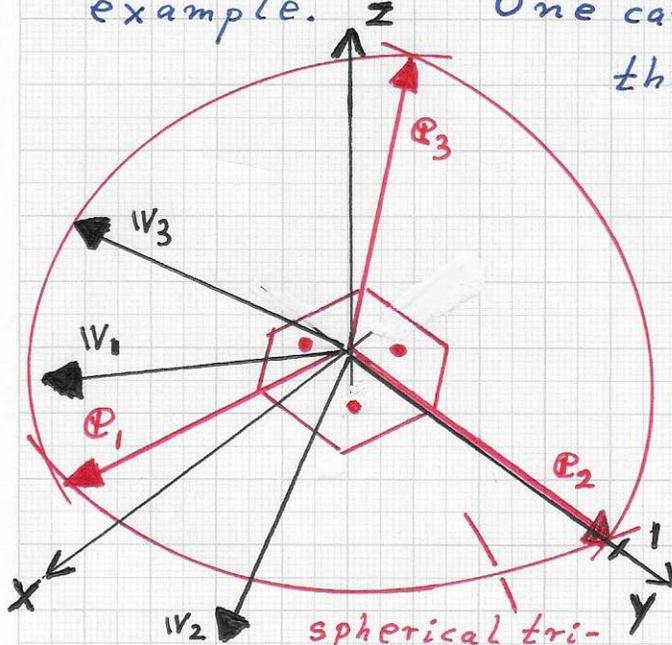


OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

• Laplacian eigenfunctions and neural networks: The Note included on the previous page is relevant: In the 2D setting the "duality" between an orthonormal \mathcal{Q} -eigensystem and the needed "optimal" u_1 -system, defined by orthonormal vectors u_1 and u_2 , is obvious. Therefore, it is of interest to explore whether this fact can be exploited in the general D -dimensional setting. The three orthonormal eigenvectors $\mathcal{Q}_1, \mathcal{Q}_2$ and \mathcal{Q}_3 provided on the previous page concern a specific 3D example. One can view the calculation of the needed u_1 -system as an optimization problem - a "morphing" problem - that is concerned with the mapping of the PCA-generated \mathcal{Q} -eigensystem to the given set of normalized, non-orthogonal set $\{w_1, w_2, w_3\}$ - minimizing "system distance" and requiring minimal "mapping energy", see left figure.



spherical triangle defined by 3 \mathcal{Q} -system arcs

$$w_1 = (\sqrt{3}/2, -1/2, 0)^T, \quad \mathcal{Q}_1 = (.96, 0, .29)^T,$$

$$w_2 = (\sqrt{3}/2, 1/2, 0)^T, \quad \mathcal{Q}_2 = (0, 1, 0)^T,$$

$$w_3 = (\sqrt{2}/2, 0, \sqrt{2}/2)^T, \quad \mathcal{Q}_3 = (-.29, 0, .96)^T$$

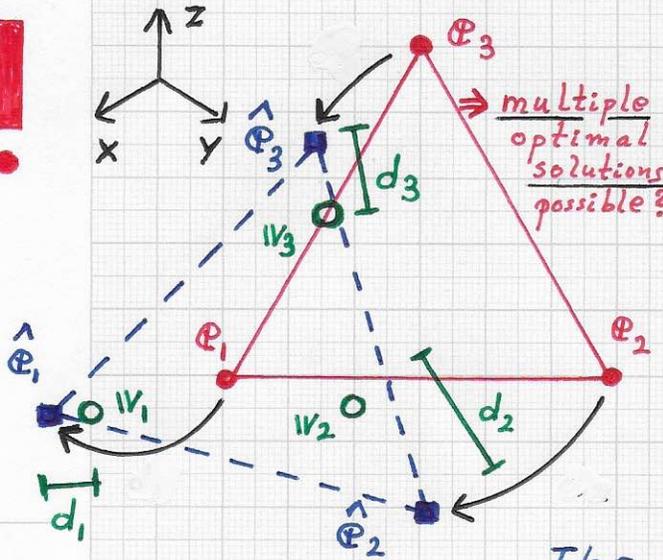
A minimal energy mapping for morphing the \mathcal{Q} - to the w -system must be defined.

minimizing "system distance" and requiring minimal "mapping energy", see left figure.

■ OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

- Laplacian eigenfunctions and neural networks:...

One can understand the mapping of the PCA-generated orthonormal eigen-system $\{\Phi_1, \Phi_2, \Phi_3\}$ to the desired "optimal" orthonormal system $\{\hat{\Phi}_1, \hat{\Phi}_2, \hat{\Phi}_3\}$ as a mapping that leads to an "optimal" placement of the vectors $\hat{\Phi}_1, \hat{\Phi}_2$ and $\hat{\Phi}_3$ such that "distance" is minimized.



The left figure illustrates this mapping for the considered 3D example, showing the involved unit vectors in a 2D projection plane as points \bullet , \circ or \blacksquare . The parameters d_1, d_2 and d_3 represent a measure for "distance" between the given vectors Ψ_i and the "optimal" vectors $\hat{\Phi}_i$. For example, one could consider the value of the sum of the squared "distances" d_i to be minimized, i.e., $\sum_{i=1}^3 d_i^2 \rightarrow \text{MIN}$.

One can also view this mapping as a mapping that maps the orthonormal matrix with column vectors Φ_1, Φ_2 and Φ_3 to the orthonormal matrix with column vectors $\hat{\Phi}_1, \hat{\Phi}_2$ and $\hat{\Phi}_3$, subject to leading to a best (matrix) approximation of the matrix with non-orthogonal column vectors Ψ_1, Ψ_2 and Ψ_3 .

Stratovan■ OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

- Laplacian eigenfunctions and neural networks... Concerning the 3D case, one can define the approximation

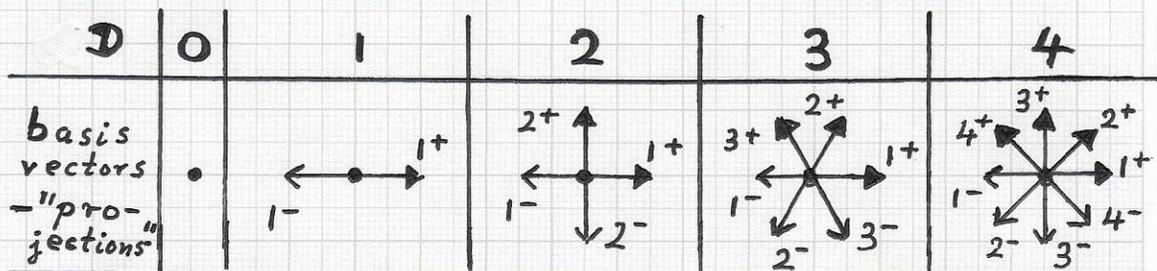
problem also as follows: Given unit vectors \mathbf{w}_1 , \mathbf{w}_2 and \mathbf{w}_3 (not mutually orthogonal to each other), determine unit and mutually orthogonal vectors $\hat{\mathbf{e}}_1$, $\hat{\mathbf{e}}_2$ and $\hat{\mathbf{e}}_3$ that approximate the given vectors in a best-approximation sense, i.e., in an error-minimization sense. Another possible

problem definition is using matrices: Given a 3-by-3 matrix V with unit column vectors \mathbf{w}_1 , \mathbf{w}_2 and \mathbf{w}_3 , i.e., $V = [\mathbf{w}_1 \ \mathbf{w}_2 \ \mathbf{w}_3]$, determine a 3-by-3 matrix \mathbb{F} with unit and mutually orthogonal vectors $\hat{\mathbf{e}}_1$, $\hat{\mathbf{e}}_2$ and $\hat{\mathbf{e}}_3$, i.e., $\mathbb{F} = [\hat{\mathbf{e}}_1 \ \hat{\mathbf{e}}_2 \ \hat{\mathbf{e}}_3]$, such that \mathbb{F} is a best matrix approximation of V - minimizing a chosen measure for the "distance" between V and \mathbb{F} , i.e., "distance(V, \mathbb{F}) = MIN."

When understanding this problem as an approximation problem, several related topics and solution approaches come to mind: (i) least-squares approximation and normal equations; (ii) orthogonal, orthonormal and rotation matrices; (iii) best approximation with constraints and method of Lagrange multipliers; (iv) approximation with energy-minimizing splines, e.g., thin-plate spline (TPS) mappings/deformations; (v) linear equation system resulting from minimization of quadratic error. ...

■ OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

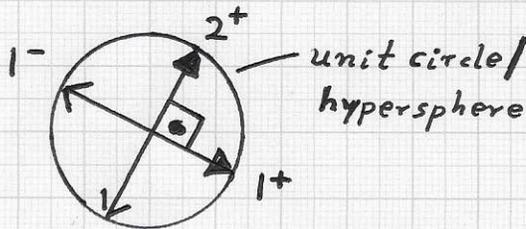
• Laplacian eigenfunctions and neural networks:... The optimal orthonormal coordinate system for a given set of linearly independent unit (but not mutually orthogonal) vectors v_1, \dots, v_D is not unique. The optimization problem concerned with the determination of orthonormal coordinate system basis vectors has as its solution a finite set, of sets of D vectors each, that defines allowable, equally optimal coordinate system basis vector solutions. This fact is a consequence of the possibility to accept either the "positive" (+) or "negative" (-) direction / orientation of each basis vector. In the following, we discuss this aspect in detail for low-dimensional cases that are helpful for understanding the general D -dimensional setting. It is possible to analyze this issue purely from a combinatorial perspective. The figure shown here



summarizes in an abstract way the unit vector sets — for dimensions $D = 0, 1, 2, 3, 4$ — from which one can/must select D to define an allowable basis.

OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

• Laplacian eigenfunctions and neural networks:...



Four unit vectors from which one must select 2.
 $D=2$

Thus, one must pick a subset consisting of D unit and mutually orthogonal vectors from the set of candidate vectors, called in this discussion $1^+, 2^+, \dots, D^+$, $1^-, 2^-, \dots, D^-$. The set of candidate vectors contains

$2D$ unit vectors, and every subset consisting of D mutually orthogonal unit vectors is an optimal set of coordinate system basis vectors. By definition, an optimal set never contains both the vector d^+ and d^- , $d \in \{1, 2, \dots, D\}$, as $d^- = -d^+$. The top-left figure illustrates the 2-dimensional case. From the combinatorics perspective, one is interested in all allowable optimal solutions and the number of them. The

D	0	1	2	3
ortho-normal systems	•		

figure included here shows the possible optimal orthonormal basis vector sets for dimensions $D=0, 1, 2$.

For example, for $D=2$ one pair of orthogonal lines defines the shown four optimal solutions, resulting from the two possible orientations (+, -) for each line. ...