The Kabsch algorithm (I)

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Vilnius, 2024

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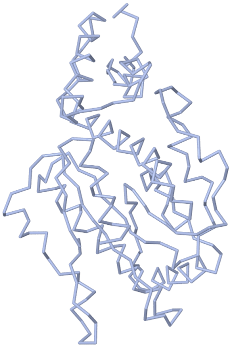
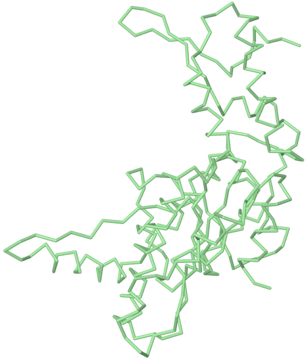
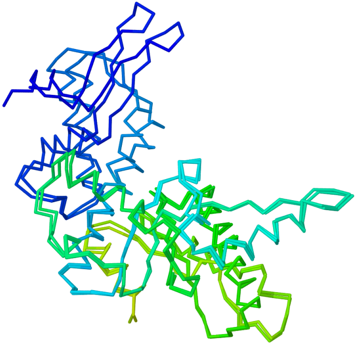
Questions?





- Are these molecules similar?
- Which parts of these molecules are similar?
- How similar they are?

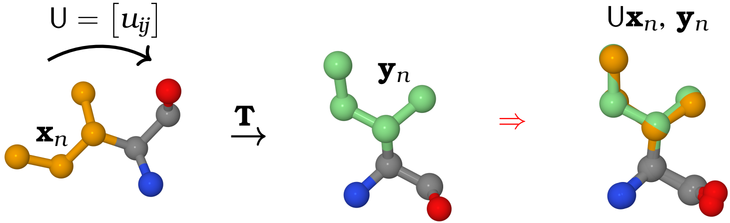
Questions?



- Are these molecules similar?
- Which parts of these molecules are similar?
- How similar they are?

The problem

Find a rigid body movement to superimpose two sets of atoms:



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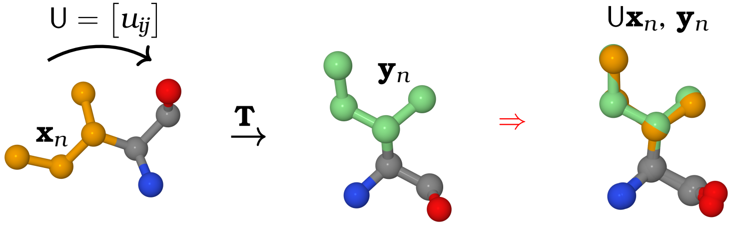

Such that

$$E = \frac{1}{2} \sum_{n=1}^{N} w_n (\mathsf{U}\mathbf{x}_n - \mathbf{y}_n)^2 \to \min$$

$$\text{where } \mathsf{U} = [u_{ij}]_O$$

The paper

Acta Cryst. (1976). A**32**, 922

A solution for the best rotation to relate two sets of vectors. By WOLFGANG KABSCH, *Max–Planck-Institut für Medizinische Forschung*, 6900 *Heidelberg*, *Jahnstrasse* 29, *Germany* (*BRD*)

(*Received* 23 *February* 1976; *accepted* 12 *April* 1976)

A simple procedure is derived which determines a best rotation of a given vector set into a second vector set by minimizing the weighted sum of squared deviations. The method is generalized for any given metric constraint on the transformation.

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Methods

- Least squares method
- Function minimisation;
- Method of Lagrange multipliers;
- Eigenvalue theory

The least squares method

$$E = \frac{1}{2} \sum_{n} w_n (\mathsf{U}\mathbf{x}_n - \mathbf{y}_n)^2 \rightarrow \min$$

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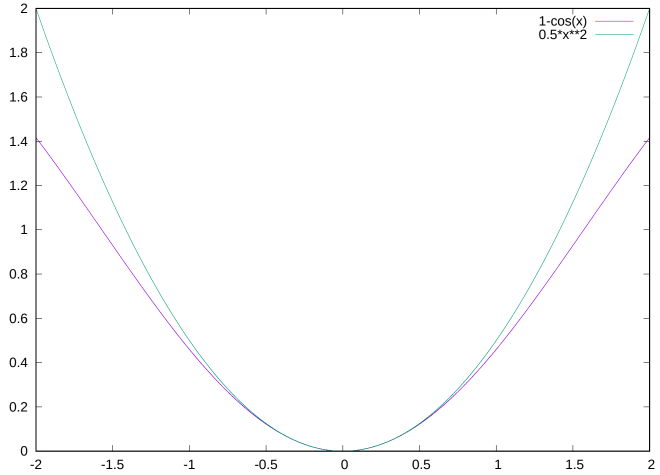
Subject to a constraint:

$$\mathsf{U}^T\mathsf{U} = \mathsf{I}, \;\; \mathsf{U} = \left[u_{ij}\right], \;\; \mathsf{I} = \left[\delta_{ij}\right]$$

i.e.

$$\sum_k u_{ki} u_{kj} - \delta_{ij} = 0$$

Function minimisation (1 variable)



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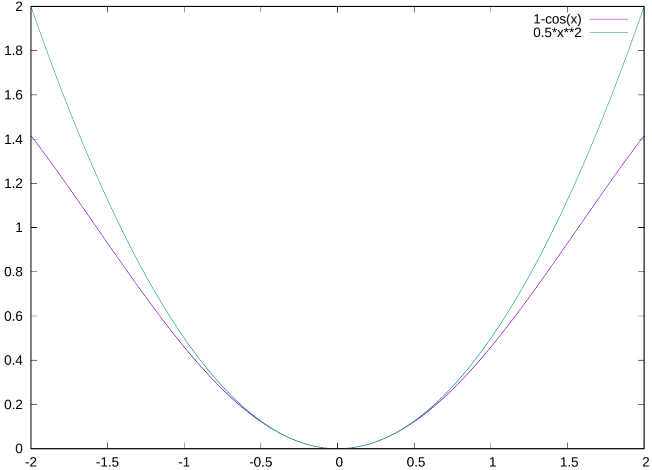
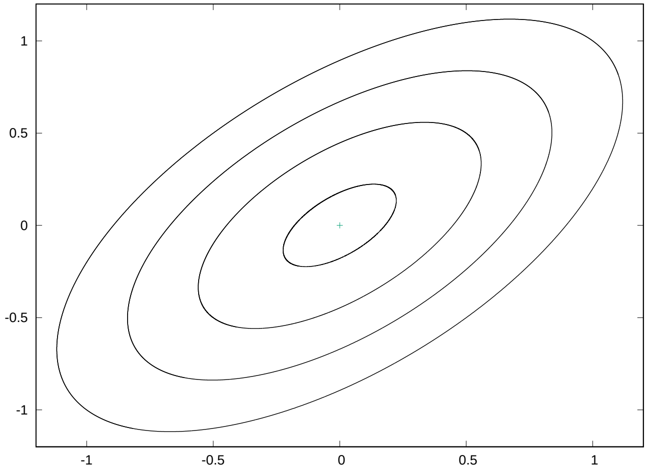


$$f(x) = f(x_0) + f'(x_0)\Delta x + \frac{1}{2} f''(x_0)\Delta x^2 + o(\Delta x^2)$$

Function of multiple variables



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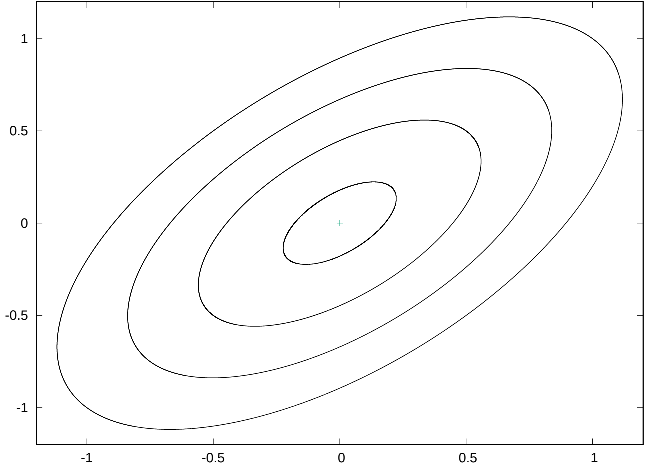
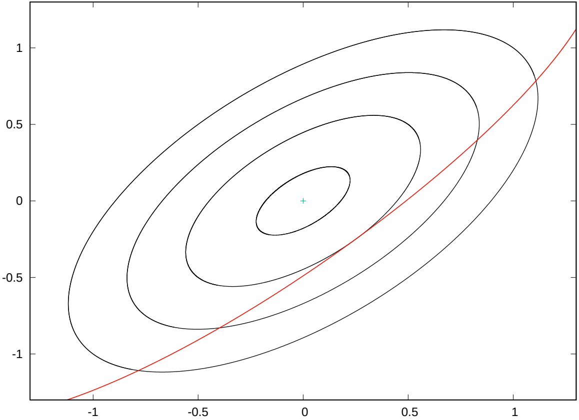


$$E(u_1, u_2) = E|_{0,0} + (\vec{\nabla} E|_{0,0} \cdot \Delta\mathbf{u}) + \frac{1}{2}\left[\Delta u_i\right]^T H\left|_{0,0}\right.\left[\Delta u_j\right] + o(||\Delta\mathbf{u}||^2)$$

Lagrange multiplier method



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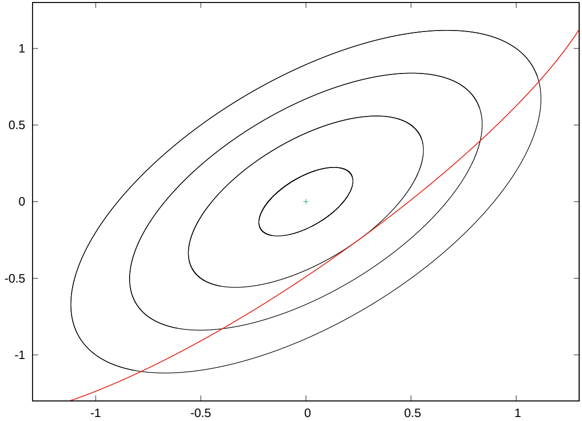
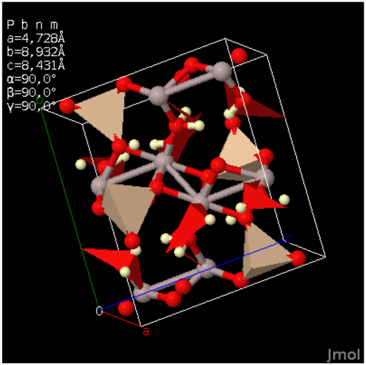


$$\vec{\nabla} E = -\lambda \vec{\nabla} F$$

Thank you!



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Original IUCr paper	HTML

http://en.wikipedia.org/wiki/Topaz

http://www.crystallography.net/2207377.html

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