Rationalizing Foot and Ankle Measurements to Conform to a Rigid Body Model

Suliman Al-Homidan* Roger Fletcher†

January 4, 2006

Abstract

Accurate estimation of the *in vivo* locations of skeletal landmarks plays an integral role in several biomechanical research techniques. Because of rounding errors caused by instruments or skin movement, the data obtained through cinematography are usually not accurate and rise to a distance matrix which, because of the data errors, may not be Euclidean. The aim of this paper is to find the best Euclidean distance matrix (EDM) that approximates the distance matrix and then, an accurate estimation of the locations of skeletal landmarks. A useful scheme for parametrizing an orthogonal matrix is also described.

Keywords: Ankle; Bone markers; EDM; Errors; Foot; Quasi-Newton method; Skin displacement.

1 Introduction

Data obtained through cinematography are usually derived from the coordinates of skin-mounted markers positioned over specific skeletal points. The

*Department of Mathematical Sciences, King Fahd University of Petroleum and Minerals, Dhahran 31261, PO Box 119, Saudi Arabia Email homidan@kfupm.edu.sa

†Department of Mathematics, University of Dundee, Dundee DD1 4HN, Scotland, UK. Email fletcher@maths.dundee.ac.uk

errors in the accuracy of such data are therefore dependent upon either instrumental errors representing the errors with which marker coordinates are reconstructed in a global frame or skin displacements mostly associated with the interposition of both passive and active soft tissues, and caused by the relative movement between the marker and the underlying bone. This is a major source of error because when the calculations are being carried out on the data, we are assuming that the body parts are rigid and the movement of the skin goes against this assumption. As can be seen in Figure 1, the foot is made up of many individual joints, resulting in a considerable amount of movement within the foot.

The experimental data are measurements of squared distances between markers positioned over specific skeletal points in a Euclidean space. Such distances are referred to as Euclidean distance matrices. However, because of experimental errors, these matrices are not exactly Euclidean and it is desirable to find the 'best' Euclidean distance matrix which approximates the non-Euclidean matrix. The aim of this paper is to reduce the errors in the experimental data. In doing this, it is hoped that subsequent calculations for finding the location of the axes in relation to each other will produce more accurate results.

An $n \times n$ symmetric matrix $D = (d_{ij})$ with nonnegative elements and zero diagonal is called a *distance matrix.* In addition, if there exist points $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ in $\mathbb{R}^r$ such that

$$d_{ij} = \|\mathbf{x}_i - \mathbf{x}_j\|_2^2, \qquad i, j = 1, 2, \ldots, n, \tag{1.1}$$

then D is called an *Euclidean distance matrix.* The smallest value of r is called the *embedding dimension* of D, also $r = rank(A)$. Let F be a distance matrix representing the experimental data and let $\|F\|_F = \sqrt{trace F^T F}$ denote the Frobenius norm of F. We consider the objective function

$$f(D) = \|F - D\|_F^2, \tag{1.2}$$

The *nearest Euclidean distance matrix problem* is

$$\text{(EDM)} \qquad \begin{array}{ll} \text{minimize} & f(D) \\ \text{subject to} & D \in \mathcal{E} \end{array} \tag{1.3}$$

where $\mathcal{E}$ denotes the cone of Euclidean distance matrices.

We consider two problems which generalize (1.3). First, given a set of frames, each frame F_k is a set of coordinate points in the Euclidean space.

All frames should generate identical EDMs but because of errors in reading, they are a little different. Thus, we need to find the best Euclidean distance matrix of all frames, i.e.

$$\text{(GEDM)} \qquad \begin{array}{ll} \text{minimize} & \sum_{k=1}^{m} \|F_k - D\|_F^2 \\ \text{subject to} & D \in \mathcal{E}. \end{array} \tag{1.4}$$

After the best Euclidean distance matrix D has been found, a second problem is to fit D to each frame of data. This will enable the original frame coordinates to be replaced by coordinates whose distance matrices are consistent with the best distance matrix obtained from (1.4). Hence, the problem can be expressed as: given a frame with the coordinate points $\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_n$, the problem can be expressed as

$$\text{(FEDM)} \qquad \begin{array}{ll} \text{minimize} & \sum_{k=1}^{n} \|\mathbf{p}_k - \mathbf{x}_k\|_2^2 \\ \text{subject to} & \|\mathbf{x}_i - \mathbf{x}_j\|_2^2 = d_{ij}, \end{array} \tag{1.5}$$

where $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ are the unknown coordinate points representing the desired frame that fits D.

Theoretical properties of Euclidean distance matrices (1.3) can be found in, e.g. [2, 3, 9, 10, 12, 20]. This includes characterizations, solutions, as well as graph-theoretic conditions for EDM problem. More information can be found in a recent survey article by Laurent [15].

Applications of Euclidean distance matrices abound: e.g., molecular conformation problems in chemistry [7]; multidimensional scaling and multivariate analysis problems in statistics [16, 17]; genetics, geography, and others [1].

In medicine where our problem arises, Stanhope et. al. [24] have presented experimental results whereby the bone-embedded frame of reference was obtained using halo pins inserted into the periosteum of the tibia of three volunteer subjects who walked on the level. Karlsson et. al. [14] report results obtained using markers mounted on a cortical pins. In a study of skin displacement, Maslen et. al. [18] refer to the fact that the extent and direction of this displacement can vary according to the specific location of the markers and the nature of the movement.

Lately, Cappozzo et. al. [6, 5] have studied the position and orientation in space of bones during movement. In order to analyze the ankle joint in movement in three-dimensions, they determine the instantaneous position and orientation of the system of axes, which they consider to be rigid with the bone under analysis. Some references that consider problem (1.5) are [4, 8, 11, 13, 22, 23, 25, 27]. Woltring [26] considers parametrisation of rotations matrices. Some of them are only relevant when the dimension r equals 3. However, Many of the above applications require a low embedding dimension, e.g. $r = 3$.

2 Solving the EDM

In this section, we describe a method to solve (1.4). This problem has been formed as an unconstrained optimization problem and then solved by the quasi-Newton method [2]. However, recently, [21] considered an organized way to calculate the gradient of the objective function so that efficient classical optimization techniques can be applied. The main idea is to replace (1.4) by a smooth unconstrained optimization problem in order to use super-linearly convergent quasi-Newton methods. In what follows, we describe the original problem, and the gradient of the objective function.

Given a set of frames where each frame represents coordinate points in $\mathbb{R}^3$, problem (1.4) is to find the best Euclidean distance matrix of all frames, or equivalently

$$\begin{array}{ll} \text{minimize} & \sum_{k=1}^{m}\{\sum_{i,j=1}^{n}(f_{ij_k} - d_{ij})^2\} \\ \text{subject to} & D \ \in \mathcal{E}. \end{array} \tag{2.1}$$

The following theorem is needed to explain the method; its proof can be found in [2].

Theorem 2.1 *The distance matrix $D \in \mathbb{R}^{n\times n}$ is a Euclidean distance matrix if and only if the $n-1 \times n-1$ symmetric matrix A defined by*

$$a_{ij} = \tfrac{1}{2}[d_{1i} + d_{1j} - d_{ij}] \qquad (2 \le i, j \le n) \tag{2.2}$$

is positive semi–definite, and D is irreducibly embeddable in $\mathbb{R}^r (r < n)$. Moreover, consider the spectral decomposition $A = U\Lambda U^T$. Let Λ_r be the *matrix of non–zero eigenvalues in* Λ *and define* X *by*

$$X = U_r \Lambda_r^{1/2}, \quad \textit{then} \quad A = XX^T, \tag{2.3}$$

where $\Lambda_r^{1/2} \in \mathbb{R}^{r\times r}$ *and* $U_r \in \mathbb{R}^{n-1\times r}$ *comprises the corresponding columns of* U. *Then the columns of* X^T *furnish coordinate choices for* $\mathbf{p}_2, \mathbf{p}_3, \ldots, \mathbf{p}_n$ *with* $\mathbf{p}_1 = \mathbf{0}$.

It is possible to express (2.1) as a smooth unconstrained optimization problem. The unknowns in the problem are chosen to be the elements of the matrix X introduced in (2.3). From (1.1), $d_{ij} = \|\mathbf{x}_i - \mathbf{x}_j\|_2^2$, therefore (2.1) is replaced by an unconstrained optimization problem in rn variables as follows:

$$\text{minimize} \quad \phi(\mathbf{x}) \; = \; \sum_{k=1}^{m}\{\sum_{i,j=1}^{n}(f_{ij_k} - \|\mathbf{x}_i - \mathbf{x}_j\|_2^2)^2\}. \tag{2.4}$$

Let $t_{ij_k} \; = \; f_{ij_k} - \|\mathbf{x}_i - \mathbf{x}_j\|_2^2$, then we can express problem (2.4) as

$$\text{minimize} \quad \phi(\mathbf{x}) \; = \; \sum_{k=1}^{m}\sum_{i,j=1}^{n} t_{ij_k}^2. \tag{2.5}$$

If the elements t_{ij_k} are put in a matrix T_k, then (2.5) becomes

$$\text{minimize} \quad \phi(\mathbf{x}) \; = \; \sum_{k=1}^{m} \textit{trace} \;\; T_k^2. \tag{2.6}$$

The expressions for the first partial derivatives of ϕ are given by

$$\frac{\partial \phi}{\partial x_{rs}} = 2 \sum_{k=1}^{m}\sum_{i,j=1}^{n} t_{ij_k} \frac{\partial t_{ij_k}}{\partial x_{rs}}, \tag{2.7}$$

where

$$\frac{\partial t_{ij_k}}{\partial x_{rs}} \; = \; \left\{ \begin{array}{cccc} 0 & \textit{if} & s \neq i \quad \& & s \neq j \\ 2(x_{rs} - x_{ri}) & \textit{if} & s = j & \\ 2(x_{rs} - x_{rj}) & \textit{if} & s = i & \end{array} \right\} \tag{2.8}$$

which is equivalent in matrix notation to

$$[\, \tfrac{\partial \phi}{\partial x_{rs}} \,] \; = \; 8X \sum_{k=1}^{m}(D_k - T_k), \tag{2.9}$$

where $D_k = diag(\mathbf{d}_k)$, $\mathbf{d}_k = T_k\mathbf{e}$ and $\mathbf{e} = (1, \ldots, 1)^T \in \mathrm{I\!R}^n$.

An extreme case occurs when the initial matrix $X = 0$ is chosen, and $\sum F_k \neq 0$. It can be seen from (2.8) that the components of the gradient vector are all zero, so that $X = 0$ is a stationary point, but not a minimizer. A gradient method will usually terminate in this situation, and so fail to find a solution. A reliable method for initializing X is to use the construction suggested by (2.2) and (2.3). Thus, we define the elements of A from the averge elements of F_k by

$$a_{ij} = \sum_{k=1}^{m} \{\tfrac{1}{2}(f_{ijk} - f_{1ik} - f_{1jk})\}/m \qquad i \geq 2, \quad j \geq 2. \tag{2.10}$$

The first row and column of A are zero and are ignored. We then find the spectral decomposition $U\Lambda U^T$ of the nontrivial part of A. Finally, X is initialized to the matrix $\Lambda_r^{1/2} U_r^T$, where $\Lambda_r = \mathrm{diag}(\lambda_i),\ i = 1, \ldots, r$ is composed of the r largest eigenvalues in Λ, and columns of U_r are the corresponding eigenvectors.

3 Fitting the frames

In the first part of the problem, an EDM D is found which best fits the data given by all the frames Y_k in the least squares sense. Columns of matrix X provide a coordinate system from which D can be calculated. The procedure in the second part is to fit X to each frame of data Y_k. That is, we find the nearest coordinate system Y to Y_k (in some sense) such that Y has the same EDM D as X. We can always express

$$Y = \mathbf{v}\mathbf{e}^T + Q(X - X\mathbf{e}\mathbf{e}^T/n), \tag{3.1}$$

where Q is an orthogonal matrix, which is the result of a translation and a rotation about the centroid of points in X. This is necessary because the coordinate system X is arbitrary and has no relation to the coordinate system in which the experimental data are expressed.

In what follows, two methods of finding $\mathbf{v}$ and Q are suggested. The first is a direct method which is readily implemented in say matlab. The second is an optimal method which requires the application of an unconstrained minimization technique. We stress that these calculations must be repeated for every frame of data, so it is important to find an efficient method. However, there are some potential difficulties that can arise when working with an orthogonal matrix. Hence, we introduce a section on a stable parametrization of an orthogonal matrix.

3.1 On the Stable Parametrization of an Orthogonal Matrix

In various optimization problems there are variables which are elements of an orthogonal matrix, and hence are subject to nonlinear orthogonality normalization constraints. It can be efficient to parameterise the problem in a different way so as to remove these constraints. However it is important that this is done in a stable way.

A well known parameterization is the Cayley transform

$$Q = (I - S)(I + S)^{-1} \tag{3.2}$$

which parameterises $Q \in \mathbb{R}^{n \times n}$ in terms of a skew-symmetric matrix S. This is a minimal representation in that S has $\frac{1}{2}n(n-1)$ independent parameters, which is the appropriate number, since Q has n^2 elements and there are $\frac{1}{2}n(n-1)$ orthogonality conditions and n normalization conditions. The inverse representation

$$S = (I - Q)(I + Q)^{-1} \tag{3.3}$$

enables S to be calculated from a given orthogonal matrix Q.

Unfortunately, not every orthogonal matrix can be expressed in this way. Orthogonal matrices may be classified as *proper* or *improper* according to whether $\det(Q)$ is $+1$ or -1. Clearly $\det(Q) = 1$ in (3.2) so the Cayley transform cannot be used for an improper orthogonal matrix. In 2 or 3 dimensions, proper orthogonal matrices are associated with rotation operations (see e.g. Mirsky [19]). However, a rotation through an angle π in 2D gives rise to the proper orthogonal matrix $Q = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$, which also cannot be transformed using (3.3). Moreover, for angles close to π, the resulting matrix S is large, giving rise to possible numerical instability.

We suggest a procedure which is applicable to both proper and improper orthogonal matrices, and which always yields a finite S matrix. It uses the transformation

$$QP = (I - S)(I + S)^{-1} \tag{3.4}$$

where P is a nonsingular matrix consisting of columns from $[I, -I]$, i.e. P incorporates column permutations and sign changes in Q. The inverse transformation is

$$S = (I - QP)(I + QP)^{-1}. \tag{3.5}$$

The problem therefore is, given an orthogonal matrix Q, find P and S such that Q is given by (3.4). In the algorithm we describe below, we need to calculate factors

$$(I + QP) = LU \tag{3.6}$$

where L is unit lower triangular, U is upper triangular with positive diagonal elements, and P is determined during the factorization process. These factors can then be used to compute S from (3.5).

To describe the process, here is an algorithm that computes U and L:

Algorithm 3.1 *Let U represent a stored matrix, which will finally become the upper triangular matrix in (3.6).*
Initialization: $U = Q$, $P = I$.
for $i = 1 : n$
  Set $k = \operatorname{argmax}_{k \geq i} |u_{ik}|$
  Interchange columns i and k of U
  Interchange columns i and k of P
  if $u_{ii} < 0$
    change the signs of column i of U and of P
  end
  Set $u_{ii} = u_{ii} + 1$
  for $j = i + 1 : n$
    Set $l_{ji} = u_{ji}/u_{ii}$
    Subtract $l_{ji}\times$ *row i of U from j of U*
  end
end

Essentially the algorithm implements column pivoting with sign change to make the pivot positive. At this stage the unit element of I is added into the pivot. To illustrate the procedure in Algorithm 3.1, we consider the following example:

Example 3.2 *Let*

$$S = \begin{pmatrix} 0 & N & N \\ -N & 0 & N \\ -N & -N & 0 \end{pmatrix}. \tag{3.7}$$

As $N \longrightarrow \infty$, *it is readily observed that* Q *in (3.2) converges to*

$$Q = \frac{1}{3} \begin{pmatrix} -1 & -2 & 2 \\ -2 & -1 & -2 \\ 2 & -2 & -1 \end{pmatrix}. \tag{3.8}$$

Clearly, the inverse calculation (3.3) fails for this Q. *We first illustrate how the new procedure calculates LU factors as in (3.6). Initially,* $U = Q$ *and column 2 is chosen as a pivot with sign change, the unit value is added in, and columns 1 and 2 are interchanged. After eliminating the subdiagonal, we have*

$$L = \begin{pmatrix} 1 & 0 & 0 \\ 1/5 & 1 & 0 \\ 2/5 & 0 & 1 \end{pmatrix}, P = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, U = \begin{pmatrix} 5/3 & -1/3 & 2/3 \\ 0 & -3/5 & -4/5 \\ 0 & 4/5 & -3/5 \end{pmatrix}$$

On stage 2, column 3 is chosen with sign change, giving

$$L = \begin{pmatrix} 1 & 0 & 0 \\ 1/5 & 1 & 0 \\ 2/5 & 1/3 & 1 \end{pmatrix}, P = \begin{pmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}, U = \begin{pmatrix} 5/3 & -2/3 & -1/3 \\ 0 & 9/5 & -3/5 \\ 0 & 0 & 1 \end{pmatrix}$$

On stage 3, column 3 is necessarily chosen, but there is no sign change. However, we still add unity into u_{33} *giving*

$$U = \begin{pmatrix} 5/3 & -2/3 & -1/3 \\ 0 & 9/5 & -3/5 \\ 0 & 0 & 2 \end{pmatrix}.$$

L *and* U *are now the factors* $I + QP = LU$. *The resulting skew-symmetric matrix in (3.5) is*

$$S = \begin{pmatrix} 0 & 1/3 & 1/3 \\ -1/3 & 0 & 1/3 \\ -1/3 & -1/3 & 0 \end{pmatrix}.$$

We now return to the second problem of fitting the best configuration with EDM D to each of the frames F_k. We use some aspects of the ideas previously presented. What we have is a set of coordinates (columns of a matrix X) which has the best EDM D as calculated in Section 2. We also have coordinates Y_k for frame F_k. Because Y_k does not have the optimal EDM D, Y_k cannot be obtained from X by using (3.1). We therefore need to develop a procedure for transforming X to be as close as possible to Y_k.

3.2 A Direct Method

In this method, we first translate X and Y_k to have a zero common centroid, giving matrices $\bar{X} = X - X\mathbf{e}\mathbf{e}^T/n$ and $\bar{Y_k} = Y_k - Y_k\mathbf{e}\mathbf{e}^T/n$. Next, we find an orthogonal matrix Q such that

$$\bar{Y} = Q\bar{X} \tag{3.9}$$

is close to $\bar{Y_k}$. Were it to exist, a general linear transformation of $\bar{X}$ to $\bar{Y_k}$ could be written

$$M\bar{X} = \bar{Y_k}. \tag{3.10}$$

However, because $\bar{Y_k}$ has many more columns than rows, these equations are overdetermined and an exact solution for M does not usually exist. Even if it were to exist, it is unlikely that M would be an orthogonal matrix. Our strategy is to find the matrix M which best fits (3.10), and then find an orthogonal matrix Q which is close to M. The best solution of (3.10) may be expressed as $M = \bar{Y_k}\bar{X}^\dagger$, where $\bar{X}^\dagger$ is the *Moore-Penrose* generalized inverse of $\bar{X}$, although it is most efficiently calculated from QR factors of $\bar{X}^T$. First, we check whether $\det(M)$ is close to $+1$, which indicates that the Cayley transform

$$Q = (I - S)(I + S)^{-1}, \tag{3.11}$$

is applicable. The inverse of this transformation is

$$S = (I - Q)(I + Q)^{-1} \tag{3.12}$$

which determines a skew-symmetric matrix from an orthogonal matrix. We apply (3.12) to the matrix M to get

$$P = (I - M)(I + M)^{-1}.$$

If M were close to an orthogonal matrix, then P should be close to a skew-symmetric matrix. Thus, we calculate the nearest skew symmetric matrix to P from

$$S = (P - P^T)/2,$$

and then use (3.11) to determine Q. If S were very large, then we would use the procedure outlined in Section 3.1 to make it smaller. Finally, we translate $\bar{Y}$ in (3.9), giving a matrix $Y = \bar{Y} + \mathbf{v}\mathbf{e}^T$ which has the same centroid as Y_k. This is achieved by defining

$$\mathbf{v} = (Y_k\mathbf{e} - \bar{Y}\mathbf{e})/n.$$

A similar method is investigated in the project report of Smith [21] where a translation has been done first and then the rotation. However, we think that the method used in [21] has a flaw as it does not do the rotation about the common centroid.

3.3 An Optimal Method

The main disadvantage of our method described in Section 3.2 is that it does not provide an optimal choice of $\mathbf{v}$ and Q. This is the subject of this section. Given a frame with the coordinate points $\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_n$, the problem can be expressed as

$$\begin{aligned} \text{minimize} \quad & \sum_{k=1}^{n} \|\mathbf{p}_k - \mathbf{x}_k\|_2^2 \\ \text{subject to} \quad & \|\mathbf{x}_i - \mathbf{x}_j\|_2^2 = d_{ij}, \end{aligned} \tag{3.13}$$

where $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ are the unknown coordinate points representing the desired frame that fits D. In our problem, the embedding dimension is $r = 3$.

Now, if the matrix X is rotated by the matrix S and transformed by the vectoer $\mathbf{v} \in \mathbb{R}^3$ to fit the best Euclidean distance matrix, then (3.13) can be expressed as

$$\text{minimize} \quad \phi, \tag{3.14}$$

where

$$\begin{aligned} \phi(\mathbf{v}, S) &= \sum_{k=1}^{n} \|\mathbf{p}_k - \mathbf{y}_k\|^2 \\ &= \sum_{k=1}^{n} \sum_{i=1}^{3} (p_{ki} - y_{ki})^2 \end{aligned} \tag{3.15}$$

and y_{ki} are the elements of the matrix

$$Y = Q\bar{X} \ + \ \mathbf{v}\mathbf{e}^T,$$

where

$$\bar{X} = X - X\mathbf{e}\mathbf{e}^T/n, \quad \mathbf{v} = [v_1, \ v_2, \ v_3]^T$$

and

$$Q \ = \ (I - S)(I + S)^{-1}, \ \ S \ = \ \begin{bmatrix} 0 & s_{12} & s_{13} \\ -s_{12} & 0 & s_{23} \\ -s_{13} & -s_{23} & 0 \end{bmatrix}.$$

This problem is equivalent to (3.13) but with only six variables. A gradient method requires expressions for the first partial derivatives of ϕ with respect to s_{ij} which are given from (3.15) by

$$\frac{\partial \phi}{\partial s_{ij}} = 2 \sum_{k=1}^{n} \sum_{i=1}^{3} (y_{ki} - p_{ki}) \frac{\partial y_{ki}}{\partial s_{ij}}, \tag{3.16}$$

where

$$\frac{\partial Y}{\partial s_{ij}} \ = \ \frac{\partial Q}{\partial s_{ij}} \bar{X} \tag{3.17}$$

We can express Q implicitly by $Q(I + S) = (I - S)$. Then, the implicit derivative of Q with respect to s_{ij} is

$$\frac{\partial Q}{\partial s_{ij}}(I + S) + QE_{ij} \ = \ - E_{ij}, \tag{3.18}$$

where E_{ij} is the matrix representing the derivative of $I + S$ with respect to s_{ij}, i.e. $E_{ij} \ = \ \mathbf{e}_i\mathbf{e}_j^T - \mathbf{e}_j\mathbf{e}_i^T$. Hence,

$$\frac{\partial Q}{\partial s_{ij}} \ = \ - (I + Q)E_{ij}(I + S)^{-1}. \tag{3.19}$$

The expressions for the first partial derivatives of ϕ with respect to v_i is given by

$$\frac{\partial \phi}{\partial v_i} = 2 \sum_{k=1}^{n} \sum_{i=1}^{3} (y_{ki} - p_{ki}) \frac{\partial y_{ki}}{\partial v_i}, \tag{3.20}$$

where

$$\frac{\partial Y}{\partial v_1} = \begin{bmatrix} \mathbf{e}^T \\ 0 \\ 0 \end{bmatrix}, \quad \frac{\partial Y}{\partial v_2} = \begin{bmatrix} 0 \\ \mathbf{e}^T \\ 0 \end{bmatrix}, \quad \frac{\partial Y}{\partial v_3} = \begin{bmatrix} 0 \\ 0 \\ \mathbf{e}^T \end{bmatrix}, \tag{3.21}$$

and $\mathbf{e}^T = [1 \;\; 1 \;\; \ldots \;\; 1] \in \mathbb{R}^n$.

Algorithm 3.1 can be used to recalculate P and S if the elements of S become large.

4 Computational Results

In this section, we will explain how the data are generated. Thereafter, the data analysis for all the methods in Sections 2 and 3 will be considered.

Recently, there has been a study by the Ninewells Teaching Hospital, Dundee, Scotland, on the location of the axes in the ankle joint, where the data are analyzed in the form of distance matrices. The subjects in this study are patients that have some form of ankle deformity or injury. Five markers are fixed on the skin of the lower leg and six on the foot of the patient and then they walk down the middle of a large room. As they walk, cameras are taking reading of the markers. The markers are fixed to the skin to estimate the position of the underlying skeletal structure. Figures 1 and 2 are idealized models of the lower leg and foot.

The ankle joint is connected by two axes about which it can rotate, one axis allows for up and down movement and the other allows for movement from side to side. The aim of this study is to determine where these axes are, but more specifically, determine how far apart these axes are from each other. Hence, to calculate where these axes are in relation to each other so that the appropriate corrective footware can be prescribed or, if necessary surgery can be carried out.

We are grateful to the *Gait Laboratory* at Ninewells Hospital for supplying a test set of data for us to analyze. The data are in the form of a matrix with 34 columns and 363 rows each row represent a frame and contains the frame number and the coordinate components for the eleven markers namely, STA1, STA2, PCAL, LCAL, MCAL, P2MT, TTUB, LEPC, MEPC, LMAL, MMAL. The first six are markers on the foot and the rest are markers on the leg. All the data measurements in this section are in decimeters.

All numerical experiments in this section were executed in Matlab 6.1 on a 2.0GHz Pentium IV PC with 512 MB memory running MS-Windows XP.

4.1 Best EDM

The best EDM of all 363 frames of data has been found by the algorithm in Section 2, using both conjugate gradient and quasi-Newton methods. Both give exactly the same results in almost the same CPU time with tolerance= 10^{-12}. Figure 3 shows the best coordinate points for the foot markers and Figure 4 shows the best coordinate points for both foot and leg markers. Table 4.1 shows the value of the objective function, the gradient $\|\mathbf{g}^{(k)}\|_2^2$ and the CPU time in seconds for the best EDM for the leg, foot and both leg and foot.

	ϕ	$\|\mathbf{g}^{(k)}\|_2^2$	CPU time
Leg	247.2982	1.6889e-007	14.8410
Foot	12.2281	5.3879e-009	12.2770
Leg and Foot	1.2377e+004	2.7674e-006	100.9160

Table 1: This table shows the value of the objective function, the gradient and the CPU time in seconds for the best EDM for the leg, foot and both leg and foot.

The best EDM for both leg and foot approximated to four digits is given by $D =$

$$\begin{bmatrix}
0 & 0.6031 & 0.6130 & 12.646 & 10.335 & 15.703 & 11.286 & 13.314 & 15.727 & 14.964 & 13.574 \\
0.6031 & 0 & 1.2477 & 14.540 & 13.219 & 17.824 & 14.537 & 15.445 & 18.040 & 18.194 & 16.869 \\
0.6130 & 1.2477 & 0 & 14.431 & 11.368 & 16.926 & 12.994 & 14.116 & 17.573 & 16.053 & 16.333 \\
12.646 & 14.540 & 14.431 & 0 & 0.900 & 0.3478 & 1.0918 & 0.4330 & 0.1980 & 0.9271 & 1.4267 \\
10.335 & 13.219 & 11.368 & 0.900 & 0 & 1.2024 & 0.2487 & 0.7059 & 1.1656 & 0.4336 & 1.3068 \\
15.703 & 17.824 & 16.926 & 0.3478 & 1.2024 & 0 & 1.6766 & 0.1666 & 0.1854 & 0.6406 & 2.3656 \\
11.286 & 14.537 & 12.994 & 1.0918 & 0.2487 & 1.6766 & 0 & 1.3841 & 1.2221 & 0.5976 & 0.4689 \\
13.314 & 15.445 & 14.116 & 0.4330 & 0.7059 & 0.1666 & 1.3841 & 0 & 0.5069 & 0.5431 & 2.5133 \\
15.727 & 18.040 & 17.573 & 0.1980 & 1.1656 & 0.1854 & 1.2221 & 0.5069 & 0 & 0.6350 & 1.3901 \\
14.964 & 18.194 & 16.053 & 0.9271 & 0.4336 & 0.6406 & 0.5976 & 0.5431 & 0.6350 & 0 & 1.4281 \\
13.574 & 16.869 & 16.333 & 1.4267 & 1.3068 & 2.3656 & 0.4689 & 2.5133 & 1.3901 & 1.4281 & 0
\end{bmatrix}$$

4.2 Fitting the frames

In Section 3, two methods have been described for finding the best fitting to each frame. In Table 4.2, the direct method explained in Section 3.1 and the optimal method explained in Section 3.2 are compared. We fit all 363 frames using these two methods, both satisfying the constraints $\|\mathbf{x}_i - \mathbf{x}_j\| = d_{ij}$. However, the optimal method is the best in terms of fitting the data to the nearest best coordinate points. As shown in Table 4.2, the frame Y_{387} fits the best EDM with $\sqrt{\phi} = 0.1248$ and the average $\sqrt{\phi}$ of all frames is 0.3427, while the direct method is far from these minimum values as can be seen in Table 4.2. Figure 5 shows frame Y_{181} as the center of the circles. The best fitting for the two methods is given by dot for the optimal method, and cross for the direct method. It is clear from the figure that the dots are nearer to the center of the circles from the crosses. Figure 6 shows a similar example but this time only for the foot with frame Y_{332}.

	$\sqrt{\phi}$ Direct	$\sqrt{\phi}$ Optimal	CPU for Direct	CPU for OP1	CPU for OP2
Average	0.58456	0.3427	0.00259	0.01285	0.1166
Maximum	1.01262	0.5403	0.01	0.04	0.921
Minimum	0.166134	0.1248	0	0	0.02

Table 2: Comparison between the direct method and the optimal method

In the contrast of Section 3.1, we found from the numerics by both methods, the direct method and optimal method that S contains small entries between -0.2 and 0.2, the determinant of Q is always one and the determinants of M range from 1.0409 and 0.90261, i.e. $\det(Q) = 1$, $\det(M) \approx 1$. This means we have a very stable orthogonal matrix. However, if we have a data with unstable matrix M, then we switch to the Algorithm 3.1.

Table 4.2 shows the amount of computations by both methods. In Table 4.2, OP1 means that the initial data for the optimal method are the solution obtained from the direct method while OP2 means that the initial data are remote from the optimal solution, specifically by choosing $v^{(0)} = \mathrm{P2MT}^T$ and $S^{(0)} = 0$. These CPU times are very small; however, in practice, considering the huge number of frames involved, fitting these frames will add up time and become large. It is clear from Table 4.2 that the direct method is almost 4 times faster than the OP1 and is almost 40 times faster than the OP2. The initial choice for OP2 will slow it down almost 10 times from OP1. These observations suggest that we always start with the direct method then we switch to the optimal method saving the data as an initial data for optimal method. These procedures are needed especially if we need high accuracy and they will reduce the amount of computations almost 10 times. If high accuracy is not required, then we can stop with the solution found by the direct method which can be found in almost no time.

5 Summery

This paper describes methods for rectifying the frame of markers from noisy point data. We were able to determine the best EDM for all the frames, and then fitted each frame to this best EDM. The methods were fast, reliable and able to remove the errors in the experimental data and gives the exact location of each marker with respect to the frame to which it was assigned. In conclusion, our methods were able to reconstruct orientation for each frame. Using this quantity directly from markers without correction is an unreliable process. By fitting each frame to the best EDM, our methods provide a much more reliable means of finding orientation.

References

[1] S. Al-Homidan. *Hybrid methods for optimization problems with positive semidefinite matrix constraints.* PhD thesis, University of Dundee, 1993.

[2] S. Al-Homidan and R. Fletcher. Hybrid methods for finding the nearest Euclidean distance matrix. In D. Du, L. Qi, and R. Womersley, editors, *Recent Advances in Nonsmooth optimization*, pages 1–7. World Scientific Publishing Co. Pte. Ltd., 1995.

[3] S. Al-Homidan and H.Wolkowicz. Approximate and exact completion problems for Euclidean distance matrices using semidefinite programming. *Linear Algebra Appl.*, 406:109–141, 2005.

[4] K.S. Arun, T.S. Huang, and S.D. Blostein. Least-Squares Fitting of Two 3-D Point Sets. *IEEE Trans. Patt. Anal. Machine Intell.*, Pami-9:698–700, 1987.

[5] A. Cappozzo, F. Catani, U. D. Croce, and A. Leardini. Position and orientation in space of bones during movement: anatomical frame definition and determination. *Clinical Biomechanics*, 10(4):171–178, 1995.

[6] A. Cappozzo, F. Catani, A. Leardini, M. G. Benedetti, and U. D. Croce. Position and orientation in space of bones during movement: experimental artefacts. *Clinical Biomechanics*, 11(2):99–100, 19962.

[7] G.M. Crippen and T.F. Havel. *Distance Geometry and Molecular Conformation*. Wiley, New York, 1988.

[8] D.W. Eggert, A. Lorusso, and R.B. Fisher. Estimating 3-D Rigid Body Transformations: A Comparison of Four Major Algorithms. *Machine Vision and Applications*, 9:272–290, 1997.

[9] W. Glunt, L. Hayden, S. Hong, and L. Wells. An alternating projection algorithm for computing the nearest Euclidean distance matrix. *SIAM J. Matrix Anal. Appl.*, 11(4):589–600, 1990.

[10] J. C. Gower. Properties of euclidean and non-euclidean distance matrices. *Linear Algebra Appl.*, 67:81–97, 1985.

[11] R.J. Hanson and M.J. Norris. Analysis of Measurements Based on the Singular Value Decomposition. *SIAM J. Sci. Stat. Comput.*, 2:363–373, 1981.

[12] T.L. Hayden, J. Wells, W-M. Liu ., and P. Tarazaga. The cone of distance matrices. *Linear Algebra Appl.*, 144:153–169, 1991.

[13] K. Kanatani. Analusis of 3-D Rotation Fitting. *IEEE Transaction on Pattern Analysis and Machine Intelligence*, 16:543–549, 1994.

[14] D. Karlsson and A. Lundberg. Accuracy estimation of kinematic data derived from bone anchored external markers. pages 27–30, Stockholm, Sweden, 1994. Proc. of the Third International Symposium on 3-D Analysis of Human Movement.

[15] M. Laurent. A tour d'horizon on positive semidefinite and Euclidean distance matrix completion problems. In *Topics in Semidefinite and Interior-Point Methods*, volume 18 of *The Fields Institute for Research in Mathematical Sciences, Communications Series*, pages 51–76, Providence, Rhode Island, 1998. American Mathematical Society.

[16] J. De Leeuw and W. Heiser. Theory of multidimensional scaling. In P. R. Krishnaiah and L. N. Kanal, editors, *Handbook of Statistics*, volume 2, pages 285–316. North-Holland, 1982.

[17] S. Lele. Euclidean distance matrix analysis (edma): Estimation of mean form and mean form difference.

[18] B. A. Maslen and T. R. Ackland. Radiographic study of skin displacement erors in the foot and ankle during standing. *Clinical Biomechanics*, 9(5):291–296, 1994.

[19] L. Mirsky. *An introduction to linear algebra.* Dover Publications Inc., New York, 1990. Reprint of the 1972 edition.

[20] I.J. Schoenberg. Remarks to Maurice Frechet's article: Sur la definition axiomatique d'une classe d'espaces vectoriels distancies applicables vectoriellement sur l'espace de Hilbert. *Ann. Math*, 36:724–732, 1935.

[21] N. Smith. Distance matrix and the euclidean distance matrix problem. Master's thesis, University of Dundee, 2003.

[22] I. Söderkvist and P.-Å. Wedin. Determining the Movements of the Skeleton Using Well-Configured Markers. *Journal of Biomechanics*, 26(12):1473–1477, 1993.

[23] C.W. Spoor and F.E Veldpaus. Rigid Body Motion Calculated from Spatial Coordinates of Markers. *Journal of Biomechanics*, 13:391–393, 1980.

[24] S. Stanhope, J. Holden, and J. Orsini. Effect of target attachment techniques on estimates of shank skeletal motion. *Gait & Posture*, 2:58, 1994.

[25] S. Umeyama. Least squares estimation of transformation parameters between two point patterns. *IEEE Trans. Pattern Anal. Mach. Intelligence*, PAMI-13:376–380, 1991.

[26] H.J Woltring. Representation and calculation of 3-D joint movement. *Human Movement Science*, 10:603–616, 1991.

[27] J. Young and R. Chellopa. 3-d motion estimation using a sequence of noisy stereo images: Models, estimation, and uniqueness results. *IEEE Transaction on Pattern Analysis and Machine Intelligence*, 12:735–759, 1990.

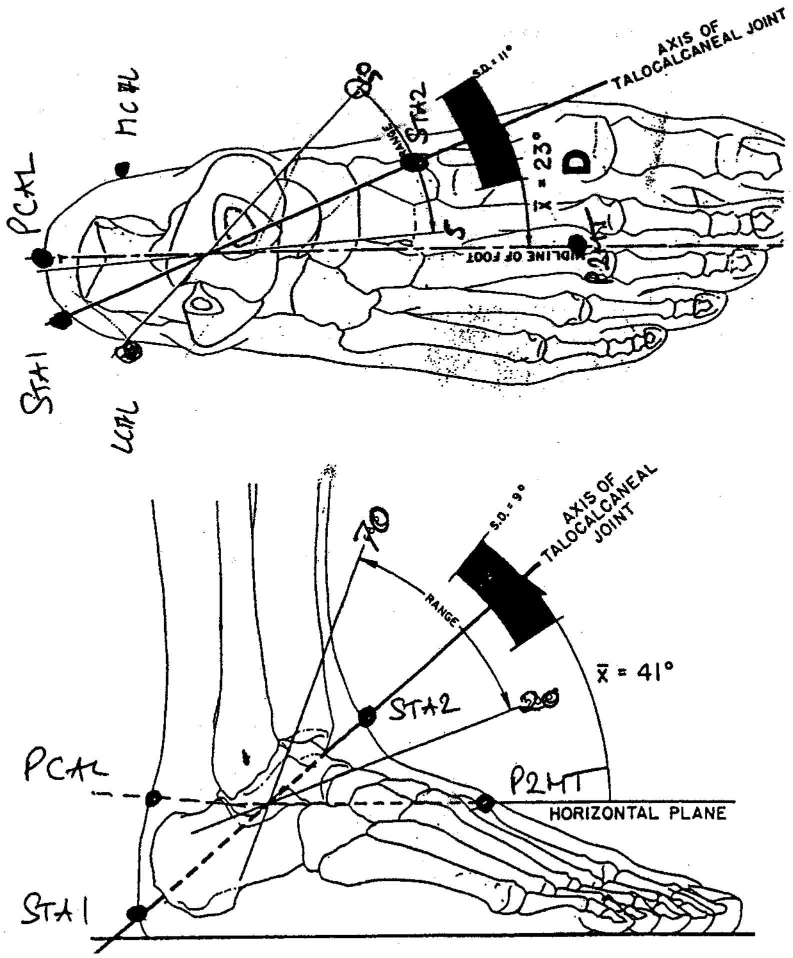

Figure 1: Shows a side view of the foot and a view from above with all six of the foot markers labeled to indicate where they would be ideally placed.

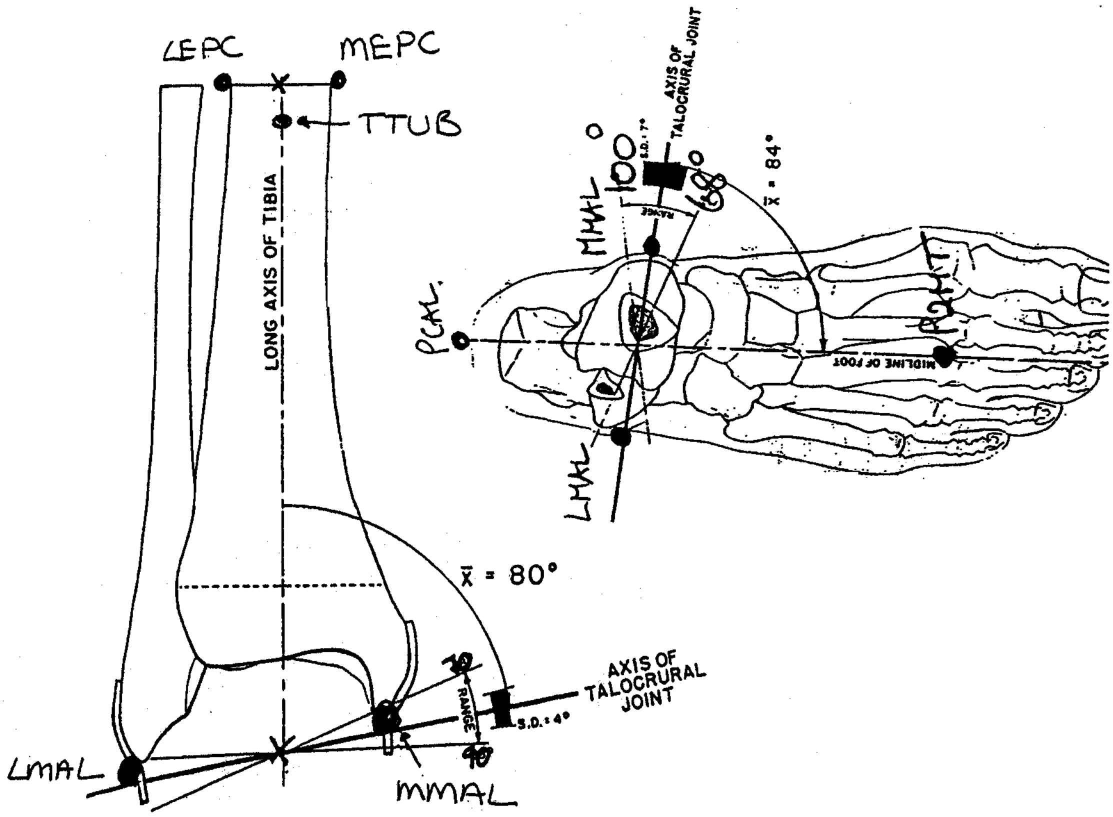

Figure 2: Shows a front view of the lower leg and a view from above the foot, with labels indicating where the leg markers are ideally placed in relation to the foot.

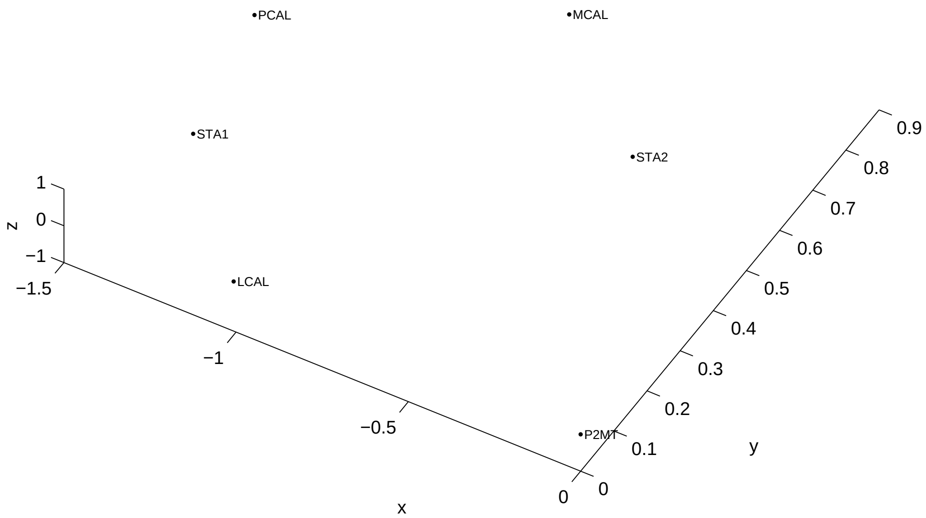

Figure 3: The best coordinate points for the foot markers

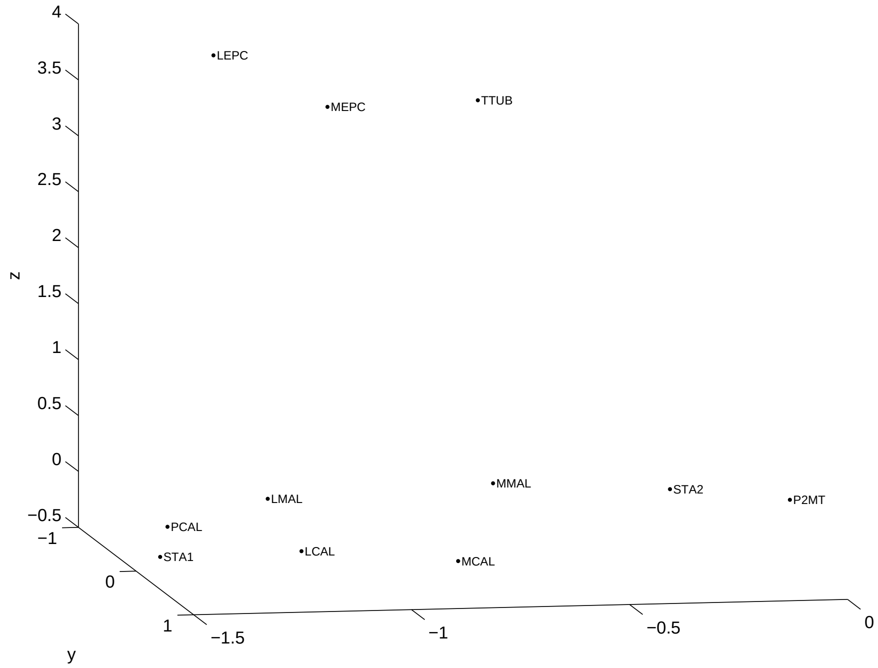

Figure 4: The best coordinate points for both foot and leg markers

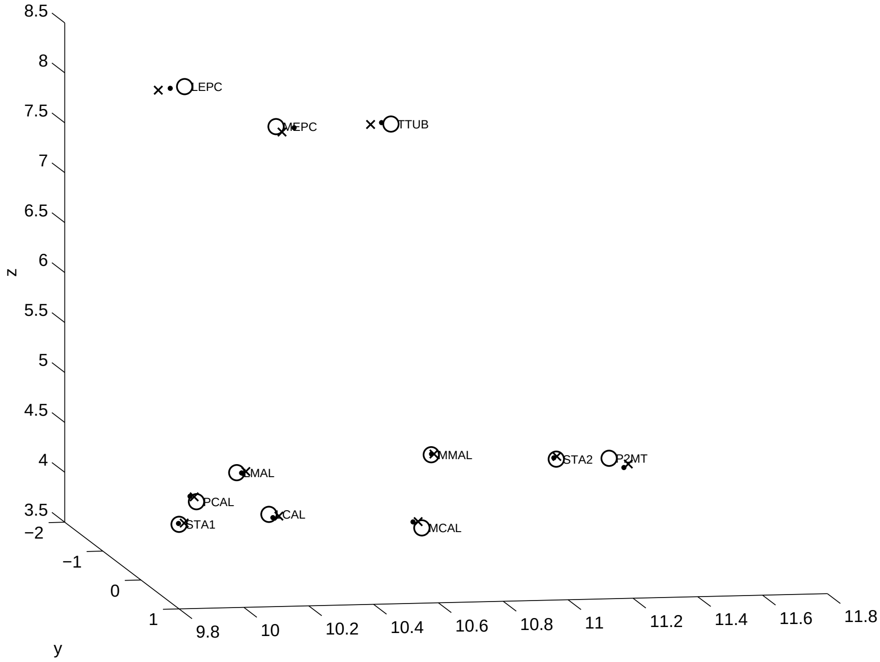

Figure 5: The best fitting for frame Y_{181}.

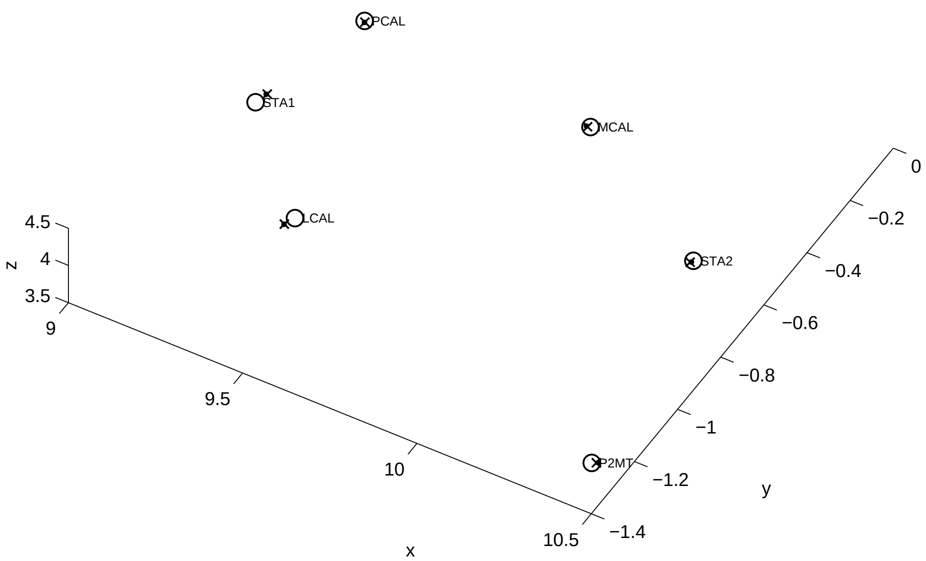

Figure 6: The best fitting for frame Y_{332} in the foot.