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**On the six-dimensional orthogonal tensor representation of the rotation in three dimensions: A simplified approach**

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## Abstract

The six-dimensional orthogonal tensor representation of the rotation about an axis in three dimensions was first proposed by (Mehrabadi et al. 1995). In this brief note, a simple and coherent approach is presented to construct the six-dimensional orthogonal tensor representation of the rotation of any parametrization in three dimensions and to prove its orthogonality.

## INTRODUCTION

The essence of the Euler's theorem regarding the representation of a  $3 \times 3$  rotation (orthogonal) matrix,  $\mathbf{Q}$ , generated from a rotation about an axis along a unit vector,  $\mathbf{p} \equiv [p_1, p_2, p_3]^T$  (the superscript  $T$  denotes matrix or vector transposition), with an angle,  $\theta$ , is encapsulated in the following expression, see (Mehrabadi et al. 1995) and references therein:

$$\mathbf{Q} = \mathbf{I} + \sin(\theta)\mathbf{P} + (1 - \cos(\theta))\mathbf{P}^2 = \exp(\theta\mathbf{P}), \quad (1)$$

where  $\mathbf{P}$  is a skew-symmetric matrix made up of the components of the unit vector,  $\mathbf{p}$ ,

$$\mathbf{P} = \begin{pmatrix} 0 & -p_3 & p_2 \\ p_3 & 0 & -p_1 \\ -p_2 & p_1 & 0 \end{pmatrix}. \quad (2)$$

In their extension of the Euler's theorem to the six dimensional matrix case, (Mehrabadi et al. 1995) relied upon the matrix exponential of a  $6 \times 6$  skew-symmetric matrix to establish the orthogonality of the six-dimensional matrix analogue of the rotation matrix,  $\mathbf{Q}$ , which was denoted by  $\hat{\mathbf{Q}}$  in (Mehrabadi et al. 1995).

In this brief note, a simple construction of the six-dimensional matrix analogue of the rotation matrix  $\mathbf{Q}$  and the proof of its orthogonality are presented.

## METHODS

Let us define  $\mathbf{Q}$  to be a  $3 \times 3$  orthogonal matrix, i.e.,  $\mathbf{Q}\mathbf{Q}^T = \mathbf{Q}^T\mathbf{Q} = \mathbf{I}$ , given by

$$\mathbf{Q} \equiv \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix}, \quad (3)$$

$\mathbf{D}$  to be a  $3 \times 3$  nonsingular symmetric matrix given by

$$\mathbf{D} \equiv \begin{pmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{xy} & D_{yy} & D_{yz} \\ D_{xz} & D_{yz} & D_{zz} \end{pmatrix}, \quad (4)$$

and  $\mathbf{A}$  to be another  $3 \times 3$  nonsingular symmetric matrix given by

$$\mathbf{A} = \begin{pmatrix} \lambda_1 & \lambda_4 & \lambda_6 \\ \lambda_4 & \lambda_2 & \lambda_5 \\ \lambda_6 & \lambda_5 & \lambda_3 \end{pmatrix}. \quad (5)$$

Then, the effect of rotating  $\mathbf{D}$  by  $\mathbf{Q}$  through a similarity transformation, which results in  $\mathbf{A}$ , can be given simply as:

$$\mathbf{A} = \mathbf{Q}^T \mathbf{D} \mathbf{Q}. \quad (6)$$

We should note that the off-diagonal elements of  $\mathbf{A}$  are generally nonzero except when each column vector of  $\mathbf{Q}$  is an eigenvector of  $\mathbf{D}$ .

Equation (6) can be vectorized using the following convention:

$$\tilde{\lambda} \equiv \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \lambda_4 \\ \lambda_5 \\ \lambda_6 \end{pmatrix} = \tilde{\mathbf{H}}\tilde{\mathbf{d}} = \tilde{\mathbf{H}} \begin{pmatrix} D_{xx} \\ D_{yy} \\ D_{zz} \\ D_{xy} \\ D_{yz} \\ D_{xz} \end{pmatrix}, \quad (7)$$

where  $\tilde{\mathbf{H}}$  is a six dimensional matrix made up of the elements of  $\mathbf{Q}$ . This convention, however, does not preserve the Euclidean vector norm and the Frobenius matrix norm. In other words, the Euclidean vector norm and the Frobenius matrix norm do not coincide under this convention, i.e.,

$$\tilde{\lambda}^T \cdot \tilde{\lambda} \neq \text{Tr}(\mathbf{A}^T \mathbf{A}), \quad (8)$$

where  $\text{Tr}(\cdot)$  denotes the matrix trace operation.

Fortunately, the Euclidean vector norm and the Frobenius matrix norm can be easily made to coincide under a slightly different but important convention of vectorization due to (Mehrabadi and Cowin 1990) and (Rychlewski 1984), (hereafter Mehrabahdi-Cowin-Rychlewski convention or MCR convention for short), i.e.:

$$\lambda \equiv \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \sqrt{2}\lambda_4 \\ \sqrt{2}\lambda_5 \\ \sqrt{2}\lambda_6 \end{pmatrix} \text{ and } \mathbf{d} = \begin{pmatrix} D_{xx} \\ D_{yy} \\ D_{zz} \\ \sqrt{2}D_{xy} \\ \sqrt{2}D_{yz} \\ \sqrt{2}D_{xz} \end{pmatrix}. \quad (9)$$

Under the MCR convention, Eq. (7) can be rearranged as:

$$\lambda = \mathbf{H}\mathbf{d}, \quad (10)$$

where the six dimensional matrix,  $\mathbf{H}$ , can be expressed as:

$$\mathbf{H} = \begin{pmatrix} Q_{11}^2 & Q_{21}^2 & Q_{31}^2 & \sqrt{2}Q_{11}Q_{21} & \sqrt{2}Q_{21}Q_{31} & \sqrt{2}Q_{11}Q_{31} \\ Q_{12}^2 & Q_{22}^2 & Q_{32}^2 & \sqrt{2}Q_{12}Q_{22} & \sqrt{2}Q_{22}Q_{32} & \sqrt{2}Q_{12}Q_{32} \\ Q_{13}^2 & Q_{23}^2 & Q_{33}^2 & \sqrt{2}Q_{13}Q_{23} & \sqrt{2}Q_{23}Q_{33} & \sqrt{2}Q_{13}Q_{33} \\ \sqrt{2}Q_{11}Q_{12} & \sqrt{2}Q_{21}Q_{22} & \sqrt{2}Q_{31}Q_{32} & Q_{11}Q_{22} + Q_{21}Q_{12} & Q_{21}Q_{32} + Q_{31}Q_{22} & Q_{11}Q_{32} + Q_{31}Q_{12} \\ \sqrt{2}Q_{12}Q_{13} & \sqrt{2}Q_{22}Q_{23} & \sqrt{2}Q_{32}Q_{33} & Q_{12}Q_{23} + Q_{22}Q_{13} & Q_{22}Q_{33} + Q_{32}Q_{23} & Q_{12}Q_{33} + Q_{32}Q_{13} \\ \sqrt{2}Q_{11}Q_{13} & \sqrt{2}Q_{21}Q_{23} & \sqrt{2}Q_{31}Q_{33} & Q_{11}Q_{23} + Q_{21}Q_{13} & Q_{21}Q_{33} + Q_{31}Q_{23} & Q_{11}Q_{33} + Q_{31}Q_{13} \end{pmatrix}. \quad (11)$$

To show that  $\mathbf{H}$  is orthogonal, i.e.,  $\mathbf{H}^{-1} = \mathbf{H}^T$ , the key step is to realize that  $\mathbf{H}^{-1}$  can be easily constructed by rearranging Eq.(6), namely:

$$\mathbf{D} = \mathbf{Q}\mathbf{A}\mathbf{Q}^T. \quad (12)$$

Vectorizing Eq.(12) using the MCR convention again, we have

$$\mathbf{d} = \mathbf{R}\boldsymbol{\lambda}, \quad (13)$$

where the six dimensional matrix,  $\mathbf{R}$ , which is the inverse of  $\mathbf{H}$ , is given by:

$$\mathbf{R} \equiv \mathbf{H}^{-1} = \begin{pmatrix} Q_{11}^2 & Q_{12}^2 & Q_{13}^2 & \sqrt{2}Q_{11}Q_{12} & \sqrt{2}Q_{12}Q_{13} & \sqrt{2}Q_{11}Q_{13} \\ Q_{21}^2 & Q_{22}^2 & Q_{23}^2 & \sqrt{2}Q_{21}Q_{22} & \sqrt{2}Q_{22}Q_{23} & \sqrt{2}Q_{21}Q_{23} \\ Q_{31}^2 & Q_{32}^2 & Q_{33}^2 & \sqrt{2}Q_{31}Q_{32} & \sqrt{2}Q_{32}Q_{33} & \sqrt{2}Q_{31}Q_{33} \\ \sqrt{2}Q_{11}Q_{21} & \sqrt{2}Q_{12}Q_{22} & \sqrt{2}Q_{13}Q_{22} & Q_{11}Q_{22} + Q_{12}Q_{21} & Q_{12}Q_{23} + Q_{13}Q_{22} & Q_{11}Q_{23} + Q_{13}Q_{21} \\ \sqrt{2}Q_{21}Q_{31} & \sqrt{2}Q_{22}Q_{32} & \sqrt{2}Q_{23}Q_{33} & Q_{21}Q_{32} + Q_{22}Q_{31} & Q_{22}Q_{33} + Q_{23}Q_{32} & Q_{21}Q_{33} + Q_{23}Q_{31} \\ \sqrt{2}Q_{11}Q_{31} & \sqrt{2}Q_{12}Q_{32} & \sqrt{2}Q_{13}Q_{33} & Q_{11}Q_{32} + Q_{12}Q_{31} & Q_{12}Q_{33} + Q_{13}Q_{32} & Q_{11}Q_{33} + Q_{13}Q_{31} \end{pmatrix}. \quad (14)$$

Based on Eq.(11) and Eq.(14), it is clear that  $\mathbf{H}^{-1} = \mathbf{H}^T$ .

For most applications, Eq.(11) can be constructed simply and directly from the components of  $\mathbf{Q}$ , regardless of the parametrization of  $\mathbf{Q}$ ; that is,  $\mathbf{Q}$  may be represented as in Eq.(1) or may be expressed in terms of the Euler angles.

## DISCUSSION

The goal of this work is to convey the simplicity of the idea, of the construction and of the proof of the six-dimensional orthogonal tensor representation of the rotation in three

dimensions to interested readers. In brief, the orthogonality of the six-dimensional orthogonal tensor representation of the rotation is a direct consequence of the invariance of a rotation-based similarity-transformed tensor in two different norms—the Euclidean norm and the Frobenius norm. It should be clear that the construction can be easily extended to orthogonal matrices in higher dimensions using a higher dimensional generalization of the MCR convention.

In practice, it may be more convenient to construct the six-dimensional orthogonal tensor representation of the rotation in three dimensions directly from the elements of the three dimensional rotation matrix regardless of the parametrization used to represent the rotation matrix. In other cases, the matrix exponential formalism as presented in (Mehrabadi et al. 1995) may be of value, e.g., (Balendran and Nemat-Nasser 1995).

The relevance of the MCR convention and of the six dimensional orthogonal tensor representation of the rotation in three dimensions can be gleaned from recent publications ranging from elasticity to imaging, (Basser and Pajevic 2007; Moakher 2006; Moakher and Norris 2006). Specifically, we note that the analysis of optimal experimental designs and the propagation of errors (Koay et al. 2007; Koay et al. 2008) through the nonlinear least squares objective function (Koay et al. 2006) in diffusion tensor imaging (Basser et al. 1994) will be greatly facilitated under the MCR convention.

We should note that the similarity transformation through an orthogonal matrix used in the construction of the six-dimension orthogonal tensor representation is a well known technique for transforming tensors or for diagonalizing tensors. This technique is

very useful in many areas of research, e.g. (Golub and Van Loan 1996; Koay et al. 2006). Finally, we hope this brief note prepare interested readers to appreciate the simplicity of the idea and the construction behind the six-dimension orthogonal tensor representation of the rotation in three dimensions as well as the elegance of the matrix exponential formalism of (Mehrabadi et al. 1995).

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### References

- Balendran, B., and Nemat-Nasser, S. (1995). "Integration of inelastic constitutive equations for constant velocity gradient with large rotation." *Applied Mathematics and Computation*, 67(1-3), 161-195.
- Basser, P. J., Mattiello, J., and Le Bihan, D. (1994). "MR diffusion tensor spectroscopy and imaging." *Biophys. J.*, 66(1), 259-267.
- Basser, P. J., and Pajevic, S. (2007). "Spectral decomposition of a 4th-order covariance tensor: Applications to diffusion tensor MRI." *Signal Processing*, 87(2), 220-236.
- Golub, G. H., and Van Loan, C. F. (1996). *Matrix computation*, The Johns Hopkins University Press, Baltimore.
- Koay, C. G., Chang, L.-C., Carew, J. D., Pierpaoli, C., and Basser, P. J. (2006). "A unifying theoretical and algorithmic framework for least squares methods of estimation in diffusion tensor imaging." *Journal of Magnetic Resonance*, 182(1), 115-125.
- Koay, C. G., Chang, L. C., Pierpaoli, C., and Basser, P. J. (2007). "Error propagation framework for diffusion tensor imaging via diffusion tensor representations." *IEEE Transactions on Medical Imaging*, 26(8), 1017-1034.
- Koay, C. G., Nevo, U., Chang, L.-C., Pierpaoli, C., and Basser, P. J. (2008). "The elliptical cone of uncertainty and its normalized measures in diffusion tensor imaging." *IEEE Transactions on Medical Imaging*, 27(6), 834-846.
- Mehrabadi, M. M., and Cowin, S. C. (1990). "Eigensensors of linear anisotropic elastic materials." *Quarterly Journal of Mechanics and Applied Mathematics*, 43, 15-41.
- Mehrabadi, M. M., Cowin, S. C., and Jaric, J. (1995). "Six-dimensional orthogonal tensor representation of the rotation about an axis in three dimensions." *International Journal of Solids and Structures*, 32(3-4), 439-449.
- Moakher, M. (2006). "On the Averaging of Symmetric Positive-Definite Tensors." *Journal of Elasticity*, 82(3), 273-296.
- Moakher, M., and Norris, A. (2006). "The Closest Elastic Tensor of Arbitrary Symmetry to an Elasticity Tensor of Lower Symmetry." *Journal of Elasticity*, 85(3), 215-263.
- Rychlewski, J. (1984). "On Hooke's law." *Prikl. Mat. Meh.*, 48, 303-314.