Protein Folding

Planar Configuration Spaces of Disk Arrangements and Hinged Polygons

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Protein Folding

Protein folding is the process in which a protein chain acquires its 3-dimensional structure.

* Proteins in an organism fold into a specific geometric pattern (sometimes referred as its *native state*).
* Geometric patterns can determine a protein's function and behavior.

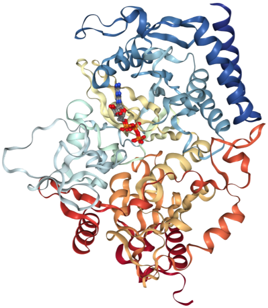

Figure: The structure of rat cytosolic PEPCK variant E89A in complex with oxalic acid and GTP [**?**].

Hinged Dissections

* asdf
* asdfasd

Figure: blah

Problem

Consider three realizability problems when the union of the polygons (resp., disks) in the desired configuration is simply connected (i.e., contractible). That is, the contact graph of the disks is a tree, or the "hinge graph" of the polygonal linkage is a tree (the vertices in the *hinge graph* are the polygons in $\mathcal{P}$, and edges represent a hinge between two polygons). Our main result is that realizability remains NP-hard when restricted to simply connected structures.

Problem 1

Theorem

It is strongly NP-hard to decide whether a polygonal linkage whose hinge graph is a tree can be realized.

Problem 2

A bit more information about this

Theorem

It is strongly NP-hard to decide whether a polygonal linkage whose hinge graph is a tree can be realized with counter-clockwise orientation.

Problem 3

A bit more information about this

Theorem

It is NP-Hard to decide whether a given ordered tree with positive vertex weights is the contact graph of a disk arrangements with specified radii.

Graphs and Drawings

Graph	Vertices	Edges
G_1	$\{a, b, c, d, e\}$	$\{(a, b), (b, c), (c, d), (d, e), (e, a)\}$
G_2	$\{1, 2, 3, 4, 5\}$	$\{(1, 2), (2, 3), (3, 4), (4, 5), (5, 1)\}$

Table: Two graphs that are isomorphic with the alphabetical isomorphism $f(a) = 1$, $f(b) = 2$, $f(c) = 3$, $f(d) = 4$, $f(e) = 5$.

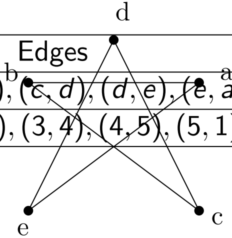

Figure: This figure depicts the graph isomorphism shown in Table 1 between V_1 and V_2.