge 0 \text{ for } \mathbf{a} \ne 0.$$

Like in [4] one can draw some analogy to mechanics using the inertia tensor. However, we shall not do it now. We just note that like any quadratic form $Q(\mathbf{a}, \mathbf{a})$ diagonalizes in some orthonormal basis associated with its primary axes.

Let's introduce the following notation analogous to (2.6) in [4]:

$$\mathbf{r}_{\rm cm} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{r}_i. \tag{4.8}$$

The vector \mathbf{r}_{cm} in (4.8) is the radius-vector of the center of mass of a group of points X_1, \ldots, X_n if assume that unit masses are placed at each of these points. In terms of (4.8) the formula (4.5) is written as

$$\mathbf{b} = [\mathbf{r}_{\rm cm}, \mathbf{a}]. \tag{4.9}$$

Comparing (4.9) with $\mathbf{b} = [\mathbf{r}_0, \mathbf{a}]$, we conclude that the optimal line should pass through the center of mass of a group of points. Its direction is determined by the non-linearity form $Q(\mathbf{a}, \mathbf{a})$ according to the following theorem.

Theorem 4.1. A line is an optimal root mean square line for a group of points if and only if it passes through the center of mass of these points and if its direction vector \mathbf{a} is directed along the primary axis of the non-linearity form Q of these points corresponding to its minimal eigenvalue.

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5. Conclusion.

Theorem 4.1 solves the linear regression problem formulated in Section 3. Its proof is obvious from the consideration preceding it. Practically this theorem means that in order to find a line best fitting a group of points in three-dimensional Euclidean space one should find their center of mass and diagonalize the symmetric matrix associated with their non-linearity form (4.7). In some cases this matrix can have two minimal eigenvalues $\lambda_1 = \lambda_2 < \lambda_3$. In these cases the shape of the group of points resembles a disc and hence there is no preferable direction for the optimal line within the plane of this disc.

If $\lambda_1 = \lambda_2 = \lambda_3$, the shape of the group of points resembles a ball. In this case we have no preferable direction for the optimal line at all.

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