

Applied Informatics

CM09 – Optimization

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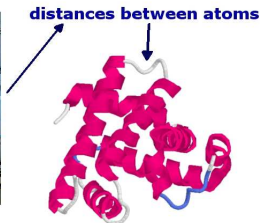
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Distance geometry

Experiments of **Nuclear Magnetic Resonance (NMR)** are able to provide estimates of some of the distances between pairs of atoms forming a molecule.



These distances can be used for finding the three-dimensional conformation of the molecule:

- 1 a **set of constraints** based on the available distances can be defined,
- 2 the three-dimensional conformation of the molecule **must satisfy** all such constraints,
- 3 this problem is known as **Molecular Distance Geometry Problem (MDGP)**.

The **M**oleculer **D**istance **G**eometry **P**roblem.

Find a molecular conformation

$$x = (x_1, x_2, \dots, x_n)$$

such that the following constraints are all satisfied:

$$\|x_i - x_j\| = d_{ij},$$

where

- $\|x_i - x_j\|$ is the computed distance between two atoms in the conformation x ,
- d_{ij} is the known distance between the two atoms.

By its nature, this is a **constraint satisfaction** problem.

A penalty function to optimize

The set of constraints on the distances is usually transformed in a **penalty function**:

$$LDE(x) = \frac{1}{m} \sum_{\{i,j\}} \frac{||x_i - x_j|| - d_{ij}}{d_{ij}}.$$

where m is the number of available distances.

Some remarks:

- If the set of given distances is feasible, then a conformation x is solution for the MDGP if and only if $LDE(x) = 0$;
- Solutions can be found by minimizing the function $LDE(x)$;
- This is an **unconstrained continuous global optimization problem**.

The **MDGP** has been widely studied in recent years.

- **DGSOL**, by J. Moré, Argonne National Laboratory.
It is based on the idea of approximating the function with a sequence of *smoother* functions.
- **SDP-based facial reduction method**, by N. Krislock, INRIA.
Particularly designed for solving sensor network localization problems.
- **MD-jeep**, by myself and other colleagues,
(more info available on my website).
It is based on a combinatorial reformulation of the problem which allows the employment of a Branch & Prune algorithm for the solution of the problem.

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Optimization

General form on an **optimization problem**:

$$\min_{x \in A} f(x)$$

subject to a set of **constraints**:

$$\begin{cases} \forall x \in B & g(x) = 0 \\ \forall x \in C & h(x) \leq 0 \end{cases}$$

where

- $f(x)$ is the **objective function**
- $g(x)$ represents the **equality constraints**
- $h(x)$ represents the **inequality constraints**

Deterministic methods (may require some assumptions to be satisfied)

- Simplex method
- Branch & Bound
- Branch & Prune
- ...

Heuristic methods (no guarantees for optimality)

- Simulated Annealing
- Genetic Algorithms
- Tabu Search
- Variable Neighbourhood Search
- ...



The end

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Distance
geometry

The MDGP

Optimization

Some approaches

Optimization

Definition

Common methods

The end

The End