CDIO

Continuous Distribution of Interdomain Orientations

User Manual

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Contents

Chapter 1

Introduction

CDIO is the first fitting program to determine a continuous interdomain orientation distribution from motionally decoupled dynamic NMR data. CDIO is our first step on a sound mathematical ground to reconstruct the conformational distribution of biological macromolecules. Underlying the MATLAB code of CDIO, there are two key components, a continuous model that describes a broad spectrum of interdomain motions and a *de novo* Branch-and-Bound algorithm that guarantees to find the best-fit. CDIO is applicable to the study of interdomain motions in protein, RNA or DNA molecules. CDIO only requires two alignment tensors of each domain calculated either from residual dipolar couplings or pseudo-contact shifts to determine the best-fit interdomain orientation distribution. CDIO is developed jointly in the lab of Prof. Bruce Donald and the lab of Prof. Terrence Oas at Duke University.

The primary contributors to this version of the CDIO distribution are: Yang Qi, Terrence Oas and Bruce Donald.

1.1 Motional Decoupling and Saupe Tensors

1.2 The Bingham Distribution on $SO(3)$

1.3 The Branch and Bound Algorithm

Chapter 2

Setting up and Running CDIO

CDIO requires MATLAB to run, but it does not require any MATLAB toolboxes. MATLAB R2013 or any later version should be sufficient. To install MATLAB, please follow the official instructions(`http://www.mathworks.com/help/install/ug/install-mathworks-software.html`).

In the CDIO distribution, the *mhg* function and its associated files are included. The copyright of the the *mhg* function belongs to Dr. Plamen Koev in San Jose State University [6]. You may want to recompile the *mhg.c* file before running. To compile the *mhg.c* file, type the following command at the MATLAB prompt:

mex mhg.c

The main function of the CDIO program is *BnBmain*. The inputs to the main function are two 2×5 matrices containing a total of four Saupe tensors. Given the Saupe tensor of the reference domain (Domain I) from two independent alignments, S^1_{I} and S^2_{I} and the Saupe tensors of the other domain (Domain II) from the two alignments, S^1_{II} and S^2_{II}, the inputs **s1** and **s2** are formatted as:

s1 = [S^1_{I}**(1,1)**, S^1_{I}**(2,2)**, S^1_{I}**(1,2)**, S^1_{I}**(1,3)**, S^1_{I}**(2,3)**;S^2_{I}**(1,1)**, S^2_{I}**(2,2)**, S^2_{I}**(1,2)**, S^2_{I}**(1,3)**, S^2_{I}**(2,3)**];

s2 = [S^1_{II}**(1,1)**, S^1_{II}**(2,2)**, S^1_{II}**(1,2)**, S^1_{II}**(1,3)**, S^1_{II}**(2,3)**; S^2_{II}**(1,1)**, S^2_{II}**(2,2)**, S^2_{II}**(1,2)**, S^2_{II}**(1,3)**, S^2_{II}**(2,3)**];

To run the program, type the following command at the MATLAB prompt:

BnBmain(s1,s2)

When no input arguments or incorrect arguments are supplied, the program sets the input as the SpA-N data automatically. If you only want to reproduce the SpA-N result, drop the arguments and simply type:

BnBmain

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