МАТЕМАТИКА И МАТЕМАТИЧЕСКО ОБРАЗОВАНИЕ, 2013
MATHEMATICS AND EDUCATION IN MATHEMATICS, 2013
Proceedings of the Forty Second Spring Conference
of the Union of Bulgarian Mathematicians
Borovetz, April 2–6, 2013

VECTOR DECOMPOSITION OF HALF TURNS*

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This study concerns the special case of the symmetric three-dimensional orthogonal matrices and here we suggest a direct method for a representation of any such matrix as a consecutive composition of rotations about three almost arbitrarily chosen axes. Using a suitable representation the task is reduced to solving of a system of quadratic equations for the scalar parameters of the rotations in the decomposition. Then a comparison of the matrix entries selects the actual solutions and dismisses the fake ones. The algorithm is explained in detail and illustrated at the end of the paper via an example.

1. Introduction. The necessity of decomposing the complex rotational motions into two or three successive rotations is dictated by the practical needs of industry and engineering sciences. It is worth to mention that the factorizations of orthogonal matrices play an important role in modern navigation and control of aircrafts, submarines, and communication satellites [8], crystallography and diffractometry [2], or digital image processing [6] and optics [10]. In any of these areas it is necessary to perform several successive displacements in order to obtain the desired setting. Besides, one must construct a framework which is logically and physically free of some constraints because everything happens in the ordinary Euclidean space. It is exactly this fact which explains why the group of the orthogonal matrices in $\mathbb{R}^3$ is somewhat special not only because its various physical applications, but also because for $n = 3$ we have an isomorphism between one-forms and two-forms given by the *Hodge* duality $* : \Lambda^k(\mathbb{R}^n) \to \Lambda^{n-k}(\mathbb{R}^n)$. In this particular case it can be interpreted as a one-to-one correspondence between the vectors and the skew-symmetric matrices in $\mathbb{R}^3$. Since the latter constitute the Lie algebra $\mathfrak{so}(3)$, this allows the standard representation of the rotation generators to be given by the exceptional formula $* : \mathbf{c} \to \mathcal{A}(\mathbf{c}) = \mathbf{c}^\times$, or in components $(\mathbf{c}^\times)_{ij} = \varepsilon_{ilj} c_l$, where ε_{ilj} are the entries of the *Levi-Civita* symbol and the summation is performed over repeated indices following *Einstein* convention. In this way any skew-symmetrical matrix $\mathcal{A}$ can be easily written in the form

$$\mathcal{A}(\mathbf{c}) = \begin{pmatrix} 0 & -c_3 & c_2 \\ c_3 & 0 & -c_1 \\ -c_2 & c_1 & 0 \end{pmatrix}.$$

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*2000 Mathematics Subject Classification: 22E15, 22E70, 81R05.
Key words: Euler angles, vector parametrization, factorization.

Geometrically the so-called *vector parameter* $\mathbf{c}$ determines the axis of rotation and its magnitude is connected to the angle of rotation φ by the simple formula

$$\mathbf{c} = \tan\frac{\varphi}{2}\,\hat{\mathbf{n}}, \qquad \hat{\mathbf{n}}^2 = 1. \tag{1}$$

Then the actual matrix of the corresponding orthogonal operator can be obtained in the standard way as $\mathcal{R} = \exp\mathcal{A}$, or alternatively by *Rodrigues'* formula [11]

$$\mathcal{R}(\hat{\mathbf{n}}\,,\varphi) = \cos\varphi\,\mathcal{I} + (1-\cos\varphi)\,\hat{\mathbf{n}}\otimes\hat{\mathbf{n}}^t + \sin\varphi\,\hat{\mathbf{n}}^{\times} \tag{2}$$

which, in combination with the trigonometric *Euler* substitution $|\mathbf{c}| = \tan\frac{\varphi}{2}$, leads to

$$\mathcal{R}(\mathbf{c}) = \frac{(1-\mathbf{c}^2)\,\mathcal{I} + 2\,\mathbf{c}\otimes\mathbf{c}^t + 2\,\mathbf{c}^{\times}}{1+\mathbf{c}^2} \tag{3}$$

where $\mathbf{c}\otimes\mathbf{c}^t$ stands for the usual tensor product of vectors used for the construction of projectors in components $(\mathbf{c}\otimes\mathbf{c}^t)_{ij} = \mathbf{c}_i\mathbf{c}_j$ and $\mathcal{I}$ is the identity operator.
The above expression can also be written in components as

$$\mathcal{R}(\mathbf{c}) = \frac{2}{1+\mathbf{c}^2}\begin{pmatrix} 1+c_1^2 & c_1c_2 - c_3 & c_1c_3 + c_2 \\ c_1c_2 + c_3 & 1+c_2^2 & c_2c_3 - c_1 \\ c_3c_1 - c_2 & c_3c_2 + c_1 & 1+c_3^2 \end{pmatrix} - \mathcal{I}. \tag{4}$$

There is a composition law for the vector parameters (sometimes called also *Rodrigues'* or *Gibbs* parameters) which is thoroughly described in [3], that comes quite handy for our considerations. Namely, from the group properties of the $\mathsf{SO}(3)$ matrices it can be derived an explicit formula about the composition of the vector parameters producing the vector parameter corresponding to the compound rotation, i.e., $\mathcal{R}(\mathbf{a})\,\mathcal{R}(\mathbf{b}) = \mathcal{R}(\langle\,\mathbf{a},\mathbf{b}\rangle)$. The group low in the space of vector parameters is remarkably simple , i.e.,

$$\langle\,\mathbf{a},\mathbf{b}\rangle = \frac{\mathbf{a}+\mathbf{b}+\mathbf{a}\times\mathbf{b}}{1-(\,\mathbf{a}\,,\mathbf{b})}\cdot \tag{5}$$

In the above formula " $\times$ ", respectively $(\cdot,\cdot)$ denote the cross and dot products of the vectors in $\mathbb{R}^3$. It is not so hard to obtain a similar formula for the composition of three rotations. In that case it can be shown that the compound vector parameter of $\mathcal{R}(\mathbf{a})\,\mathcal{R}(\mathbf{b})\,\mathcal{R}(\mathbf{c})$ is just

$$\langle\langle\,\mathbf{a},\mathbf{b}\rangle,\mathbf{c}\rangle = \frac{\mathbf{a}+\mathbf{b}+\mathbf{c}+\mathbf{a}\times\mathbf{b}+\mathbf{a}\times\mathbf{c}+\mathbf{b}\times\mathbf{c}+(\,\mathbf{a}\times\mathbf{b})\times\mathbf{c}-(\,\mathbf{a}\,,\mathbf{b})\,\mathbf{c}}{1-(\,\mathbf{a}\,,\mathbf{b})-(\,\mathbf{a}\,,\mathbf{c})-(\,\mathbf{b}\,,\mathbf{c})-(\,\mathbf{a}\,,\mathbf{b}\times\mathbf{c})}\,. \tag{6}$$

Note that this operation is associative, but not commutative unless the vectors are parallel.

2. Technicalities. We concentrate our effort on the particular case of a symmetric orthogonal matrix of the type

$$\mathcal{O}(\hat{\mathbf{n}}) = 2\,\hat{\mathbf{n}}\otimes\hat{\mathbf{n}} - \mathcal{I} \tag{7}$$

that is basically a rotation by an angle π about the axis specified by the unit vector $\hat{\mathbf{n}}$. It is easy to see that just like in the plane, $-\mathcal{O}(\mathbf{n})$ is a mirror reflection with respect to the plane, normal to $\hat{\mathbf{n}}$. Let us choose three unit vectors $\hat{\mathbf{c}}_k$, possibly coplanar, but such that $\hat{\mathbf{c}}_2$ is not parallel to any of the other two. These will play the role of axes of rotations in our decomposition

$$\mathcal{O}(\hat{\mathbf{n}}) = \mathcal{R}_3(w\hat{\mathbf{c}}_3)\mathcal{R}_2(v\hat{\mathbf{c}}_2)\mathcal{R}_1(u\hat{\mathbf{c}}_1). \tag{8}$$

In order to find the equations for u, v and w we use (8) and suitably chosen scalar products (see also [7]). Let us start with

$$(\hat{\mathbf{c}}_3, \mathcal{O}(\hat{\mathbf{n}})\, \hat{\mathbf{c}}_1) = (\hat{\mathbf{c}}_3, \mathcal{R}_3(w\hat{\mathbf{c}}_3)\mathcal{R}_2(v\hat{\mathbf{c}}_2)\mathcal{R}_1(u\hat{\mathbf{c}}_1)\, \hat{\mathbf{c}}_1) = (\hat{\mathbf{c}}_3, \mathcal{R}_2(v\hat{\mathbf{c}}_2)\, \hat{\mathbf{c}}_1)$$

where we use the fact that $\hat{\mathbf{c}}_1$ is an eigenvector of $\mathcal{R}_1$ with eigenvalue equal to one and so is $\hat{\mathbf{c}}_3$ for $\mathcal{R}_3$ for any value of their scalar parameters. In combination with (3), this leads to a quadratic equation for v in the form

$$(\rho_1\rho_3 - \kappa_{12}\kappa_{23})\, v^2 + \omega\, v + \rho_1\rho_3 - \kappa_{13} = 0 \tag{9}$$

in which for simplicity we use the notation $\kappa_{ij} = (\hat{\mathbf{c}}_i, \hat{\mathbf{c}}_j)$ for the components of the *Gram* matrix of the vectors $\hat{\mathbf{c}}_k$, $\rho_i = (\hat{\mathbf{n}}, \hat{\mathbf{c}}_i)$ for the scalar products with $\hat{\mathbf{n}}$ and $\omega = (\hat{\mathbf{c}}_1, \hat{\mathbf{c}}_2 \times \hat{\mathbf{c}}_3)$ stands for their triple product. This equation has real solutions whenever its discriminant is non-negative, that is

$$\omega^2 = \det(\kappa) \geq 4\, (\rho_1\rho_3 - \kappa_{12}\kappa_{23})\, (\rho_1\rho_3 - \kappa_{13})\,.$$

Taking into account that κ is symmetric with diagonal elements equal to one, we may easily write its determinant as

$$\det(\kappa) = 1 + 2\kappa_{12}\kappa_{23}\kappa_{13} - \kappa_{12}^2 - \kappa_{13}^2 - \kappa_{23}^2$$

which allows for expressing the above inequality as

$$4\, (\rho_1\rho_3 - \kappa_{12}\kappa_{23} - \kappa_{13})\, \rho_1\rho_3 \leq 1 - 2\kappa_{12}\kappa_{23}\kappa_{13} - \kappa_{12}^2 - \kappa_{13}^2 - \kappa_{23}^2. \tag{10}$$

Thus we recover the condition

$$\left(\hat{\mathbf{c}}_1, (\mathcal{O}(\hat{\mathbf{n}}) - \hat{\mathbf{c}}_2 \otimes \hat{\mathbf{c}}_2^t)\, \hat{\mathbf{c}}_3\right)^2 \leq \left(1 - (\hat{\mathbf{c}}_1, \hat{\mathbf{c}}_2)^2\right) \left(1 - (\hat{\mathbf{c}}_3, \hat{\mathbf{c}}_2)^2\right) \tag{11}$$

given in [9]. The reader will find there the derivation of this inequality and the proof why it should be considered as a necessary and sufficient condition for the existence of the decomposition (8).

If it is fulfilled, we may solve the above equation for v and use the two roots $v_\pm$ for the computation of the matrix entries of $\mathcal{R}_1$ in a very similar way

$$(\hat{\mathbf{c}}_3, \mathcal{O}(\hat{\mathbf{n}})\, \hat{\mathbf{c}}_2) = (\hat{\mathbf{c}}_3, \mathcal{R}_3(w\hat{\mathbf{c}}_3)\mathcal{R}_2(v_\pm\hat{\mathbf{c}}_2)\mathcal{R}_1(u\hat{\mathbf{c}}_1)\, \hat{\mathbf{c}}_2) = (\hat{\mathbf{c}}_3, \mathcal{R}_2(v_\pm\hat{\mathbf{c}}_2)\mathcal{R}_1(u\hat{\mathbf{c}}_2)\, \hat{\mathbf{c}}_2)$$

which leads to a pair of quadratic equations for the scalar parameter u

$$\left(\rho_2\rho_3(v_\pm^2 + 1) + \kappa_{12}\nu_\pm\right) u^2 + \mu_\pm u + (\rho_2\rho_3 - \kappa_{23})\, (v_\pm^2 + 1) = 0 \tag{12}$$

where

$$\begin{aligned} \nu_\pm &= \kappa_{13}(v_\pm^2 - 1) - 2\kappa_{12}\kappa_{23}v_\pm^2 + 2\omega\, v_\pm \\ \mu_\pm &= \omega(v_\pm^2 - 1) + 2(\kappa_{12}\kappa_{23} - \kappa_{13})v_\pm. \end{aligned}$$

Hence we have four solutions for u. Now it remains to determine only the value of w by exploiting the equality

$$\begin{aligned} (\hat{\mathbf{c}}_2, \mathcal{O}(\hat{\mathbf{n}})\, \hat{\mathbf{c}}_1) &= (\hat{\mathbf{c}}_2, \mathcal{R}_3(w\hat{\mathbf{c}}_3)\mathcal{R}_2(v_\pm\hat{\mathbf{c}}_2)\mathcal{R}_1(u\hat{\mathbf{c}}_1)\, \hat{\mathbf{c}}_1) \\ &= (\hat{\mathbf{c}}_2, \mathcal{R}_3(w\hat{\mathbf{c}}_3)\mathcal{R}_2(v_\pm\hat{\mathbf{c}}_2)\, \hat{\mathbf{c}}_1) \end{aligned}$$

from which we derive the corresponding quadratic equations

$$\left(\rho_1\rho_2(v_\pm^2 + 1) + \kappa_{23}\nu_\pm\right) w^2 + \mu_\pm w + (\rho_1\rho_2 - \kappa_{12})\, (v_\pm^2 + 1) = 0. \tag{13}$$

In this way we end up with eight candidates for *Euler* decomposition, since each of the three quadratic equations has two solutions in the generic case. To choose the actual

solution or solutions to the problem among these eight possibilities one may simply compare their matrix entries with the corresponding entries of $\mathcal{O}(\hat{\mathbf{n}})$.
However, we may use another trick here. Note that representation (4) should be possible for any special orthogonal transformation, in particular for a matrix of the type (7). In order to make (4) symmetric is one has only two options - either set the vector parameter equal to zero and obtain the identity matrix or take the limit $|\,\mathbf{c}\,| \to \infty$ in (4) and end up with a half turn of the type (7). Since this limiting procedure yields a vanishing denominator for the composed vector parameters in (6), we have another independent condition that in our notation reads

$$(\,\mathbf{c}_1\,,\,\mathbf{c}_2) + (\,\mathbf{c}_1\,,\,\mathbf{c}_3) + (\,\mathbf{c}_2\,,\,\mathbf{c}_3) - (\,\mathbf{c}_1\,,\,\mathbf{c}_2 \times \mathbf{c}_3) = 1$$

which can be rewritten for the scalar parameters as

$$\kappa_{12}uv + \kappa_{13}uw + \kappa_{23}vw - \omega uvw = 1. \tag{14}$$

The above formula can be successfully used in the algorithm as an additional condition for the system of quadratic equations (9), (12) and (13), or as a base for an alternative approach.

3. The algorithm. We start our calculations with an input of four vectors: $\mathbf{c}_1, \mathbf{c}_2, \mathbf{c}_3$ and $\mathbf{n}$. First we make all vectors with unit length by a simple re-scaling $\mathbf{v} \to \hat{\mathbf{v}} = \dfrac{\mathbf{v}}{|\,\mathbf{v}\,|}\cdot$
Next we construct the operator $\mathcal{O}(\hat{\mathbf{n}}) = 2\,\hat{\mathbf{n}} \otimes \hat{\mathbf{n}}^t - \mathcal{I}$, calculate all scalar products involved in the equations (9), (12) and (13) – that is ω, κ_{ij}, σ_{ij} and ξ_i and then, after obtaining the solutions $v_\pm$ of (9), do the same for $v_\pm^2 \pm 1$, $\nu_\pm$ and $\mu_\pm$, so that these expressions do not have to be computed repeatedly. Then we construct a procedure to calculate the matrices $\mathcal{R}_1(u\hat{\mathbf{c}}_1)$, $\mathcal{R}_2(v\hat{\mathbf{c}}_2)$ and $\mathcal{R}_3(w\hat{\mathbf{c}}_3)$ based on formula (4).
Before moving on we need to check whether the necessary and sufficient conditions for the existence of a generalized *Euler* representation are fulfilled, namely that the vector $\hat{\mathbf{c}}_2$ is not parallel to any of the other two vectors $\hat{\mathbf{c}}_1$ and $\hat{\mathbf{c}}_3$ together with the inequality for the discriminant (11), or better its more convenient form (10). If the conditions are satisfied, we proceed to solving the equation (9), then substituting its roots $v_\pm$ in (12) and (13) to solve for u and w. Each time we obtain a new solution, we calculate each of the matrices $\mathcal{R}_k$ using the previously designed for this procedure, obtain the product $\mathcal{R}_3\,\mathcal{R}_2\,\mathcal{R}_1$ and check whether it has the same matrix entries as $\mathcal{O}(\hat{\mathbf{n}})$ or, as we did in our routine, if the norm of $\mathcal{O} - \mathcal{R}_3\,\mathcal{R}_2\,\mathcal{R}_1$ vanishes (within the machine precision as far as numerical operations are involved). If not, we continue searching for a true solution, if so – we stop there, remember the parameters and calculate the corresponding generalized *Euler* angles using formula (1). Since the solution may not be unique, and in fact typically there are two of them, corresponding to v_+ and v_-, for practical reasons it is convenient to choose the most "economic" one. As a measure in this case (i.e., a cost or penalty function) we can use the sum of squares $u^2 + v^2 + w^2$ of the computed scalar parameters.

4. An example. Let us consider now the application of this method for obtaining the *Euler* and *Bryan* decomposition of the symmetric orthogonal matrix

$$\mathcal{O}(\hat{\mathbf{n}}) = \frac{1}{3}\begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix} \tag{15}$$

which plays an essential role in the construction of the *minimal atlas* for the rotation group SO(3) [5]. First of all, let us note that since (15) is symmetric, and due to the axis-angle representation of rotations (2), we have $\varphi = k\,\pi,\ k = 0, \pm 1, \pm 2, \ldots$, so it is either the identity matrix, or a half turn in which case the above formula reduces to

$$\mathcal{R}(\mathbf{n}\,,\pi) = \mathcal{O}(\hat{\mathbf{n}}) = 2\,\hat{\mathbf{n}} \otimes \hat{\mathbf{n}}^t - \mathcal{I}.$$

We may use the latter to determine, up to a sign, the unit vector along the axis from the matrix entries. Using the diagonal elements we can find the squared values of the vector components from

$$2\,\hat{n}_k^2 = \mathcal{O}(\hat{\mathbf{n}})_{kk} + 1.$$

Then the procedure demands either division or taking square root and therefore one needs to select the component with highest absolute value in order to avoid the problem of small denominators. We take it with a positive sign and form the off-diagonal elements of $\mathcal{O}(\hat{\mathbf{n}})$ retrieve the other components by division since $\mathcal{O}(\hat{\mathbf{n}})_{ij} = 2\,\hat{n}_i\hat{n}_j$ for $i \neq j$ and we have our vector. Note that the vector $-\hat{\mathbf{n}}$ is also a solution since all matrix entries are quadratic functions of the vector components.

In the above example we have $\hat{\mathbf{n}} = \left(\dfrac{1}{\sqrt{3}}, \dfrac{1}{\sqrt{3}}, \dfrac{1}{\sqrt{3}}\right)$ and because all off-diagonal entries are positive we may conclude that the signs are either all positive, or all negative. We may take the positive one without loss of generality, since the equations involved in the procedure are quadratic in the components of the axis $\hat{\mathbf{n}}$.

Now we exploit our algorithm to obtain the *Euler* and *Bryan* decompositions of the matrix in (15), when $\hat{\mathbf{c}}_1$, $\hat{\mathbf{c}}_2$ and $\hat{\mathbf{c}}_3$ are chosen to be the unit vectors along the coordinate axes OZ, OX, OZ (*Euler*) and OX, OY, OZ (*Bryan*) respectively. Their definitions and history can be traced in the review article by Fraiture [4].

In the first case we obtain two solutions (u_+, v_+, w_+) and (u_-, v_-, w_-) and therefore two decompositions

$$\mathcal{O}(\hat{\mathbf{n}}) = \mathcal{R}_3^+\,\mathcal{R}_2^+\,\mathcal{R}_1^+ = \mathcal{R}_3^-\,\mathcal{R}_2^-\,\mathcal{R}_1^- \tag{16}$$

where $\mathcal{R}_1^{\pm} = \mathcal{R}_1(u_{\pm}\hat{\mathbf{c}}_1)$, $\mathcal{R}_2^{\pm} = \mathcal{R}_2(v_{\pm}\hat{\mathbf{c}}_2)$ and $\mathcal{R}_3^{\pm} = \mathcal{R}_3(w_{\pm}\hat{\mathbf{c}}_3)$.

Using formula (1), we find also the so called generalized *Euler* and *Bryan* angles [1] corresponding to these pairs of decompositions, i.e.,

$$(\phi_{\pm}, \theta_{\pm}, \psi_{\pm}) = (2\ \arctan u_{\pm},\ 2\ \arctan v_{\pm},\ 2\ \arctan w_{\pm})\,. \tag{17}$$

For the chosen matrix (15) we obtain

$$(\phi_+, \phi_-) = (\ \frac{\pi}{4},\ -\frac{3\pi}{4}\ ), \qquad \theta_{\pm} = \pm 2\arctan\sqrt{2}, \qquad (\psi_+, \psi_-) = (\ \frac{3\pi}{4},\ -\frac{\pi}{4}\ )$$

and the corresponding rotations about the fixed axes are

$$\mathcal{R}_1^{\pm} = \begin{pmatrix} \pm\frac{1}{\sqrt{2}} & \mp\frac{1}{\sqrt{2}} & 0 \\ \pm\frac{1}{\sqrt{2}} & \pm\frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \end{pmatrix},\ \mathcal{R}_2^{\pm} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{3} & \mp\frac{2\sqrt{2}}{3} \\ 0 & \pm\frac{2\sqrt{2}}{3} & -\frac{1}{3} \end{pmatrix},\ \mathcal{R}_3^{\pm} = \begin{pmatrix} \mp\frac{1}{\sqrt{2}} & \mp\frac{1}{\sqrt{2}} & 0 \\ \pm\frac{1}{\sqrt{2}} & \mp\frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

As for the *Bryan* decomposition of (15) we have

$$\phi_{\pm} = -2\arctan\frac{-1 \pm \sqrt{5}}{2}, \qquad \theta_{\pm} = -2\arctan\frac{3 \pm \sqrt{5}}{2}, \qquad \psi_{\pm} = \phi_{\pm}$$

with matrices of rotation

$$\mathcal{R}_1^{\pm} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \pm\frac{1}{\sqrt{5}} & \pm\frac{2}{\sqrt{5}} \\ 0 & \mp\frac{2}{\sqrt{5}} & \pm\frac{1}{\sqrt{5}} \end{pmatrix}, \ \mathcal{R}_2^{\pm} = \begin{pmatrix} \mp\frac{\sqrt{5}}{3} & 0 & -\frac{2}{3} \\ 0 & 1 & 0 \\ \frac{2}{3} & 0 & \mp\frac{\sqrt{5}}{3} \end{pmatrix}, \ \mathcal{R}_3^{\pm} = \begin{pmatrix} \pm\frac{1}{\sqrt{5}} & \pm\frac{2}{\sqrt{5}} & 0 \\ \mp\frac{2}{\sqrt{5}} & \pm\frac{1}{\sqrt{5}} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The algorithm we have described here is realized also as a MAPLE routine.

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ВЕКТОРНО РАЗЛАГАНЕ НА СИМЕТРИЧНИ ОРТОГОНАЛНИ МАТРИЦИ

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Тук предлагаме алгоритъм за реализиране на обобщено разлагане на тримерни ортогонални матрици, като осите на въртене са почти произволно избрани. Спрели сме се на частния случай на симетрични матрици, задаващи въртене на ъгъл π около ос в пространството, която може лесно да бъде определена от конкретните матрични елементи.
В подходящо представяне задачата се свежда до намиране решенията на система от три квадратни уравнения за скаларните параметри на трите въртения в разлагането. След сравнение на съответните матрични елементи се елиминират псевдо-решенията. Подходът е илюстриран детайлно чрез пример.