Kabšo algoritmas (I)

Saulius Gražulis

Vilnius, 2024

Vilniaus universitetas, Matematikos ir informatikos fakultetas

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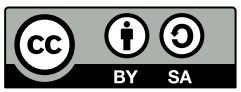
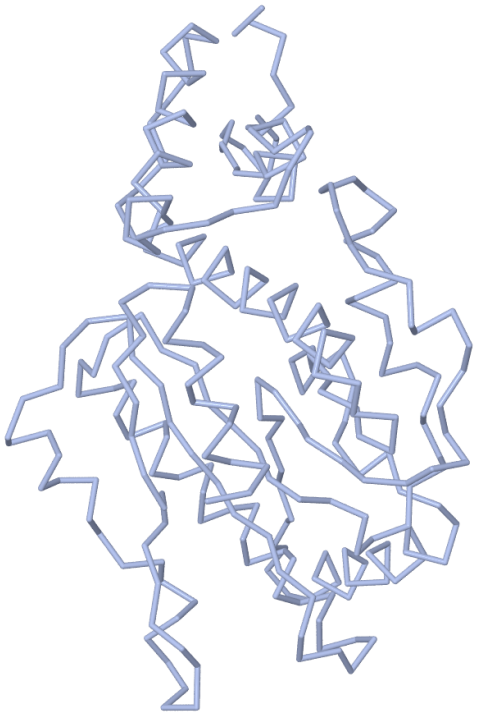
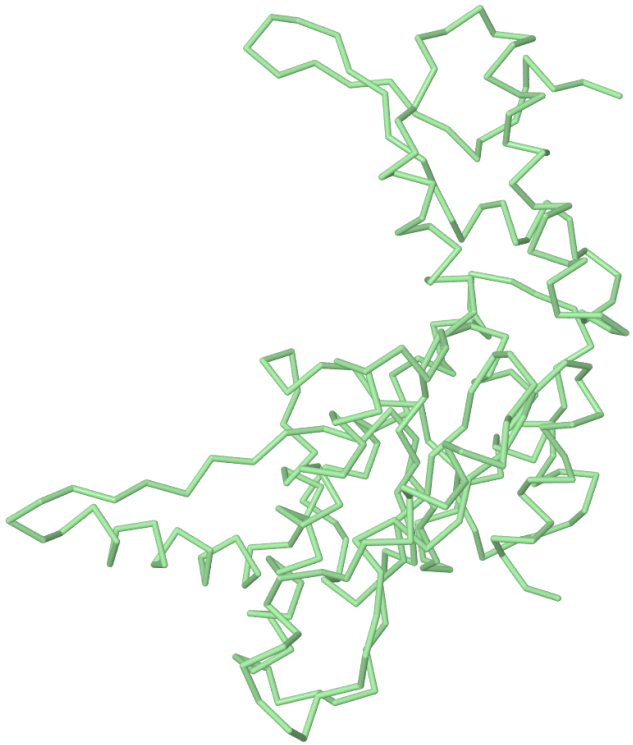


Klausimai





- Ar šios molekulės panašios?
- Kurios molekulių dalys yra panašios?
- Kiek jos panašios?

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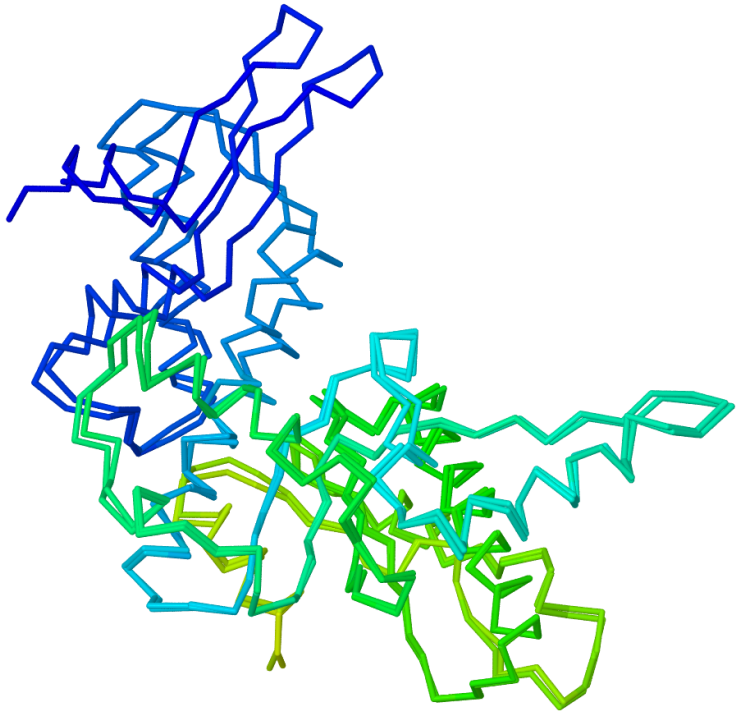

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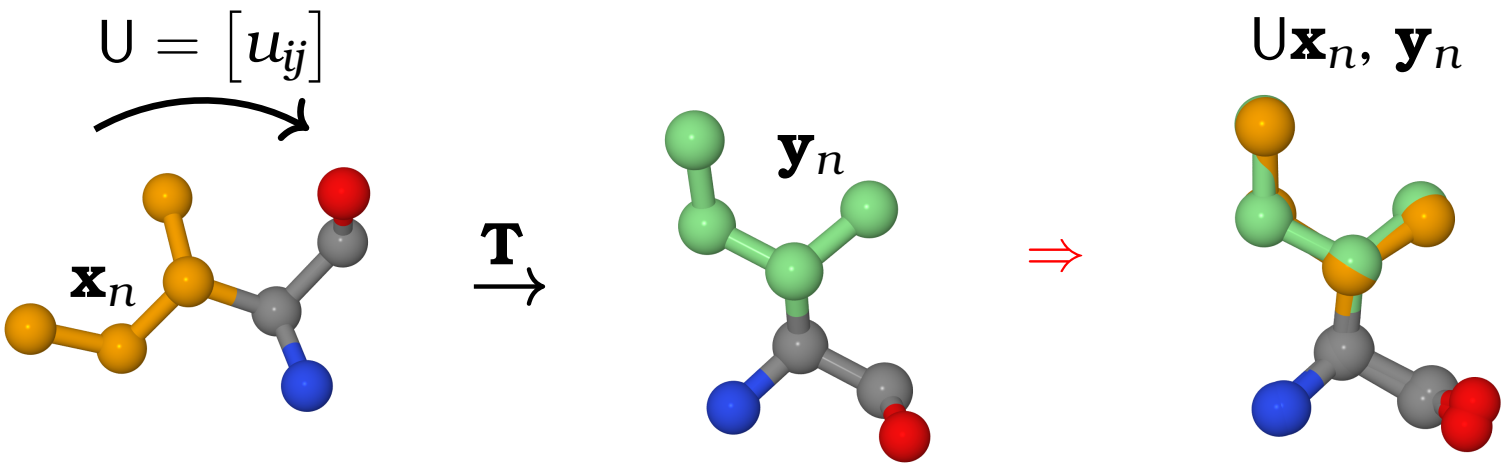
Uždavinys

Rasti kieto kūno judesį, sutapatinantį du atomų rinkinius:



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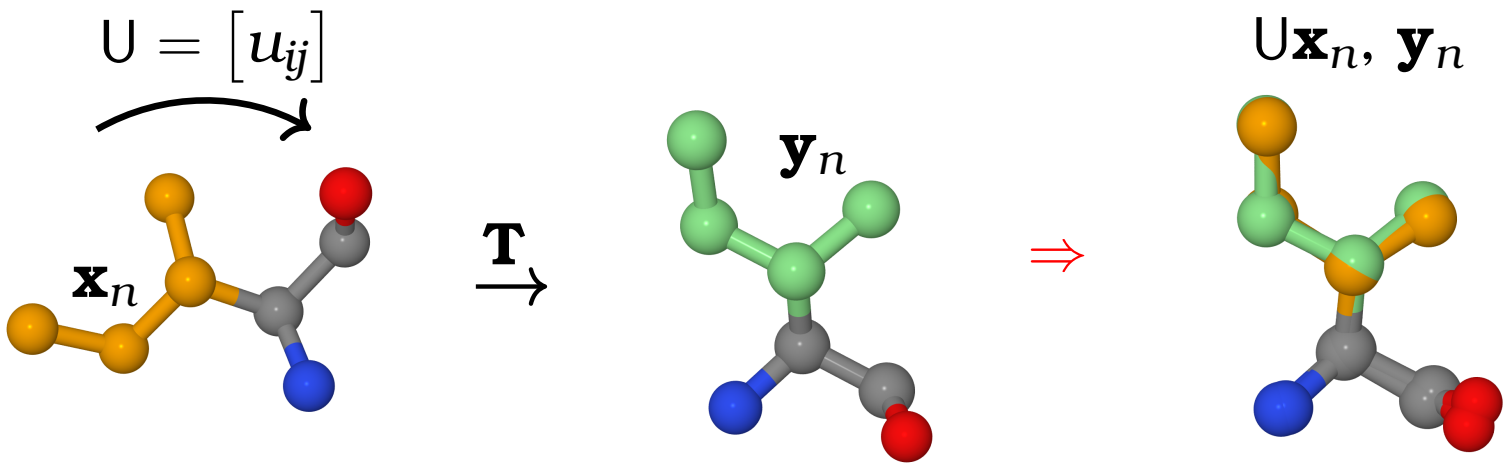

Taip, kad

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

$$\text{kur } \mathsf{U} = \left[u_{ij}\right]_O$$

Straipsnis

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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Taikymo sritys

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- Theobald ir kt. (2012) “Optimal simultaneous superpositioning of multiple structures with missing data” *Bioinformatics*

Metodai

- Mažiausių kvardratų metodas;
- Funkcijos minimizavimas;
- Lagranžo koeficientų metodas;
- Tikrinių (nuosavųjų) verčių teorija;

Mažiausių kvadratų metodas

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

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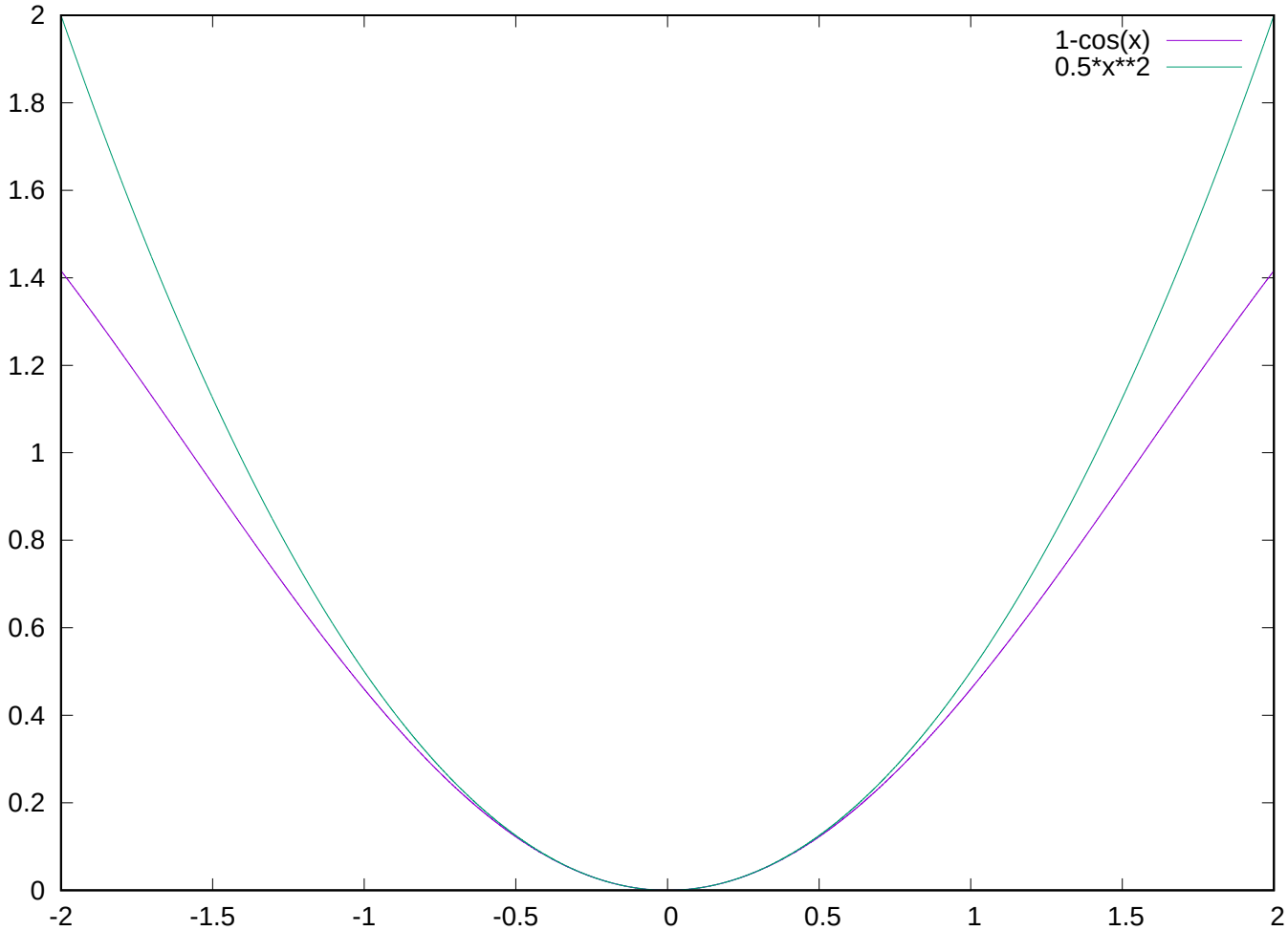
Su apribojimu:

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

t.y.

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

Funkcijos minimizavimas (1 kintamasis)



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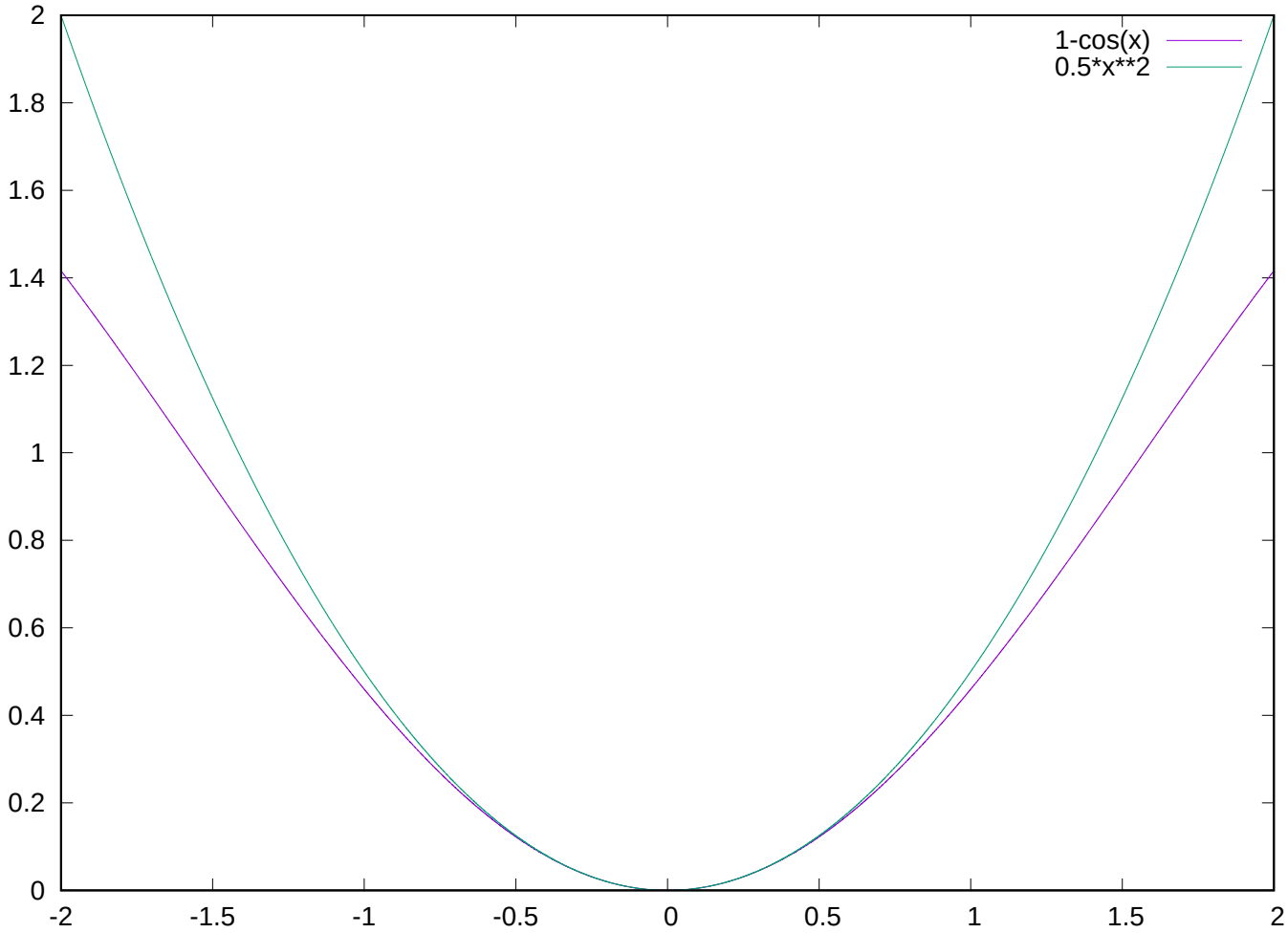
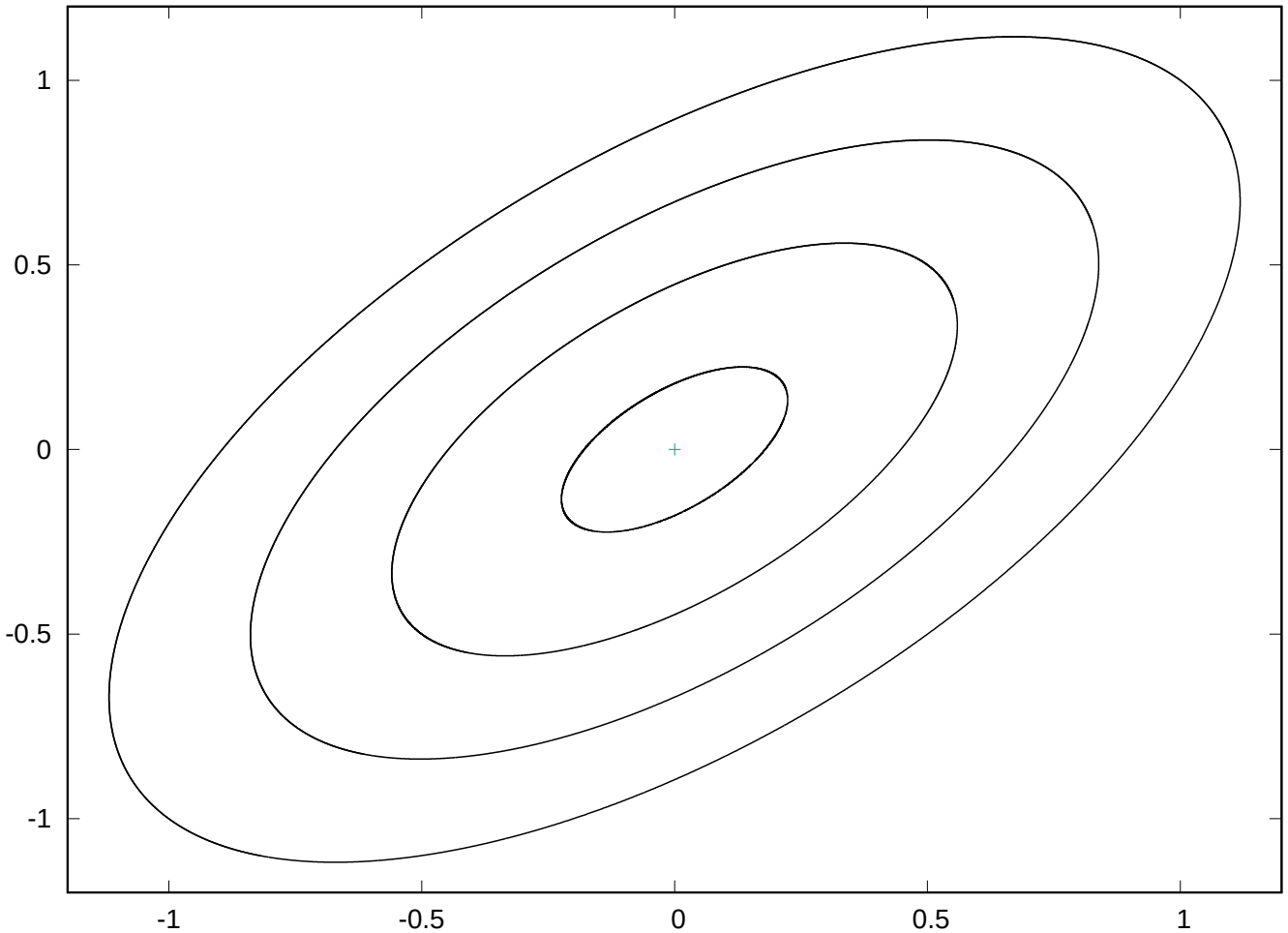
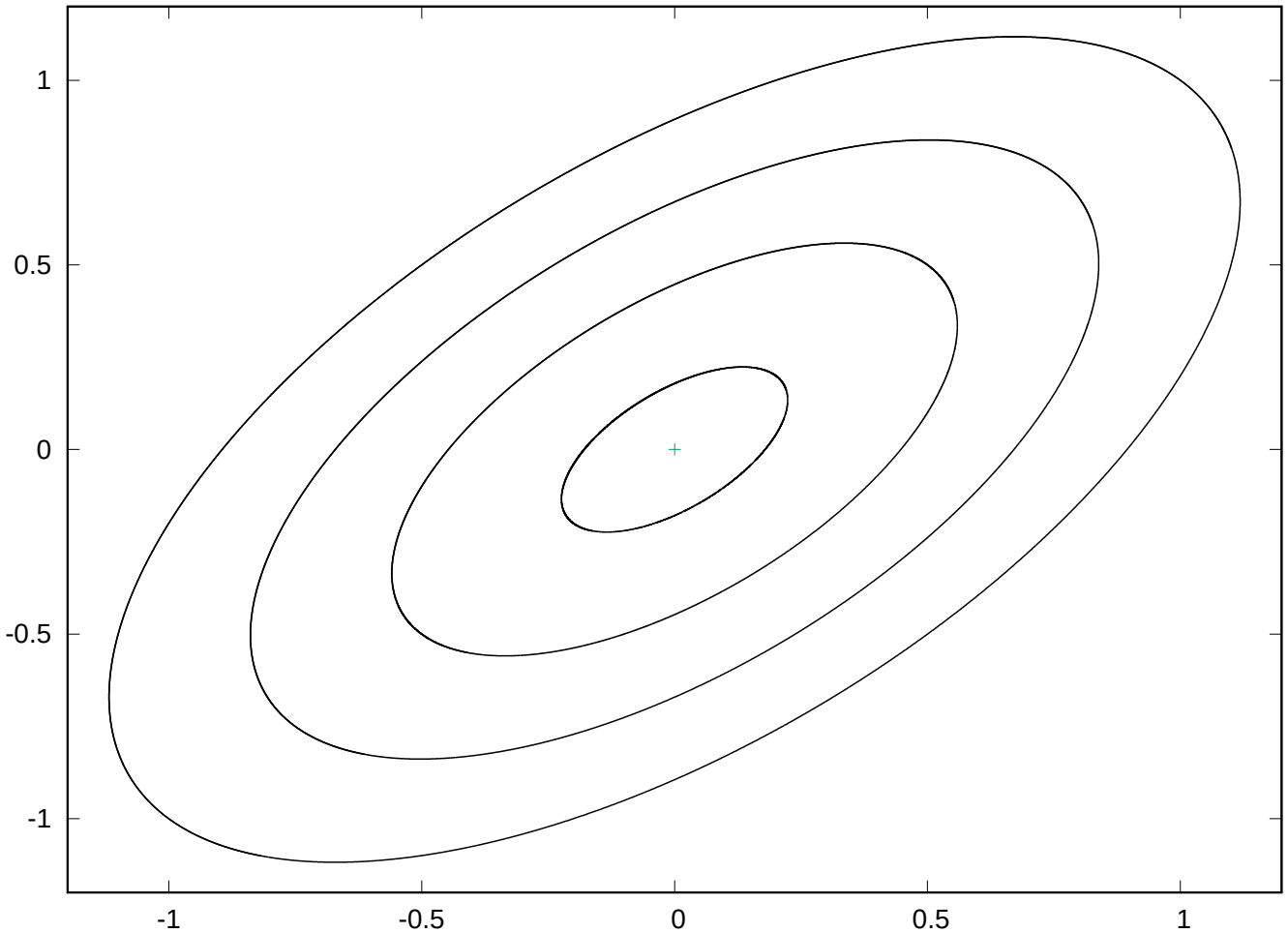


$$f(x) = f(x_0) + f'(x_0)\Delta x + \frac{1}{2} f''(x_0)\Delta x^2 + o(\Delta x^2)$$

Daugelio kintamųjų f-ja

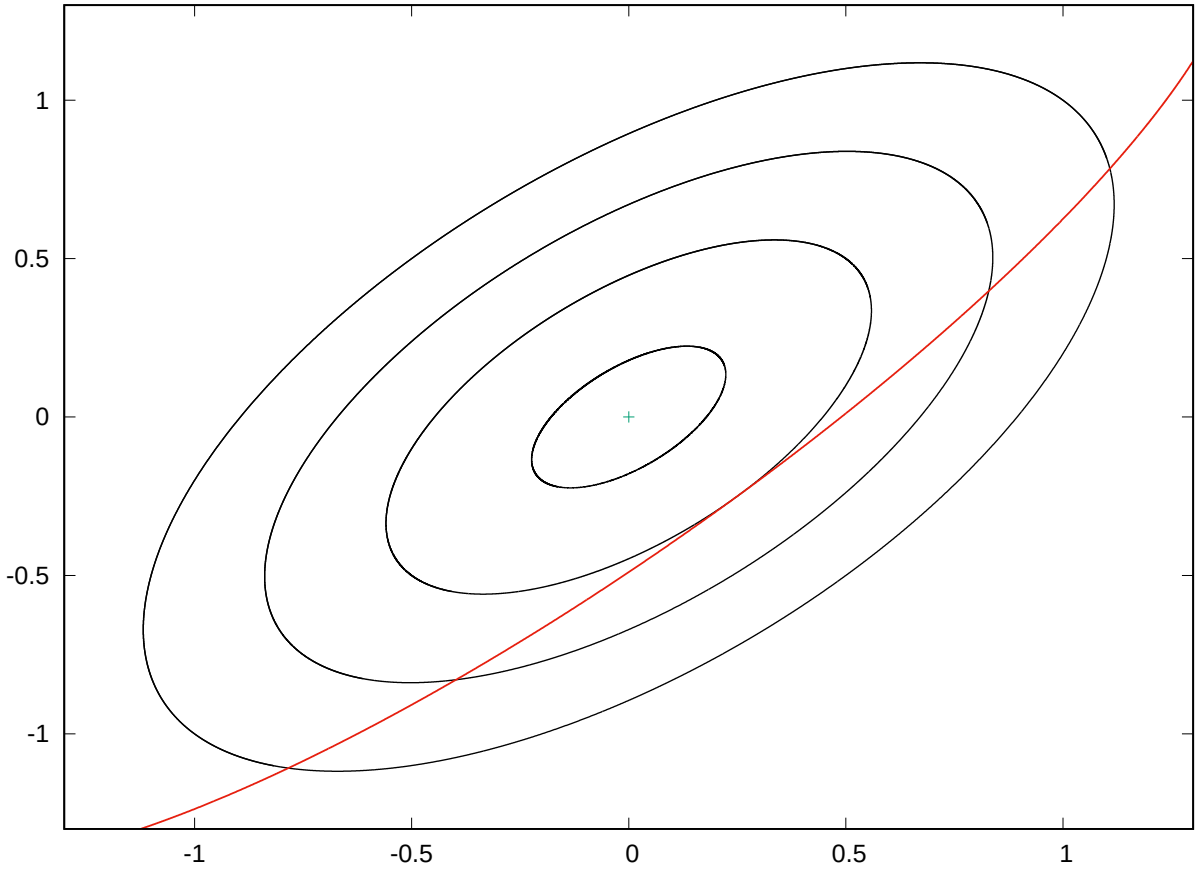


Daugelio kintamųjų f-ja



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

Lagranžo koeficientų metodas



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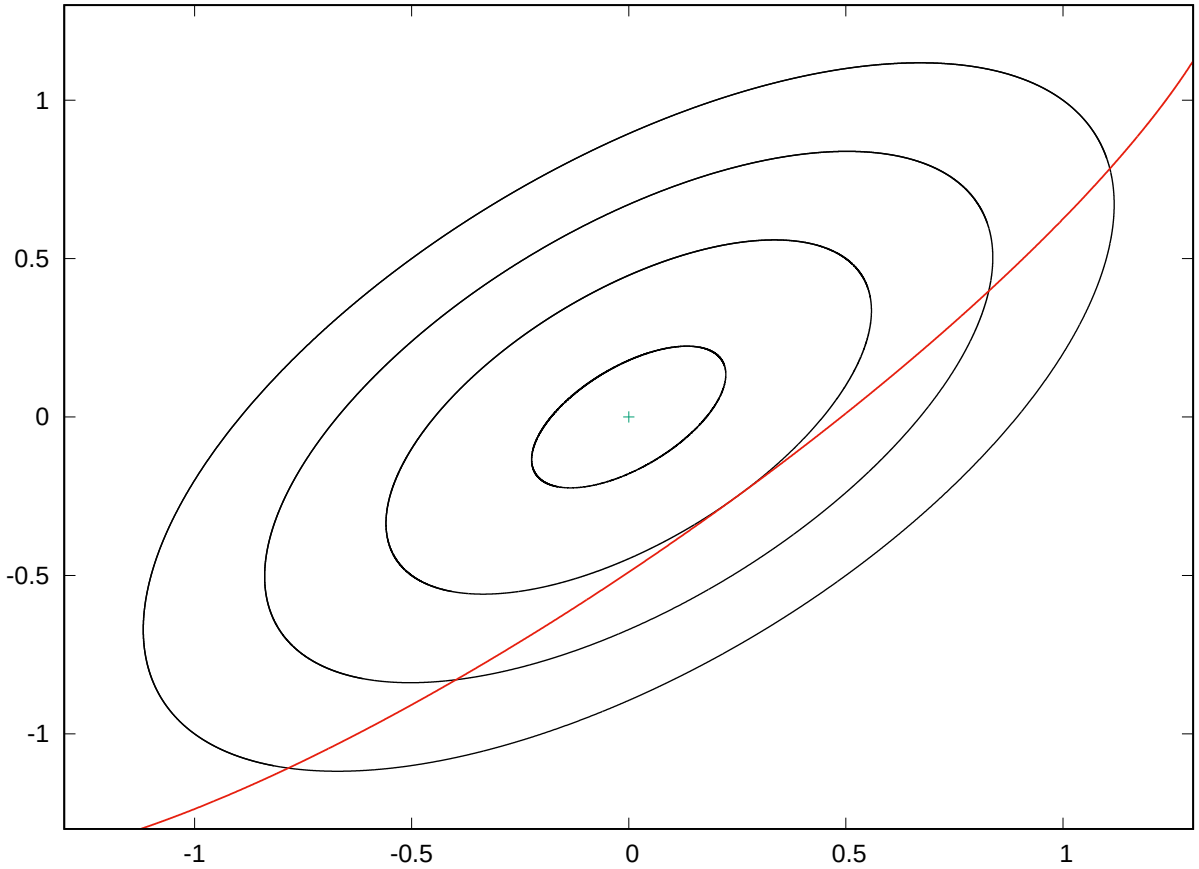
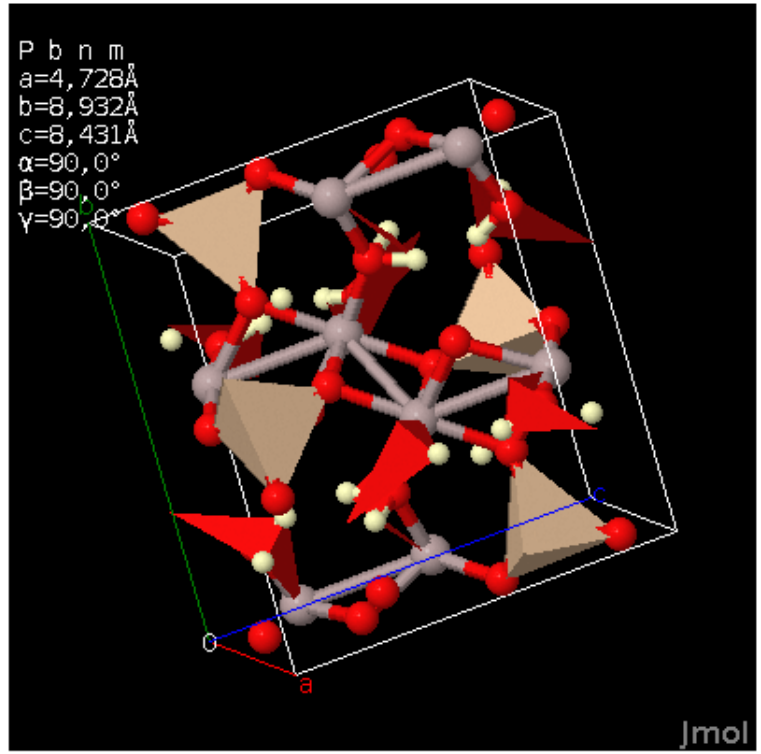


$$\vec{\nabla} E = -\lambda \vec{\nabla} F$$

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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