Main page
Contents
Featured content
Current events
Random article
Donate to Wikipedia
Wikipedia store

Interaction
Help
About Wikipedia
Community portal
Recent changes
Contact page

Tools
What links here
Related changes
Upload file
Special pages
Permanent link
Page information
Wikidata item
Cite this page

Print/export
Create a book
Download as PDF
Printable version

Languages
Add links

Kabsch algorithm

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The **Kabsch algorithm**, named after Wolfgang Kabsch, is a method for calculating the optimal rotation matrix that minimizes the RMSD (root mean squared deviation) between two paired sets of points. It is useful in graphics, cheminformatics to compare molecular structures, and also bioinformatics for comparing protein structures (in particular, see root-mean-square deviation (bioinformatics)).

The algorithm only computes the rotation matrix, but it also requires the computation of a translation vector. When both the translation and rotation are actually performed, the algorithm is sometimes called partial Procrustes superimposition (see also orthogonal Procrustes problem).

Description [edit]

The algorithm starts with two sets of paired points, *P* and *Q*. Each set of points can be represented as an *N*×3 matrix. The first row is the coordinates of the first point, the second row is the coordinates of the second point, the *N*th row is the coordinates of the *N*th point.

$$\begin{pmatrix} x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ \vdots & \vdots & \vdots \\ x_N & y_N & z_N \end{pmatrix}$$

The algorithm works in three steps: a translation, the computation of a covariance matrix, and the computation of the optimal rotation matrix.

Translation [edit]

Both sets of coordinates must be translated first, so that their centroid coincides with the origin of the coordinate system. This is done by subtracting from the point coordinates the coordinates of the respective centroid.

Computation of the covariance matrix [edit]

The second step consist of calculating a covariance matrix *A*. In matrix notation,

$$A = P^T Q$$

or, using summation notation,

$$A_{ij} = \sum_{k=1}^{N} P_{ki} Q_{kj},$$

Computation of the optimal rotation matrix [edit]

It is possible to calculate the optimal rotation *U* based on the matrix formula $U = (A^T A)^{1/2} A^{-1}$ but implementing a numerical solution to this formula becomes complicated when all special cases are accounted for (for example, the case of *A* not having an inverse).

If singular value decomposition (SVD) routines are available, the optimal rotation, *U*, can be calculated using

the following simple algorithm.

First, calculate the SVD of the covariance matrix *A*.

$$A = VSW^T$$

Next, decide whether we need to correct our rotation matrix to ensure a right-handed coordinate system

$$d = \mathrm{sign}(\det(WV^T))$$

Finally, calculate our optimal rotation matrix, *U*, as

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

Coutsias, Seok, and Dill[1] have found an equivalent method that uses quaternions. Expressing the optimal rotation matrix with a quaternion goes back to 1999: see appendix in [2] and was generalized in 2002 to probability distributions (continuous or not): see appendix A.5 in.[3]

Generalizations [edit]

The algorithm was described for points in a three-dimensional space. The generalization to *D* dimensions is immediate.

External links [edit]

This SVD algorithm is described in more detail at http://cnx.org/content/m11608/latest/

A Matlab function is available at http://www.mathworks.com/matlabcentral/fileexchange/25746-kabsch-algorithm

A C++ implementation (and unit test) using Eigen

A Python script is available at https://github.com/charnley/rmsd

A free PyMol plugin easily implementing Kabsch is Cealign. VMD uses the Kabsch algorithm for its alignment.

See also [edit]

Wahba's Problem

References [edit]

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