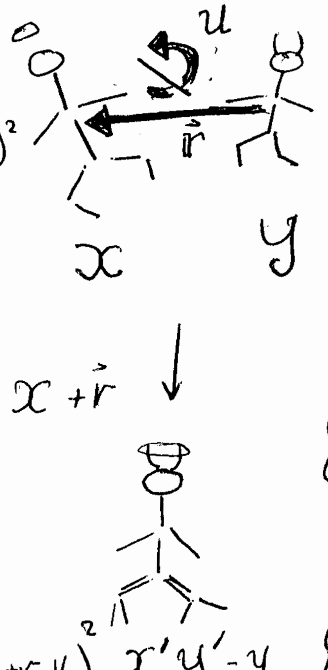
The optimal superposition problem

$E = \frac{1}{N}\sum_1^N (\vec{x}_k - \vec{y}_k)^2$

$\parallel$

$E\{x, y\}$



$x' = ux + \vec{r}$

$\min E\{x', y\} =$

$= \min_{u, \vec{r}} \sum (ux_k + r - y_k)^2 \quad x', y' = y$

"Given an ordered set of vectors $\{\vec{y}_k\}_{k=1}^N$ (target) and

$\{y_k, k = 1, \ldots, N\}$

& a second set $\{\vec{x}_k\}_{k=1}^N$ (model)

find an orthogonal transformation U and translation $\vec{r}$ such that the residual

$$E := \frac{1}{N}\sum_{k=1}^N |U\vec{x}_k + \vec{r} - \vec{y}_k|^2 \qquad (1)$$

is minimized. "

(1) Minimize E with respect to $\vec{r}$:

$$\nabla E = \frac{2}{N}\sum_1^N (U\vec{x}_k + \vec{r} - \vec{y}_k) = 0 \Rightarrow U\Big(\underbrace{\frac{1}{N}\sum_1^N \vec{x}_k}_{\bar{x}}\Big) + \vec{r} - \Big(\underbrace{\frac{1}{N}\sum \vec{y}_k}_{\bar{y}}\Big) = 0$$

$\bar{x} \leftarrow$ barycenter $\rightarrow \bar{y}$

$$\Rightarrow \vec{r} = -(U\bar{x} + \bar{y})$$

Therefore, if we shift both sets so that their barycenters $\bar{x}, \bar{y}$ are placed at the origin, (i.e. they coincide) then they will be optimally placed with respect to translations. We assume $\bar{x} = \bar{y} = 0$ and we focus on the second problem:

(2) Minimize E with respect to all orthogonal matrices U, given $\bar{x} = \bar{y} = 0$.

We have (see Horn & Johnson, Matrix Analysis, p. 431)

$$NE = \sum_{k=1}^{N} |x_k' - y_k|^2 = \mathrm{Tr}\left\{(\mathcal{X}'-\mathcal{Y})^T(\mathcal{X}'-\mathcal{Y})\right\}$$

$$= \mathrm{Tr}\ \mathcal{X}'^T\mathcal{X}' + \mathrm{Tr}\ \mathcal{Y}'^T\mathcal{Y}' - 2\,\mathrm{Tr}\ \mathcal{Y}^T\mathcal{X}'$$

$$= \underbrace{\sum_{k=1}^{N} |x_k'|^2}_{\sum_{k=1}^{N}|x_k|^2} + \sum_{k=1}^{N} |y_k|^2 - 2\,\mathrm{Tr}\ \mathcal{Y}^T\mathcal{X}' \qquad (2)$$

(since $\mathcal{U}$ preserves norms)

$$|\mathbf{x}_k'|^2 = |\mathcal{U}\mathbf{x}_k|^2 = x_k^T\mathcal{U}^T\mathcal{U}x_k = x_k^T\mathbf{x}_k = |\mathbf{x}_k|^2$$

So, the problem of minimizing the residual has now become to maximize the trace $\mathrm{Tr}\,\mathcal{Y}^T\mathcal{X}'$

We can show:

Problem 1: Show that $\mathrm{Tr}\,AB = \mathrm{Tr}\,BA$

Then, using the result of problem (1),

$$\mathrm{Tr}(\mathcal{Y}^T\mathcal{X}') = \mathrm{Tr}(\mathcal{Y}^T\mathcal{U}\mathcal{X}) = \mathrm{Tr}(\mathcal{X}\mathcal{Y}^T\mathcal{U}) \qquad (3)$$

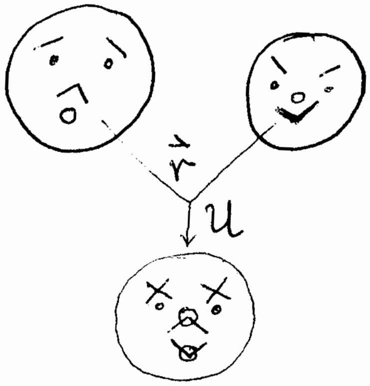
Definition: The correlation matrix of the two sets, $\mathcal{R}$, is defined as

$$\mathcal{R} = \mathcal{X}\mathcal{Y}^T \qquad (4)$$

Pictorially:

$$\mathcal{X} = (\vec{x}_1, \ldots \vec{x}_N), \quad \mathcal{Y} = (\vec{y}_1, \ldots, \vec{y}_N) \quad (3\times N)$$

$$\mathcal{R} := \mathcal{X}\mathcal{Y}^T = \sum_{k=1}^{N} x_k y_k^T \qquad (5)$$



$$(\vec{x}_1 \cdots \vec{x}_N)\begin{pmatrix}\vec{y}_1^T \\ \vdots \\ \vec{y}_N^T\end{pmatrix}$$

That is, $\mathcal{R}_{ij} = \sum_{k=1}^{N} x_{ik} y_{jk} \; ; \; i,j = 1,2,3$

Now, consider the SVD of $\mathcal{R} = V \Sigma W^T$. Then

$$\mathrm{Tr}(\mathcal{R}\mathcal{U}) = \mathrm{Tr}(V\Sigma W^T \mathcal{U}) = \mathrm{Tr}(\Sigma W^T \mathcal{U} V) = \sum_{i=1}^{3} \sigma_i w_i^T \mathcal{U} v_i$$

$$=: \sum_{1}^{3} \sigma_i T_{ii} \qquad (6)$$

where we introduce the orthonormal matrix

$$T := W^T \mathcal{U} V \qquad (7)$$

<u>Problem (2)</u> Show that the diagonal elements of T,

$T_{ii} = w_i^T \mathcal{U} v_i$ (all as defined above) satisfy

$$|T_{ii}| \leq 1 \qquad (8)$$

<u>Hint</u>: $\vec{w}_i$, $\vec{v}_i$ are ~~an~~ column vectors of the orthogonal matrices W, V, i.e. they are unit vectors.

~~Problem (3)~~

As a consequence of (8), $\mathrm{Tr}(\mathcal{Y}^T \mathcal{X}') \leq \sum_{1}^{3} \sigma_i$

$\mathrm{Tr}\, \cancel{\mathcal{X}\mathcal{Y}}$

The minimal residual is found if the above expression is maximized, i.e. T becomes the identity. This happens if the matrix $\mathcal{U}$ rotates the vectors v_i onto the w_i. If the two sets have the same chirality (i.e. both right or left handed) then this can be done with a proper rotation, otherwise an improper rotation (i.e. a rotation-reflection) is required:

$$T = \sum w_i^T \mathcal{U} v_j = W^T \mathcal{U} V = I$$

$$\Rightarrow \underline{\mathcal{U} = W V^T}$$

if $\det W = \det V$ then $\mathcal{U}$ is proper, else it is improper.

If we want to minimize the residual subject to only proper rotations, then the best rotation is found as $\underline{\mathcal{U} = W \begin{pmatrix} 1 & & \\ & 1 & \\ & & \pm 1 \end{pmatrix} V^T}$

and the minimal residual is

$$E = \frac{1}{N}\left(\Sigma |x_k|^2 + \Sigma |y_k|^2 - 2 \sum_{i=1}^{3} \chi_i \sigma_i \right)$$

$\chi_1 = 1, \chi_2 = 1, \chi_3 = \pm 1$