OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:... When understanding the computation of the optimal quaternion q_{rot} as an optimization problem to be addressed via Lagrange multipliers, the function to be MAXIMIZED is the function $F(\alpha,u,v,w) = \sum_{i=1}^{n} \langle R\mathbf{y}_i, \mathbf{x}_i \rangle$, subject to the NORMALIZATION CONSTRAINT $\|q_{rot}\| = 1 = (c\frac{\alpha}{2})^2 + (s\frac{\alpha}{2})^2(u^2+v^2+w^2) = G(\alpha,u,v,w)$. The gradient of F is $\text{grad}\,F = (\partial/\partial\alpha\,F, \partial/\partial u\,F, \partial/\partial v\,F, \partial/\partial w\,F) = (F_\alpha, F_u, F_v, F_w)$; the gradient of G is $\text{grad}\,G = (\partial/\partial\alpha\,G, \partial/\partial u\,G, \partial/\partial v\,G, \partial/\partial w\,G) = (G_\alpha, G_u, G_v, G_w)$. Specifically, $\text{grad}\,G = (0, 2u(s\frac{\alpha}{2})^2, 2v(s\frac{\alpha}{2})^2, 2w(s\frac{\alpha}{2})^2) = \ldots = (0, u(1-c\alpha), v(1-c\alpha), w(1-c\alpha))$. Following the method of Lagrange multipliers, one must determine λ-values that satisfy the equation

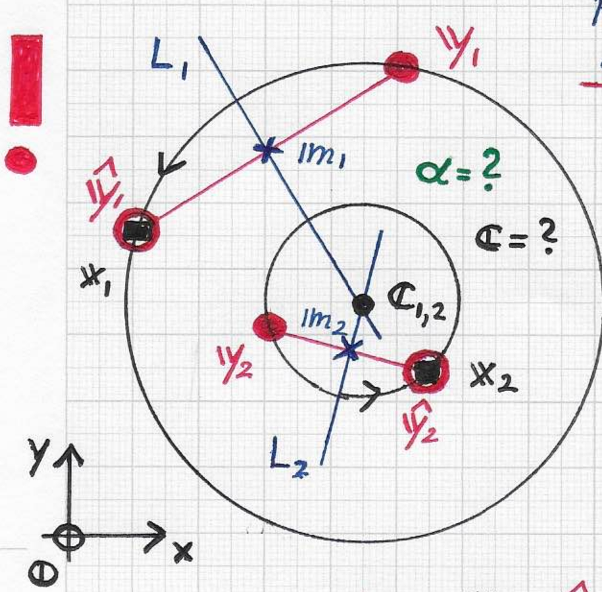
$$\boxed{\begin{array}{l} \text{grad}\,F = \lambda\,\text{grad}\,G \\ \Leftrightarrow \quad (F_\alpha, F_u, F_v, F_w) = \lambda(0, u(1-c\alpha), v(1-c\alpha), w(1-c\alpha)), \\ \qquad\qquad \text{where } u^2+v^2+w^2 = 1 . \end{array}}$$

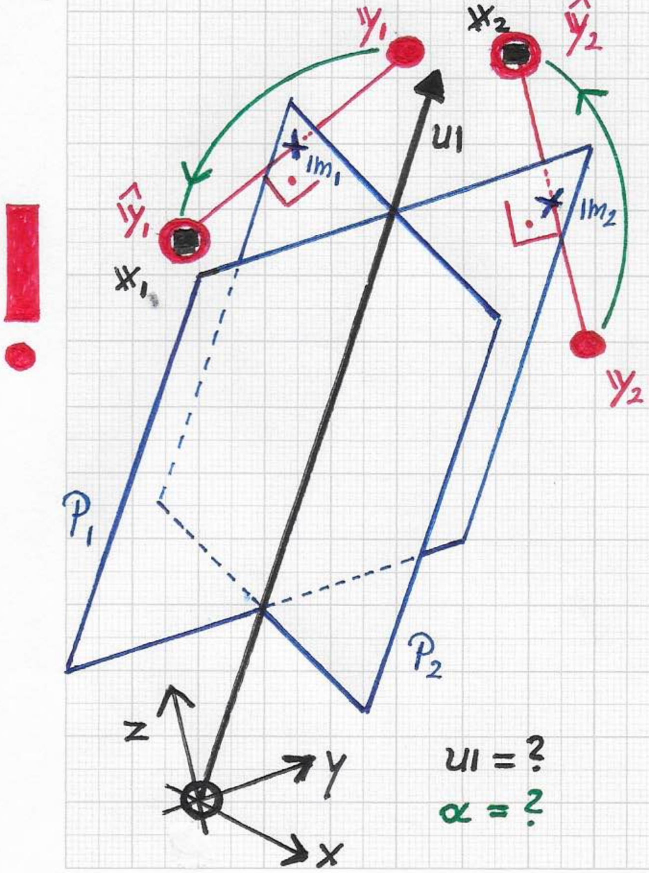
Considering this equation and constraint $\|\mathbf{u}\| = 1$, the method of Lagrange multipliers determines all "formally allowable" values for λ, α, u, v and w. Subsequentially, one must employ additional tests necessary to derive the (one) "geometrically correct" solution — i.e., the optimal angle α and optimal rotation axis direction vector $\mathbf{u}$, $\|\mathbf{u}\| = 1$.

...

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks: ...





• **Note.** It is possible to solve the problem with a slightly different approach that combines geometrical and least-squares, best approximation methods. Again, the problem is concerned with the best-possible rotation that maps a given set of points $\{\mathbf{y}_i\}_{i=1}^n$ to an image set of points $\{\hat{\mathbf{y}}_i\}_{i=1}^n$, where $\mathbf{y}_i \mapsto \hat{\mathbf{y}}_i$, such that $\sum_{i=1}^n \|\hat{\mathbf{y}}_i - \mathbf{x}_i\|^2$ has minimal value – where the "target point set" $\{\mathbf{x}_i\}_{i=1}^n$ is also provided. The top-left figure shows a simple, ideal scenario for the 2D case: Points $\mathbf{y}_1$, $\mathbf{y}_2$, $\mathbf{x}_1$ and $\mathbf{x}_2$ are given; the goal is to calculate the optimal center of rotation $\mathbf{c}$ and optimal rotation angle α that map $\mathbf{y}_i$ to $\hat{\mathbf{y}}_i$ such that the sum $\|\hat{\mathbf{y}}_1 - \mathbf{x}_1\|^2 + \|\hat{\mathbf{y}}_2 - \mathbf{x}_2\|^2$ has minimal value. The figure sketches a "perfect problem" where a rotation exists that maps $\mathbf{y}_i$ to $\hat{\mathbf{y}}_i = \mathbf{x}_i$. The relevant geometry is shown. ...

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• **Laplacian eigenfunctions and neural networks:...** The figure on the previous page illustrating the 2D case includes the following provided or computed geometrical primitives:

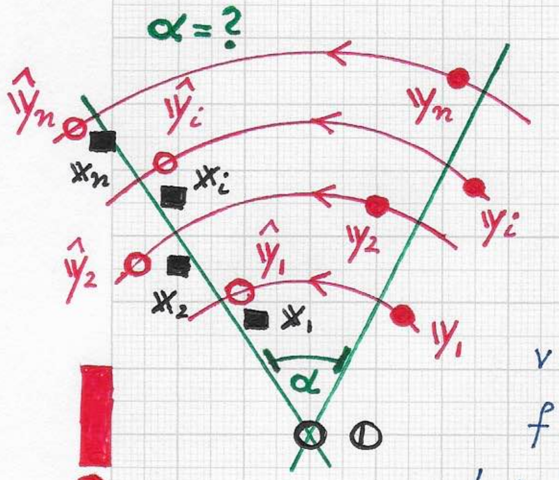
- $\overline{\mathbb{y}_i \mathbb{x}_i}$ — Line segments connecting a given point $\mathbb{y}_i$ and associated target point $\mathbb{x}_i$
- $\mathbb{m}_i$ — midpoints of line segments $\overline{\mathbb{y}_i \mathbb{x}_i}$
- L_i — lines passing through $\mathbb{m}_i$ and being orthogonal to $\overline{\mathbb{y}_i \mathbb{x}_i}$
- $\mathbb{c}_{i,j}$ — intersection points of lines L_i and L_j ("assumed to be close to the optimal center of rotation $\mathbb{c}$")
- $\hat{\mathbb{y}}_i$ — image points of given points $\mathbb{y}_i$, resulting from rotating $\mathbb{y}_i$ around the optimal rotation center $\mathbb{c}$ by the optimal rotation angle α
- $\mathbb{c}, \alpha$ — optimal center of rotation and optimal rotation angle, resulting from the minimization goal $\sum_{i=1}^{n} \| \hat{\mathbb{y}}_i - \mathbb{x}_i \|^2 \rightarrow \min$

• **Note.** If one can assume that the two point sets $\{\mathbb{y}_i\}_{i=1}^n$ and $\{\mathbb{x}_i\}_{i=1}^n$ have already been pre-processed to ensure that (i) they share the origin $\mathbb{O}$ as their common center and (ii) they are "of the same scale," then it will not be necessary to view the center of rotation $\mathbb{c}$ as an unknown parameter; one will be able to simply define $\mathbb{c} := \mathbb{O}$. Thus, one must optimize the value of α only.

...

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:...



First, we briefly summarize the 2D case for two point sets, $\{\mathbf{y}_i\}_{i=1}^n$ and $\{\mathbf{x}_i\}_{i=1}^n$, both being centered around the origin $\mathbf{O}$ that they share as their common center. The left figure illustrates this case. One must determine the optimal value of rotation angle α that defines the best-possible rotation (matrix) mapping the points $\mathbf{y}_i$ to the image points $\hat{\mathbf{y}}_i$ — such that the image points are as close as possible to the target points $\mathbf{x}_i$, minimizing the sum of squared distances. These are the computations:

- $\mathbf{y}_i = (y_1^i, y_2^i)^T$, $\hat{\mathbf{y}}_i = (\hat{y}_1^i, \hat{y}_2^i)^T$, $\mathbf{x}_i = (x_1^i, x_2^i)^T$
- $\hat{\mathbf{y}}_i = R \cdot \mathbf{y}_i = (y_1^i c\alpha - y_2^i s\alpha,\ y_1^i s\alpha + y_2^i c\alpha)^T$; $R = \begin{bmatrix} c\alpha & -s\alpha \\ s\alpha & c\alpha \end{bmatrix}$
- $\|\hat{\mathbf{y}}_i - \mathbf{x}_i\|^2 = (\hat{y}_1^i - x_1^i)^2 + (\hat{y}_2^i - x_2^i)^2 = \ldots =$

$$= (x_1^i)^2 + (x_2^i)^2 + (y_1^i)^2 + (y_2^i)^2$$
$$+ 2\,(s\alpha\,(x_1^i y_2^i - x_2^i y_1^i) - c\alpha\,(x_1^i y_1^i + x_2^i y_2^i))$$
$$= \|\mathbf{x}_i\|^2 + \|\mathbf{y}_i\|^2 - 2\,(s\alpha\,\langle \mathbf{x}_i, \mathbf{y}_i^{\perp}\rangle + c\alpha\,\langle \mathbf{x}_i, \mathbf{y}_i\rangle)\ ;$$
$$\mathbf{y}_i^{\perp} = (-y_2^i, y_1^i)^T$$

- $\Sigma_{i=1}^n \|\hat{\mathbf{y}}_i - \mathbf{x}_i\|^2 = \ldots$; extremum condition: $\frac{d}{d\alpha} \Sigma_{i=1}^n \|\ldots\|^2 = 0$
- $\frac{d}{d\alpha}\left(\|\mathbf{x}_i\|^2 + \|\mathbf{y}_i\|^2 - 2\,(s\alpha\,\langle \mathbf{x}_i, \mathbf{y}_i^{\perp}\rangle + c\alpha\,\langle \mathbf{x}_i, \mathbf{y}_i\rangle)\right) =$

$$= 2\,(s\alpha\,\langle \mathbf{x}_i, \mathbf{y}_i\rangle - c\alpha\,\langle \mathbf{x}_i, \mathbf{y}_i^{\perp}\rangle)$$

- $\Rightarrow \frac{d}{d\alpha} \Sigma_{i=1}^n \|\ldots\|^2 = 2\, \Sigma_{i=1}^n (s\alpha\,\langle \mathbf{x}_i, \mathbf{y}_i\rangle - c\alpha\,\langle \mathbf{x}_i, \mathbf{y}_i^{\perp}\rangle) \overset{!}{=} 0$

$\Rightarrow \ldots$

...

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks: ...

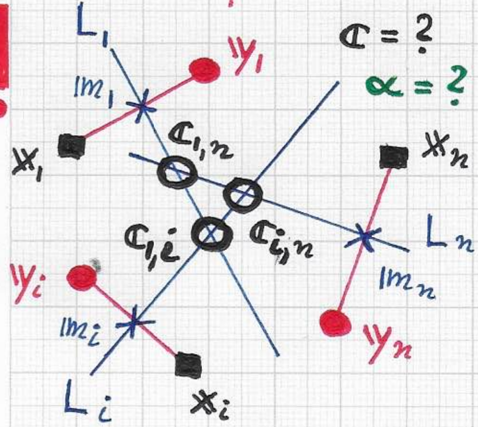
• $\Rightarrow \sum_{i=1}^{n} s\alpha \langle x_i, y_i \rangle = \sum_{i=1}^{n} c\alpha \langle x_i, y_i^{\perp} \rangle$

$\Leftrightarrow s\alpha \sum_{i=1}^{n} \langle x_i, y_i \rangle = c\alpha \sum_{i=1}^{n} \langle x_i, y_i^{\perp} \rangle$

• Thus, the optimal value of α can be computed by using the following two equations:

$$\boxed{\begin{aligned} s\alpha / c\alpha &= \underline{\tan\alpha} = \sum_{i=1}^{n} \langle x_i, y_i^{\perp} \rangle \Big/ \sum_{i=1}^{n} \langle x_i, y_i \rangle \,, \\ c\alpha / s\alpha &= \underline{\cot\alpha} = \sum_{i=1}^{n} \langle x_i, y_i \rangle \Big/ \sum_{i=1}^{n} \langle x_i, y_i^{\perp} \rangle \,. \end{aligned}}$$

One obtains the value of α by using the arctan or arccot function. In singular, degenerate cases (division by zero) one can only use one of these two inverse functions.



Second, we consider the more general case sketched in the left figure. Here, the origin $\mathbf{0}$ is not / cannot be used as the (optimal) center of rotation ($\mathbf{C}$). One can consider the shown lines L_i, $i=1 \ldots n$, and their pairwise intersections in a solution approach for determining an optimal rotation center $\mathbf{C}$. (It should also be noted that a solution approach for this 2D case can also guide an approach needed for the 3D case, where one must determine an optimal unit axis direction vector $\mathbf{u}$, see bottom figure on page 7 (2-14-2024). The vector $\mathbf{u}$ should be constructed via an approach that employs the shown planes P_i and their intersections.) •••