■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:... In fact, the problem of calculating a best (least-squares) approximation of a given non-orthogonal set of basis vectors by an orthonormal basis was stated by **Grace Wahba** in 1965 in **SIAM** Review, Vol. 7, No. 3 as follows:

[Problem 65-1, A Least Squares Estimate of Satellite Attitude, by Grace Wahba (IBM Corp.)]

• "Given two sets of n points, $\{\mathbb{v}_1, \dots, \mathbb{v}_n\}$ and $\{\mathbb{v}_1^*, \dots, \mathbb{v}_n^*\}$, where $n \geq 2$, find the rotation matrix M, i.e., the orthogonal matrix with determinant $+1$, which brings the first set into the best least squares coincidence with the second. That is, find M which minimizes

$$\sum_{i=1}^{n} \| \mathbb{v}_i^* - M \mathbb{v}_i \|^2 .$$

This problem has arisen in the estimation of the attitude of a satellite ..."

This problem statement includes as a special "sub-problem" the best approximation of a non-orthogonal basis $\{\mathbb{b}_i^*\}_{i=1}^n$ by mapping an orthonormal basis $\{\mathbb{b}_i\}_{i=1}^n$ via an orthogonal rotation matrix M such that $\sum_{i=1}^n \|\mathbb{b}_i^* - M\mathbb{b}_i\|^2$ is minimal — where $\mathbb{b}_1 = (1, 0, \dots, 0)^T, \dots, \mathbb{b}_n = (0, \dots, 0, 1)^T$.

A solution to Grace Wahba's problem concerns the n-dimensional case, and it would be applicable to our n-dimensional classification case.

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks: ... Geometric algebra is concerned with algebraic operations/operators applied to "geometrical objects." Geometric algebra provides effective methods for the "computation with geometrical objects" — and is therefore advantageous for object-oriented problem solving and programming when computations must be performed for complex geometry. A good reference is:

Geometric Algebra for Computer Science (Revised Edition), by Leo Dorst, Daniel Fontijne and Stephen Mann, Morgan Kaufman, 2009.

This book, and geometric algebra in general, is covering topics including: rotors; rotation; Clifford Algebra; versors; orthogonal mappings; quaternions; Grassmann Algebra; Hamiltonian quaternions etc. It turns out that several of these topics and associated computational methods apply directly to our best approximation problem regarding the optimal orientation of an approximating orthonormal basis.

First, we provide a brief summary of only the most important and relevant definitions and rules for QUATERNIONS (Hamilton numbers) needed for the representation of rotations.

...

■ OBJECT AND MATERIAL EIGENFUNCTIONS — Cont'd.

• Laplacian eigenfunctions and neural networks: … QUATERNIONS. Basic definitions and rules for quaternion-based representation and calculations are provided in the following. A quaternion is defined as the LINEAR COMBINATION

$$q = x_0 + x_1 i + x_2 j + x_3 k \,, \quad x_0, x_1, x_2, x_3 \in \mathbb{R}, \text{ BASIS } \{1, i, j, k\}.$$

The addition of two quaternions is defined as

$$(x_0 + x_1 i + x_2 j + x_3 k) + (y_0 + y_1 i + y_2 j + y_3 k) = $$
$$= (x_0 + y_0) + (x_1 + y_1) i + (x_2 + y_2) j + (x_3 + y_3) k \,.$$

The multiplication of two quaternions can be defined in several ways; we consider this definition:

$$(x_0 + x_1 i + x_2 j + x_3 k) \cdot (y_0 + y_1 i + y_2 j + y_3 k) =$$
$$= (x_0 y_0 - x_1 y_1 - x_2 y_2 - x_3 y_3) +$$
$$+ (x_0 y_1 + x_1 y_0 + x_2 y_3 - x_3 y_2) i +$$
$$+ (x_0 y_2 - x_1 y_3 + x_2 y_0 + x_3 y_1) j +$$
$$+ (x_0 y_3 + x_1 y_2 - x_2 y_1 + x_3 y_0) k \,.$$

(Note. $q_1 \cdot q_2 \neq q_2 \cdot q_1$.)

The matrix representation of $q = x_0 + x_1 i + x_2 j + x_3 k$ is

$$M(q) = \begin{bmatrix} x_0 & -x_1 & x_3 & -x_2 \\ x_1 & x_0 & -x_2 & -x_3 \\ -x_3 & x_2 & x_0 & -x_1 \\ x_2 & x_3 & x_1 & x_0 \end{bmatrix}.$$

Rules are:

$$\boxed{\begin{array}{l} i \cdot j = k \,, \; j \cdot k = i \,, \; k \cdot i = j \,, \\ j \cdot i = -k \,, \; k \cdot j = -i \,, \; i \cdot k = -j \,, \\ i^2 = j^2 = k^2 = i \cdot j \cdot k = -1 \,. \end{array}}$$

Quaternions can be used to represent a rotation in 3D space ("representation of q as linear combination or as matrix") and to perform a rotation of a point around an axis (via quaternion multiplication). To represent a rotation, the quaternion q_{rot} must be normalized, i.e., $\|q_{rot}\| = 1$.

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:... The length of a quaternion q is defined as $\|q\| = (x_0^2 + x_1^2 + x_2^2 + x_3^2)^{1/2}$.

Thus, the quaternion q becomes the normalized quaternion q_{norm} by computing $q_{norm} = q / \|q\|$, i.e.,

$$q_{norm} = x_0/\|q\| + x_1/\|q\|\, i + x_2/\|q\|\, j + x_3/\|q\|\, k.$$

Another relevant operation is conjugation: The quaternion $q = x_0 + x_1 i + x_2 j + x_3 k$ has the associated conjugated quaternion $\overline{q} = x_0 - x_1 i - x_2 j - x_3 k$. One can show that $q_{norm} \cdot \overline{q_{norm}} = \overline{q_{norm}} \cdot q_{norm} = 1$.

Rotation in 3D space via normalized quaternions. Given a point $(x, y, z)^T$, a rotation of this point around an axis passing through the origin can be represented as

$$p' = (x', y', z')^T = q \cdot p \cdot \overline{q} = q_{norm} \cdot p \cdot \overline{q_{norm}},$$

where $p = (x, y, z)^T$. One can express this rotation in vector notation as the product

$$p' = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \cdot \begin{bmatrix} 0 \\ x \\ y \\ z \end{bmatrix} \cdot \begin{bmatrix} x_0 \\ -x_1 \\ -x_2 \\ -x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ x' \\ y' \\ z' \end{bmatrix}.$$

The resulting 3D matrix-based representation is

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} x_0^2 + x_1^2 - x_2^2 - x_3^2 & 2(-x_0 x_3 + x_1 x_2) & 2(x_0 x_2 + x_1 x_3) \\ 2(x_0 x_3 + x_1 x_2) & x_0^2 - x_1^2 + x_2^2 - x_3^2 & 2(-x_0 x_1 + x_2 x_3) \\ 2(-x_0 x_2 + x_1 x_3) & 2(x_0 x_1 + x_2 x_3) & x_0^2 - x_1^2 - x_2^2 + x_3^2 \end{bmatrix} \cdot \begin{bmatrix} x \\ y \\ z \end{bmatrix}.$$

Thus, using these formulas it is possible to convert a quaternion-based representation of a rotation to its matrix representation and vice versa. ...

OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks: … **Converting quaternion representation to matrix representation (of a rotation) and vice versa.**

! • From quaternion to matrix representation:
Given the rotation quaternion $q_{norm} = x_0 + x_1 i + x_2 j + x_3 k$, the rotation is represented equivalently by the matrix

$$M = \begin{bmatrix} 1-2(x_2^2+x_3^2) & 2(-x_0x_3+x_1x_2) & 2(x_0x_2+x_1x_3) \\ 2(x_0x_3+x_1x_2) & 1-2(x_1^2+x_3^2) & 2(-x_0x_1+x_2x_3) \\ 2(-x_0x_2+x_1x_3) & 2(x_0x_1+x_2x_3) & 1-2(x_1^2+x_2^2) \end{bmatrix}.$$

! • From matrix to quaternion representation:
Given the orthogonal rotation matrix M, where

$$M = \begin{bmatrix} r_{11} & r_{12} & r_{13} \\ r_{21} & r_{22} & r_{23} \\ r_{31} & r_{32} & r_{33} \end{bmatrix},$$

the rotation is represented equivalently by the quaternion

$q_{norm} = x_0 + x_1 i + x_2 j + x_3 k$, where $x_0 = (1 + r_{11}^2 + r_{22}^2 + r_{33}^2)^{1/2}/2 = c$, and $x_1 = (r_{32} - r_{23})/(4c)$, $x_2 = (r_{13} - r_{31})/(4c)$, $x_3 = (r_{21} - r_{12})/(4c)$.

NOT ortho-gonal

$$N = \begin{bmatrix} n_{11} & n_{12} & n_{13} \\ n_{21} & n_{22} & n_{23} \\ n_{31} & n_{32} & n_{33} \end{bmatrix}$$

Many solution approaches to Wahba's problem have been published. The paper "New Method

$$\hat{N} = \begin{bmatrix} n_{11}-n_{22}-n_{33} & n_{12}+n_{21} & n_{13}+n_{31} & n_{23}-n_{32} \\ n_{21}+n_{12} & n_{22}-n_{11}-n_{33} & n_{23}+n_{32} & n_{31}-n_{13} \\ n_{31}+n_{13} & n_{32}+n_{23} & n_{33}-n_{11}-n_{22} & n_{12}-n_{21} \\ n_{23}-n_{32} & n_{31}-n_{13} & n_{12}-n_{21} & n_{11}+n_{22}+n_{33} \end{bmatrix} \cdot \frac{1}{3}$$

! for Extracting the Quaternion from a Rotation Matrix" (I.Y. Bar-Itzhack, J. Guidance, Control and Dynamics 23(6), p. 1085) proposes a method for deriving a symmetric 4x4 matrix $\hat{N}$ from a given non-orthogonal matrix N (3×3). THE EIGENVECTOR ASSOCIATED WITH $\hat{N}$'S LARGEST EIGENVALUE IS THE BEST-APPROXIMATION QUATERNION OF N.

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