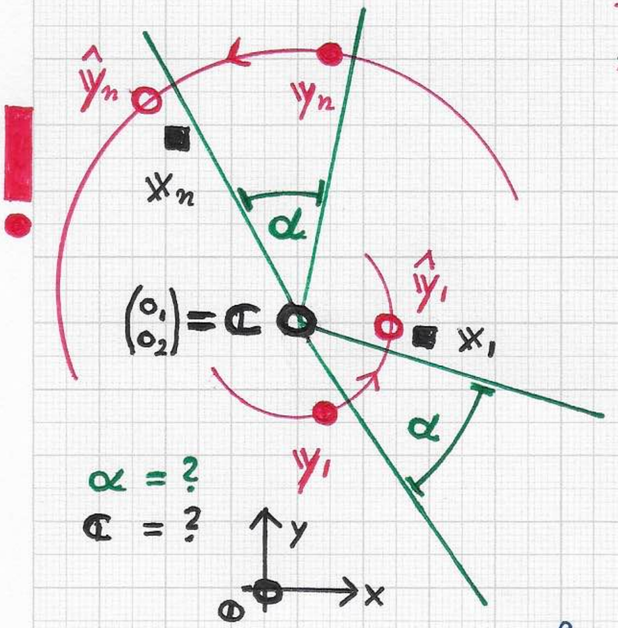
■ OBJECT AND MATERIAL EIGENFUNCTIONS — Cont'd.

• Laplacian eigenfunctions and neural networks: …



It is also possible to set up an optimization problem that simultaneously considers the parameters α and $\mathbb{C} = (o_1, o_2)^T$. The left figure sketches this case. Here, one must solve a "trivariate optimization problem," where the goal is to **minimize** an error/cost function having α, o_1 and o_2 as its independent variables for which optimal values must be computed. As before, the value of $\sum_{i=1}^{n} \| \hat{\mathbb{y}}_i - \mathbb{x}_i \|^2$ must be minimal. The value of $\hat{\mathbb{y}}_i$ is the result of the concatenation of three mappings of $\mathbb{y}_i$: First, $\mathbb{y}_i$ is translated by $-\vec{\mathbb{C}} = (-o_1, -o_2)^T$; second, the intermediate result is rotated by α around the global origin $\mathbb{O} = (0,0)^T$; third, the intermediate result of the rotation is translated by $\vec{\mathbb{C}} = (o_1, o_2)^T$, yielding the point $\hat{\mathbb{y}}_i$. Thus, the point $\hat{\mathbb{y}}_i$ is defined as

$$\hat{\mathbb{y}}_i = \begin{bmatrix} \hat{y}_1^i \\ \hat{y}_2^i \end{bmatrix} = \begin{bmatrix} \cos(y_1^i - o_1) - \sin(y_2^i - o_2) + o_1 \\ \sin(y_1^i - o_1) + \cos(y_2^i - o_2) + o_2 \end{bmatrix}.$$

We use the abbreviations $c = \cos$ and $s = \sin$ in the following. The essential term for the minimization is $\| \hat{\mathbb{y}}_i - \mathbb{x}_i \|^2$, where

$$\| \hat{\mathbb{y}}_i - \mathbb{x}_i \|^2 = \left(c(y_1^i - o_1) - s(y_2^i - o_2) + o_1 - x_1^i \right)^2 + \left(s(y_1^i - o_1) + c(y_2^i - o_2) + o_2 - x_2^i \right)^2 = \ldots$$

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OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

- **Laplacian eigenfunctions and neural networks:...**

$$= \left(c(y_1^i-o_1) - s(y_2^i-o_2)\right)^2 + 2\left(c(y_1^i-o_1)-s(y_2^i-o_2)\right)(o_1-x_1^i) + (o_1-x_1^i)^2$$

$$+\left(s(y_1^i-o_1)+c(y_2^i-o_2)\right)^2 + 2\left(s(y_1^i-o_1)+c(y_2^i-o_2)\right) \cdot (o_2-x_2^i) + (o_2-x_2^i)^2 = \ldots$$

$$= c^2\left((y_1^i)^2 - 2o_1y_1^i + o_1^2\right) - 2sc\left(y_1^iy_2^i - o_2y_1^i - o_1y_2^i + o_1o_2\right) + s^2\left((y_2^i)^2 - 2o_2y_2^i + o_2^2\right)$$
$$+2\left(cy_1^i - co_1 - sy_2^i + so_2\right)(o_1 - x_1^i)$$
$$+o_1^2 - 2o_1x_1^i + (x_1^i)^2$$
$$+s^2\left((y_1^i)^2 - 2o_1y_1^i + o_1^2\right) + 2sc\left(y_1^iy_2^i - o_2y_1^i - o_1y_2^i + o_1o_2\right) + c^2\left((y_2^i)^2 - 2o_2y_2^i + o_2^2\right)$$
$$+2\left(sy_1^i - so_1 + cy_2^i - co_2\right)(o_2 - x_2^i)$$
$$+o_2^2 - 2o_2x_2^i + (x_2^i)^2 =$$

$s^2+c^2=1$ $\quad$ $=$ $\quad$ $0=$ $\quad$ $=$

$$= (y_1^i)^2 - 2o_1y_1^i + o_1^2 + (y_2^i)^2 - 2o_2y_2^i + o_2^2$$
$$+2\left(co_1y_1^i - cx_1^iy_1^i - co_1^2 + co_1x_1^i - so_1y_2^i + sx_1^iy_2^i + so_1o_2 - so_2x_1^i\right)$$
$$+2\left(so_2y_1^i - sx_2^iy_1^i - so_1o_2 + so_1x_2^i + co_2y_2^i - cx_2^iy_2^i - co_2^2 + co_2x_2^i\right)$$
$$+o_1^2 - 2o_1x_1^i + (x_1^i)^2 + o_2^2 - 2o_2x_2^i + (x_2^i)^2 =$$

$$= \|\mathbf{y}_i\|^2 - 2\langle \mathbf{o}, \mathbf{y}_i\rangle + \|\mathbf{o}\|^2$$
$$+2\left(c\langle \mathbf{o},\mathbf{y}_i\rangle - c\langle \mathbf{x}_i,\mathbf{y}_i\rangle - c\|\mathbf{o}\|^2 + c\langle \mathbf{o},\mathbf{x}_i\rangle + s\langle \mathbf{o},\mathbf{y}_i^\perp\rangle - s\langle \mathbf{x}_i,\mathbf{y}_i^\perp\rangle - s\langle \mathbf{o},\mathbf{x}_i^\perp\rangle\right)$$
$$+\|\mathbf{o}\|^2 - 2\langle \mathbf{o},\mathbf{x}_i\rangle + \|\mathbf{x}_i\|^2 =$$

/* where $\mathbf{x}_i^\perp = (-x_2^i, x_1^i)^T$ and $\mathbf{y}_i^\perp = (-y_2^i, y_1^i)^T$ */

$$= \|\mathbf{y}_i\|^2 - 2\langle \mathbf{o},\mathbf{y}_i\rangle + \|\mathbf{o}\|^2$$
$$+\|\mathbf{x}_i\|^2 - 2\langle \mathbf{o},\mathbf{x}_i\rangle + \|\mathbf{o}\|^2$$
$$+2\left(c\left(\langle \mathbf{o},\mathbf{x}_i\rangle + \langle \mathbf{o},\mathbf{y}_i\rangle - \langle \mathbf{o},\mathbf{o}\rangle\right) - c\langle \mathbf{x}_i,\mathbf{y}_i\rangle + s\left(\langle \mathbf{o},\mathbf{y}_i^\perp\rangle - \langle \mathbf{o},\mathbf{x}_i^\perp\rangle\right) - s\langle \mathbf{x}_i,\mathbf{y}_i^\perp\rangle\right) =$$

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$$= \|\mathbf{y}_i\|^2 - 2\langle \mathbf{o},\mathbf{y}_i\rangle + \|\mathbf{o}\|^2 + \|\mathbf{x}_i\|^2 - 2\langle \mathbf{o},\mathbf{x}_i\rangle + \|\mathbf{o}\|^2$$
$$+2\left(c\langle \mathbf{o}, -\mathbf{o}+\mathbf{x}_i+\mathbf{y}_i\rangle + s\langle \mathbf{o}, \mathbf{y}_i^\perp - \mathbf{x}_i^\perp\rangle - c\langle \mathbf{x}_i,\mathbf{y}_i\rangle - s\langle \mathbf{x}_i,\mathbf{y}_i^\perp\rangle\right) = \ldots$$

/* where $\langle \mathbf{o},\mathbf{x}\rangle + \langle \mathbf{o},\mathbf{y}\rangle = \langle \mathbf{o},\mathbf{x}+\mathbf{y}\rangle$ */

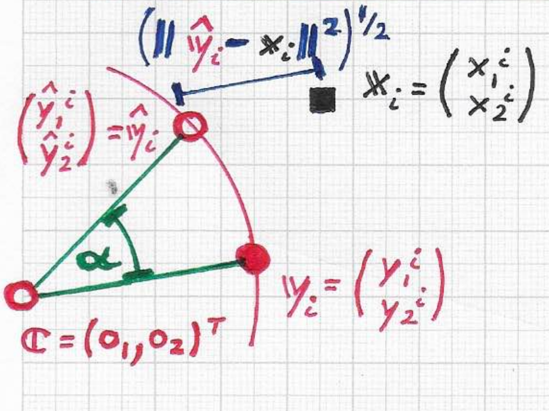
...

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• **Laplacian eigenfunctions and neural networks:...** $= \|\mathbf{y}_i\|^2 - 2\langle \mathbf{c}, \mathbf{y}_i\rangle + \|\mathbf{c}\|^2$
$+ \|\mathbf{x}_i\|^2 - 2\langle \mathbf{c}, \mathbf{x}_i\rangle + \|\mathbf{c}\|^2$
$+2\left(c\langle \mathbf{c}, \mathbf{x}_i + \mathbf{y}_i - \mathbf{c}\rangle - s\langle \mathbf{c}, (\mathbf{x}_i - \mathbf{y}_i)^\perp\rangle - c\langle \mathbf{x}_i, \mathbf{y}_i\rangle - s\langle \mathbf{x}_i, \mathbf{y}_i^\perp\rangle\right)$.

/* where $\langle \mathbf{c}, \mathbf{x}^\perp + \mathbf{y}^\perp\rangle = \langle \mathbf{c}, (\mathbf{x}+\mathbf{y})^\perp\rangle$ and $\langle \mathbf{c}, -\mathbf{x}\rangle = -\langle \mathbf{c}, \mathbf{x}\rangle$ */

This is the squared distance between $\hat{\mathbf{y}}_i$ and $\mathbf{x}_i$, when adopting a "point" interpretation, or the squared length of the difference vector of $\hat{\mathbf{y}}_i$ and $\mathbf{x}_i$, when adopting a "vector" interpretation, i.e., $\|\hat{\mathbf{y}}_i - \mathbf{x}_i\|^2$; it depends on three independent variables — α, o_1, o_2 — and, to solve the minimization problem, the three partial derivatives of $\|\hat{\mathbf{y}}_i - \mathbf{x}_i\|^2$ must be considered. The



left figure summarizes the relevant data/variables that define the minimization problem. Again, the objective is the minimization of $D = D(\alpha, o_1, o_2) = \sum_{i=1}^n \|\hat{\mathbf{y}}_i - \mathbf{x}_i\|^2 = \sum_{i=1}^n d_i = \sum_{i=1}^n d_i(\alpha, o_1, o_2)$. Thus, the needed partial derivatives of $D(\alpha, o_1, o_2)$ are:

$$\partial/\partial\alpha\, D = \sum_{i=1}^n \left(\partial/\partial\alpha\, d_i(\alpha, o_1, o_2)\right) = D_\alpha,$$

$$\partial/\partial o_1\, D = \sum_{i=1}^n \left(\partial/\partial o_1\, d_i(\alpha, o_1, o_2)\right) = D_{o_1},$$

$$\partial/\partial o_2\, D = \sum_{i=1}^n \left(\partial/\partial o_2\, d_i(\alpha, o_1, o_2)\right) = D_{o_2}.$$

...

■ OBJECT AND MATERIAL EIGENFUNCTIONS - Cont'd.

• Laplacian eigenfunctions and neural networks: ...

● **Note.** The equation at the top of the previous page "reduces" to $\ldots = \|\mathbb{y}_i\|^2 + \|\mathbb{x}_i\|^2 - 2(c\langle \mathbb{x}_i, \mathbb{y}_i\rangle + s\langle \mathbb{x}_i, \mathbb{y}_i^\perp\rangle)$ when defining $\mathbb{C} = (0,0)^T = \mathbb{O}$. This result is thus in agrement with the equation for $\|\mathbb{x} - \hat{\mathbb{y}}\|^2$ provided on page 24 (2-9-2024), where the global origin $\mathbb{O}$ is used to define and solve the minimization problem. This is a consequence of the fact that all inner products of the form $\langle \mathbb{C}, \cdot \rangle$ have the value zero for $\mathbb{C} = \mathbb{O}$.

For the more general minimization problem, where the optimal center of rotation is to be calculated, one must calculate and use the partial derivatives of the summands $d_i = d_i(\alpha, o_1, o_2)$. We denote the derivatives as $d_\alpha^i = \partial/\partial\alpha \, d_i$, $d_{o_1}^i = \partial/\partial o_1 \, d_i$ and $d_{o_2}^i = \partial/\partial o_2 \, d_i$.

● **Note.** The solution approach for this more general minimization problem mentioned briefly on page 10 (2-17-2024) — "Second, we consider ..." — suggests a "two-step method": In a first step, one determines a "quasi-optimal" center of rotation (based on line-pair intersections), and in a second step, one determines the optimal angle of rotation. The first step of this method has the advantage that plane-pair intersections can be used to define a rotation axis.

...

OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• **Laplacian eigenfunctions and neural networks:...** Therefore, one method considers the "simultaneous" computation of optimal values for α, o_1 and o_2 via minimization of the trivariate function $D(\alpha, o_1, o_2)$, while an alternative "two-step method" first determines a rotation center and subsequently a rotation angle — "first $\mathbb{C} = (o_1, o_2)^T$, then α."

For the minimization of $D(\alpha, o_1, o_2)$, we calculate the algebraic definitions of the three partial derivatives of its summands $d_i(\alpha, o_1, o_2) = \|\hat{\mathbb{y}}_i - \mathbb{x}_i\|^2 =$

$$= \|\mathbb{y}_i\|^2 + \|\mathbb{x}_i\|^2 + 2\big((1-c)\langle \mathbb{C}, \mathbb{C} - \mathbb{x}_i - \mathbb{y}_i\rangle - s\langle \mathbb{C}, (\mathbb{x}_i - \mathbb{y}_i)^\perp\rangle - c\langle \mathbb{x}_i, \mathbb{y}_i\rangle - s\langle \mathbb{x}_i, \mathbb{y}_i^\perp\rangle\big).$$

Differentiation yields the following derivatives:

$$d^i_\alpha = 2\big(s\langle \mathbb{C}, \mathbb{C} - \mathbb{x}_i - \mathbb{y}_i\rangle - c\langle \mathbb{C}, (\mathbb{x}_i - \mathbb{y}_i)^\perp\rangle + s\langle \mathbb{x}_i, \mathbb{y}_i\rangle - c\langle \mathbb{x}_i, \mathbb{y}_i^\perp\rangle\big),$$

$$d^i_{o_1} = 2\big((1-c)\,\partial/\partial o_1 \langle \mathbb{C}, \mathbb{C} - \mathbb{x}_i - \mathbb{y}_i\rangle - s\,\partial/\partial o_1 \langle \mathbb{C}, (\mathbb{x}_i - \mathbb{y}_i)^\perp\rangle\big) = 2\big((1-c)(2o_1 - x^i_1 - y^i_1) - s(y^i_2 - x^i_2)\big),$$

$$d^i_{o_2} = 2\big((1-c)\,\partial/\partial o_2 \langle \mathbb{C}, \mathbb{C} - \mathbb{x}_i - \mathbb{y}_i\rangle - s\,\partial/\partial o_2 \langle \mathbb{C}, (\mathbb{x}_i - \mathbb{y}_i)^\perp\rangle\big) = 2\big((1-c)(2o_2 - x^i_2 - y^i_2) - s(x^i_1 - y^i_1)\big).$$

The necessary condition for $D(\alpha, o_1, o_2)$, understood as a smooth analytical function, is given by the requirement that all three partial derivatives of D must be zero, i.e., $D_\alpha = D_{o_1} = D_{o_2} = 0 \Leftrightarrow \Sigma^n_{i=1} d^i_\alpha = \Sigma^n_{i=1} d^i_{o_1} = \Sigma^n_{i=1} d^i_{o_2} = 0$. The manual derivation of the solution of the resulting equations is rather complex, and one must use a symbolic solver.

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