MAX PLANCK INSTITUTE FOR INTELLIGENT SYSTEMS
Empirical Inference Department (Prof. Bernhard Schölkopf)
Learning and Dynamical Systems Group (Dr. Michael Muehlebach)

Master Thesis Project

Optimization Algorithms for Applications in Chemistry (Distance Geometry)

A distance geometry description of a molecular system consists of chirality constraints and a list of pairwise distances between different atoms. Starting from such a description it is often desirable to compute the molecular conformation, i.e. the coordinates of the atoms in a global reference frame. The global configuration is important for biological applications as it determines the function of the molecular system.

Determining possible molecular conformations is an inverse problem, and can be formulated as a high-dimensional, non-convex mathematical optimization problem, whereby constraints are of considerable importance.

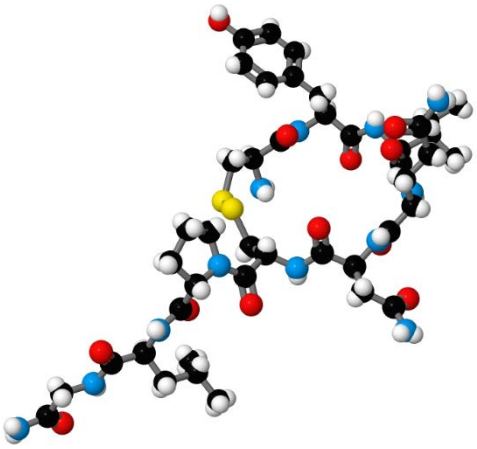

Figure 1: 3D rendering of the Oxytocin molecule.

The project aims at designing optimization algorithms that are tailored to distance geometry applications. For example, one could evaluate whether newly proposed optimization algorithms from machine learning and statistics, which likewise deal with high-dimensional problems, could be applied. Other interesting avenues of research would be to find numerically efficient treatments of the constraints, since traditional projection-based approaches might not be adequate. To that extent, we have recently developed a new projection-free optimization routine, which is likely to perform well. The project will be hosted at the Empirical Inference Department and the group for Learning and Dynamical Systems at the Max Planck Institute for Intelligent Systems.

Empirical Inference Department (https://ei.is.mpg.de/)
The Empirical Inference Department is headed by Prof. B. Schölkopf and part of the Max Planck Institute for Intelligent Systems located in Tübingen, Germany. The Max Planck Institute for Intelligent Systems and ETH Zurich are in close collaboration, for example via the Max Planck ETH Center for Learning Systems. Accommodation at the institute's guest house may be available for the duration of the project, and travel to international conferences can be supported if the project leads to a publication.

Prerequisites
Strong analytical skills and programming experience (Python, MATLAB, C/C++ or similar). Background in machine learning, control theory, statistics, or mathematical optimization is a plus.

Contact
If you have any questions do not hesitate to contact us. When applying for a project, please include your CV, bachelor's and master's transcripts, and a one-page letter of motivation describing your research interests and educational background.

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