OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• **Laplacian eigenfunctions and neural networks:...** The first derivative of $D(\alpha)$, $d/d\alpha\, D(\alpha)$, is the function

$$D'(\alpha) = 2 s\alpha \sum_{i=1}^{n} \langle x_i, y_i \rangle - 2 c\alpha \sum_{i=1}^{n} \langle x_i, y_i^{\perp} \rangle .$$

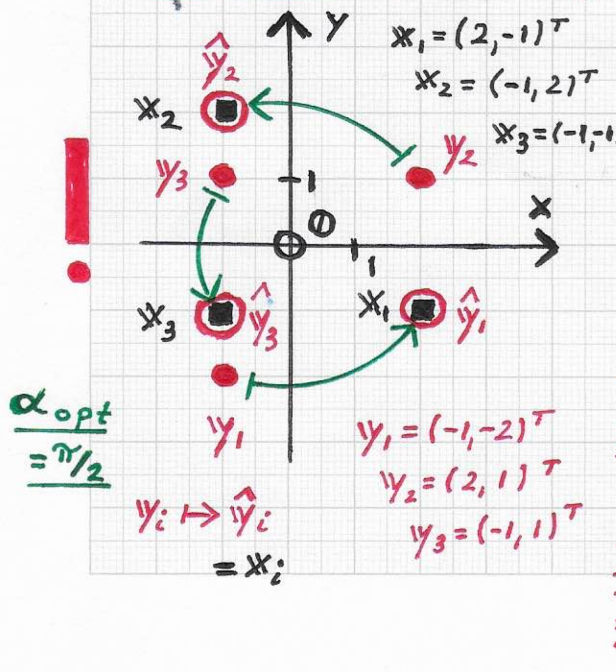
Since $D'(\alpha)$ must be zero, one obtains:

$$\tan\alpha = \frac{1}{\cot\alpha} = \frac{s\alpha}{c\alpha} = \sum_{i=1}^{n} \langle x_i, y_i^{\perp} \rangle \Big/ \sum_{i=1}^{n} \langle x_i, y_i \rangle$$

$$\Rightarrow \alpha = \arctan\left(\sum_{i=1}^{n} \langle x_i, y_i^{\perp} \rangle / \sum_{i=1}^{n} \langle x_i, y_i \rangle \right) \quad \text{or}$$

$$\alpha = \operatorname{arccot}\left(\sum_{i=1}^{n} \langle x_i, y_i \rangle / \sum_{i=1}^{n} \langle x_i, y_i^{\perp} \rangle \right) .$$

We consider a simple example for $n=3$, where it is possible to determine a rotation angle α that leads to a sum-of-squared-distances error with value zero. In general, the sum-of-squared-distances error can be used to define a measure of "similarity" or "shape match" for the point sets $\{x_i\}_{i=1}^{n}$ and $\{y_i\}_{i=1}^{n}$.



The left figure illustrates the example. The two point data sets $\{x_i\}_{i=1}^{3}$ and $\{y_i\}_{i=1}^{3}$ share the same center (0), achieved by mean subtraction, for example, and they "have the same scale". For the given points one obtains $\sum_{i=1}^{3} \langle x_i, y_i \rangle = 0$ and $\sum_{i=1}^{3} \langle x_i, y_i^{\perp} \rangle = 12$. Thus, $\alpha = \operatorname{arccot}(0/12) = \pi/2$. In this case, $\hat{y}_i = x_i$, $i = 1 \ldots 3$, and a "zero-error shape match" results.

...

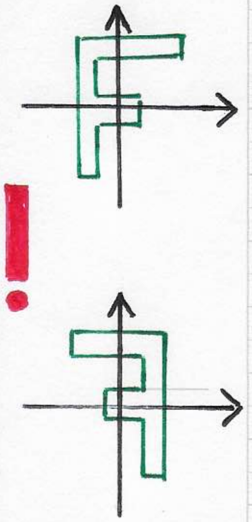
Bernd Hamann
Stratovan

2/11/2024

OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

- Laplacian eigenfunctions and neural networks:...

Note. It is important to keep in mind that the "orientation of the coordinate system" (right-handed vs. left-handed system) must be considered for geometrical "shape matching" and computing a "shape similarity" measure. FUNDAMENTALLY, A ROTATION **MATRIX** IS AN ORTHONORMAL MATRIX WITH DETERMINANT VALUE **+1**. Thus, the desribed optimization method for calculating an optimal rotation angle α yielding the minimal sum-of-squared-distances approximation error value MIGHT NOT LEAD TO THE BEST-POSSIBLE SHAPE MATCH! Therefore, one must consider the representation of a data set $\{y_i\}_{i=1}^{n}$ with respect to both a right-handed and left-handed coordinate system.

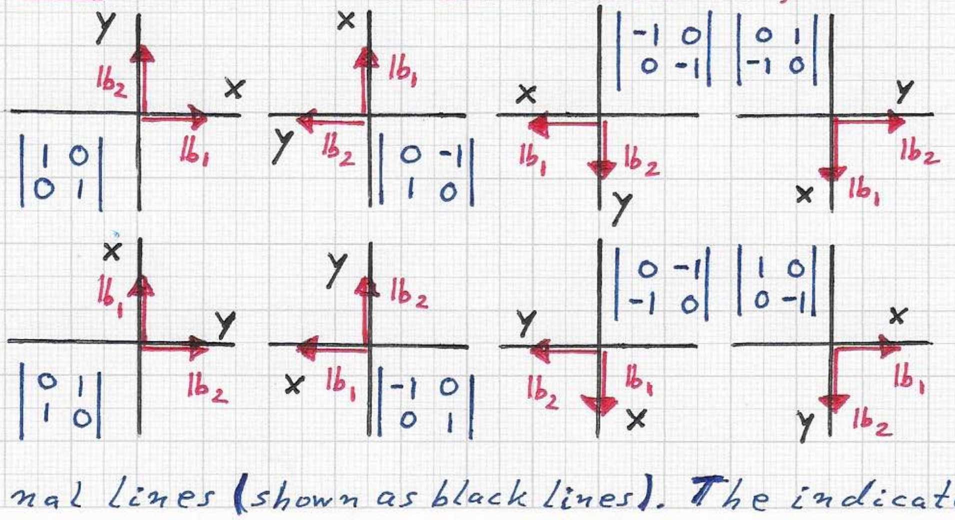


"Mirror images" (reflections) of the "same shape" must be handled!

For example, the left figure shows sketches of eight possible coordinate systems for two given orthogonal lines (shown as black lines).

DET=+1

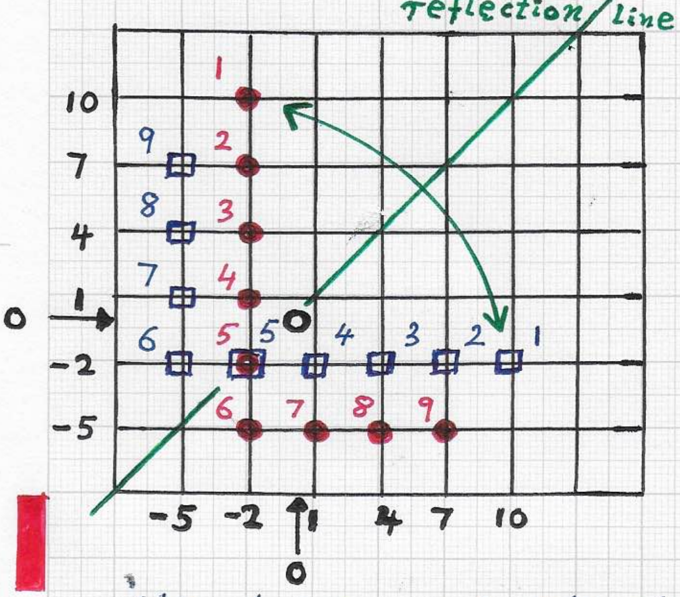
DET=−1



The indicated axis basis vectors $\mathbb{b}_1$ and $\mathbb{b}_2$ are orthonormal and define four right-handed systems (top, DET=1) and four left-handed systems (bottom, DET=−1)...

OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

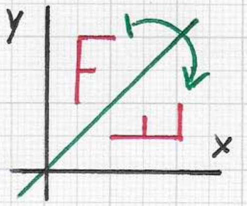
• Laplacian eigenfunctions and neural networks:... AS A CONSEQUENCE, ONE MUST PROCESS "TWO VERSIONS" OF THE DATA SET $\{y_i\}_{i=1}^n$, E.G., $\{(y_1^i, y_2^i)^T\}_{i=1}^n$ AND $\{(-y_1^i, y_2^i)^T\}_{i=1}^n$ (reflected with respect to the second axis; first coordinate with opposite sign). The "most extreme case" is illustrated in the left figure.



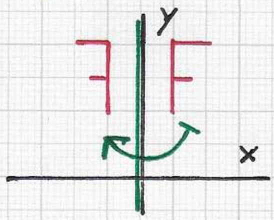
Two data sets are shown, $\{\bullet_i\}_{i=1}^9$ and $\{\square_i\}_{i=1}^n$. When ignoring the indices indicated next to the points, the two point sets are "reflections of each other." The line / is the line of reflection. Further, the chosen point sets share the origin **o** as shared centroid (mean) and "have the same scale." **BUT:** Despite the fact that both point sets represent "the same discrete version of the letter **L**, i.e., **L** and a "mirror image" **⅃**, it is NOT POSSIBLE TO USE AN ORTHONORMAL ROTATION (MATRIX WITH DETERMINANT +1) THAT YIELDS THE "DESIRED MAPPING WITH APPROXIMATION ERROR ZERO," INDICATING "PERFECT MATCH." This example simply serves the purpose of emphasizing that **A RIGHT-HANDED AND LEFT-HANDED (=reflected) VERSION OF $\{y_i\}_{i=1}^n$ ARE NEEDED.** ...

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

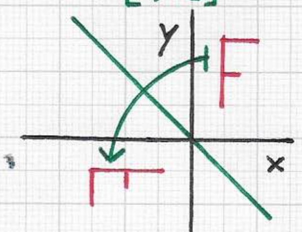
• **Laplacian eigenfunctions and neural networks:...** The figure on page 2 (2-11-2024) provides sketches of four reflections, defined by orthonormal transformation matrices with determinant value −1 (shown in the four bottom illustrations). Fundamentally, these reflections can be used to create "mirror images" of a given shape, i.e., a shape induced by a discrete point set. In summary, one must use a right- and left-handed version of a given point data set $\{y_i\}_{i=1}^n$ and calculate the TWO optimal rotation angle VALUES that define the best-possible rotations of the two versions, i.e., lead to the two minimal rotation approximation errors, relative to the target point data set $\{x_i\}_{i=1}^n$. The FINAL MEASURE OF POINT SET SIMILARITY IS THE SMALLER OF THE TWO ROTATION APPROXIMATION ERRORS. The figure on this page shows "abstract representations" of four reflections mapping the letter F to its mirror image, ꟻ. The associated reflection matrices, Ref, are provided.



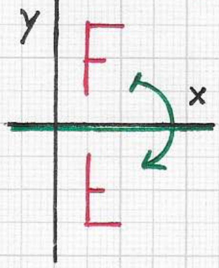
$\text{Ref} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$



$\text{Ref} = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$



$\text{Ref} = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}$

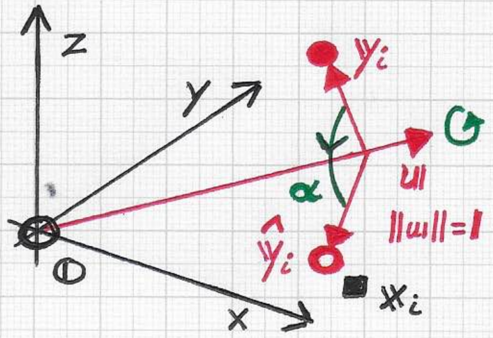


$\text{Ref} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

...

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:… The detailed discussion of optimal rotation in the 2D plane, including its representation with complex numbers, serves the purpose of obtaining a better understanding of optimal rotation in 3D space via quaternions — with the ultimate goal of obtaining "distances," "similarity measures" or "shape match probabilities" for two point sets that have been optimally registered to each other via an optimal quaternion-based mapping. Page 19 (2-5-2024) summarizes conditions for such an optimal "four-dimensional quaternion" q_{rot}.



The left figure succintly summarizes the relevant data involved. One must determine an optimal unit rotation axis direction vector $\mathbf{u}$ and optimal rotation angle α, $0 \leq \alpha < 2\pi$, such that the points $\mathbf{y}_i$, $i=1 \ldots n$, can be mapped to the corresponding image points $\hat{\mathbf{y}}_i$, $i=1 \ldots n$, minimizing the sum of squared distances $\|\hat{\mathbf{y}}_i - \mathbf{x}_i\|^2$. Again, the necessary conditions are:

$$\Sigma_{i=1}^{n} (\mathbf{x}_i^T U \mathbf{y}_i) = 0 \; ; \; (\Sigma_{i=1}^{n} \mathbf{x}_i^T Y_1^i)\,\mathbf{u} = 0 \; ;$$
$$(\Sigma_{i=1}^{n} \mathbf{x}_i^T Y_2^i)\,\mathbf{u} = 0 \; ; \; (\Sigma_{i=1}^{n} \mathbf{x}_i^T Y_3^i)\,\mathbf{u} = 0 \text{ and}$$
$$\|\mathbf{u}\|^2 = \|(u,v,w)^T\|^2 = u^2+v^2+w^2 = 1 \text{ (unit constraint).}$$

One can use numerical optimization programs to calculate the implied UNIT QUATERNION $c\frac{\alpha}{2} + (iu+jv+kw)\,s\frac{\alpha}{2} = q_{rot}$.

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