Homework #1

“Optimal orthogonal transformation”

Mathematical Modelling

Dmytro Tkachenko

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Task 1

Equation: $\boldsymbol{Q} * \boldsymbol{x_i} + \boldsymbol{b} = \boldsymbol{y_i}, where\ i = 1, .., n$

Given matrices X and Y:

$$X = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -1 & 0 \\ 0 & -1 \\ 1 & 1 \\ -1 & 1 \\ -1 & -1 \\ 1 & -1 \end{bmatrix} \quad Y = \begin{bmatrix} 1.007 & 0.207 \\ -0.407 & 0.207 \\ -0.407 & -1.207 \\ 1.007 & -1.207 \\ 0.3 & 0.914 \\ -1.114 & -0.5 \\ 0.3 & -1.914 \\ 1.714 & -0.5 \end{bmatrix}$$

Matrix Q and vector b after naïve approach:

$$Q = \begin{bmatrix} 0.70711 & 0.70711 \\ -0.70711 & 0.70711 \end{bmatrix} \quad b = [0.3 \quad -0.5]$$

Task 2

My function ***naive(X, Y)*** takes matrices X, Y of the same dimension **n** x **k** and returns square matrix Q and vector b, as it is specified in a specification.

<u>Overview of my solution</u>

My idea is to simplify the work and to bring the expression

$$\boldsymbol{Q}\boldsymbol{x_i} + \boldsymbol{b} = \boldsymbol{y_i}, where\ i = 1, .., n$$

into the $Ax = b$ format to improve flexibility and increase the number of possibilities I can do to get the matrix Q and vector b from the new "unknowns" matrix B.

After converting the system to the form I am comfortable with and finding the unknowns matrix B, I can easily get the rotation matrix Q and displacement vector b out of it.

In the last step, I will apply QR decomposition to make sure that the resulting Q matrix is square and orthogonal (which is what the rotation matrix should be).

Detailed Principle of action

1. Matrix Preparation. Let's move a little bit backwards in solving the problem. Let's imagine that we already have our convenient form $\boldsymbol{X} * \boldsymbol{B} = \boldsymbol{Y}$. Now if we look more carefully, we see that in order for the left side of the expression to also represent a sum where the second operand (vector b) is not multiplied by a vector from matrix X, we need to add a column of ones to matrix X.
2. Obtaining the matrix of unknowns. Then, to solve our equation and get the unknowns matrix B from the equation $\boldsymbol{X} * \boldsymbol{B} = \boldsymbol{Y}$, we need to multiply both parts by the Moore Penrose inverse matrix **X.** $\boldsymbol{B} = \boldsymbol{X}^{\dagger} * \boldsymbol{Y}$**.**
3. Getting the values, we are looking for. Cut the matrix B. The last row of matrix B will be the vector b to be searched, and the rest of it will be matrix Q.
4. Ensure that Q is orthogonal. Use QR decomposition to obtain a new matrix Q which is exactly orthogonal.

Task 3

$$\boldsymbol{C} = \boldsymbol{U} * \boldsymbol{S} * \boldsymbol{V}^{\boldsymbol{T}}$$

From the Theorem Multiplication Theorem: **det(AB) = det(A) * det(B)**. We can use the same principle in our equation**:** $\boldsymbol{det}(\boldsymbol{C}) = \boldsymbol{det}(\boldsymbol{U}) * \boldsymbol{det}(\boldsymbol{S}) * \boldsymbol{det}(\boldsymbol{V}^{\boldsymbol{T}})$.

As U and V matrices are orthogonal, then their determinants equal to +/-1

S matrix is a diagonal matrix of singular values. It means that det(S) equals to the product of singular value that are greater or equals 0, because singular value is a square root of eigenvalue.

Now we can see that as det(S) is always positive as the product of non-negative numbers, then the sign of determinant of matrix C relies on a sign of a determinant of the product of U and V^T matrices.

Task 4

The function ***kabsch(X, Y)*** takes matrices X, Y of the same dimension **n** x **k** and returns square matrix Q and vector b, as it is specified in a specification.

Overview of my solution

In implementing the function, I followed the tasks in the function specification behind this reference step by step.

Detailed Principle of action

1. Creation of matrices of centroids X and Y, where each matrix element is equal to the difference of mean of the corresponding matrix, corresponding measurement and matrix value at the specified position matrix X.
2. Obtaining the covariance C of a k x k matrix. C = ...
3. Applying Singular Value Decomposition on matrix C to partition it into 3 matrices U, S and V^T
4. Creating a diagonal matrix D with dimensions k x k, where the rightmost lower element is 1 or -1 depending on the sign of the matrix determinant of C or $U * V^T$
5. Obtaining the sought matrix Q by multiplication of matrices U, D and V^T
6. Obtaining the sought vector b from the formula: $\boldsymbol{b} = \overline{\boldsymbol{y}} - \boldsymbol{Q} * \overline{\boldsymbol{x}}$

References

1. Wikipedia. Linear Least Squares: https://en.wikipedia.org/wiki/Linear_least_squares
2. Wikipedia. QR Decomposition: https://en.wikipedia.org/wiki/QR_decomposition
3. Wikipedia. Kabsch Algorithm: https://en.wikipedia.org/wiki/Kabsch_algorithm