Absolute Orientation and Kabsch Algorithm

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Given two point sets $\mathcal{P} = \{\boldsymbol{p}_i\}$ and $\mathcal{Q} = \{\boldsymbol{q}_i\}$ with one-to-one correspondence, find the rotate $\boldsymbol{R}$(and translation $\boldsymbol{T}$) to make the RMSD(root mean squared deviation) minimum.

$$\min E = \sum ||\boldsymbol{R}\boldsymbol{p}_i + \boldsymbol{T} - \boldsymbol{q}_i||_2^2$$

Translation can be got directly and $\mathcal{P}$ and $\mathcal{Q}$ must be translated first so that their centroid coincides with the origin of the coordinate system. The centroid of $\mathcal{P}$ and $\mathcal{Q}$ are

$$\boldsymbol{p}_o = \frac{1}{n_p} \sum \boldsymbol{p}_i, \boldsymbol{p}_i \in \mathcal{P}$$
$$\boldsymbol{q}_o = \frac{1}{n_q} \sum \boldsymbol{q}_i, \boldsymbol{q}_i \in \mathcal{Q}$$

The translation $\boldsymbol{T}$ is

$$\boldsymbol{T} = \boldsymbol{q}_o - \boldsymbol{p}_o$$

$\mathcal{P}$ should be tranlated $-\boldsymbol{p}_o$ so that the centroid coincides of $\mathcal{P}$ coincides with the origin of the coordinate system. So does $\mathcal{Q}$

$$\mathcal{P}' = \{\boldsymbol{p}'_i = \boldsymbol{p}_i - \boldsymbol{p}_o | \boldsymbol{p}_i \in \mathcal{P}\}$$
$$\mathcal{Q}' = \{\boldsymbol{q}'_i = \boldsymbol{q}_i - \boldsymbol{q}_o | \boldsymbol{q}_i \in \mathcal{Q}\}$$

The point set can be represented by the matrix with dimension 3*N.

$$\boldsymbol{P}' = \begin{pmatrix} \boldsymbol{p}'_0 & \boldsymbol{p}'_1 & \cdots & \boldsymbol{p}'_{n_p} \end{pmatrix}$$
$$\boldsymbol{Q}' = \begin{pmatrix} \boldsymbol{q}'_0 & \boldsymbol{q}'_1 & \cdots & \boldsymbol{q}'_{n_q} \end{pmatrix}$$

and the covariance matrix can be calculated as

$$H = \boldsymbol{P}'\boldsymbol{Q}'^T$$

The SVD decomposition can be computed on H

$$H = U \Lambda V^T$$

The rotate matrix is

$$R = V \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & d \end{pmatrix} U^T$$

where $d = \text{sign}(\det(VU^T))$

Matrix trace and determinante

$$
\begin{aligned}
||A||_F^2 &= tr(A^T A) \\
tr(AB) &= tr(BA) \\
det(A) &= det(A^T)
\end{aligned}
$$

$$\text{RMSD} = \sqrt{\frac{1}{m}\sum_{i=1}^{m}(h(x_i) - y_i)}$$

$$\text{MSE} = \frac{1}{m}\sum_{i=1}^{m}(h(x_i) - y_i)$$

$$\text{MAE} = \frac{1}{m}\sum_{i=1}^{m}|h(x_i) - y_i|$$

$$\text{SD} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_i - avg(x))}$$

Derivation

Given $\mathcal{P}$ and $\mathcal{Q}$, find $\boldsymbol{R}$ and $\boldsymbol{T}$ such that

$$\min E = \sum ||\boldsymbol{R}\boldsymbol{p}_i + \boldsymbol{T} - \boldsymbol{q}_i||_2^2$$

Translate the point sets so that their centroid coincides with the origin of the coordinate system and represent it in matrix form.

$$
\begin{aligned}
\boldsymbol{P'} &= \begin{pmatrix}\boldsymbol{p}_0 - \boldsymbol{p}_o & \boldsymbol{p}_1 - \boldsymbol{p}_o & \cdots & \boldsymbol{p}_{n_p} - \boldsymbol{p}_o\end{pmatrix} \\
\boldsymbol{Q'} &= \begin{pmatrix}\boldsymbol{q}_0 - \boldsymbol{q}_o & \boldsymbol{q}_1 - \boldsymbol{q}_o & \cdots & \boldsymbol{q}_{n_q} - \boldsymbol{q}_o\end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
\min E = \sum ||\boldsymbol{RP'} - \boldsymbol{Q'}||_F^2 &= tr((\boldsymbol{RP'} - \boldsymbol{Q'})^T(\boldsymbol{RP'} - \boldsymbol{Q'})) \\
&= tr(\boldsymbol{P'}^T\boldsymbol{R}^T\boldsymbol{RP'}) + tr(\boldsymbol{Q'}^T\boldsymbol{Q'}) - 2tr(\boldsymbol{Q'}^T\boldsymbol{RP'}) \\
&= tr(\boldsymbol{P'}^T\boldsymbol{P'}) + tr(\boldsymbol{Q'}^T\boldsymbol{Q'}) - 2tr(\boldsymbol{Q'}^T\boldsymbol{RP'})
\end{aligned}
$$

E is minimum when $tr(\boldsymbol{Q'}^T\boldsymbol{RP'})$ is maximum.

$$
\begin{aligned}
\max E' &= tr(\boldsymbol{Q'}^T\boldsymbol{RP'}) \\
&= tr(\boldsymbol{Q'}^T\boldsymbol{P'R}) \\
&= tr(\boldsymbol{P'Q'}^T\boldsymbol{R})
\end{aligned}
$$

Do SVD on $\boldsymbol{P'Q'}^T$, and

$$\max E' = tr(\boldsymbol{P'Q'}^T\boldsymbol{R}) = tr(\boldsymbol{U}\,\Sigma\,\boldsymbol{V}^T\boldsymbol{R}) = tr(\Sigma\,\boldsymbol{UV}^T\boldsymbol{R}) = tr(\Sigma\,\boldsymbol{T}) \leq \sum \sigma_i T_{ii}$$

Where $\boldsymbol{T} = \boldsymbol{UV}^T\boldsymbol{R}$, $\boldsymbol{T}$ is a orthogonal matrix therefore $T_{ii} \leq 1$. So E' is maximum when $\boldsymbol{UV}^T\boldsymbol{R} = \boldsymbol{Id}$,

$$\boldsymbol{R} = \boldsymbol{VU}^T$$

To make sure $\boldsymbol{R}$ is in right-handed coordinate system

$$\boldsymbol{R} = \boldsymbol{V}\begin{pmatrix}1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & d\end{pmatrix}\boldsymbol{U}^T$$

where $d = \text{sign}(\text{det}(VU^T))$