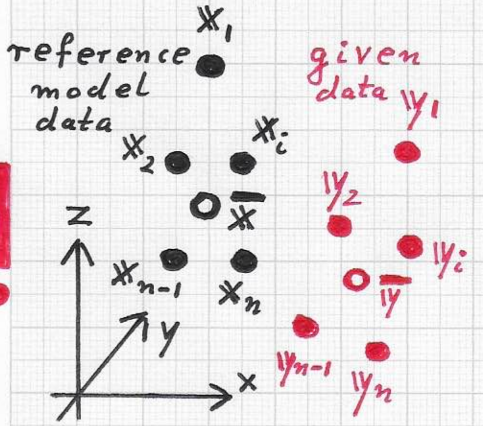
■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:... Our overarching material classification problem treats objects/materials to be characterized and classified as sets of voxels with various 3D, volumetric characteristics/features, mainly based on the notion of a trivariate object "density" function. Nevertheless, for certain types of objects – e.g., various classes of knives – one should also consider **GEOMETRIC SHAPE CHARACTERISTICS AND SIMILARITY** for classification purposes. Geometry features become particularly relevant when one is concerned with the recognition/classification of rather "rigid and non-deformable" objects. Point data registration and shape matching are crucial for determining degree of similarity of geometry and class-membership probabilities. Quaternions offer an alternative to 3-by-3 rotation matrices for solving the registration problem, i.e., determining the best rotation that – when applied to a given shape (a point set) – minimizes the least-squares error between to-be-registered shape and some reference shape model. Quaternions can be used to represent point data, rotation axis and rotation angle to set up the optimization problem elegantly. ...

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:... The topics "point data registration" and "quaternions for registration" are covered in many papers. (For example, the notes "Quaternions and Rotations" by Yan-Bin Jia provide a succinct introductory overview of quaternions. These notes present many of the concepts summarized in the following.)



Here, we do not assume that the point sets $\{\mathbb{x}_i\}_{i=1}^n$ and $\{\mathbb{y}_i\}_{i=1}^n$ have an associated point connectivity; we consider only meshless point data ("no topology"), see left figure. We do assume index correspondence, i.e., a to-be-registered point $\mathbb{y}_i$ corresponds to standard, reference model point $\mathbb{x}_i$. Further, since the points have no associated connectivity, they can, in principle, represent single, isolated points (of dimension 0), points on a curve (of dimension 1), points of a surface (of dimension 2) or points in the interior of a volumetric object (of dimension 3). By eliminating scaling as an allowable transformation and considering only translation and rotation, one must determine optimal translation and rotation for $\{\mathbb{y}_i\}_{i=1}^n$ ...

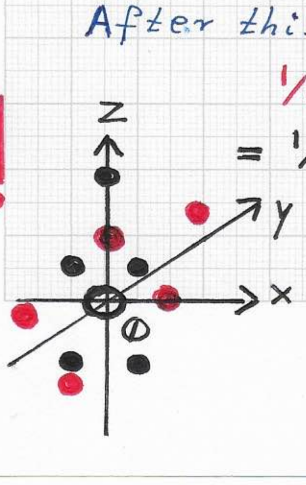
OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:… Registration is relevant for object recognition and classification. Determining the best-possible mapping of the given point set $\{\mathbf{y}_i\}_{i=1}^n$ to the reference model point set $\{\mathbf{x}_i\}_{i=1}^n$ yields a minimal approximation error. If this error is smaller than some tolerance, then one will be able to assume that the "shape" represented by $\{\mathbf{y}_i\}_{i=1}^n$ matches the "shape" represented by $\{\mathbf{x}_i\}_{i=1}^n$, i.e., the reference model is "matched and recognized." If this error is larger than that tolerance, then the two "shapes" will not be matching. We summarize the steps involved in optimally mapping $\{\mathbf{y}_i\}_{i=1}^n$ to $\{\mathbf{x}_i\}_{i=1}^n$. First, one determines the centroids/means of the point sets, called $\bar{\mathbf{x}} = 1/n \sum_{i=1}^n \mathbf{x}_i$ and $\bar{\mathbf{y}} = 1/n \sum_{i=1}^n \mathbf{y}_i$, and translates $\mathbf{y}_i$, $i=1\ldots n$, by the vector $\bar{\mathbf{x}} - \bar{\mathbf{y}}$. This step effectively ensures that all point sets have the same centroid/mean, i.e., $\bar{\mathbf{x}}$:

$$\mathbf{y}_i \mapsto \mathbf{y}_i + (\bar{\mathbf{x}} - \bar{\mathbf{y}}) = \mathbf{y}_i + \left(1/n \sum_{i=1}^n \mathbf{x}_i - 1/n \sum_{i=1}^n \mathbf{y}_i\right).$$

After this mapping (translation), the centroid is

$$1/n \left(\sum_{i=1}^n \mathbf{y}_i + n \, 1/n \sum_{i=1}^n \mathbf{x}_i - n \, 1/n \sum_{i=1}^n \mathbf{y}_i \right) =$$
$$= 1/n \sum_{i=1}^n \mathbf{x}_i = \bar{\mathbf{x}}.$$



In a subsequent step, one can map both point sets by subtracting the positional vector $\bar{\mathbf{x}}$ from all points, thus making the origin $\mathbf{0}$ the shared centroid, see left figure.

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■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• **Laplacian eigenfunctions and neural networks:...** In the following, it is assumed that the point sets $\{\mathbf{x}_i\}_{i=1}^n$ and $\{\mathbf{y}_i\}_{i=1}^n$ share the origin $\mathbf{0}$ as their common centroid. Using standard matrix representation and algebra, the objective is the calculation of the optimal 3-by-3 rotation matrix R — being an orthonormal matrix satisfying $\det R = 1$ — that, when applied to the given data, yields minimal approximation error (least squares), i.e.,

$$E = E(R) = \sum_{i=1}^n \|\mathbf{x}_i - R\mathbf{y}_i\|^2,$$

the sum of the squared lengths of the difference vectors $\mathbf{x}_i - R\mathbf{y}_i$, has the smallest possible value. The value of the error can be calculated via matrix algebra:

$$\begin{aligned} E(R) &= \sum_{i=1}^n \|\mathbf{x}_i - R\mathbf{y}_i\|^2 = \sum_{i=1}^n \langle \mathbf{x}_i, \mathbf{x}_i \rangle - 2\sum_{i=1}^n \langle \mathbf{x}_i, R\mathbf{y}_i \rangle \\ &\quad + \sum_{i=1}^n \langle R\mathbf{y}_i, R\mathbf{y}_i \rangle = \sum_{i=1}^n \left(\|\mathbf{x}_i\|^2 + \|R\mathbf{y}_i\|^2\right) \\ &\quad - 2\sum_{i=1}^n \langle \mathbf{x}_i, R\mathbf{y}_i \rangle \\ &= \sum_{i=1}^n \left(\|\mathbf{x}_i\|^2 + \|\mathbf{y}_i\|^2\right) - 2\sum_{i=1}^n \langle \mathbf{x}_i, R\mathbf{y}_i \rangle. \end{aligned}$$

(Note. Since R only affects orientation of the "shape" but not scale, $\|R\mathbf{y}_i\|^2 = \|\mathbf{y}_i\|^2$.)

Thus, in order to minimize the value of $E(R)$, one must maximize the value of the second term in the definition of $E(R)$, i.e., $2\sum_{i=1}^n \langle \mathbf{x}_i, R\mathbf{y}_i \rangle$, since the first term is a constant $\left(\sum_{i=1}^n \left(\|\mathbf{x}_i\|^2 + \|\mathbf{y}_i\|^2\right)\right)$.

The optimal rotation matrix R that maximizes the value of $\sum_{i=1}^n \langle \mathbf{x}_i, R\mathbf{y}_i \rangle$.

...

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:... Solving this optimization problem via standard matrix algebra und using the 3-by-3 rotation matrix R as unknown is "not advantageous": The matrix R does not have 9 degrees of freedom; R is an orthonormal matrix and $\det R = +1$. As a consequence, R provides only (the sufficient number of) 4 degrees of freedom. The number 4 is also the number that is necessary and sufficient to represent a rotation axis passing through the origin (via a unit axis direction vector $\mathbb{d} = (d_x, d_y, d_z)^T$) and a rotation angle α. A quaternion makes it possible to represent precisely this data.

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• **Note.** Since this optimization problem is defined as a least-squares optimization problem, it can be solved via the standard approach: (i) establish a quadratic function (to calculate extremal value for), where the function's independent variables are the variables whose values must be determined for the optimization problem; (ii) calculate the gradient (vector) of this function; (iii) determine where the gradient vanishes (necessary condition for an extremum); (iv) compute the value of the function where its gradient vanishes; (v) this value is the function's needed extremal value. ...

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