The Geometry and Topology of Random Polygons

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Topology Seminar
LSU
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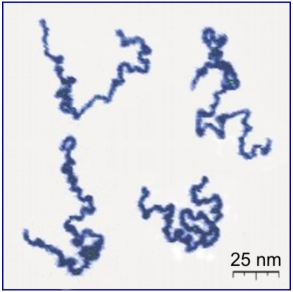
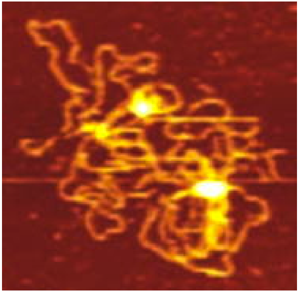
Physics Question

What is the average shape of a polymer in solution?





Protonated P2VP
Roiter/Minko
Clarkson University

Plasmid DNA
Alonso-Sarduy, Dietler Lab
EPF Lausanne

Physics Question

What is the average shape of a polymer in solution?

Physics Answer

> *Modern polymer physics is based on the analogy between a polymer chain and a random walk.*
> *—Alexander Grosberg, NYU.*

Random Polygons (and Geometry and Topology)

Math Question

With respect to a given probability measure on closed polygons, what is the expected value of radius of gyration or total curvature?

Math Question

What fraction of 7-gons of length 2 are knotted?

Topology of cyclo-octane energy landscape
Martin, Thompson, Coutsias, Watson

Numerical Analysis Question

How can we construct random samples drawn from the space of closed space n-gons? More generally, how should we numerically integrate over the space of closed polygons?

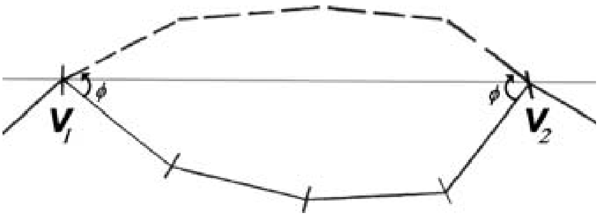


Illustration of crankshaft algorithm of Vologoskii et. al.
Benham/Mielke

Plan of Attack

Construct a mathematical structure underlying polygon spaces which makes these probability and numerical questions tractable.

- Construct a natural measure on framed polygons with edgelengths $r_1, \ldots, r_n$.

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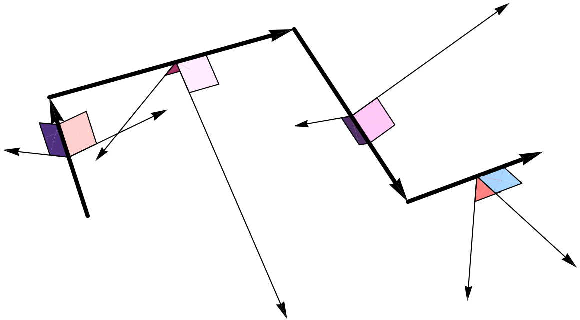
- Construct a natural measure on framed polygons with edgelengths $r_1, \ldots, r_n$.
- Assemble all these spaces with $r_1 + \cdots + r_n = 2$ into a simple space.
- Develop sampling algorithm and make explicit computations on simple space.
- (Future) Specialize back to fixed edgelength spaces.

Definition

Let $\mathrm{FArm}_3(n; r_1, \dots, r_n)$ be the space of framed n-gons with edgelengths $r_1, \dots, r_n$ (up to translation) in $\mathbb{R}^3$.



Quaternions: natural coordinates for frames

Definition

The quaternions $\mathbb{H}$ are the skew-algebra over $\mathbb{R}$ defined by adding $\mathbf{i}$, $\mathbf{j}$, and $\mathbf{k}$ so that

$$\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = -1, \quad \mathbf{ijk} = -1$$

We can identify quaternions with frames in SO(3) via the Hopf map

$$\mathrm{Hopf}(q) = (\bar{q}\mathbf{i}q, \bar{q}\mathbf{j}q, \bar{q}\mathbf{k}q),$$

where the entries turn out to be purely imaginary quaternions, and hence vectors in $\mathbb{R}^3$.

Proposition

The unit quaternions (S^3) double-cover SO(3) *via the Hopf map.*

Question

Does the space of length r orthogonal frames for $\mathbb{R}^3$ have less volume than the space of length 1 orthogonal frames? If so, how much?

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Lemma

The Hopf map takes quaternions of norm $\sqrt{r}$ to frames where each vector has norm r.

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Does the space of length r orthogonal frames for $\mathbb{R}^3$ have less volume than the space of length 1 orthogonal frames? If so, how much?

Lemma

The Hopf map takes quaternions of norm $\sqrt{r}$ to frames where each vector has norm r.

Definition

We take the measure on the space of frames of length r to be the pushforward under the Hopf map of the standard measure on the 3-sphere $S^3(\sqrt{r})$ of radius $\sqrt{r}$ inside $\mathbb{H}$.

Assembly of the measure on the space of framed arms

Definition

We take the measure on the space $\mathrm{FArm}_3(n; r_1, \ldots, r_n)$ to be the pushforward by the Hopf map

$$S^3(\sqrt{r_1}) \times \cdots \times S^3(\sqrt{r_n}) \stackrel{\text{Hopf}}{\to} r_1 \,\mathrm{SO}(3) \times \cdots \times r_n \,\mathrm{SO}(3).$$

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Definition

Let $\mathrm{FArm}_3(n)$ be the space of framed space polygons with total length 2.

$$\mathrm{FArm}_3(n) = \bigcup_{\sum r_i = 2} \mathrm{FArm}_3(n; r_1, \ldots, r_n).$$

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Proposition

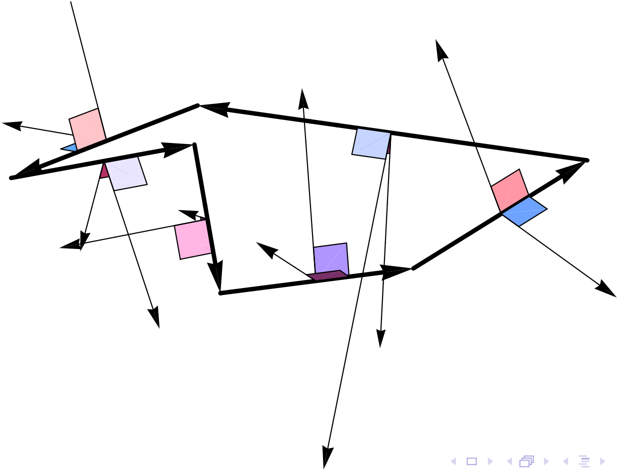
The space $\mathrm{FArm}_3(n)$ *is covered* 2^n *times by* $S^{4n-1}(\sqrt{2}) \subset \mathbb{H}^n$.

We can forget the framing to generate a natural measure on the *unframed* polygon spaces $\mathrm{Arm}_3(n; r_1, \ldots, r_n)$ and $\mathrm{Arm}_3(n)$. We call this the *symmetric* measure on $\mathrm{FArm}_3(n)$ and $\mathrm{Arm}_3(n)$ since it comes from the round sphere.

$$\begin{tikzcd}
S^3(\sqrt{r_1}) \times \cdots S^3(\sqrt{r_n}) \subset \mathbb{H}^n \arrow[r, hook] \arrow[d, "\mathrm{Hopf}"'] & S^{4n-1}(\sqrt{2}) \subset \mathbb{H}^n \arrow[d, "\mathrm{Hopf}"'] \\
\mathrm{FArm}_3(n; r_1, \ldots, r_n) \arrow[r, hook] \arrow[d, "\pi"'] & \mathrm{FArm}_3(n) \arrow[d, "\pi"'] \\
\mathrm{Arm}_3(n; r_1, \ldots, r_n) \arrow[r, hook] & \mathrm{Arm}_3(n)
\end{tikzcd}$$

Definition

Let $\mathrm{FPol}_3(n; r_1, \ldots, r_n) \subset \mathrm{FArm}_3(n; r_1, \ldots, r_n)$ be the space of **closed** framed n-gons with edgelengths $r_1, \ldots, r_n$ (up to translation) in $\mathbb{R}^3$.



From Arm Space to Closed Polygon Space

The quaternionic n-sphere $S^{4n-1}(\sqrt{2})$ is the (scaled) join $S^{2n-1} \star S^{2n-1}$ of complex n-spheres:

$$(\vec{u}, \vec{v}, \theta) \mapsto \sqrt{2}(\cos\theta \vec{u} + \sin\theta \vec{v}\mathbf{j})$$

where $\vec{u}, \vec{v} \in \mathbb{C}^n$ lie in the unit sphere and $\theta \in [0, \pi/2]$. We focus on

$$S^{4n-1}(\sqrt{2}) \supset \{(\vec{u}, \vec{v}, \pi/4) \mid \langle \vec{u}, \vec{v} \rangle = 0\} = V_2(\mathbb{C}^n)$$

Knutson and Hausmann (1997) proved:

$$\begin{tikzcd} V_2(\mathbb{C}^n) \subset \mathbb{H}^n \arrow[r, hook] \arrow[d, "\text{Hopf}"'] & S^{4n-1}(\sqrt{2}) \subset \mathbb{H}^n \arrow[d, "\text{Hopf}"'] \\ \mathrm{FPol}_3(n) \arrow[r, hook] & \mathrm{FArm}_3(n) \end{tikzcd}$$

The proof is (a computation) worth doing!

In complex form, the map $\mathrm{Hopf}_{\mathbf{i}}(q)$ can be written as

$$\mathrm{Hopf}(a + b\mathbf{j}) = \mathbf{i}(|a|^2 - |b|^2 + 2\bar{a}b\mathbf{j})$$

Thus the polygon closes $\iff$

$$\begin{aligned}
\left|\sum \mathrm{Hopf}(q_i)\right|^2 &= \Big|\sum 2|\cos\theta\, u_i|^2 - \sum 2|\sin\theta\, v_i|^2 \\
&\qquad + 4\cos\theta\sin\theta\, \sum \overline{u_i} v_i \mathbf{j}\Big|^2 \\
&= \left|2\cos^2\theta - 2\sin^2\theta\right|^2 + |4\cos\theta\sin\theta\,\langle u, v\rangle|^2 \\
&= 4\cos^2 2\theta + 4\sin^2 2\theta\, |\langle u, v\rangle|^2 = 0
\end{aligned}$$

or $\iff$ $\theta = \pi/4$ and $\vec{u}$, $\vec{v}$ are orthogonal.

Definition

The Stiefel manifold $V_k(\mathbb{C}^n)$ is the space of orthonormal k-frames in $\mathbb{C}^n$. The Grassmann manifold $G_k(\mathbb{C}^n)$ is the space of k-dimensional subspaces of $\mathbb{C}^n$.

There is a bundle

$$U(k) \to V_k(\mathbb{C}^n) \to G_k(\mathbb{C}^n)$$

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Theorem (Howard/Manon/Millson, 2011)

The action of $U(2)$ on $V_2(\mathbb{C}^n)$ in the bundle

$$U(2) \to V_2(\mathbb{C}^n) \to G_2(\mathbb{C}^n)$$

descends to the product of an action of $SO(3)$ on $\mathrm{FPol}_3(n)$ given by rotating the polygon in space and an action of S^1 on $\mathrm{FPol}_3(n)$ given by rotating all frame vectors simultaneously.

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There is a bundle

$$U(k) \to V_k(\mathbb{C}^n) \to G_k(\mathbb{C}^n)$$

Theorem (Howard/Manon/Millson, 2011)

Planes in $G_2(\mathbb{C}^n)$ are a ***Euclidean group invariant*** *representation of framed polygons.*

Proposition (with Cantarella, Deguchi)

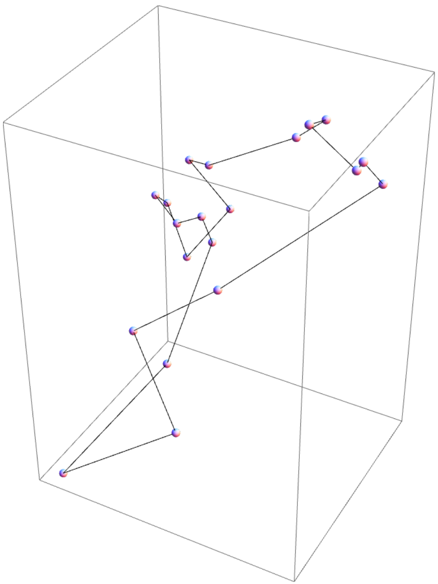
The natural (Haar) measure on $V_2(\mathbb{C}^n)$ is obtained by generating random complex n-vectors with independent Gaussian coordinates and applying (complex) Gram-Schmidt.

```
In[9]:= RandomComplexVector[n_] := Apply[Complex,
          Partition[#, 2] & /@ RandomVariate[NormalDistribution[], {1, 2 n}], {2}][[1]];

        ComplexDot[A_, B_] := Dot[A, Conjugate[B]];
        ComplexNormalize[A_] := (1 / Sqrt[Re[ComplexDot[A, A]]]) A;

        RandomComplexFrame[n_] := Module[{a, b, A, B},
            {a, b} = {RandomComplexVector[n], RandomComplexVector[n]};
            A = ComplexNormalize[a];
            B = ComplexNormalize[b - Conjugate[ComplexDot[A, b]] A];
           {A, B}
          ];
```

Now we need only apply the Hopf map to generate an edge set:

```
In[6]:= ToEdges[{A_, B_}] := {#[[2]], #[[3]], #[[4]]} & /@ (HopfMap /@ Transpose[{A, B}]);
```

Examples of 20-gons



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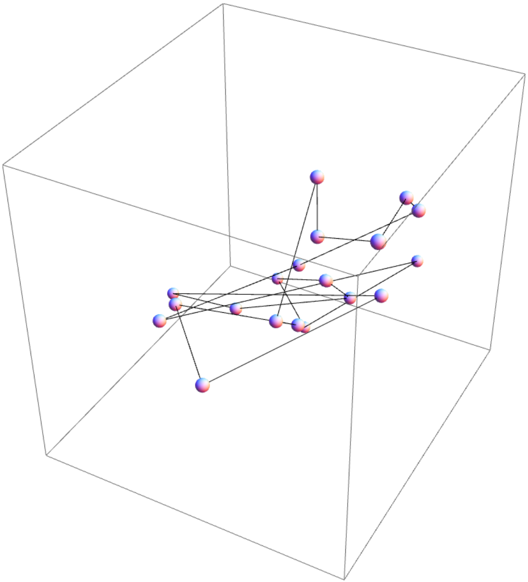

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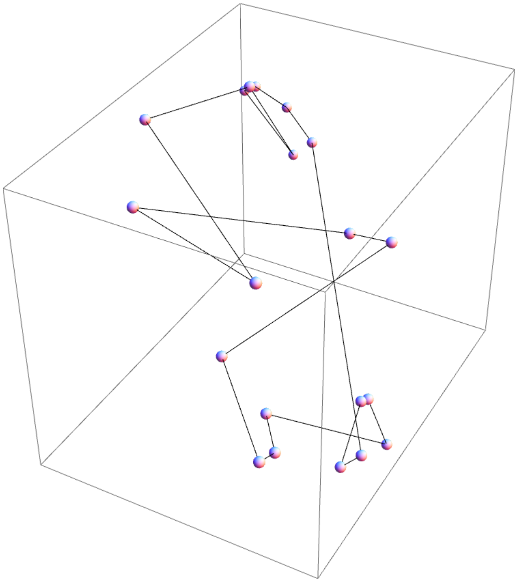

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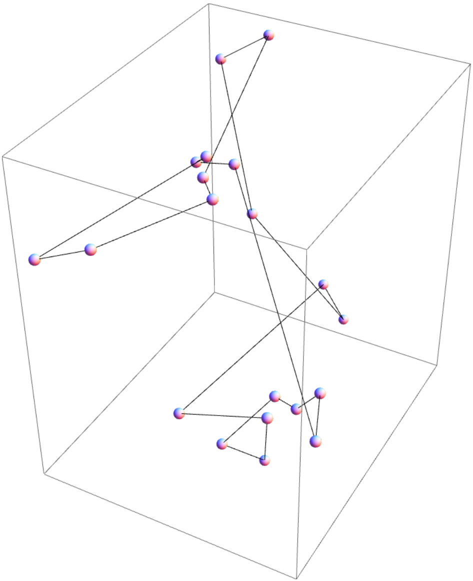

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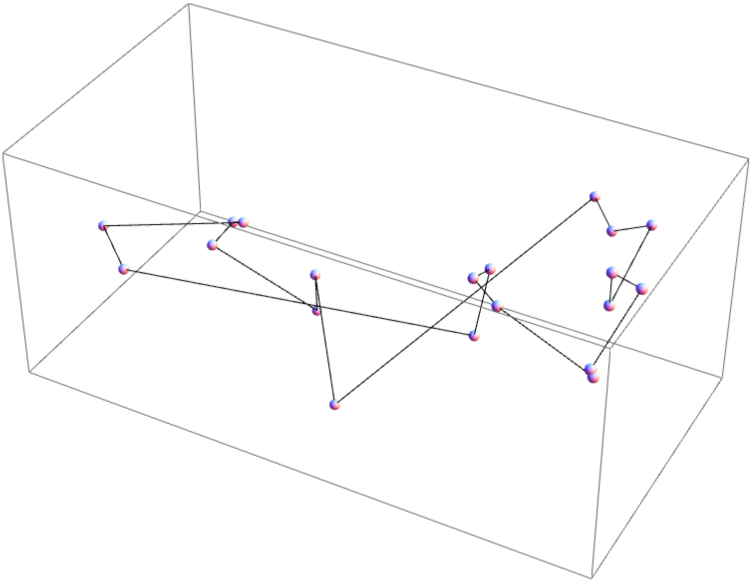
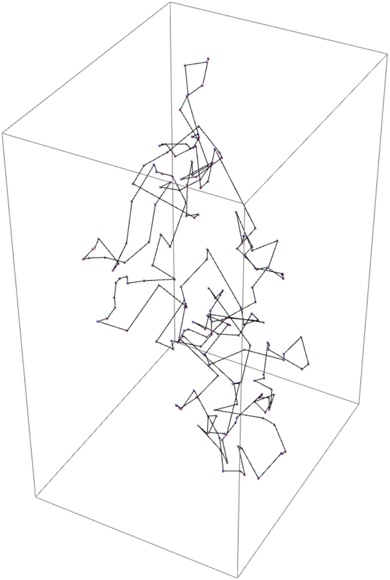
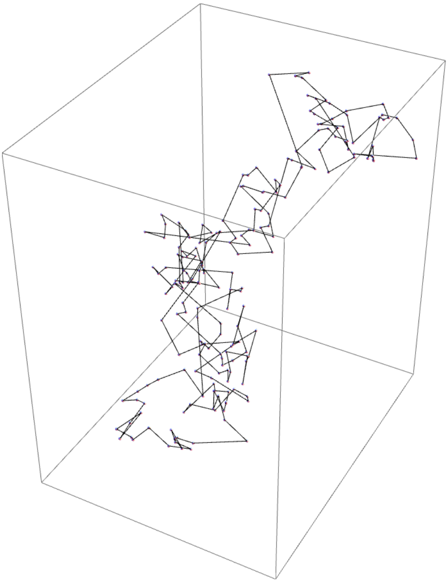


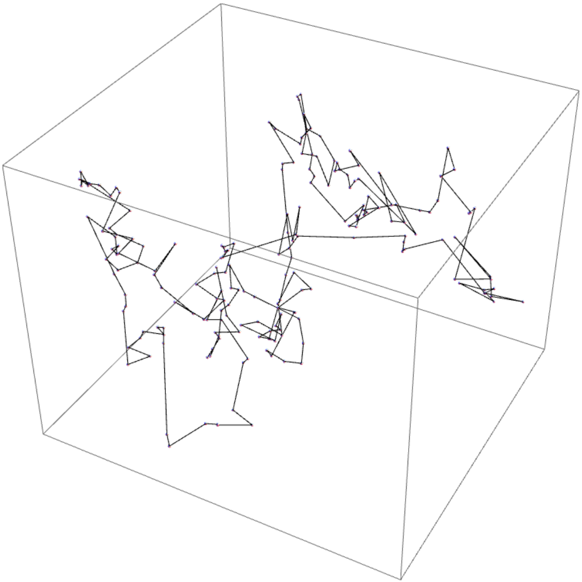
Examples of 200-gons



Examples of 200-gons



Examples of 200-gons



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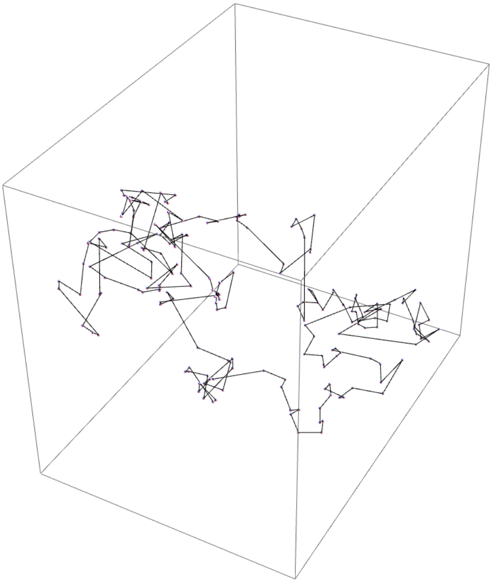
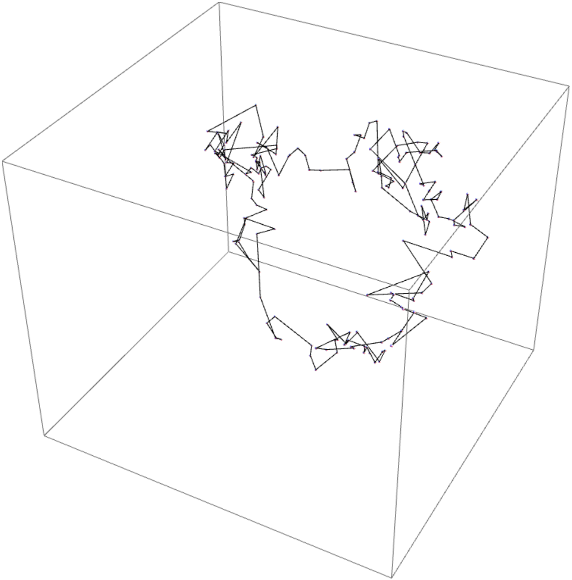
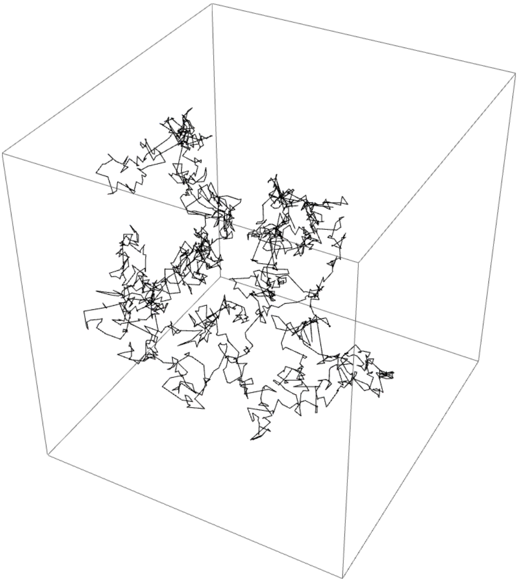




Examples of 2,000-gons



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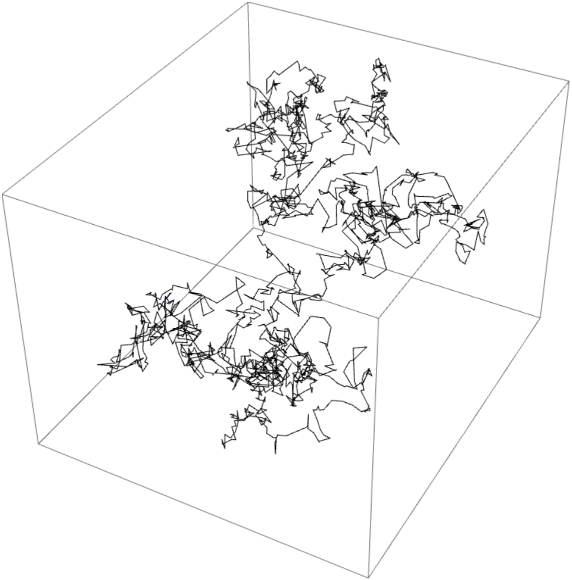

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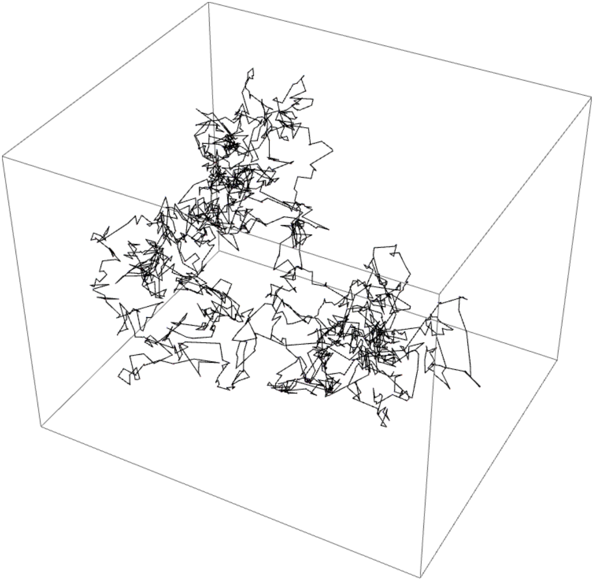
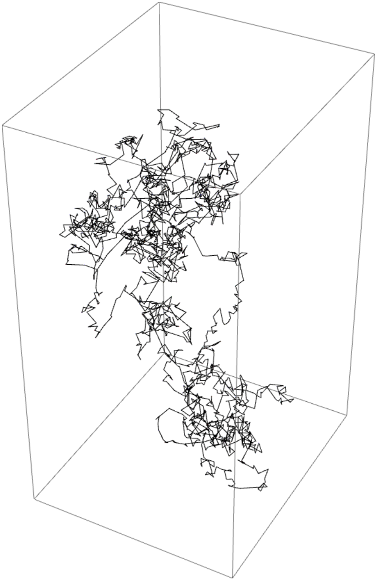
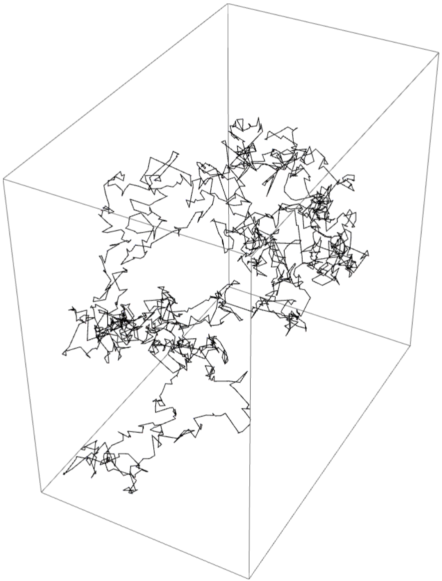


Examples of 2,000-gons



Examples of 2,000-gons



Definition

Let $\mathrm{Chord}(k)$ be the **squared** length of the chord skipping the first k edges of a polygon.

Theorem (with Cantarella, Deguchi)

The expected values for $\mathrm{Chord}(k)$ *are:*

$$E(\mathrm{Chord}(k), \mathrm{Arm}_3(n)) = \frac{6k}{n(n + {}^1\!/_2)},$$

$$E(\mathrm{Chord}(k), \mathrm{Pol}_3(n)) = \left(\frac{n-k}{n-1}\right)\frac{6k}{n(n+1)},$$

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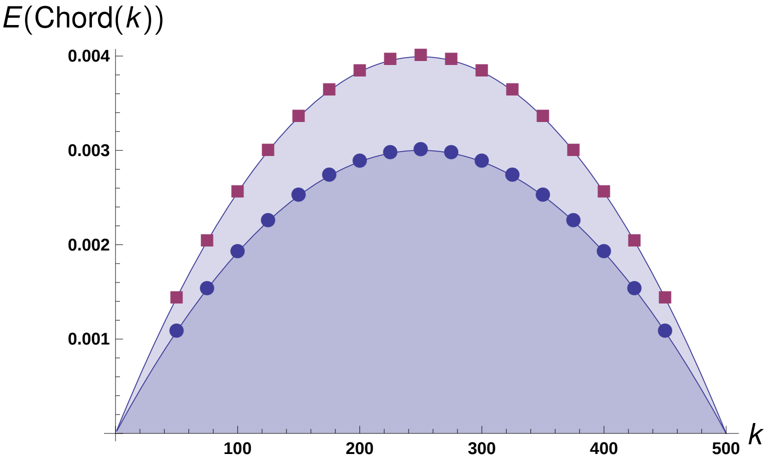
Theorem (with Cantarella, Deguchi)

The expected values for $\mathrm{Chord}(k)$ *are:*

$$E(\mathrm{Chord}(k), \mathrm{Arm}_2(n)) = \frac{8k}{n(n+1)},$$

$$E(\mathrm{Chord}(k), \mathrm{Pol}_2(n)) = \left(\frac{n-k}{n-1}\right)\frac{8k}{n(n+2)}.$$

Checking Chord Lengths against Experiment



$\mathrm{Pol}_2(500)$ and $\mathrm{Pol}_3(500)$

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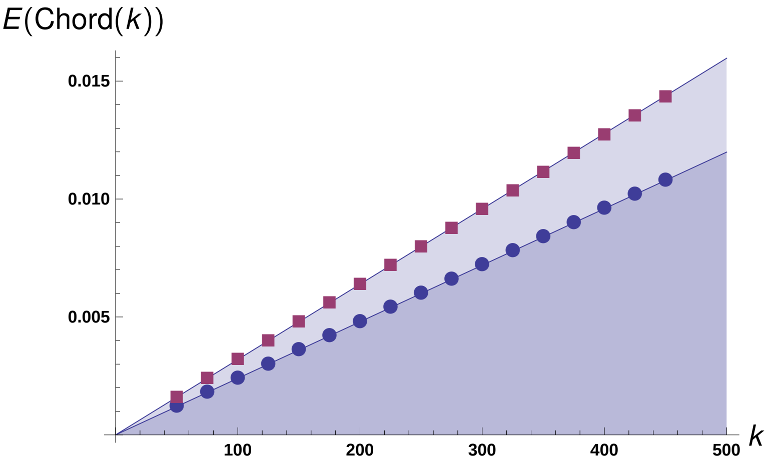


$\mathrm{Arm}_2(500)$ and $\mathrm{Arm}_3(500)$

Expected Value of Radius of Gyration

Definition

The squared radius of gyration $\mathrm{Gyradius}(P)$ is the average squared distance between any two vertices of P.

Theorem (with Cantarella, Deguchi)

The expected values of Gyradius *are*

$$E(\mathrm{Gyradius}, \mathrm{Arm}_3(n)) = \frac{n+2}{(n+1)(n+1/2)},$$
$$E(\mathrm{Gyradius}, \mathrm{Pol}_3(n)) = \frac{1}{2}\frac{1}{n},$$

Definition

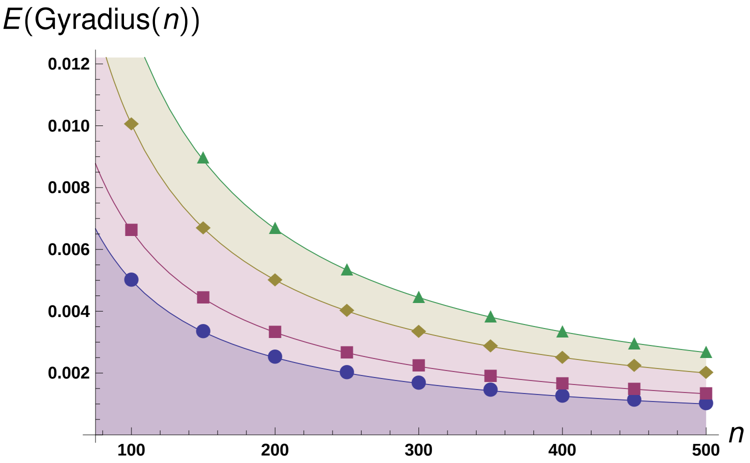
The squared radius of gyration $\mathrm{Gyradius}(P)$ is the average squared distance between any two vertices of P.

Theorem (with Cantarella, Deguchi)

The expected values of Gyradius *are*

$$E(\mathrm{Gyradius}, \mathrm{Arm}_2(n)) = \frac{4}{3}\frac{n+2}{(n+1)^2},$$
$$E(\mathrm{Gyradius}, \mathrm{Pol}_2(n)) = \frac{2}{3}\frac{n+1}{n(n+2)}.$$

Checking Gyradius against Experiment



$\text{Pol}_3(n)$, $\text{Pol}_2(n)$, $\text{Arm}_3(n)$, and $\text{Arm}_2(n)$

Definition

$\mathrm{Arm}_i(n; 2\vec{/}n)$ and $\mathrm{Pol}_i(n; 2\vec{/}n)$ are spaces of equilateral polygons (of total length 2).

Theorem (with Cantarella, Deguchi)

The expected values of Chord *and* Gyradius *for equilateral polygons:*

$$E(\mathrm{Chord}(k), \mathrm{Arm}_i(n; 2\vec{/}n)) = k\frac{4}{n^2},$$

$$E(\mathrm{Chord}(k), \mathrm{Pol}_i(n; 2\vec{/}n)) = \frac{k(n-k)}{n-1}\frac{4}{n^2},$$

Definition

$\mathrm{Arm}_i(n; 2\vec{/}n)$ and $\mathrm{Pol}_i(n; 2\vec{/}n)$ are spaces of equilateral polygons (of total length 2).

Theorem (with Cantarella, Deguchi)

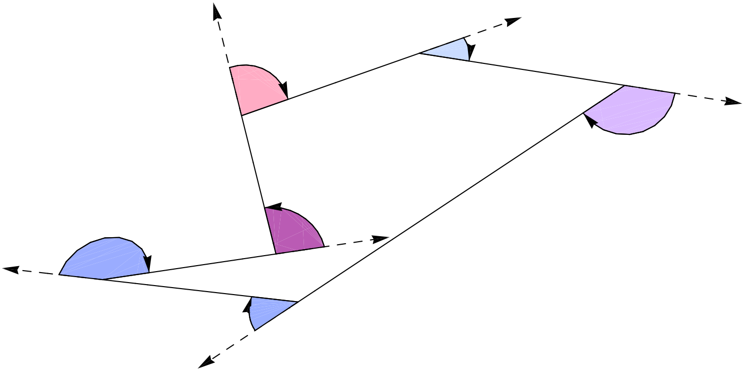
The expected values of Chord *and* Gyradius *for equilateral polygons:*

$$E(\mathrm{Gyradius}, \mathrm{Arm}_i(n; 2\vec{/}n)) = \frac{n+2}{6}\frac{4}{n(n+1)},$$

$$E(\mathrm{Gyradius}, \mathrm{Pol}_i(n; 2\vec{/}n)) = \frac{n+1}{12}\frac{4}{n^2}.$$

Definition

The total curvature κ of a space polygon is the sum of the turning angles $\theta_1, \ldots, \theta_n$.



The total curvature surplus puzzle

Lemma

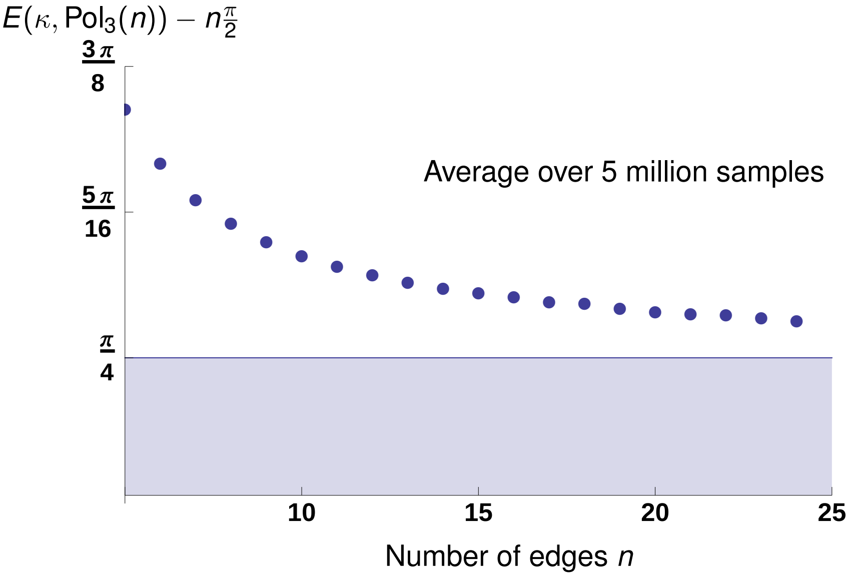
The expected total curvature of a polygon in $\mathrm{Arm}_3(n; r_1, \ldots, r_n)$ *is* $(n-1)\pi/2$.

In 2007, Plunkett et. al. sampled random equilateral closed polygons and noticed that

$$E(\kappa, \mathrm{Pol}_3(n; 1, \ldots, 1)) \to \frac{\pi}{2} n + \alpha$$

> We have observed that the normalized average total curvature and total torsion of the phantom polygons appears to be constant, approximately 1.2 and −1.2, respectively. A simple estimate derived from the inner product of the sum of the edge vectors[26] suggests an approximation of 1.0 for the excess total curvature. The case of the total torsion and the search for more accurate estimates remains an interesting research question.

Total curvature surplus in our measure on $\mathrm{Pol}_3(n)$



We can project the measure on the Stiefel manifold to a single pair of edges using the coarea formula and get an explicit probability measure on pairs of vectors in $\mathbb{R}^3$. Integrating the turning angle between the vectors with respect to this measure, we get:

Proposition (with Cantarella, Grosberg, Kusner)

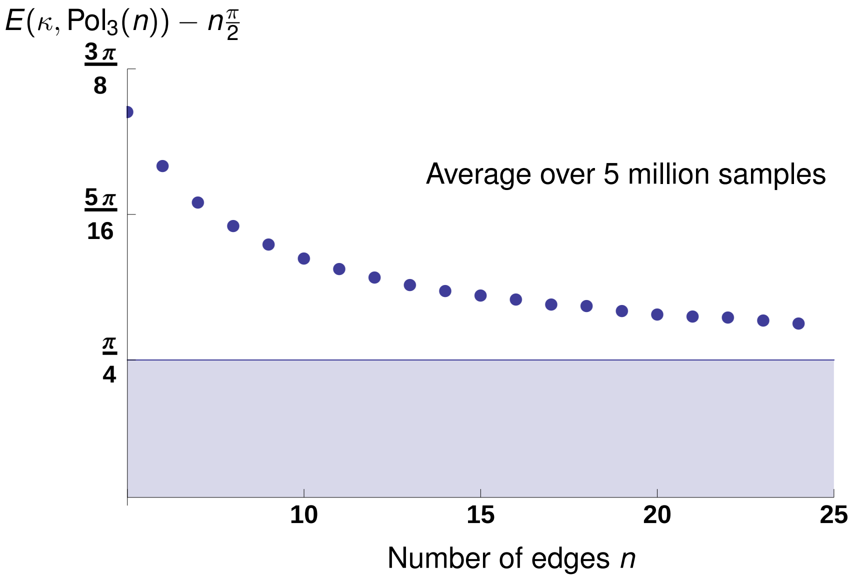
The expected value of the turning angle θ for a single pair of edges in $\mathrm{Pol}_3(n)$ is given by the formula

$$E(\theta) = \frac{\pi}{2} + \frac{\pi}{4}\frac{2}{2n-3}$$

so

$$E(\kappa, \mathrm{Pol}_3(n)) = \frac{\pi}{2}n + \frac{\pi}{4}\frac{2n}{2n-3}.$$

Checking against the numerical data



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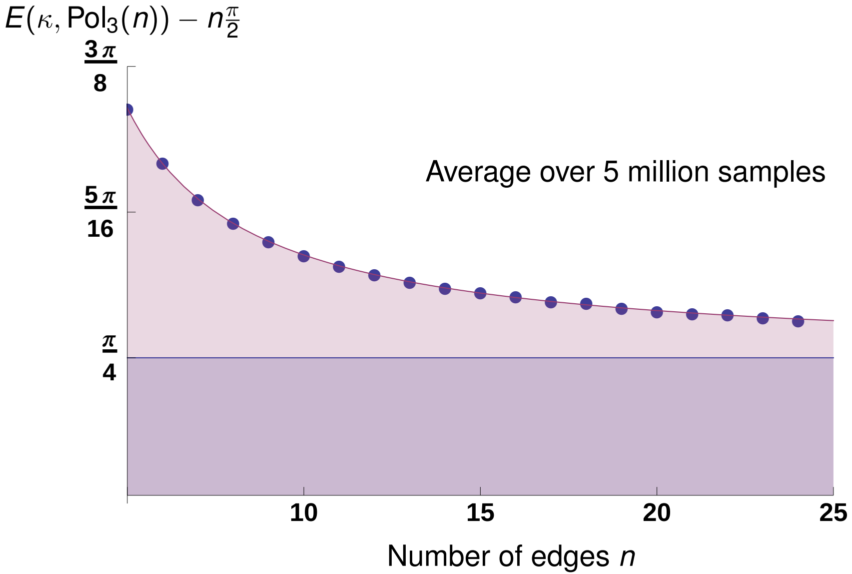

How likely is a random n-gon to be knotted?

Conjecture (Frisch-Wassermann-Delbrück, 1969)

A sufficiently large random closed n-gon is very likely to be knotted.

How likely is a random n-gon to be knotted?

Conjecture (Frisch-Wassermann-Delbrück, 1969)

A sufficiently large random closed n-gon is very likely to be knotted.

Theorem (Diao, 1995)

For n sufficiently large, the probability that a random closed equilateral n-gon is knotted is at least $1 - \exp(-n^{\epsilon})$ *for some positive constant* ϵ. *(No useful explicit bounds are known for the constant* ϵ *or for how large is sufficiently large.)*

How likely is a random n-gon to be knotted?

Conjecture (Frisch-Wassermann-Delbrück, 1969)

A sufficiently large random closed n-gon is very likely to be knotted.

Theorem (Diao, 1995)

For n sufficiently large, the probability that a random closed equilateral n-gon is knotted is at least $1 - \exp(-n^{\epsilon})$ *for some positive constant* ϵ*. (No useful explicit bounds are known for the constant* ϵ *or for how large is sufficiently large.)*

Conjecture

The probability that an element of $\mathrm{Pol}_3(n)$ *is knotted is at least* $1 - \exp(-n^{\epsilon})$ *for some positive constant* ϵ*.*

Proposition (with Cantarella, Grosberg, Kusner)

At least $1/3$ *of* $\mathrm{Pol}_3(6)$ *and* $1/11$ *of* $\mathrm{Pol}_3(7)$ *consists of unknots.*

Proposition (with Cantarella, Grosberg, Kusner)

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Proof.

Let x be the fraction of polygons in $\mathrm{Pol}_3(n)$ with total curvature greater than 4π (by the Fáry-Milnor theorem, these are the only polygons which may be knotted). The expected value of total curvature then satisfies

$$E(\kappa; \mathrm{Pol}_3(n)) > 4\pi x + 2\pi(1 - x).$$

Solving for x and using our total curvature expectation, we see that

$$x < \frac{(n-2)(n-3)}{2(2n-3)}.$$

$\square$

Some open questions

- There's a version of all this for *curves*. What can we derive about curve theory from this point of view? For plane curves, this is the Michor–Shah–Mumford–Younes metric on closed plane curves.
- What does Brownian motion on the Stiefel manifold look like? Is this a model for evolution of polygons?
- How can we get better bounds on knot probabilities? What are the constants in the Frisch–Wassermann–Delbrück conjecture? What about slipknots?

- *Probability Theory of Random Polygons from the Quaternionic Viewpoint*
  Jason Cantarella, Tetsuo Deguchi, and Clayton Shonkwiler
  arXiv:1206.3161
  To appear in *Communications on Pure and Applied Mathematics*.

- *The Expected Total Curvature of Random Polygons*
  Jason Cantarella, Alexander Y. Grosberg, Robert Kusner, and Clayton Shonkwiler
  arXiv:1210.6537.

Thank you for inviting me!