Least-Squares Rigid Motion Using SVD

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Abstract

This note summarizes the steps to computing the best-fitting rigid transformation that aligns two sets of corresponding points.

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1 Problem statement

Let $\mathcal{P} = \{\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_n\}$ and $\mathcal{Q} = \{\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_n\}$ be two sets of corresponding points in $\mathbb{R}^d$. We wish to find a rigid transformation that optimally aligns the two sets in the least squares sense, i.e., we seek a rotation R and a translation vector $\mathbf{t}$ such that

$$(R, \mathbf{t}) = \underset{R \in SO(d),\ \mathbf{t} \in \mathbb{R}^d}{\operatorname{argmin}} \sum_{i=1}^{n} w_i \left\| (R\mathbf{p}_i + \mathbf{t}) - \mathbf{q}_i \right\|^2, \tag{1}$$

where $w_i > 0$ are weights for each point pair.

In the following we detail the derivation of R and $\mathbf{t}$; readers that are interested in the final recipe may skip the proofs and go directly Section 4.

2 Computing the translation

Assume R is fixed and denote $F(\mathbf{t}) = \sum_{i=1}^{n} w_i \left\| (R\mathbf{p}_i + \mathbf{t}) - \mathbf{q}_i \right\|^2$. We can find the optimal translation by taking the derivative of F w.r.t. $\mathbf{t}$ and searching for its roots:

$$\begin{aligned} 0 &= \frac{\partial F}{\partial \mathbf{t}} = \sum_{i=1}^{n} 2w_i \left(R\mathbf{p}_i + \mathbf{t} - \mathbf{q}_i \right) = \\ &= 2\mathbf{t} \left(\sum_{i=1}^{n} w_i \right) + 2R \left(\sum_{i=1}^{n} w_i \mathbf{p}_i \right) - 2 \sum_{i=1}^{n} w_i \mathbf{q}_i. \end{aligned} \tag{2}$$

Denote

$$\bar{\mathbf{p}} = \frac{\sum_{i=1}^{n} w_i \mathbf{p}_i}{\sum_{i=1}^{n} w_i}, \quad \bar{\mathbf{q}} = \frac{\sum_{i=1}^{n} w_i \mathbf{q}_i}{\sum_{i=1}^{n} w_i}. \tag{3}$$

By rearranging the terms of (2) we get

$$\mathbf{t} = \bar{\mathbf{q}} - R\bar{\mathbf{p}}. \tag{4}$$

In other words, the optimal translation $\mathbf{t}$ maps the transformed weighted centroid of $\mathcal{P}$ to the weighted centroid of $\mathcal{Q}$. Let us plug the optimal $\mathbf{t}$ into our objective function:

$$\begin{aligned} \sum_{i=1}^{n} w_i \left\|(R\mathbf{p}_i + \mathbf{t}) - \mathbf{q}_i\right\|^2 &= \sum_{i=1}^{n} w_i \left\|R\mathbf{p}_i + \bar{\mathbf{q}} - R\bar{\mathbf{p}} - \mathbf{q}_i\right\|^2 = \qquad (5)\\ &= \sum_{i=1}^{n} w_i \left\|R(\mathbf{p}_i - \bar{\mathbf{p}}) - (\mathbf{q}_i - \bar{\mathbf{q}})\right\|^2. \qquad (6) \end{aligned}$$

We can thus concentrate on computing the rotation R by restating the problem such that the translation would be zero:

$$\mathbf{x}_i := \mathbf{p}_i - \bar{\mathbf{p}}, \quad \mathbf{y}_i := \mathbf{q}_i - \bar{\mathbf{q}}. \tag{7}$$

So we look for the optimal rotation R such that

$$R = \underset{R \in SO(d)}{\operatorname{argmin}} \sum_{i=1}^{n} w_i \left\|R\mathbf{x}_i - \mathbf{y}_i\right\|^2. \tag{8}$$

3 Computing the rotation

Let us simplify the expression we are trying to minimize in (8):

$$\begin{aligned} \left\|R\mathbf{x}_i - \mathbf{y}_i\right\|^2 &= (R\mathbf{x}_i - \mathbf{y}_i)^\top (R\mathbf{x}_i - \mathbf{y}_i) = (\mathbf{x}_i^\top R^\top - \mathbf{y}_i^\top)(R\mathbf{x}_i - \mathbf{y}_i) = \\ &= \mathbf{x}_i^\top R^\top R\mathbf{x}_i - \mathbf{y}_i^\top R\mathbf{x}_i - \mathbf{x}_i^\top R^\top \mathbf{y}_i + \mathbf{y}_i^\top \mathbf{y}_i = \\ &= \mathbf{x}_i^\top \mathbf{x}_i - \mathbf{y}_i^\top R\mathbf{x}_i - \mathbf{x}_i^\top R^\top \mathbf{y}_i + \mathbf{y}_i^\top \mathbf{y}_i. \qquad (9) \end{aligned}$$

We got the last step by remembering that rotation matrices imply $R^\top R = I$ (I is the identity matrix).

Note that $\mathbf{x}_i^\top R^\top \mathbf{y}_i$ is a scalar: $\mathbf{x}_i^\top$ has dimension $1 \times d$, $R^\top$ is $d \times d$ and $\mathbf{y}_i$ is $d \times 1$. For any scalar a we trivially have $a = a^\top$, therefore

$$\mathbf{x}_i^\top R^\top \mathbf{y}_i = (\mathbf{x}_i^\top R^\top \mathbf{y}_i)^\top = \mathbf{y}_i^\top R\mathbf{x}_i. \tag{10}$$

Therefore we have

$$\left\|R\mathbf{x}_i - \mathbf{y}_i\right\|^2 = \mathbf{x}_i^\top \mathbf{x}_i - 2\mathbf{y}_i^\top R\mathbf{x}_i + \mathbf{y}_i^\top \mathbf{y}_i. \tag{11}$$

Let us look at the minimization and substitute the above expression:

$$\begin{aligned} &\underset{R \in SO(d)}{\operatorname{argmin}} \sum_{i=1}^{n} w_i \left\|R\mathbf{x}_i - \mathbf{y}_i\right\|^2 = \underset{R \in SO(d)}{\operatorname{argmin}} \sum_{i=1}^{n} w_i (\mathbf{x}_i^\top \mathbf{x}_i - 2\mathbf{y}_i^\top R\mathbf{x}_i + \mathbf{y}_i^\top \mathbf{y}_i) = \\ &= \underset{R \in SO(d)}{\operatorname{argmin}} \left(\sum_{i=1}^{n} w_i \mathbf{x}_i^\top \mathbf{x}_i - 2\sum_{i=1}^{n} w_i \mathbf{y}_i^\top R\mathbf{x}_i + \sum_{i=1}^{n} w_i \mathbf{y}_i^\top \mathbf{y}_i \right) = \\ &= \underset{R \in SO(d)}{\operatorname{argmin}} \left(-2 \sum_{i=1}^{n} w_i \mathbf{y}_i^\top R\mathbf{x}_i \right). \qquad (12) \end{aligned}$$

$$
\begin{bmatrix} w_1 & & & \\ & w_2 & & \\ & & \ddots & \\ & & & w_n \end{bmatrix}
\begin{bmatrix} \text{—} \; \mathbf{y}_1^\mathsf{T} \; \text{—} \\ \text{—} \; \mathbf{y}_2^\mathsf{T} \; \text{—} \\ \vdots \\ \text{—} \; \mathbf{y}_n^\mathsf{T} \; \text{—} \end{bmatrix}
\begin{bmatrix} & & \\ & R & \\ & & \end{bmatrix}
\begin{bmatrix} | & | & & | \\ \mathbf{x}_1 & \mathbf{x}_2 & \dots & \mathbf{x}_n \\ | & | & & | \end{bmatrix} =
$$

$$
= \begin{bmatrix} \text{—} \; w_1\mathbf{y}_1^\mathsf{T} \; \text{—} \\ \text{—} \; w_2\mathbf{y}_2^\mathsf{T} \; \text{—} \\ \vdots \\ \text{—} \; w_n\mathbf{y}_n^\mathsf{T} \; \text{—} \end{bmatrix}
\begin{bmatrix} | & | & & | \\ R\mathbf{x}_1 & R\mathbf{x}_2 & \dots & R\mathbf{x}_n \\ | & | & & | \end{bmatrix}
= \begin{bmatrix} w_1\mathbf{y}_1^\mathsf{T}R\mathbf{x}_1 & & & * \\ & w_2\mathbf{y}_2^\mathsf{T}R\mathbf{x}_2 & & \\ & & \ddots & \\ * & & & w_n\mathbf{y}_n^\mathsf{T}R\mathbf{x}_n \end{bmatrix}
$$

Figure 1: Schematic explanation of $\sum_{i=1}^n w_i\mathbf{y}_i^\mathsf{T}R\mathbf{x}_i = \mathrm{tr}(WY^\mathsf{T}RX)$.

The last step (removing $\sum_{i=1}^n w_i\mathbf{x}_i^\mathsf{T}\mathbf{x}_i$ and $\sum_{i=1}^n w_i\mathbf{y}_i^\mathsf{T}\mathbf{y}_i$) holds because these expressions do not depend on R at all, so excluding them would not affect the minimizer. The same holds for multiplication of the minimization expression by a scalar, so we have

$$
\underset{R\in SO(d)}{\mathrm{argmin}} \left(-2\sum_{i=1}^n w_i\mathbf{y}_i^\mathsf{T}R\mathbf{x}_i \right) = \underset{R\in SO(d)}{\mathrm{argmax}} \sum_{i=1}^n w_i\mathbf{y}_i^\mathsf{T}R\mathbf{x}_i. \tag{13}
$$

We note that

$$
\sum_{i=1}^n w_i\mathbf{y}_i^\mathsf{T}R\mathbf{x}_i = \mathrm{tr}\left(WY^\mathsf{T}RX\right), \tag{14}
$$

where $W = \mathrm{diag}(w_1, \dots, w_n)$ is an $n \times n$ diagonal matrix with the weight w_i on diagonal entry i; Y is the $d \times n$ matrix with $\mathbf{y}_i$ as its columns and X is the $d \times n$ matrix with $\mathbf{x}_i$ as its columns. We remind the reader that the trace of a square matrix is the sum of the elements on the diagonal: $\mathrm{tr}(A) = \sum_{i=1}^n a_{ii}$. See Figure 1 for an illustration of the algebraic manipulation.

Therefore we are looking for a rotation R that maximizes $\mathrm{tr}\left(WY^\mathsf{T}RX\right)$. Matrix trace has the property

$$
\mathrm{tr}(AB) = \mathrm{tr}(BA) \tag{15}
$$

for any matrices A, B of compatible dimensions. Therefore

$$
\mathrm{tr}\left(WY^\mathsf{T}RX\right) = \mathrm{tr}\left((WY^\mathsf{T})(RX)\right) = \mathrm{tr}\left(RXWY^\mathsf{T}\right). \tag{16}
$$

Let us denote the $d \times d$ "covariance" matrix $S = XWY^\mathsf{T}$. Take SVD of S:

$$
S = U\Sigma V^\mathsf{T}. \tag{17}
$$

Now substitute the decomposition into the trace we are trying to maximize:

$$
\mathrm{tr}\left(RXWY^\mathsf{T}\right) = \mathrm{tr}\left(RS\right) = \mathrm{tr}\left(RU\Sigma V^\mathsf{T}\right) = \mathrm{tr}\left(\Sigma V^\mathsf{T}RU\right). \tag{18}
$$

The last step was achieved using the property of trace (15). Note that V, R and U are all orthogonal matrices, so $M = V^\mathsf{T}RU$ is also an orthogonal matrix. This means that the columns of M are orthonormal vectors, and in particular, $\mathbf{m}_j^\mathsf{T}\mathbf{m}_j = 1$ for each M's column $\mathbf{m}_j$. Therefore all entries m_{ij} of M are ≤ 1 in magnitude:

$$
1 = \mathbf{m}_j^\mathsf{T}\mathbf{m}_j = \sum_{i=1}^d m_{ij}^2 \;\Rightarrow\; m_{ij}^2 \leq 1 \;\Rightarrow\; |m_{ij}| \leq 1\,. \tag{19}
$$

So what is the maximum possible value for $tr(\Sigma M)$? Remember that Σ is a diagonal matrix with non-negative values $\sigma_1, \sigma_2, \ldots, \sigma_d \geq 0$ on the diagonal. Therefore:

$$\operatorname{tr}(\Sigma M) = \begin{pmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_d \end{pmatrix} \begin{pmatrix} m_{11} & m_{12} & \ldots & m_{1d} \\ m_{21} & m_{22} & \ldots & m_{2d} \\ \vdots & \vdots & \vdots & \vdots \\ m_{d1} & m_{d2} & \ldots & m_{dd} \end{pmatrix} = \sum_{i=1}^{d} \sigma_i m_{ii} \leq \sum_{i=1}^{d} \sigma_i. \tag{20}$$

Therefore the trace is maximized if $m_{ii} = 1$. Since M is an orthogonal matrix, this means that M would have to be the identity matrix!

$$I = M = V^{\mathsf{T}} R U \;\Rightarrow\; V = RU \;\Rightarrow\; R = VU^{\mathsf{T}}. \tag{21}$$

Orientation rectification. The process we just described finds the optimal *orthogonal* matrix, which could potentially contain reflections in addition to rotations. Imagine that the point set $\mathcal{P}$ is a perfect reflection of $\mathcal{Q}$. We will then find that reflection, which aligns the two point sets perfectly and yields zero energy in (8), the global minimum in this case. However, if we restrict ourselves to rotations only, there might not be a rotation that perfectly aligns the points.

Checking whether $R = VU^{\mathsf{T}}$ is a rotation is simple: if $\det(VU^{\mathsf{T}}) = -1$ then it contains a reflection, otherwise $\det(VU^{\mathsf{T}}) = +1$. Assume $\det(VU^{\mathsf{T}}) = -1$. Restricting R to a rotation is equivalent to restricting M to a reflection. We now want to find a reflection M that maximizes:

$$\operatorname{tr}(\Sigma M) = \sigma_1 m_{11} + \sigma_2 m_{22} + \ldots + \sigma_d m_{dd} =: f(m_{11}, \ldots, m_{dd}). \tag{22}$$

Note that f only depends on the diagonal of M, not its other entries. We now consider the m_{ii}'s as variables $(m_{11}, \ldots, m_{dd})$. This is the set of all diagonals of reflection matrices of order n. Surprisingly, it has a very simple structure. Indeed, a result by A. Horn [1] states that the set of all diagonals of rotation matrices of order n is equal to the convex hull of the points $(\pm 1, ..., \pm 1)$ with an even number of coordinates that are -1. Since any reflection matrix can be constructed by inverting the sign of a row of a rotation matrix and vice versa, it follows that the set we are optimizing on is the convex hull of the points $(\pm 1, ..., \pm 1)$ with an *uneven* number of -1's.

Since our domain is a convex polyhedron, the linear function f attains its extrema at its vertices. The diagonal $(1, 1, \ldots, 1)$ is not in the domain since it has an even number of -1's (namely, zero), and therefore the next best shot is $(1, 1, \ldots, 1, -1)$:

$$\operatorname{tr}(\Sigma M) = \sigma_1 + \sigma_2 + \ldots + \sigma_{d-1} - \sigma_d. \tag{23}$$

This value is attained at a vertex of our domain, and is larger than any other combination of the form $(\pm 1, ..., \pm 1)$ except $(1, 1, \ldots, 1)$, because σ_d is the smallest singular value.

To summarize, we arrive at the fact that if $\det(VU^{\mathsf{T}}) = -1$, we need

$$M = V^{\mathsf{T}} R U = \begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & & -1 \end{pmatrix} \quad \Rightarrow \quad R = V \begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & & -1 \end{pmatrix} U^{\mathsf{T}}. \tag{24}$$

We can write a general formula that encompasses both cases, $\det(VU^{\mathsf{T}}) = 1$ and $\det(VU^{\mathsf{T}}) = -1$:

$$R = V \begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & & \det(VU^{\mathsf{T}}) \end{pmatrix} U^{\mathsf{T}}. \tag{25}$$

4 Rigid motion computation – summary

Let us summarize the steps to computing the optimal translation $\mathbf{t}$ and rotation R that minimize

$$\sum_{i=1}^{n} w_i \left\|(R\mathbf{p}_i + \mathbf{t}) - \mathbf{q}_i\right\|^2 .$$

1. Compute the weighted centroids of both point sets:

$$\bar{\mathbf{p}} = \frac{\sum_{i=1}^{n} w_i \mathbf{p}_i}{\sum_{i=1}^{n} w_i}, \quad \bar{\mathbf{q}} = \frac{\sum_{i=1}^{n} w_i \mathbf{q}_i}{\sum_{i=1}^{n} w_i}.$$

2. Compute the centered vectors

$$\mathbf{x}_i := \mathbf{p}_i - \bar{\mathbf{p}}, \quad \mathbf{y}_i := \mathbf{q}_i - \bar{\mathbf{q}}, \qquad i = 1, 2, \ldots, n.$$

3. Compute the $d \times d$ covariance matrix

$$S = XWY^{\mathsf{T}},$$

where X and Y are the $d \times n$ matrices that have $\mathbf{x}_i$ and $\mathbf{y}_i$ as their columns, respectively, and $W = \mathrm{diag}(w_1, w_2, \ldots, w_n)$.

4. Compute the singular value decomposition $S = U\Sigma V^{\mathsf{T}}$. The rotation we are looking for is then

$$R = V \begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & & \det(VU^{\mathsf{T}}) \end{pmatrix} U^{\mathsf{T}}.$$

5. Compute the optimal translation as

$$\mathbf{t} = \bar{\mathbf{q}} - R\bar{\mathbf{p}}.$$

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References

[1] A. Horn, *Doubly stochastic matrices and the diagonal of a rotation matrix*. Amer. J. Math. 76:620–630 (1954).