

Stratovan■ OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

- Laplacian eigenfunctions and neural networks:... • Note. (i) Quaternions and their generalization, i.e., octonions, have become desirable representations for a variety of structures and phenomena encountered in several fields of science and engineering, including: calculations of satellite/planet/aircraft/ballistic dynamics and control; physical phenomena involving space and time for their mathematical description (Maxwell's equations, for example); special and general relativity; particle physics; quantum mechanics;...

(ii) Emmy Nöther (Noether) and, more recently, Cohl (Nicohl) Furey have substantially moved forward the science of quaternions and octonions, especially their use in mathematical physics and even the purely a priori derivation of the "Laws" governing elementary particle physics. See:

- C. Furey, "Standard Model Physics from an Algebra?", Ph. D. thesis, 2016.
- Willi Kafitz, "Hyperkomplexe Zahlen in Mathematik und Physik" (Hyper-complex numbers in mathematics and physics), 2023, University of Gießen (Giessen), Germany.
- Manon Bischoff, "From complex numbers to 'Tomb Raider'" (Von komplexen Zahlen zu 'Tomb Raider'), Spektrum der Wissenschaft, February 17, 2023.

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• Laplacian eigenfunctions and neural networks:... The brief summary of Wahba's Problem, quaternions and a method for deriving a quaternion from a (rotation, orthogonal or non-orthogonal) matrix (method introduced by Itzhack Y. Bar-Itzhack) serves this purpose: Our related problem (and goal) concerns the calculation of a best orthonormal basis (or orthonormal matrix) approximation for a given set of non-orthogonal basis vectors in D-dimensional space. Wahba's Problem and the method of Bar-Itzhack (for the special case of calculating a best-approximating quaternion / 3x3 orthonormal rotation matrix for a given non-orthogonal 3x3 matrix) provide ideas and approaches that might lead to a viable solution strategy for the general D-dimensional case concerned with  $D \times D$  matrices.

• Example (Bar-Itzhack method). First, we consider the simple case of reproducing an orthonormal rotation matrix from a given matrix that (already) is an orthonormal matrix. The given normalized vectors are  $w_1 = (1, 0, 0)^T$ ,

$w_2 = (0, 1, 0)^T$  and  $w_3 = (0, 0, 1)^T$ , defining the matrices  $N$  and  $\hat{N}$ , see left. The eigenvalues of  $\hat{N}$  are  $\lambda_1 = 1$  (largest) and  $\lambda_2 = \lambda_3 = \lambda_4 = -1/3$ . The eigenvector  $e_1 = (x_0, x_1, x_2, x_3)^T$  is given by  $\hat{N} \cdot e_1 = 1 \cdot e_1 \Rightarrow e_1 = (0, 0, 0, x_3)^T$ . ...

$$N = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\hat{N} = \begin{bmatrix} -1/3 & 0 & 0 & 0 \\ 0 & -1/3 & 0 & 0 \\ 0 & 0 & -1/3 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

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• Laplacian eigenfunctions and neural networks... The value of  $x_3$  must be chosen in order to normalize  $\mathcal{Q}_1$  and

to define a normalized quaternion  $q$ :

$$\|\mathcal{Q}_1\| = (\mathcal{Q}_1 \cdot \mathcal{Q}_1)^{1/2} = (x_3^2)^{1/2} = 1 \Rightarrow x_3 = \pm 1.$$

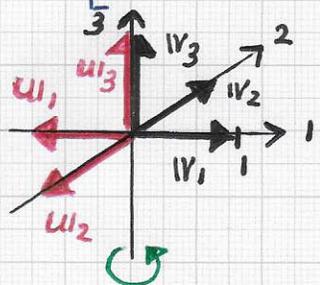
Thus, the resulting two possible quaternions are:

$$q_1 = 0 + 0i + 0j + 1k, \quad q_2 = 0 + 0i + 0j - 1k.$$

(The quaternions  $q_1$  and  $q_2$  are conjugated normalized quaternions, i.e.,  $q_2 = \bar{q}_1$  and  $q_1 = \bar{q}_2$ .)

The conversion of  $q_1$  (or  $q_2$ ) to the corresponding 3x3 matrix representation is defined on page 25 (11/25/2023); one obtains the matrix  $M$ , where

$$M = \begin{bmatrix} 1-2x_3^2 & 0 & 0 \\ 0 & 1-2x_3^2 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad \text{This means that the method does}$$



not reproduce the original basis vectors  $v_i, i=1,2,3$ , exactly; rather it produces a set of orthonormal vectors  $u_i, i=1,2,3$ , that one can

view as the result of a rotation of the given vectors around axis '3' by rotation angle  $\pi$ , see figure above. ●

The numerical 3D example provided on pp. 3 ff. (11/3/2023)

uses as non-orthogonal basis vectors  $v_1 = \sqrt{2} (2/3, 1/6, 1/6)^T$ ,

$v_2 = \sqrt{2} (1/6, 2/3, 1/6)^T$  and  $v_3 = \sqrt{2} (1/6, 1/6, 2/3)^T$  — for which the

best-approximating vectors  $b_1 = (1, 0, 0)^T$ ,  $b_2 = (0, 1, 0)^T$  and  $b_3 = (0, 0, 1)^T$

are (re-) constructed. We now apply Bar-Itzhack's method to the non-orthogonal basis  $\{v_i\}_{i=1}^3$ . ●●●

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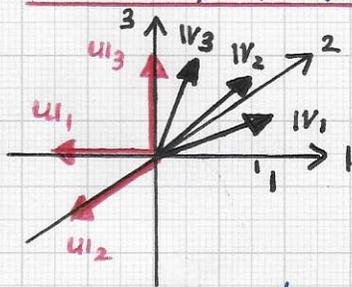
• Laplacian eigenfunctions and neural networks:... The resulting matrices for this set of vectors  $w_i, i=1,2,3$ , are:

$$\underline{N} = \sqrt{2} \begin{bmatrix} 2/3 & 1/6 & 1/6 \\ 1/6 & 2/3 & 1/6 \\ 1/6 & 1/6 & 2/3 \end{bmatrix}, \quad \underline{\hat{N}} = \begin{bmatrix} -2 & 1 & 1 & 0 \\ 1 & -2 & 1 & 0 \\ 1 & 1 & -2 & 0 \\ 0 & 0 & 0 & 6 \end{bmatrix} \cdot \sqrt{2}/9$$

The eigenvalues of  $\underline{\hat{N}}$  are  $\lambda_1 = 2\sqrt{2}/3$  (largest),  $\lambda_2 = \lambda_3 = -\sqrt{2}/3$  and  $\lambda_4 = 0$ .

Solve  $\underline{\hat{N}} \cdot \underline{e}_1 = 2\sqrt{2}/3 \cdot \underline{e}_1$

Solving the equation system for the eigenvector  $\underline{e}_1$  yields  $\underline{e}_1 = (0, 0, 0, x_3)^T$ . This is the same eigenvector  $\underline{e}_1$  as obtained in the previous example.



Thus, all subsequent calculations are the same as well, and one obtains the same orthonormal matrix  $M$ ,

having the orthonormal column vectors  $\underline{u}_1, \underline{u}_2$  and  $\underline{u}_3$  shown in the above figure together with the given non-orthogonal basis vectors  $w_1, w_2$  and  $w_3$ .

• Note. Complex numbers and their generalizations — quaternions, octonions and "hyper-complex numbers" more generally — are also becoming increasingly interesting for computational neural network applications. Thus, it is important to summarize some of the most relevant relationships between these complex numbers; rotations; orthogonal/orthonormal matrices and bases; best approximation; geometric algebra; linear and matrix algebra.

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- Laplacian eigenfunctions and neural networks:... The following list merely serves the purpose of stimulating one's

thinking about related concepts and computations:

- A complex number  $z = x + yi$  can be represented as a point/positional vector in the (complex) plane.  $\Rightarrow$  Relationship between number and geometry.

- The multiplication of two complex numbers can be understood as and visualized by a 2D rotation.

- "Rotations in 3D space around an axis are non-commutative and require a non-commutative algebra" for their algebraic representation and calculation. Quaternions have an associated algebra that involves non-commutative multiplication.

- A rotation in 3D space around an axis passing through the origin (defined via a normalized direction vector), mapping a point  $p$  to  $p'$ , can be expressed as the quaternion product  $p' = q \cdot p \cdot \bar{q}$ .

- The best approximation of a given non-orthogonal 3D basis (3x3 matrix) by an orthonormal 3D basis (3x3 rotation matrix) can be elegantly computed via quaternions: A rotation-defining  $q = x_0 + x_1i + x_2j + x_3k$  (also defining an associated orthogonal rotation matrix), i.e., its unknown "coefficients"  $x_0, x_1, x_2$  and  $x_3$ , can be calculated via a best approximation / least squares approach using as requirement the mapping of the non-orthogonal matrix to an

\* Use this equation to define the linear system for  $x_0, x_1, x_2, x_3$ , by mapping orthonormal vectors to non-orthonormal vectors.

\* orthogonal matrix.