

Fitting affine and orthogonal transformations between two sets of points

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Abstract. *Let two point sets P and Q be given in \mathbb{R}^n . We determine a translation and an affine transformation or an isometry such that the image of Q approximates P as best as possible in the least squares sense.*

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1. Introduction

Let the two sets of points P and Q be given by

$$\mathbf{p}_i = (p_{1i}, \dots, p_{ni})^T, \quad \mathbf{q}_i = (a_{1i}, \dots, a_{ni})^T \quad (i = 1, \dots, m). \quad (1)$$

We are looking for some matrix

$$\mathbf{A} = (a_{jk})_{j,k=1,\dots,n} \quad (2)$$

and some translation vector

$$\mathbf{t} = (t_1, \dots, t_n)^T \quad (3)$$

such that

$$\mathbf{p}_i \approx \mathbf{A}\mathbf{q}_i + \mathbf{t} \quad (i = 1, \dots, m). \quad (4)$$

As the number of unknowns is $n^2 + n$, we require $m > n^2 + n$. One possible objective function to be minimized is the sum of squared Euclidean distances, i. e.

$$S(\mathbf{A}, \mathbf{t}) = \sum_{i=1}^m \|\mathbf{p}_i - \mathbf{A}\mathbf{q}_i - \mathbf{t}\|_2^2. \quad (5)$$

The first solution method will consist of a generalization of the least square fitting by a straight line ($n = 1$). The second method is an iteration method that could also be applied but should not.

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If \mathbf{A} is orthogonal, we will have the $n(n+1)/2$ side conditions

$$\mathbf{A}^T \mathbf{A} = \mathbf{I}, \quad \text{i. e. } \mathbf{a}_j^T \mathbf{a}_k = \delta_{jk} \quad (j \leq k) \quad (6)$$

where \mathbf{a}_j ($j = 1, \dots, n$) are the columns of \mathbf{A} . It will turn out in *Section 3* that it is easier to manage them implicitly and that the mentioned second method can be used here. Other methods are discussed in [1, 2, 4, 5].

2. Fitting affine transformations

The necessary and – because of linearity – also sufficient conditions for (5) to be minimized are

$$\frac{\partial S}{\partial a_{jk}} = -2 \sum_{i=1}^m (\mathbf{E}_{jk} \mathbf{q}_i)^T (\mathbf{p}_i - \mathbf{A} \mathbf{q}_i - \mathbf{t}) = 0 \quad (j, k = 1, \dots, n) \quad (7)$$

$$\frac{\partial S}{\partial \mathbf{t}} = -2 \sum_{i=1}^m (\mathbf{p}_i - \mathbf{A} \mathbf{q}_i - \mathbf{t}) = 0 \quad (8)$$

In (7) we set $\mathbf{E}_{jk} = \frac{\partial \mathbf{A}}{\partial a_{jk}}$, i. e. the $n \times n$ matrix that contains 1 in the j -th row and the k -th column and 0 elsewhere. As

$$(\mathbf{E}_{jk} \mathbf{q}_i)^T = (0, \dots, 0, q_{ki}, 0, \dots, 0), \quad (9)$$

where q_{ki} is in the j -th position, the conditions (7) will read

$$\left(\sum_{i=1}^m q_{1i} q_{ki} \right) a_{j1} + \dots + \left(\sum_{i=1}^m q_{ni} q_{ki} \right) a_{jn} + \left(\sum_{i=1}^m q_{ki} \right) t_j = \sum_{i=1}^m q_{ki} p_{ji} \quad (10)$$

$$(j, k = 1, \dots, n).$$

Additionally, (8) gives

$$\left(\sum_{i=1}^m q_{1i} \right) a_{j1} + \dots + \left(\sum_{i=1}^m q_{ni} \right) a_{jn} + m t_j = \sum_{i=1}^m p_{ji} \quad (11)$$

$$(j = 1, \dots, n).$$

In order to integrate (10) and (11) we introduce

$$q_{n+1,i} = 1 \quad (i = 1, \dots, m) \quad (12)$$

and put

$$\tilde{\mathbf{q}}_i = (q_{1i}, \dots, q_{ni}, q_{n+1,i})^T \quad (i = 1, \dots, m), \quad (13)$$

$$\tilde{\mathbf{Q}} = \sum_{i=1}^m \tilde{\mathbf{q}}_i \tilde{\mathbf{q}}_i^T, \quad (14)$$

$$\tilde{\mathbf{a}}_j = (a_{j1}, \dots, a_{jn}, t_j)^T, \quad (15)$$

$$\tilde{\mathbf{c}}_j = (\tilde{c}_{j1}, \dots, \tilde{c}_{j,n+1})^T \quad \text{with } \tilde{c}_{jk} = \sum_{i=1}^m q_{ki} p_{ji} \quad (k = 1, \dots, n+1). \quad (16)$$

Then (10) and (11) can be integrated within

$$\tilde{\mathbf{Q}}\tilde{\mathbf{a}}_j = \tilde{\mathbf{c}}_j \quad (j = 1, \dots, n). \quad (17)$$

Note that $\tilde{\mathbf{Q}}$ is common to all n systems of linear equations with $n + 1$ unknowns, i. e. you need just one LU-decomposition to solve all systems. $\tilde{\mathbf{Q}}$ will normally be positively definite for $m > n^2 + n$ and thus nonsingular.

Example 1. For Q we used $m = 20$ points $\mathbf{q}_i \in \mathbb{R}^3$ given by

$$Q = \begin{pmatrix} 0 & 1 & 0 & 1 & 1 & 0 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & 0 & 1 & -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & -1 & 1 & 0 & 0 & 0 & 1 & -1 & 0 & -1 & 0 & 1 & -1 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & -1 & 1 & 1 & 0 & -1 & 1 & 0 & 1 & -1 & 0 & -1 & 1 & -1 & 1 & 1 & -1 \end{pmatrix}$$

Then we used

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & 1 \\ 1 & -1 & 0 \end{pmatrix}, \quad \mathbf{t} = \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}$$

to produce $\mathbf{p}_i = \mathbf{A}\mathbf{q}_i + \mathbf{t}$ ($i = 1, \dots, 20$). In this case the minimal solution of (5) must give $S(\mathbf{A}, \mathbf{t}) = 0$. Of course, this was done, and \mathbf{A} and \mathbf{t} were retrieved.

Example 2. We disturbed a lot of coefficients of \mathbf{p}_i and \mathbf{q}_i randomly by ± 1 to receive

$$Q = \begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & 0 & 0 & -1 & 0 & 1 & 0 & 1 & -1 & 0 \\ 1 & 1 & 1 & -1 & 0 & -1 & 0 & -1 & -1 & 1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & -1 & 1 & 1 & 0 & -1 & 1 & 0 & 1 & -1 & 0 & -1 & 1 & 0 & 0 & 1 & -1 \end{pmatrix}$$

$$P = \begin{pmatrix} -1 & 0 & -1 & 0 & 1 & -2 & -2 & -3 & -1 & -3 & -1 & -3 & -1 & -2 & -1 & -1 & -1 & -1 & -2 & 0 \\ 1 & 1 & 2 & -1 & -1 & 0 & 2 & 0 & -2 & 1 & 1 & -1 & -1 & -1 & -1 & 3 & -1 & 0 & 1 & -1 \\ 0 & 1 & 1 & 2 & 2 & 3 & -1 & 1 & 1 & 1 & -1 & 1 & 0 & 0 & 2 & 0 & 1 & 2 & 1 & 1 \end{pmatrix}$$

We received

$$\mathbf{A} = \begin{pmatrix} .6564 & .1728 & -.5658 \\ -.0028 & .7831 & 1.0776 \\ .7316 & -.3747 & -.1107 \end{pmatrix}, \quad \mathbf{t} = \begin{pmatrix} -1.1058 \\ -.2724 \\ 1.0702 \end{pmatrix}$$

and $S(\mathbf{A}, \mathbf{t}) = 32.25425$.

Now we will mention an iterative descent method that, it is true, does not exceed the straightforward and direct solution of (13) but will also be able to be applied in the next section. We can write (8) as

$$\mathbf{t} = \frac{1}{m} \sum_{i=1}^m (\mathbf{p}_i - \mathbf{A}\mathbf{q}_i) \quad (18)$$

and (7) as

$$\sum_{i=1}^m (\mathbf{E}_{jk}\mathbf{q}_i)^T \mathbf{A}\mathbf{q}_i = \sum_{i=1}^m (\mathbf{E}_{jk}\mathbf{q}_i)^T (\mathbf{p}_i - \mathbf{t}) \quad (19)$$

We consider the following algorithm:

Step 0: Give some starting value $\mathbf{A}^{(0)}$ for \mathbf{A} , e. g. $\mathbf{A}^{(0)} = \mathbf{I}$. Set $w = 0$.

Step 1: Use (18) to calculate

$$\mathbf{t}^{(w+1)} = \frac{1}{m} \sum_{i=1}^m (\mathbf{p}_i - \mathbf{A}^{(w)} \mathbf{q}_i). \quad (20)$$

Step 2: Use (19) to calculate $\mathbf{A}^{(w+1)}$, i. e. to solve

$$\sum_{i=1}^m (\mathbf{E}_{jk} \mathbf{q}_i)^T \mathbf{A}^{(w+1)} \mathbf{q}_i = \sum_{i=1}^m (\mathbf{E}_{jk} \mathbf{q}_i)^T (\mathbf{p}_i - \mathbf{t}^{(w+1)}). \quad (21)$$

Step 3: STOP, if some convergence criterion is fulfilled, otherwise set $w := w + 1$ and go back to Step 1.

This alternating method gives a descent within every iteration. For the above two examples it converged to 6 correct digits within 6 and 9 iterations, respectively, and gave the same solution as (17).

3. Fitting orthogonal transformations

Orthogonal transformations are affine transformations with the property (6). Thus to the objective function (5) one could add the side conditions (6). Instead of trying to solve a nonlinear system after introducing the LAGRANGIAN function we will describe a more effective way. It is well-known [3] that every orthogonal matrix \mathbf{A} of size $n \times n$ can be written as a product

$$\mathbf{A} = \mathbf{R}_1 \cdots \mathbf{R}_N \mathbf{B}, \quad (22)$$

where

$$\mathbf{R}_\ell = \mathbf{R}(\varphi_{jk}) \quad (\ell = 1, \dots, N = \frac{(n-1)n}{2}) \quad (23)$$

and where $\mathbf{R}(\varphi_{jk}) = (r_{is})_{i,s=1,\dots,n}$ has the elements

$$\begin{aligned} r_{jj} = r_{kk} &= \cos(\varphi_{jk}) \\ r_{jk} = -r_{kj} &= -\sin(\varphi_{jk}) \\ r_{ii} = 1 \quad (i \neq j, k), \quad r_{is} &= 0 \text{ else.} \end{aligned} \quad (24)$$

The indices ℓ uniquely correspond to pairs (j, k) with $j < k$ as indicated in the following table:

ℓ	1	2	\cdots	$n-1$	n	$n+1$	\cdots	$2n-3$	$2n-2$	\cdots	N
(j, k)	(1, 2)	(1, 3)	\cdots	(1, n)	(2, 3)	(2, 4)	\cdots	(2, n)	(3, 4)	\cdots	($n-1, n$)

Finally, $\mathbf{B} = \mathbf{I}$ (identity) for $\det \mathbf{A} = +1$ [3, 6] and $\mathbf{B} = \text{diag}(1, 1, \dots, 1, -1)$ for $\det \mathbf{A} = -1$ [3]. The angles φ_{ik} are called the EULER rotation angles. We will also write

$$\boldsymbol{\varphi} = (\varphi_1, \dots, \varphi_N)^T$$

With this notation the objective function (5) to be minimized here reads

$$S(\boldsymbol{\varphi}, \mathbf{t}) = \sum_{i=1}^m \|\mathbf{p}_i - \mathbf{R}_1 \mathbf{R}_2 \cdots \mathbf{R}_N \mathbf{B} \mathbf{q}_i - \mathbf{t}\|_2^2. \quad (25)$$

The necessary conditions for a minimum are

$$\frac{\partial S}{\partial \mathbf{t}} = -2 \sum_{i=1}^m (\mathbf{p}_i - \mathbf{R}_1 \cdots \mathbf{R}_N \mathbf{B} \mathbf{q}_i - \mathbf{t}) = 0, \quad (26)$$

$$\frac{\partial S}{\partial \varphi_\ell} = -2 \sum_{i=1}^m (\mathbf{p}_i - \mathbf{R}_1 \cdots \mathbf{R}_N \mathbf{B} \mathbf{q}_i - \mathbf{t})^T \mathbf{R}_1 \cdots \mathbf{R}_{\ell-1} \mathbf{R}'_\ell \mathbf{R}_{\ell+1} \cdots \mathbf{R}_N \mathbf{B} \mathbf{q}_i = 0 \quad (27)$$

$$(\ell = 1, \dots, N),$$

where the matrix

$$\mathbf{R}'_\ell = \frac{\partial \mathbf{R}_\ell}{\partial \varphi_{jk}} \quad (28)$$

has the coefficients

$$\begin{aligned} r'_{jj} = r'_{kk} &= -\sin(\varphi_{jk}), \\ r'_{jk} &= -r'_{kj} = -\cos(\varphi_{jk}), \\ r'_{is} &= 0 \quad \text{else.} \end{aligned} \quad (29)$$

Note that the matrix

$$\mathbf{C}_\ell = \mathbf{R}_\ell^T \mathbf{R}'_\ell = (c_{is})_{i,s=1,\dots,n} \quad (30)$$

has the elements

$$c_{jk} = -c_{kj} = -1, \quad c_{is} = 0 \quad \text{else.} \quad (31)$$

Now (26) can be written as

$$\mathbf{t} = \mathbf{t}(\boldsymbol{\varphi}) = \frac{1}{m} \sum_{i=1}^m (\mathbf{p}_i - \mathbf{R}_1 \cdots \mathbf{R}_N \mathbf{B} \mathbf{q}_i) \quad (32)$$

and (27) as

$$\begin{aligned} - \sum_{i=1}^m (\mathbf{p}_i - \mathbf{t})^T \mathbf{R}_1 \cdots \mathbf{R}'_\ell \cdots \mathbf{R}_N \mathbf{q}_i &= - \sum_{i=1}^m \mathbf{q}_i^T \mathbf{R}_N^T \cdots \mathbf{R}_1^T \mathbf{R}_1 \cdots \mathbf{R}'_\ell \cdots \mathbf{R}_N \mathbf{q}_i \\ &= - \sum_{i=1}^m \mathbf{s}_i^T \mathbf{R}_\ell^T \mathbf{R}'_\ell \mathbf{s}_i \\ &= - \sum_{i=2}^m \mathbf{s}_i^T \mathbf{C}_\ell \mathbf{s}_i \end{aligned} \quad (33)$$

where $\mathbf{s}_i = \mathbf{R}_{\ell+1} \cdots \mathbf{R}_N \mathbf{B} \mathbf{q}_i$. But because of (31) the right-hand side of (33) is zero. Thus (27) reduces to

$$-\sum_{i=1}^m (\mathbf{p}_i - \mathbf{t})^T \mathbf{R}_1 \cdots \mathbf{R}_{\ell-1} \mathbf{R}'_{\ell} \mathbf{R}_{\ell+1} \cdots \mathbf{R}_N \mathbf{B} \mathbf{q}_i = 0. \quad (34)$$

Putting

$$\begin{aligned} \mathbf{u}_i^{(\ell)T} &= (\mathbf{p}_i - \mathbf{t})^T \mathbf{R}_1 \cdots \mathbf{R}_{\ell-1}, \\ \mathbf{v}_i^{(\ell)} &= \mathbf{R}_{\ell+1} \cdots \mathbf{R}_N \mathbf{B} \mathbf{q}_i, \end{aligned} \quad (i = 1, \dots, m; \ell = 1, \dots, N) \quad (35)$$

(34) reads

$$-\sum_{i=1}^m \mathbf{u}_i^{(\ell)T} \mathbf{R}'_{\ell} \mathbf{v}_i^{(\ell)} = 0 \quad (36)$$

Using (29) this results in

$$g_{jk} \sin(\varphi_{jk}) - f_{jk} \cos(\varphi_{jk}) = 0, \quad (37)$$

where

$$\begin{aligned} f_{jk} &= \sum_{i=1}^m v_{ij}^{(\ell)} u_{ik}^{(\ell)} - v_{ik}^{(\ell)} u_{ij}^{(\ell)}, \\ g_{jk} &= \sum_{i=1}^m v_{ij}^{(\ell)} u_{ij}^{(\ell)} + v_{ik}^{(\ell)} u_{ik}^{(\ell)}. \end{aligned} \quad (38)$$

Thus $\varphi_{ik} = \varphi_{\ell}$ is given by

$$\varphi_{ik} = \operatorname{atan} \left(\frac{f_{jk}}{g_{jk}} \right). \quad (39)$$

A minimum of S w.r.t. φ_{jk} is given by (39) if

$$\frac{1}{2} \frac{\partial^2 S}{\partial \varphi_{ik}^2} = g_{jk} \cos(\varphi_{jk}) + f_{jk} \sin(\varphi_{jk}) > 0. \quad (40)$$

Otherwise φ_{jk} has to be replaced by $\varphi_{jk} + \pi$. Additionally, in order to avoid negative angles, we replace φ_{jk} by $\varphi_{jk} + 2\pi$. Altogether we can now design the following descent algorithm:

- Step 1: Give starting values $\varphi_{\ell}^{(0)}$ ($\ell = 1, \dots, N$), e.g. $\varphi_{\ell}^{(0)} = 0$. Decide whether to use $\mathbf{B} = \mathbf{I}$ or $\mathbf{B} = \operatorname{diag}(1, \dots, 1, -1)$. Set $w = 0$.
- Step 2: Calculate $\mathbf{R}_{\ell}^{(w)} = \mathbf{R}(\varphi_{\ell}^{(w)})$ ($\ell = 1, \dots, N$) corresponding to (23) and (24).
- Step 3: Set $\mathbf{F} := \mathbf{R}_2^{(w)} \cdots \mathbf{R}_N^{(w)}$ and $\mathbf{G} := \mathbf{I}$.

Step 4: Corresponding to (32) calculate

$$\mathbf{t}^{(w)} = \frac{1}{m} \sum_{i=1}^m (\mathbf{p}_i - \mathbf{R}_1^{(w)} \mathbf{F} \mathbf{q}_i)$$

Step 5: do $\ell = 1, N$

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g := 0; f := 0; if  $\ell = N$  then  $\mathbf{F} := \mathbf{I}$ 
do  $i = 1, m$ 
 $\mathbf{u}^T := (\mathbf{p}_i - \mathbf{t}^{(w)})^T \mathbf{G}$ 
 $\mathbf{v} := \mathbf{F} \mathbf{q}_i$ 
 $g := g + v_j u_k - v_k u_j$ 
 $f := f + v_j u_j + v_k u_k$ 
end  $i$ 
 $\varphi = \text{atan}(g/f)$ 
if  $(g \cos(\varphi) + f \sin(\varphi)) \leq 0$  then  $\varphi := \varphi + \pi$ 
if  $(\varphi < 0)$  then  $\varphi := \varphi + 2\pi$ 
 $\varphi_\ell^{(w+1)} := \varphi$ ;  $\mathbf{R}_\ell^{(w+1)} := \mathbf{R}(\varphi)$ 
if  $(\ell < n)$  then

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$$\mathbf{G} := \mathbf{G} \mathbf{R}_\ell^{(w+1)}; \quad \mathbf{F} := \mathbf{R}_{\ell+1}^{(w)T} \mathbf{F}$$

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end  $if$ 

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end  $\ell$ 

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Step 6: Set $w := w + 1$. If some convergence criterion is not fulfilled, then go back to Step 3; otherwise set $\mathbf{t} := \mathbf{t}^{(w)}$ and $\mathbf{A} := \mathbf{R}_1^{(w)} \cdots \mathbf{R}_N^{(w)} \mathbf{B}$ and stop.

Convergence of this algorithm to a global minimum cannot be proved. However, empirically, the global minimum was always attained independently of the starting values for $\varphi^{(0)}$. We will give some examples where we always used $\varphi_\ell^{(0)} = 0$ ($\ell = 1, \dots, N$).

Starting with a set Q of $m = 20$ points $\mathbf{a}_i \in \mathbb{R}^4$, namely

$$Q = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 2 & 2 \\ 0 & 1 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 2 & 2 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 1 & 1 & 2 & 0 & 2 & 2 & 2 \\ 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 2 & 0 \end{pmatrix}$$

and angles $\varphi_\ell = \ell$ ($\ell = 1, \dots, 6$) and a translation $\mathbf{t} = (-1, 0, 1, 2)^T$ we produced $\mathbf{p}_i = \mathbf{R}_1 \cdots \mathbf{R}_6 \mathbf{q}_i + \mathbf{t}$ ($i = 1, \dots, m = 20$).

Example 3. Using those data after 206 iterations we got $S = 0.00000$ (as expected) and $\mathbf{t} = (-1.0000, 0.0000, 1.0000, 2.0000)^T$; instead of $\varphi_\ell = \ell$ ($\ell = 1, \dots, 6$) we ended up with $\varphi_1 = 1.0000$, $\varphi_2 = 5.1416$, $\varphi_3 = .1416$, $\varphi_4 = 5.4248$, $\varphi_5 =$

1.8584, $\varphi_6 = 6.0000$. This result is right because with $(\varphi_1, \dots, \varphi_6)^T$ (among others) $(\varphi_1, \varphi_2 + \pi, \pi - \varphi_3, 3\pi - \varphi_4, \varphi_5 - \pi, \varphi_6)^T$ is also a global minimum.

Example 4. We used the same data as before but dropped all components of p_i from $d_1.d_2d_3d_4d_5d_6$ to $d_1.d_2$ thus introducing small errors. After 202 iterations we received $S = 0.07328$, $\mathbf{t} = (-.9644, -.0459, .9469, 1.9441)^T$ and $\boldsymbol{\varphi} = (.9614, 5.1497, .1431, 5.3838, 1.8640, 5.9972)^T$. As expected, these results do not differ very much from those of Example 3.

Example 5. We further dropped the components of p_i from $d_1.d_2$ to integer values d_1 getting

$$P = \begin{pmatrix} 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & -1 & -2 & 0 & -1 & 0 & -1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 1 & 3 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 0 \\ 2 & 3 & 3 & 2 & 2 & 1 & 1 & 2 & 2 & 3 & 2 & 2 & 1 & 1 & 2 & 2 & 3 & 4 & 3 & 4 \end{pmatrix}$$

After 258 iterations we got $S = 5.66304$, $\mathbf{t} = (-.5893, -.5366, .6593, 1.6014)^T$ and $\boldsymbol{\varphi} = (1.3334, 5.0294, .1224, 5.5977, 2.0565, 6.0189)^T$. Of course, these results differ more than before. Varying the starting values $\boldsymbol{\varphi}^{(0)}$ we always received the same results, i.e. hopefully a global minimum.

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