

GROMACS - Feature #2005

Full Correlation Analysis (FCA) as Trajectory Analysis Module

07/14/2016 10:15 AM - Christian Blau

Status:	New
Priority:	Normal
Assignee:	Christian Blau
Category:	analysis tools
Target version:	future
Difficulty:	uncategorized

Description

Why

Full Correlation Analysis (FCA) aids resolve conformational substates and identify actual transition pathways, usually much more successfully so than Principal Components Analysis (PCA).

Algorithm

FCA of a trajectory follows the spirit of PCA in finding important modes of motion through an orthonormal coordinate transformation and subsequent sorting of basis vectors.

While the projection of the trajectory on the subspace spanned by any two PCA basis vectors is linearly uncorrelated, they usually share mutual information (think of a circle).

The flavour of FCA to implement here, minimizes mutual information in the total system as defined by the information entropy H , $I = \sum H[x_i] - H[\{x\}]$.

It starts from an initial guess of Eigenvectors from a PCA, then iteratively minimizes Mutual Information by 2d-planes rotations of pairs of basis vectors.

Implementation

The algorithm described here has been implemented for gromacs3 by Oliver Lange and then ported to gromacs4.6 by Christian Blau. It should fit perfectly the trajectoryanalysis framework

References

Lange, Oliver F., and Helmut Grubmüller. "Full correlation analysis of conformational protein dynamics." *Proteins: Structure, Function, and Bioinformatics* 70.4 (2008): 1294-1312.

standard_sans_both.jpg

[\[\[http://www.mpibpc.mpg.de/9619680/g_fca_ver_1_3.tgz\]\]](http://www.mpibpc.mpg.de/9619680/g_fca_ver_1_3.tgz)

[\[\[http://www.mpibpc.mpg.de/9768579/g_fca_ver_2_0.tgz\]\]](http://www.mpibpc.mpg.de/9768579/g_fca_ver_2_0.tgz)

History

#1 - 03/15/2017 06:00 PM - Mark Abraham

- Target version changed from 2018 to future

not happening for 2017

#2 - 02/07/2018 02:19 PM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '1' for Issue [#2005](#).

Uploader: berenger bramas (berenger.eu@gmail.com)

Change-Id: gromacs~master~Id9f8a59a82d9ae2d0ec2a49a19de7363d13c9a44

Gerrit URL: <https://gerrit.gromacs.org/7552>