

Classifying Knots in Open Chains with Random Equilateral Polygon Closures

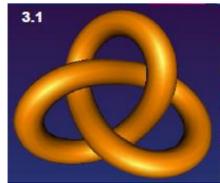


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Theory

The purpose of this project is to analyze and compare methods for classifying knots in open chains. The methods close the open knot via extending rays from the endpoints out to infinity and then connecting them, or close them with randomly generated equilateral arcs. The knot's classification is the knot type that is found most prevalently among multiple closures. The goal is to determine how the methods differ and which is preferred.

Closed Knots vs Open Knots



Closed Knot:
 A curve in Euclidean Space with no endpoints.

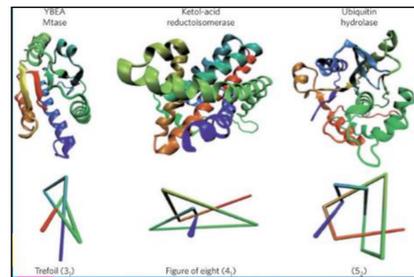


Open Knot:
 A curve in Euclidean Space with two endpoints.

Knot Theorists normally work with closed knots (left), but intuitively it seems as though open chains (right) contain knots as well. In closed curves the topology is trapped and you can study knotting mathematically. An open knot, like in a garden hose or extension cord, can always be untangled.

Why We Care?

We want a way to classify knots in open chains such as those in proteins. Proteins are made up of chains of amino acids, but have an alpha-carbon backbone. Proteins can be modeled as polygons where the alpha-carbons represent vertices.



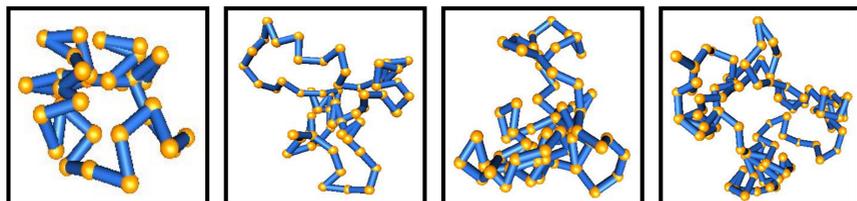
Protein folding: To knot or not to knot?
 Eugene Shakhnovich, January 2011

The protein models are intuitively comparable to randomly generated arcs. By studying knotting patterns in the random arcs, we can apply our understanding to protein structures and potentially their functions.

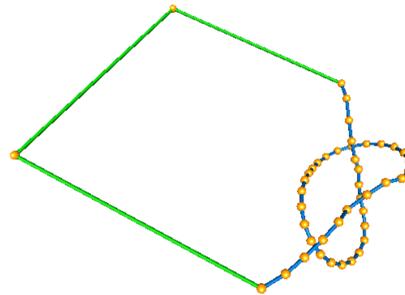
Procedure:

We first generated random equilateral knots. They were classified to acquire their actual knot types. The knots displayed below are examples of closed knots.

To begin these open-knot classifications methods, the closed knot must be opened. This is achieved by removing arcs starting at each vertex. This process produces multitudes of open chains per closed knot. These knots will be closed via the two methods and then classified.



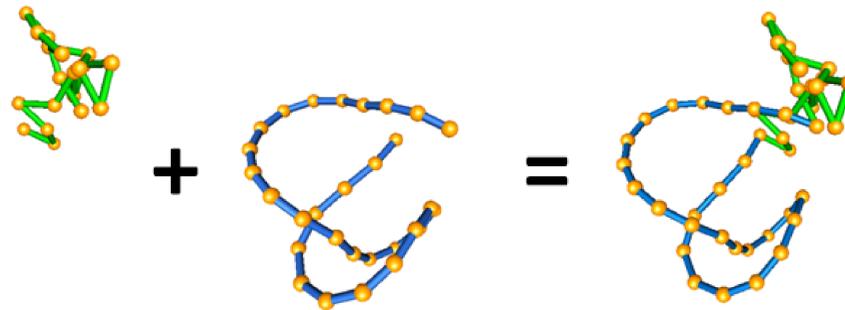
Method I: Extended Rays



Once an open knot is generated, parallel rays are extended to infinity from the open knot's endpoints and connected. This process is done for each open knot in 100 different directions, which are uniformly distributed and fixed. Each of the newly closed knots are classified. The most prevalent knot type found through this process is considered the overall classification.

Method II: Random Equilateral Arcs

This method classifies an open knot by connecting the two endpoints via a randomly generated equilateral arc. The closures are created with the same number of edges as is missing from each trimmed knot. The process is repeated 100 times and the closed knot is classified each time. Again, the knot type given to the open knot is the most commonly found knot type. This method more intuitively resembles the nature of folding proteins.



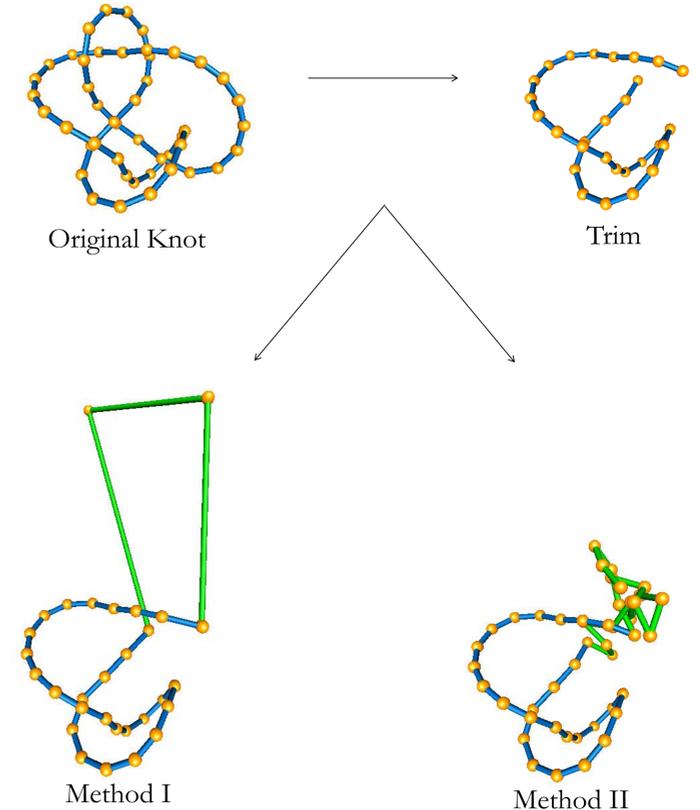
Above is a closure being concatenated with an open chain.

plCurve:

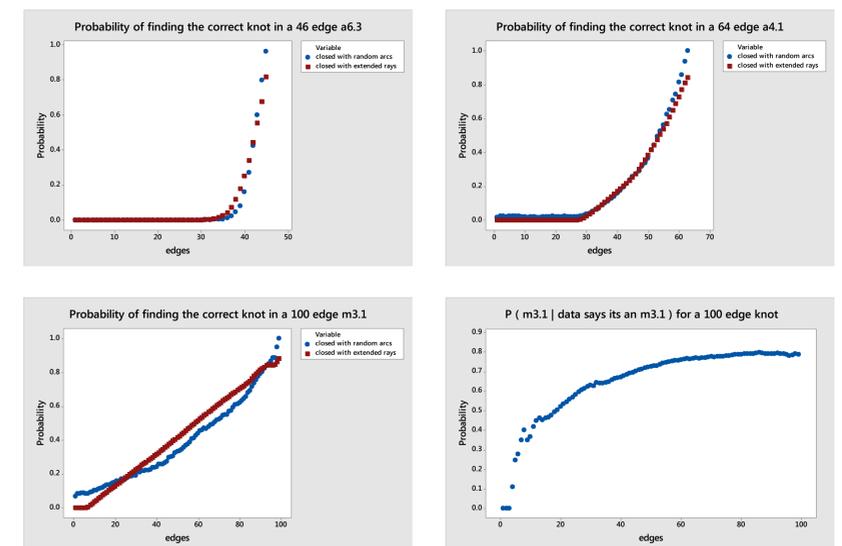
This is a library of C++ functions that are used to randomly generate the knots, delete edges, and create the random arcs used to close the knot.

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Comparison of the Methods



Comparison Analysis



- The first three graphs show the probability of a closure yielding the original knot type for each number of edges possible in the trimmed knot.
- The fourth graph shows the probability of the original knot type being what knot type is found when the knot is closed.