

# The Geometry of Random Polygons

Clayton Shonkwiler

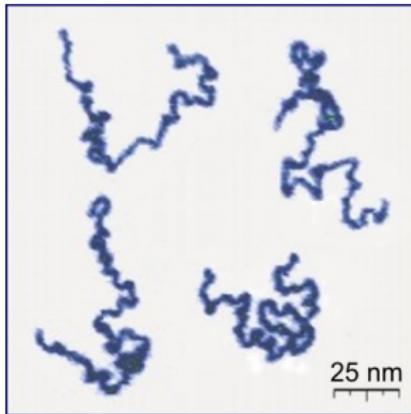
University of Georgia & Isaac Newton Institute

Geometry Seminar  
University of Manchester  
December 13, 2012

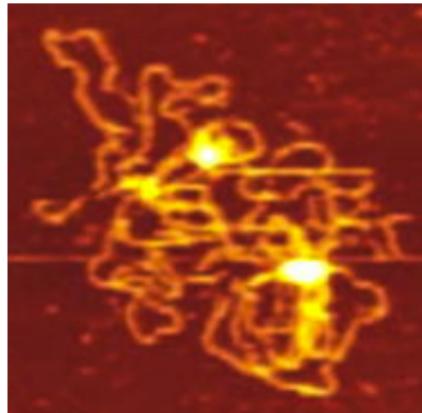
# Random Polygons (and Polymer Physics)

## 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

# Random Polygons (and Polymer Physics)

## 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.*

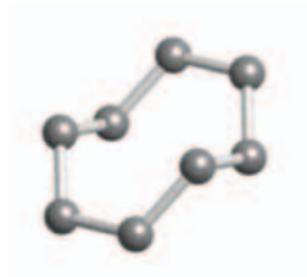
# Random Polygons (and Geometry and Topology)

## 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, Coutsiias, Watson

# Random Polygons (and Numerical Analysis)

## 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?*

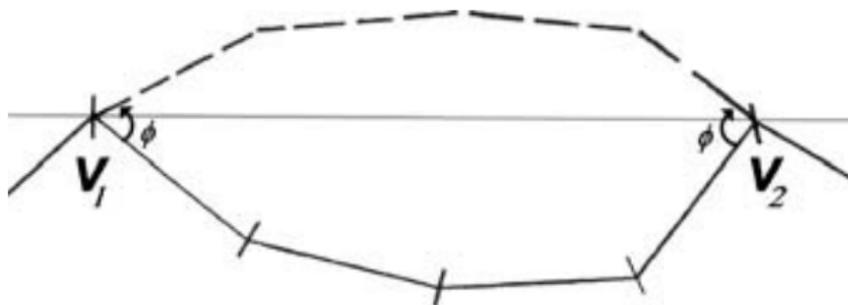


Illustration of crankshaft algorithm of Vologoskii et. al.  
Benham/Mielke

## 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  $r_1, \dots, r_n$ .

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- Assemble all these spaces with  $r_1 + \dots + r_n = 2$  into a simple space.

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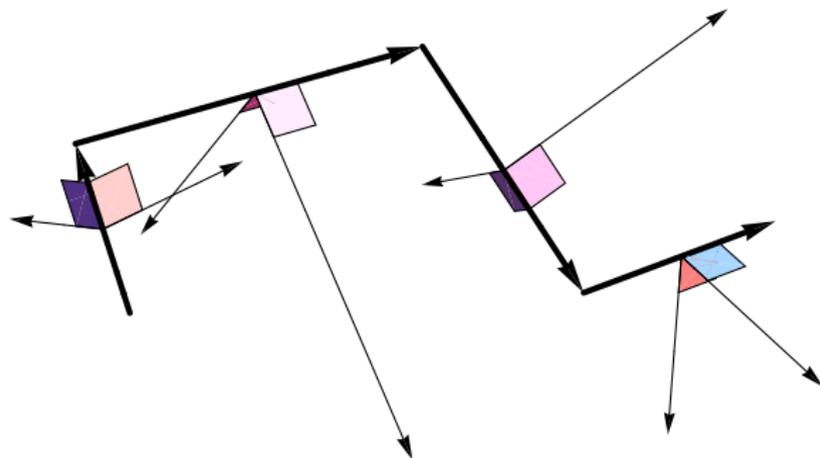
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- Assemble all these spaces with  $r_1 + \dots + r_n = 2$  into a simple space.
- Develop sampling algorithm and make explicit computations on simple space.
- (Future) Specialize back to fixed edgelength spaces.

## Definition

Let  $\text{FArm}_3(n; r_1, \dots, r_n)$  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

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

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

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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  $\text{FArm}_3(n; r_1, \dots, r_n)$  to be the pushforward by the Hopf map

$$\mathcal{S}^3(\sqrt{r_1}) \times \cdots \times \mathcal{S}^3(\sqrt{r_n}) \xrightarrow{\text{Hopf}} r_1 \text{SO}(3) \times \cdots \times r_n \text{SO}(3).$$

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## Definition

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

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

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## Proposition

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

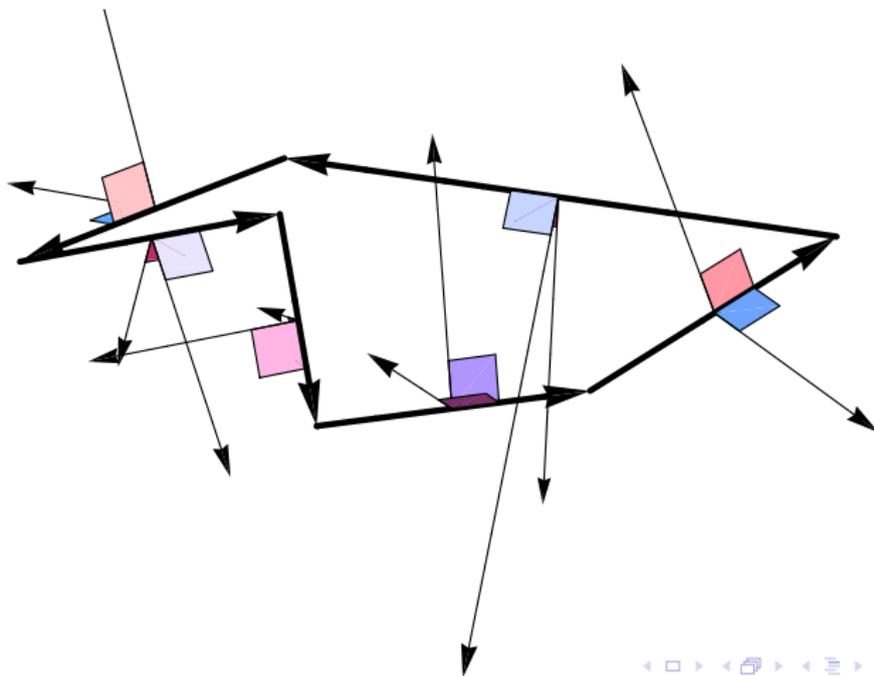
# Summary of Arm Picture

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

$$\begin{array}{ccc} \mathcal{S}^3(\sqrt{r_1}) \times \cdots \times \mathcal{S}^3(\sqrt{r_n}) \subset \mathbb{H}^n & \hookrightarrow & \mathcal{S}^{4n-1}(\sqrt{2}) \subset \mathbb{H}^n \\ \downarrow \text{Hopf} & & \downarrow \text{Hopf} \\ \text{FArm}_3(n; r_1, \dots, r_n) & \hookrightarrow & \text{FArm}_3(n) \\ \downarrow \pi & & \downarrow \pi \\ \text{Arm}_3(n; r_1, \dots, r_n) & \hookrightarrow & \text{Arm}_3(n) \end{array}$$

## Definition

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



# From Arm Space to Closed Polygon Space

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

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

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

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

Knutson and Hausmann (1997) proved:

$$\begin{array}{ccc} V_2(\mathbb{C}^n) \subset \mathbb{H}^n & \hookrightarrow & S^{4n-1} \subset \mathbb{H}^n \\ \text{Hopf} \downarrow & & \text{Hopf} \downarrow \\ \text{FPol}_3(n) & \hookrightarrow & \text{FArm}_3(n) \end{array}$$

# The proof is (a computation) worth doing!

## Proof.

In complex form, the map  $\text{Hopf}_i(q)$  can be written as

$$\text{Hopf}(u + v\mathbf{j}) = \mathbf{i}(|u|^2 - |v|^2 + 2\bar{u}v\mathbf{j})$$

Thus the polygon closes  $\iff$

$$\begin{aligned} \left| \sum \text{Hopf}(q_i) \right|^2 &= \left| \sum 2|\cos \theta u_i|^2 - \sum 2|\sin \theta v_i|^2 \right. \\ &\quad \left. + 4 \cos \theta \sin \theta \sum \bar{u}_i v_i \mathbf{j} \right|^2 \\ &= \left| 2 \cos^2 \theta - 2 \sin^2 \theta \right|^2 + |4 \cos \theta \sin \theta \langle u, v \rangle|^2 \\ &= 4 \cos^2 2\theta + 4 \sin^2 2\theta |\langle u, v \rangle|^2 = 0 \end{aligned}$$

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

# Sampling random polygons (directly!)

## 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]];

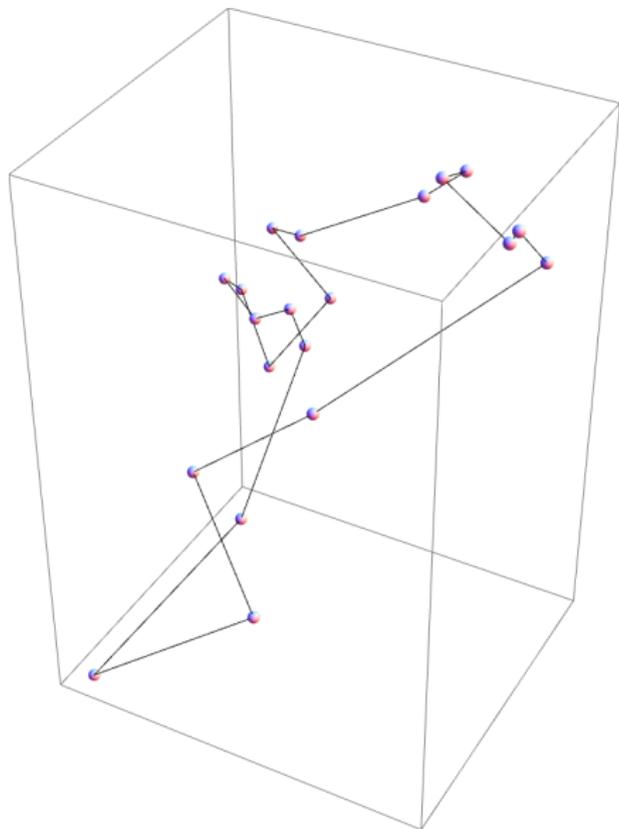
ComplexDot[A_, B_] := Dot[A, Conjugate[B]];
ComplexNormalize[A_] := (1 / Sqrt[Re[ComplexDot[A, A]]]) A;

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}
];
```

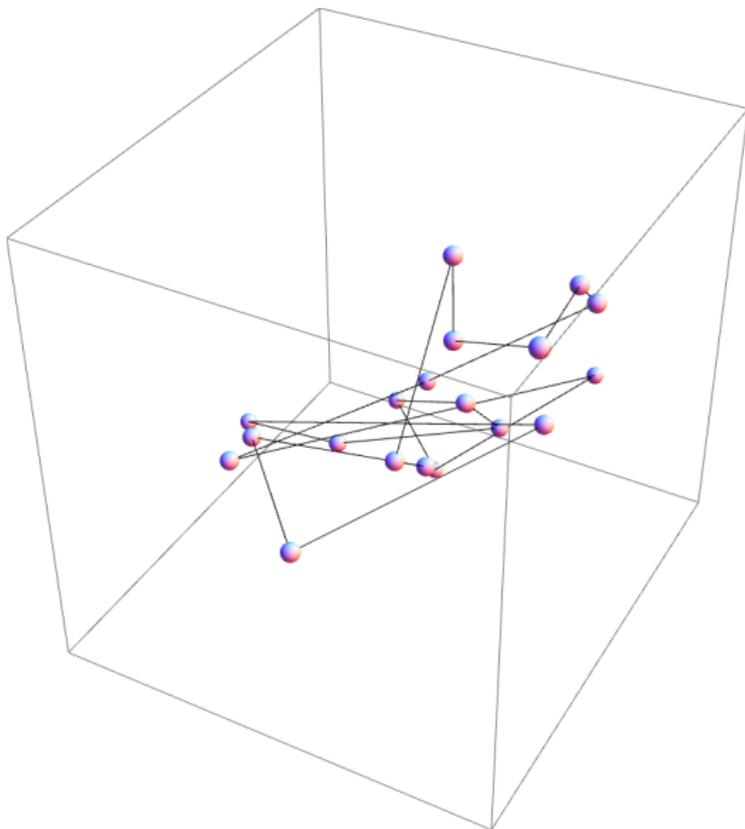
Now we need only apply the Hopf map to generate an edge set:

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

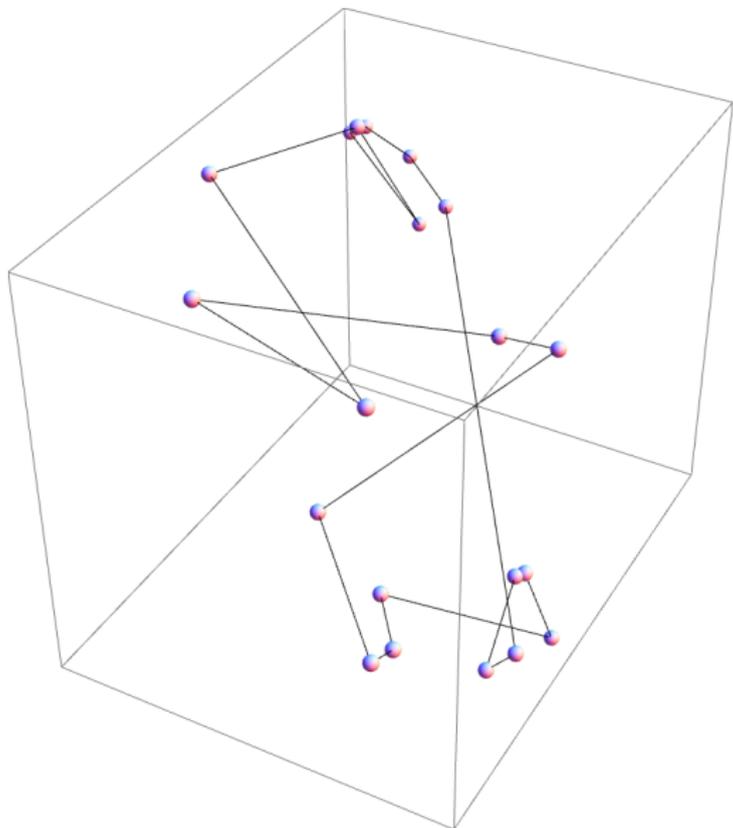
# Examples of 20-gons



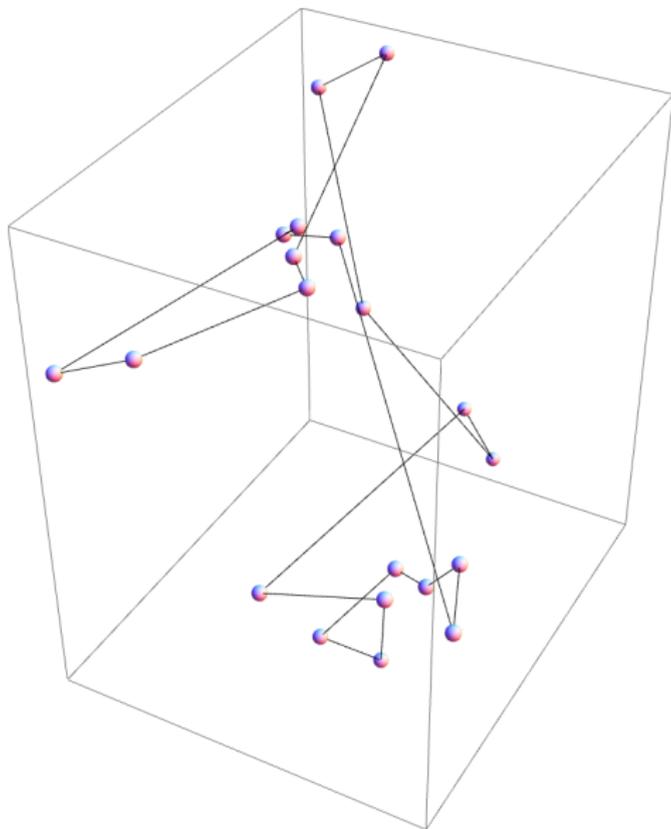
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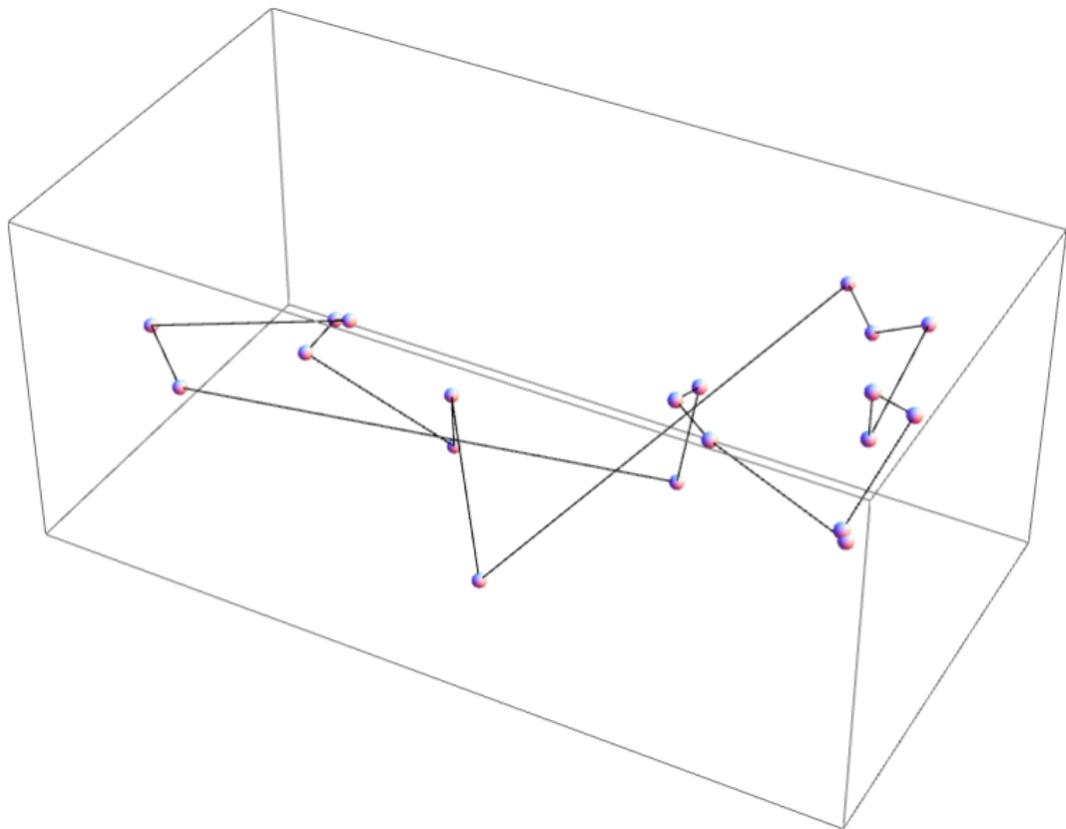
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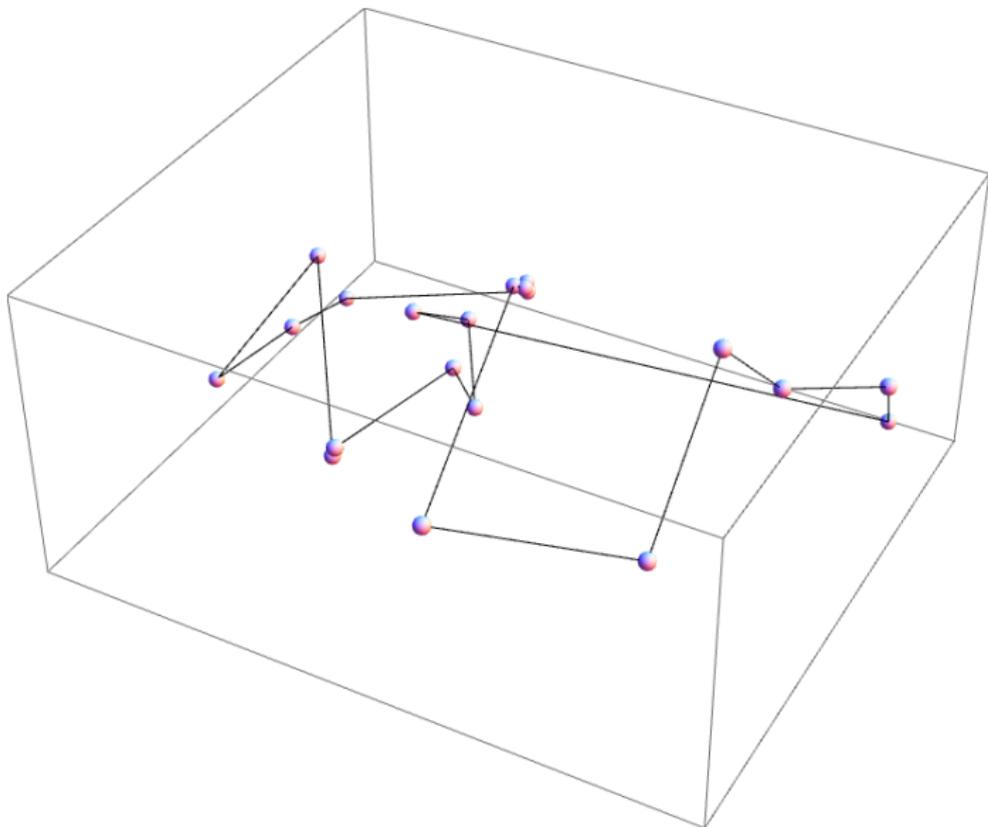
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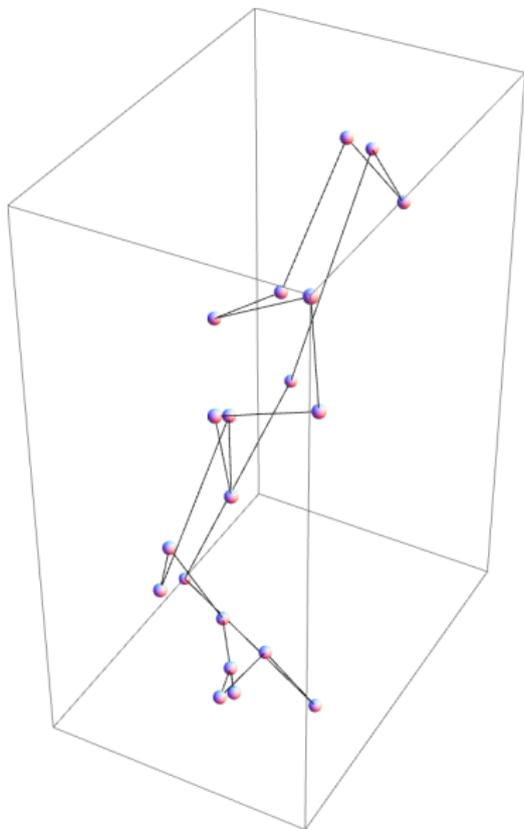
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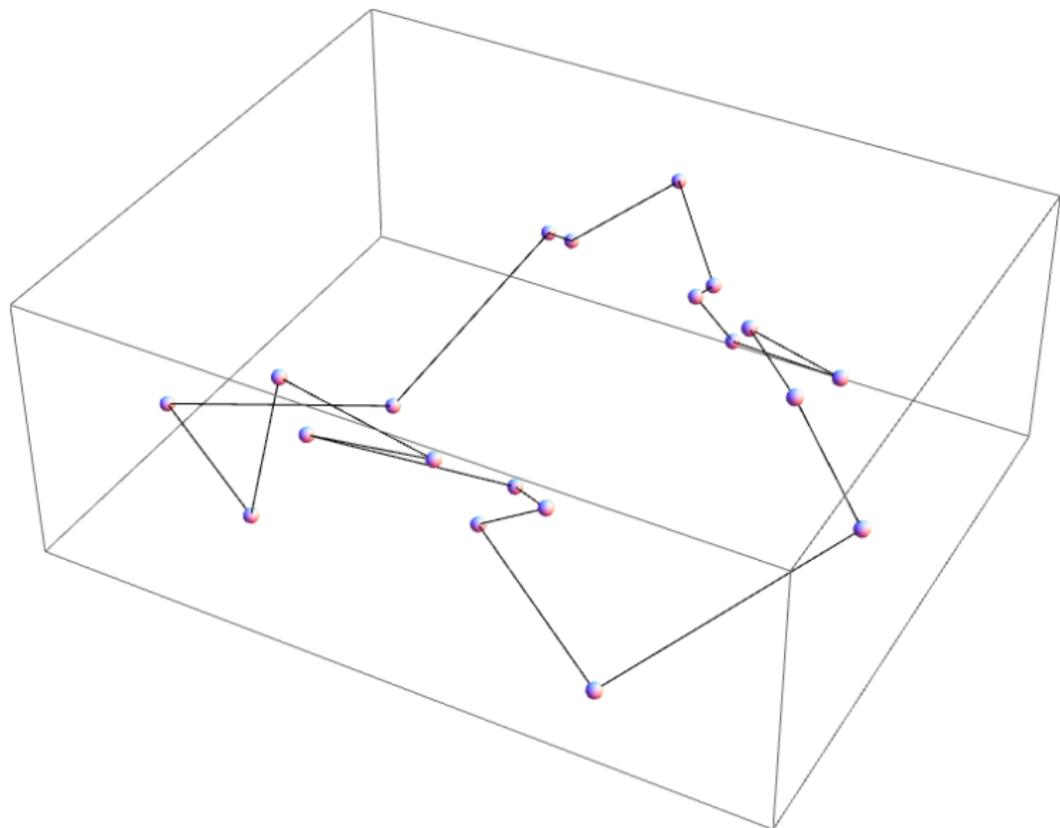
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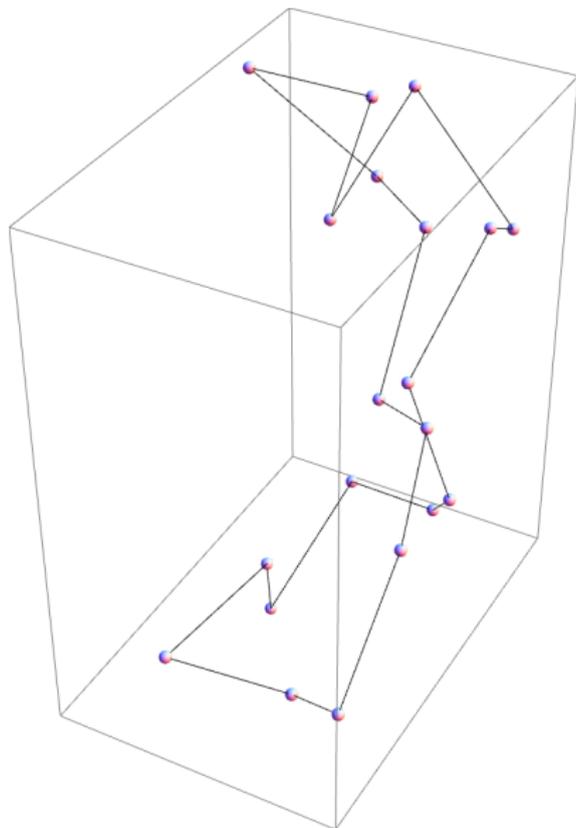
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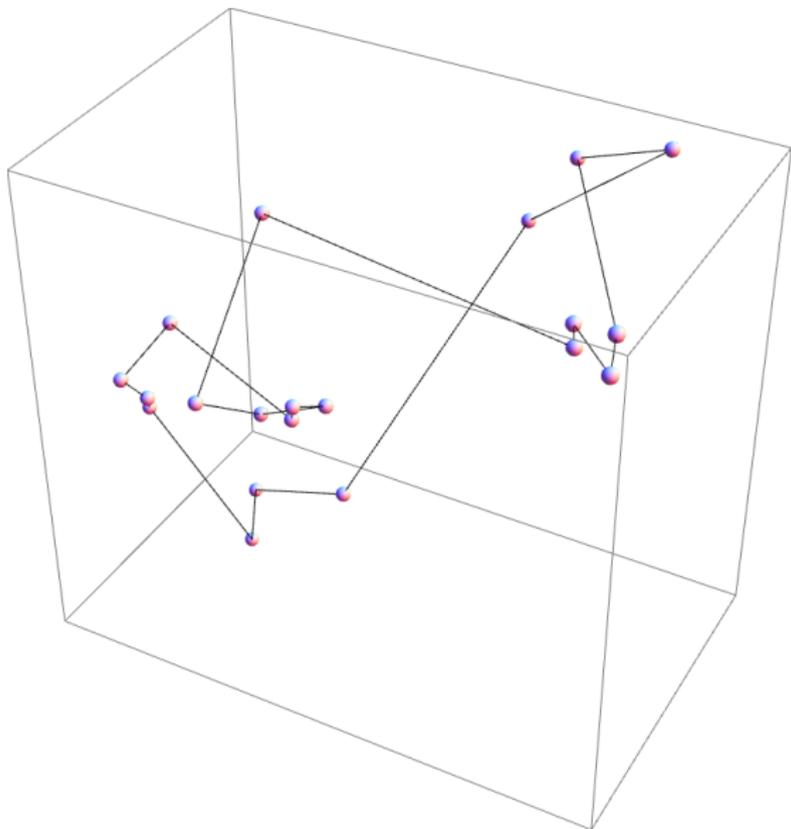
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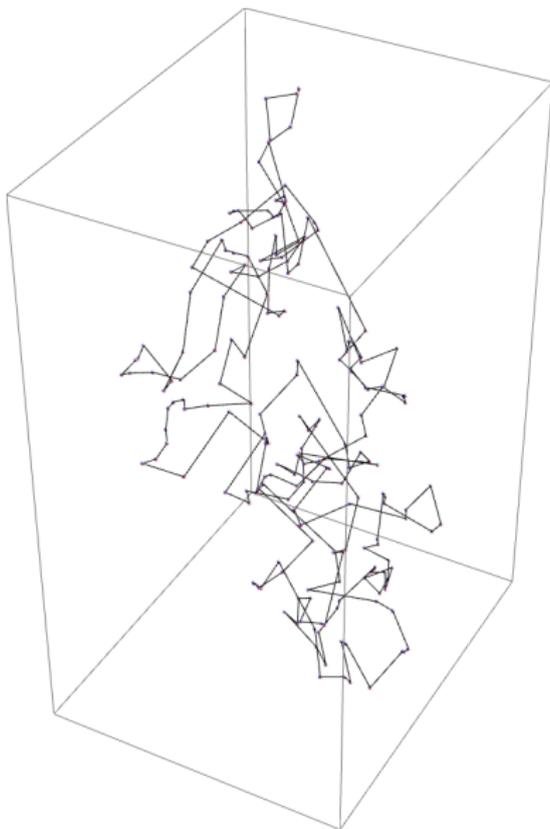
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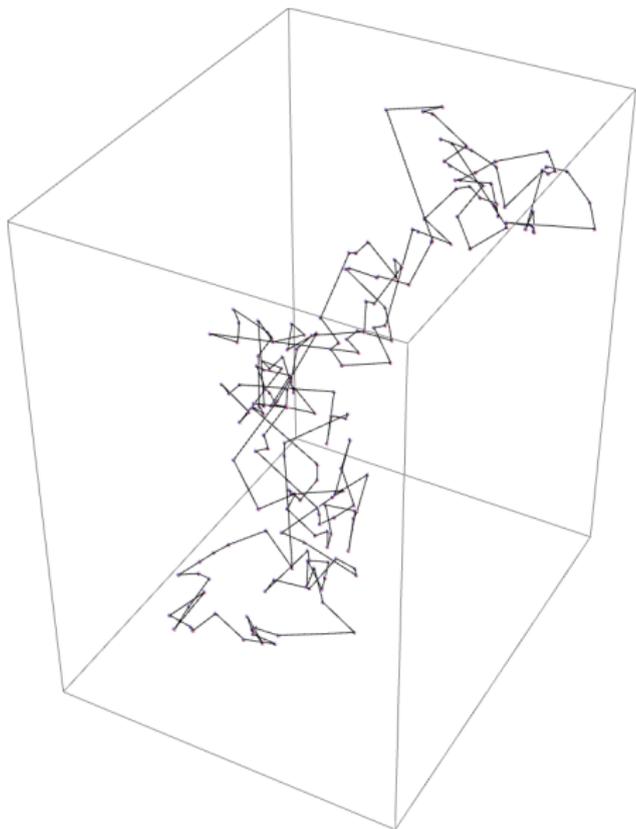
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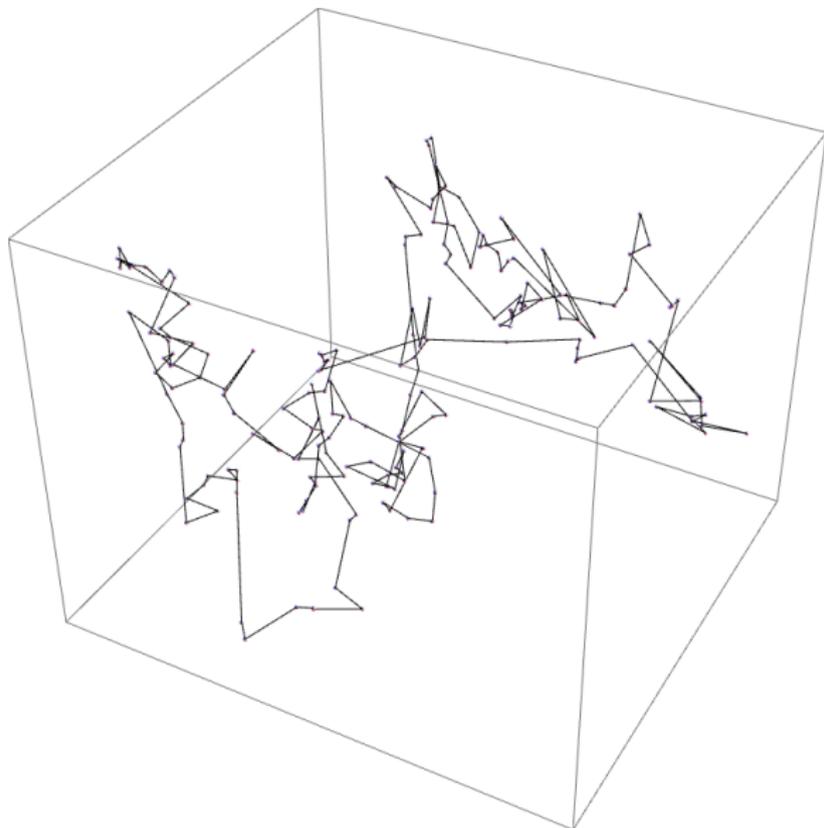
# Examples of 200-gons



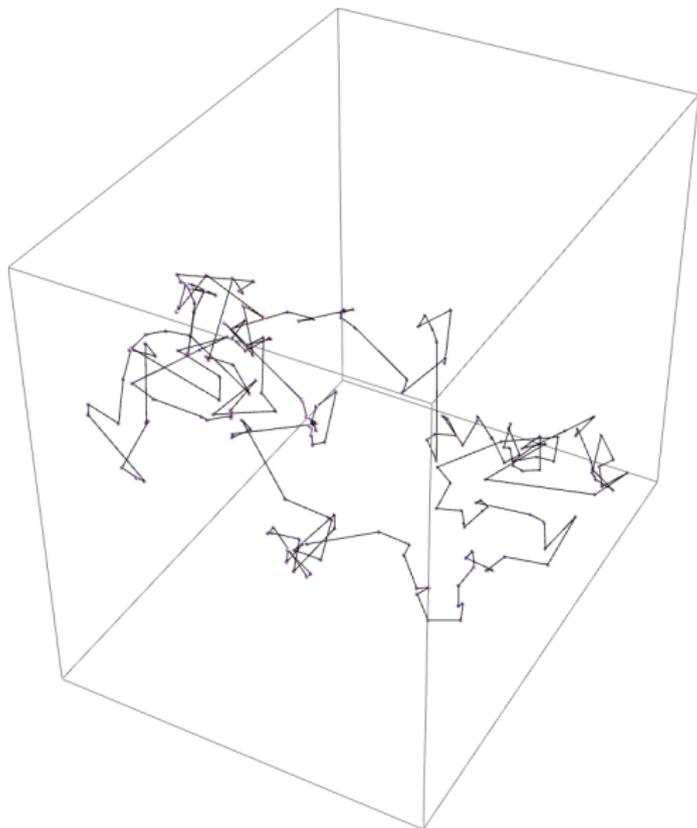
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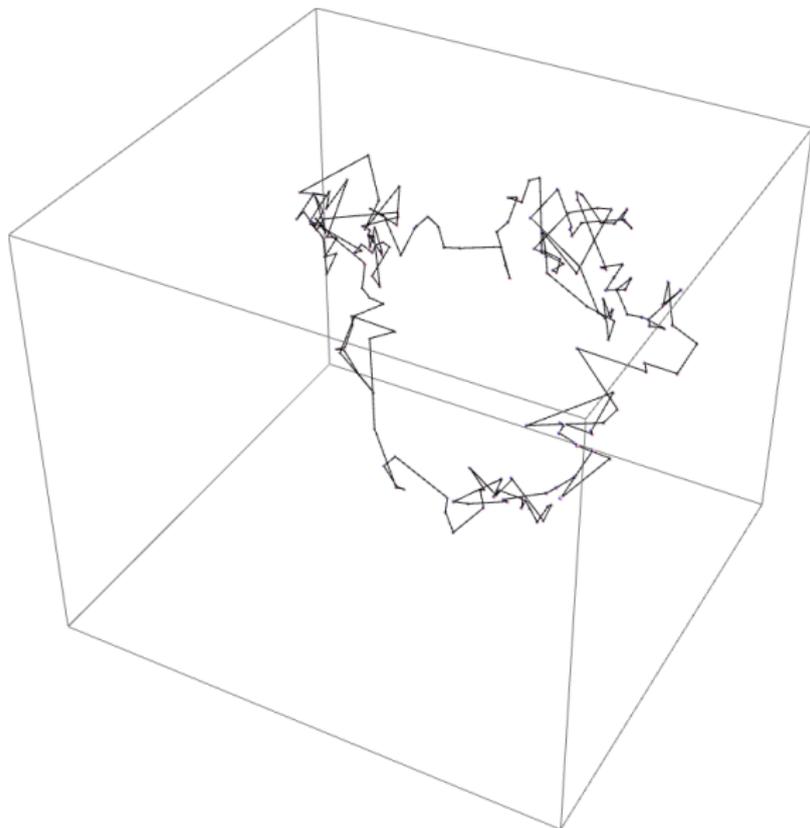
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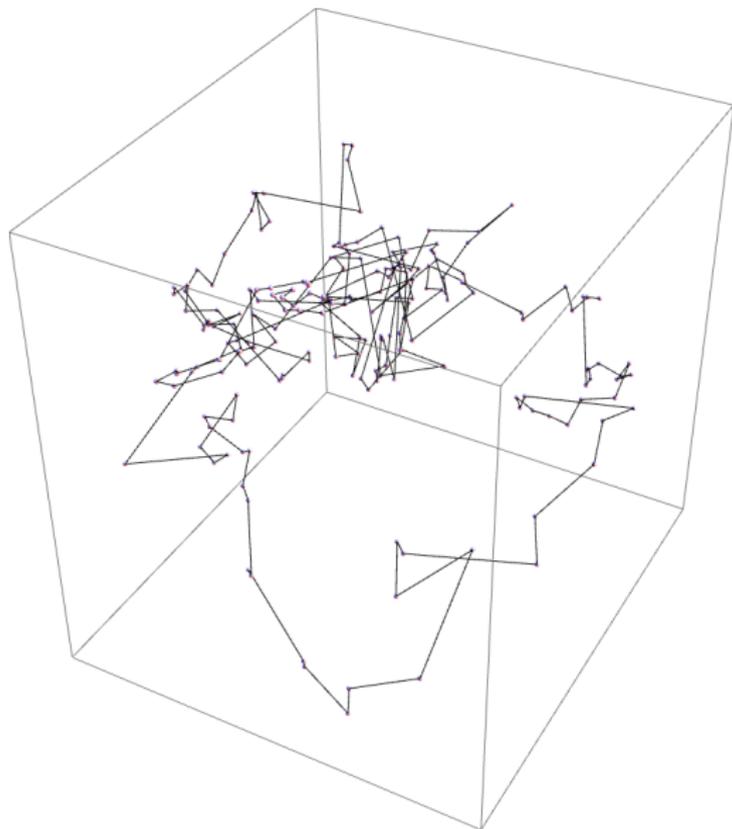
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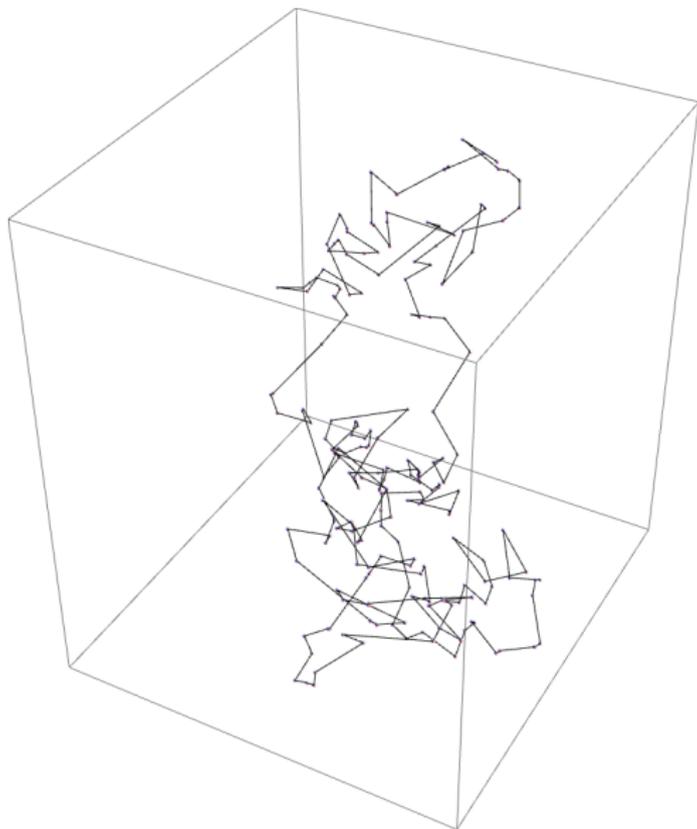
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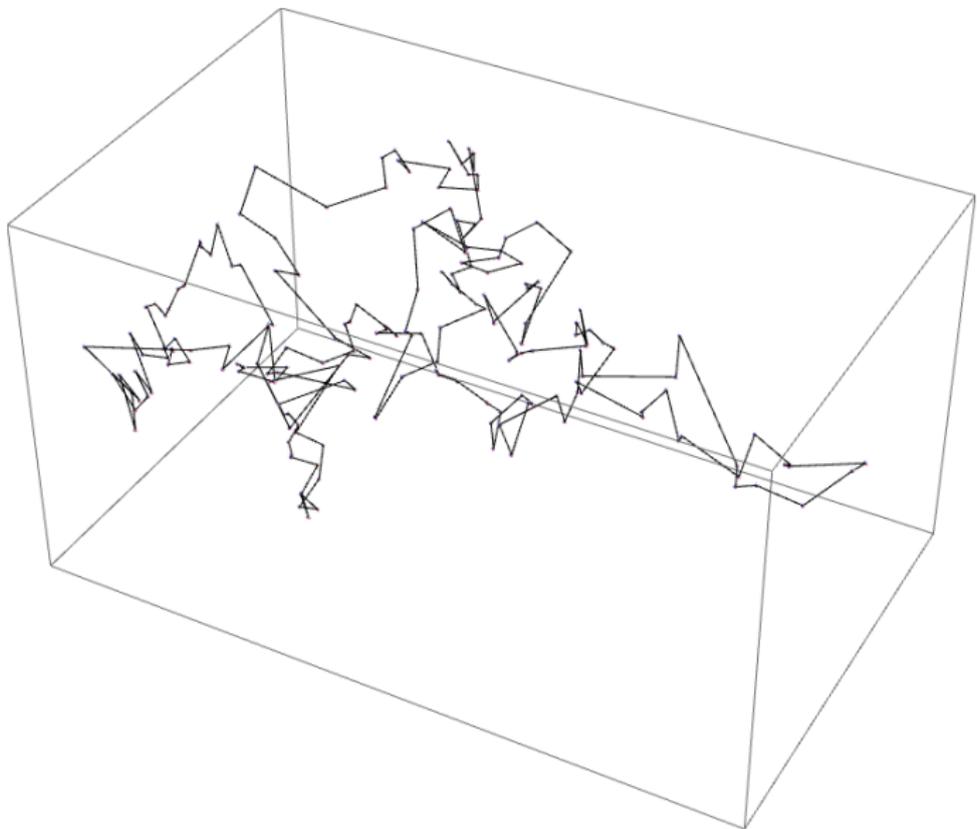
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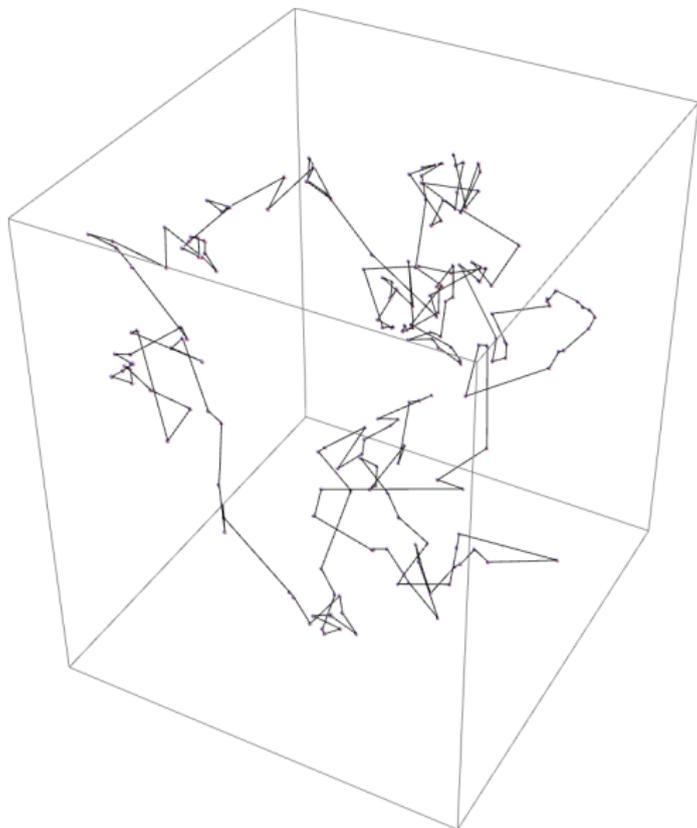
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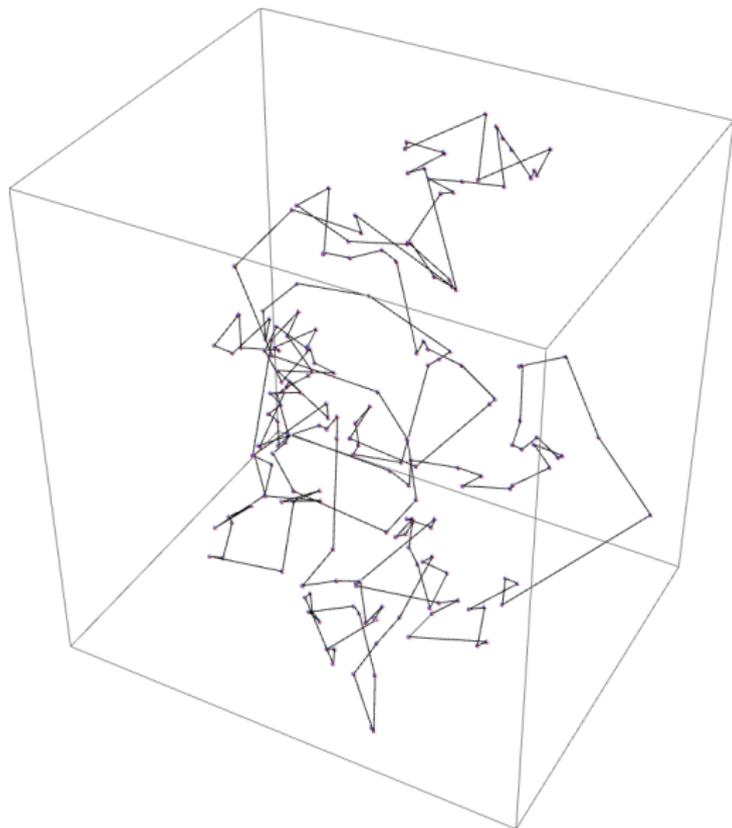
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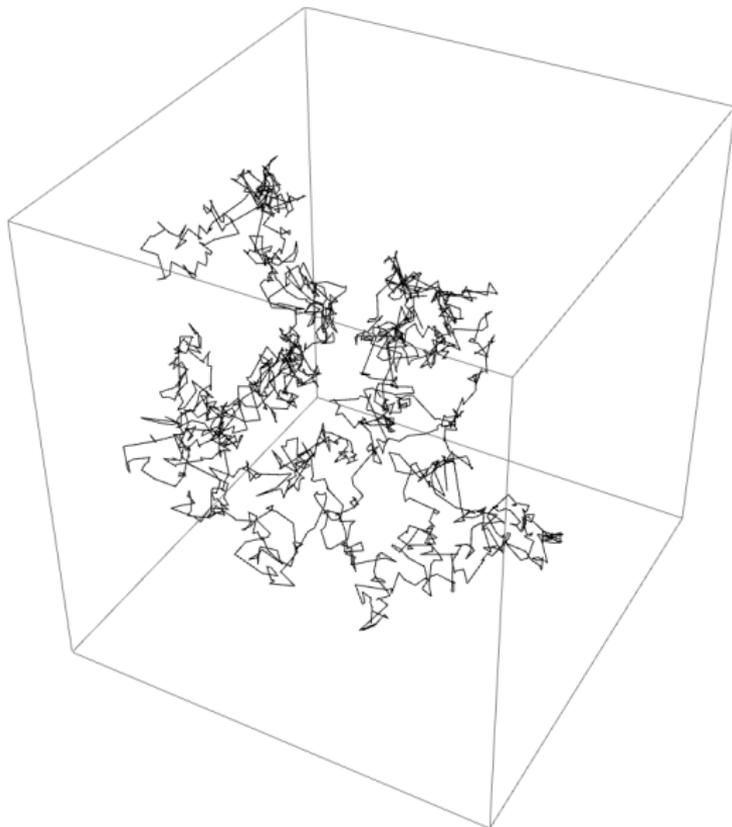
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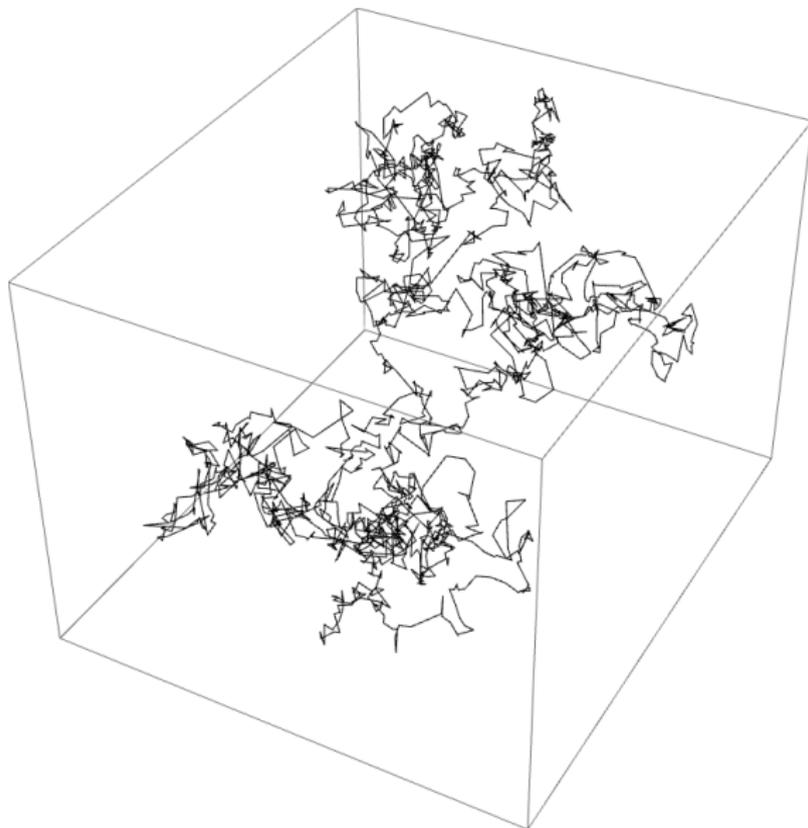
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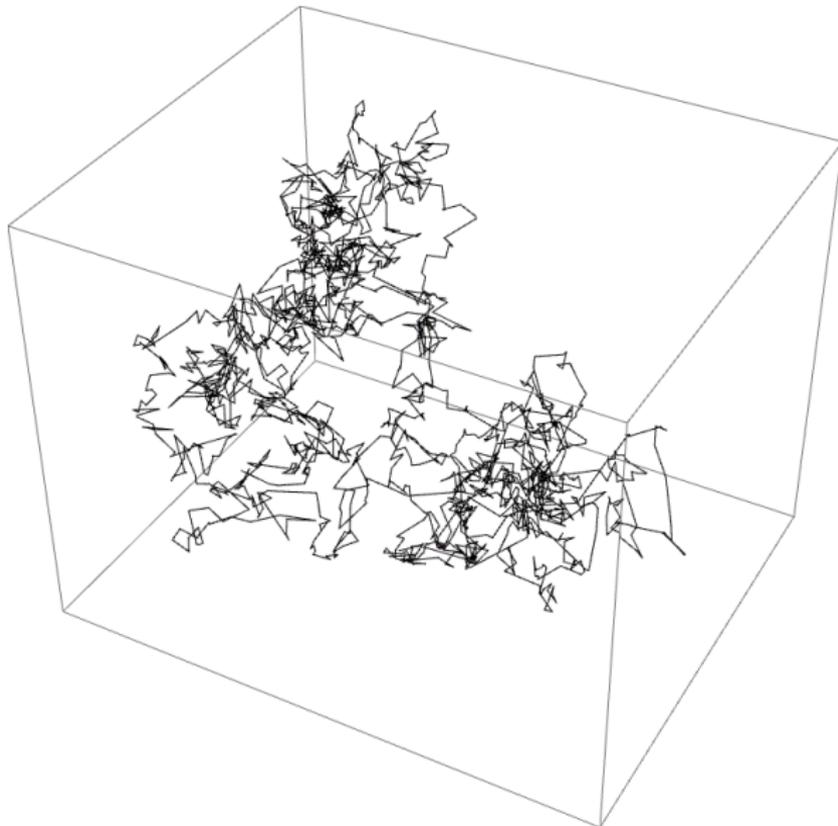
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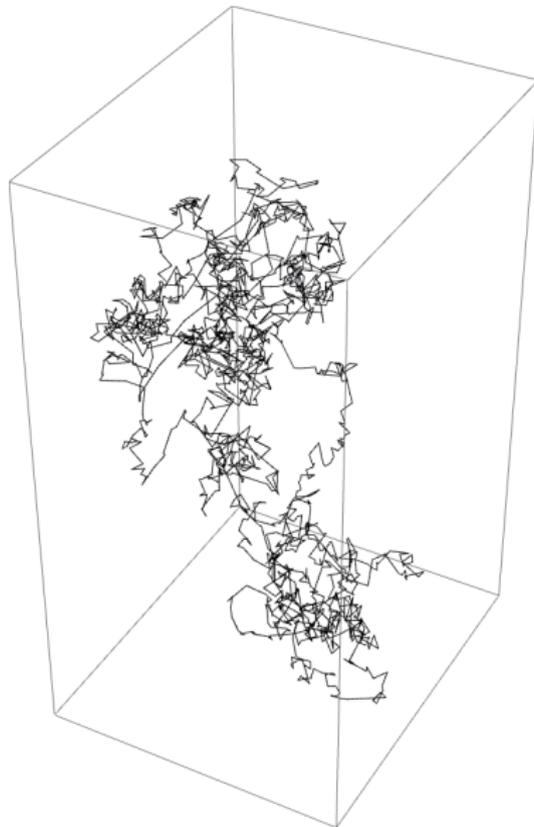
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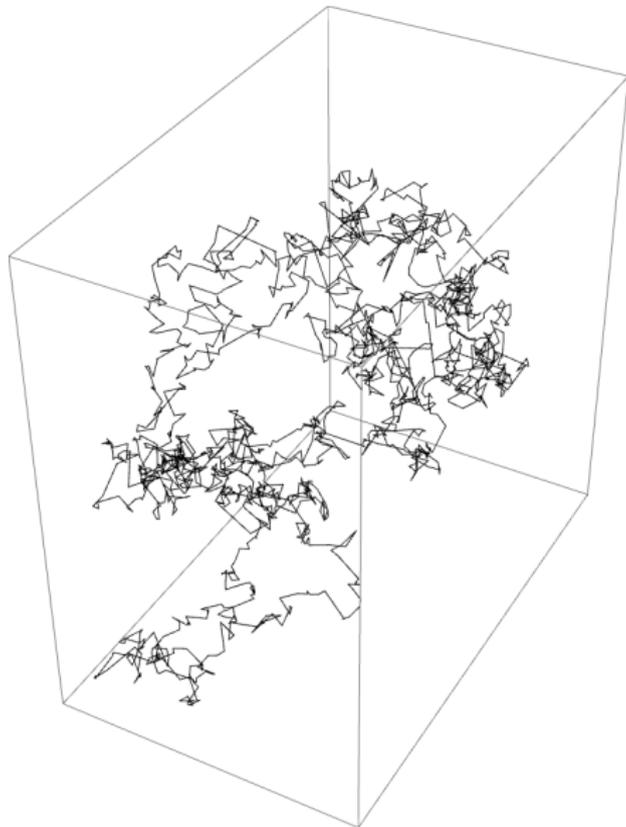
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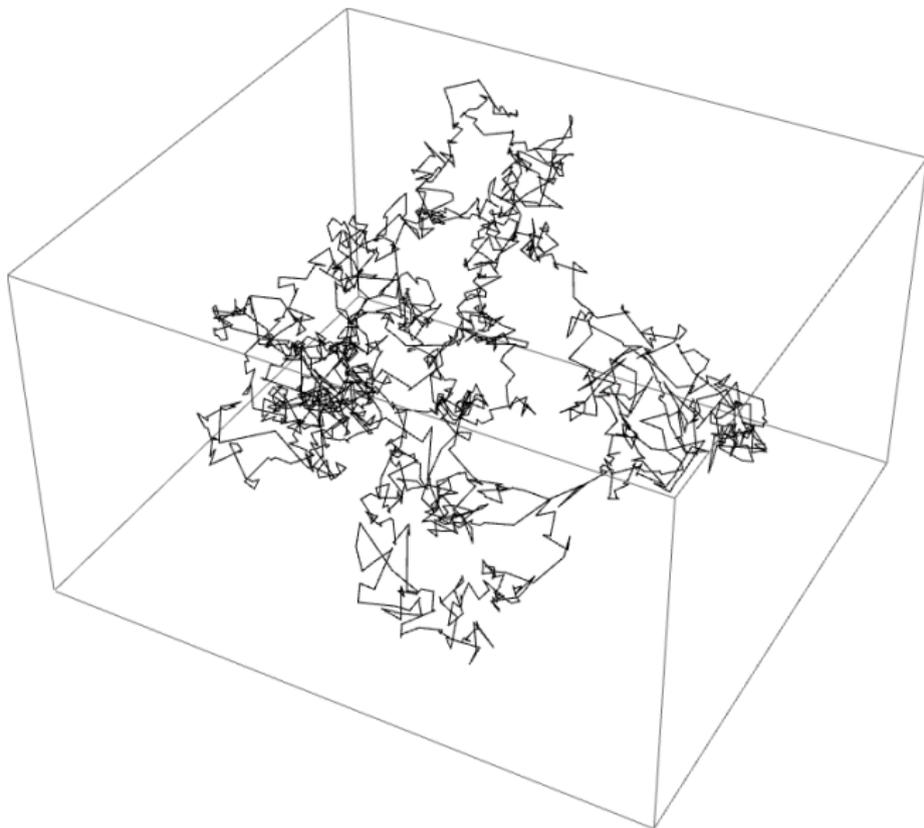
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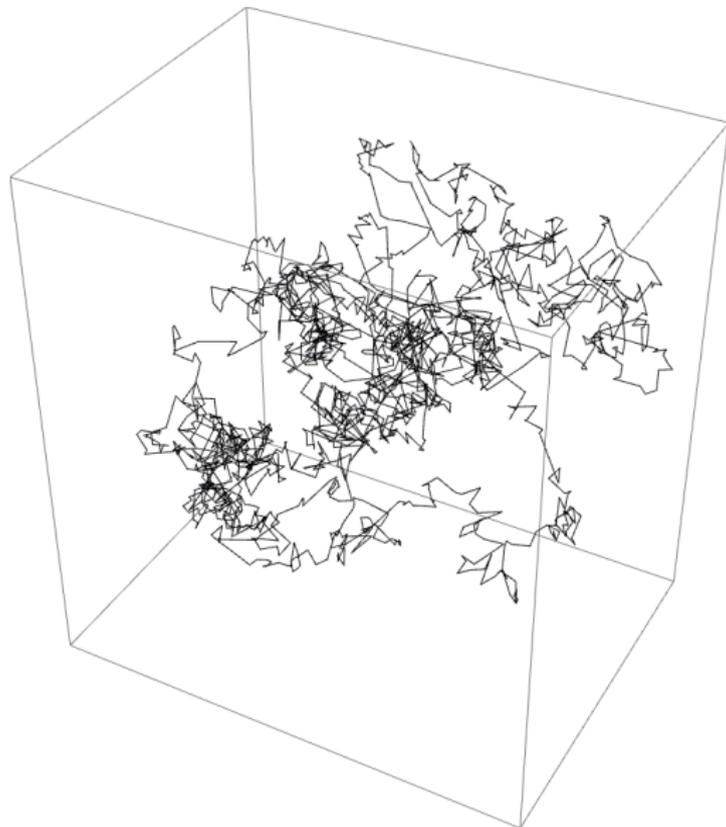
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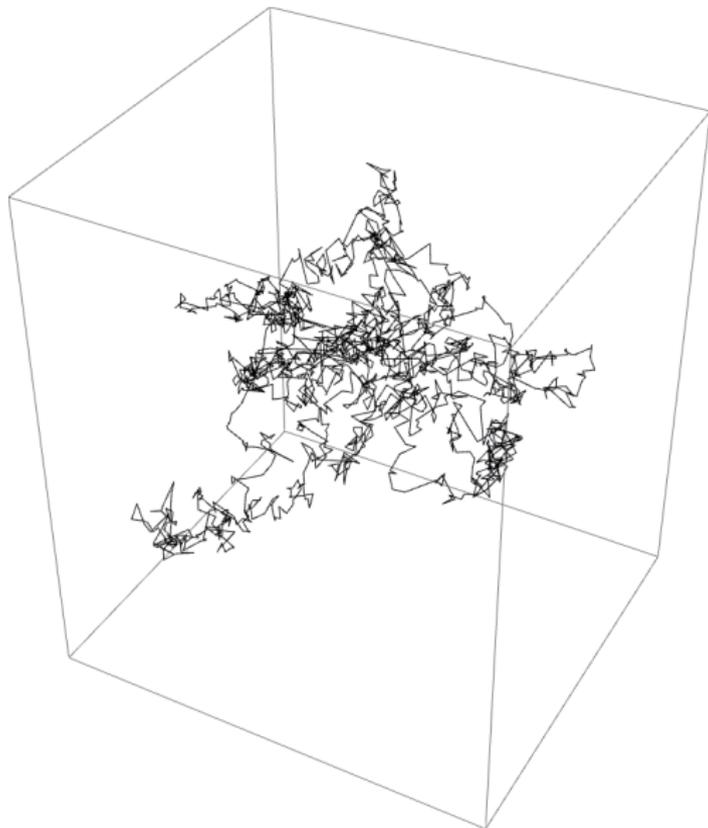
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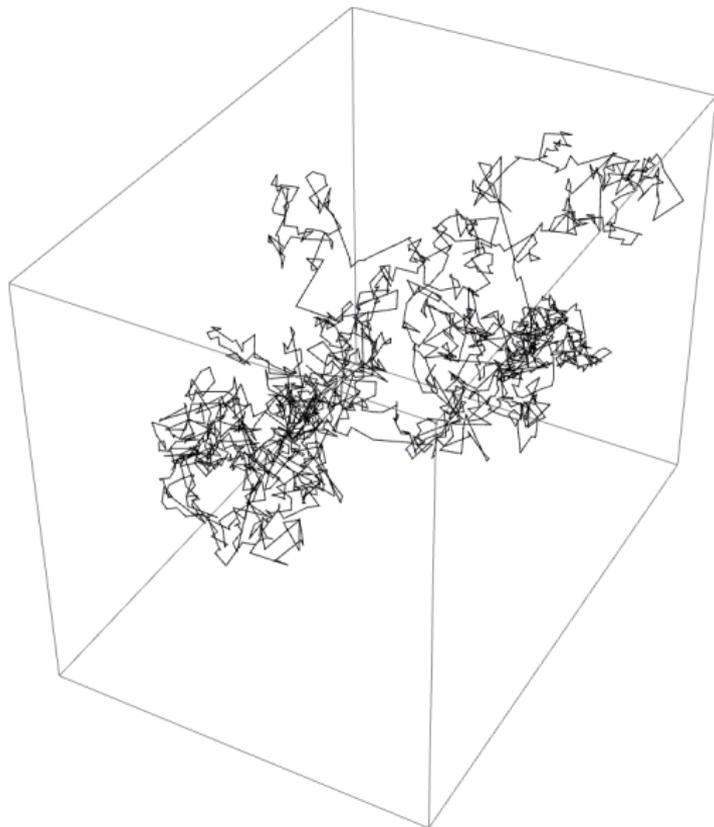
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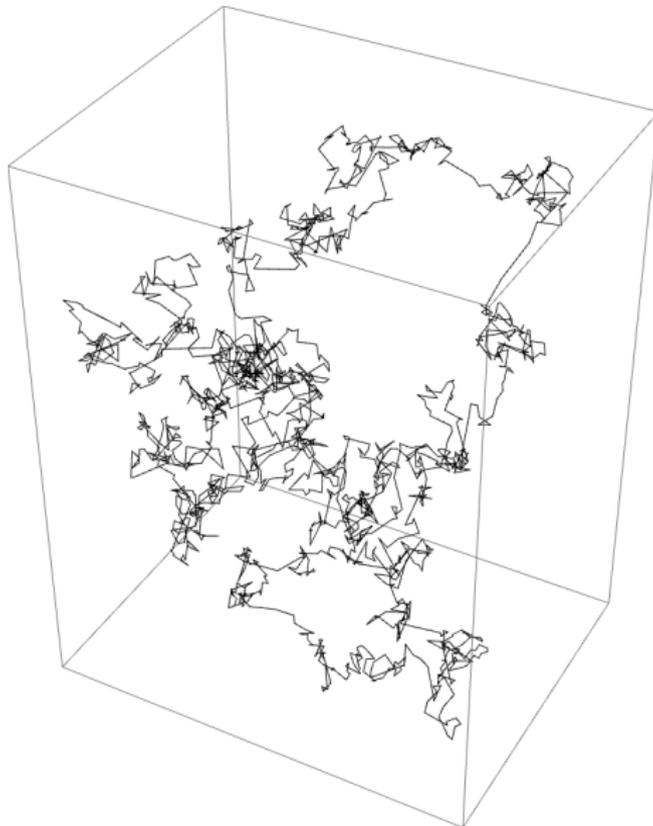
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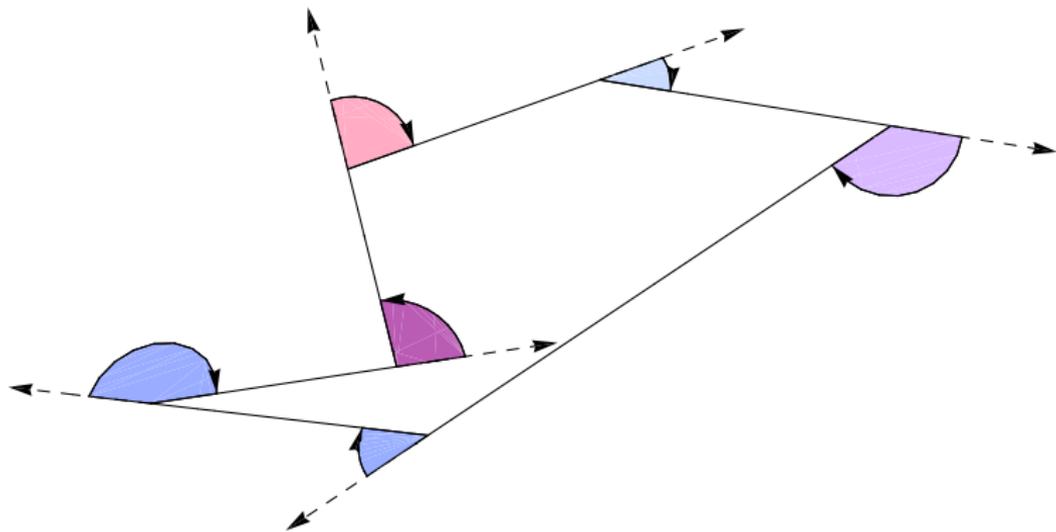
# Examples of 2,000-gons



# Total Curvature for Space Polygons

## Definition

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



# The total curvature surplus puzzle

## Lemma

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

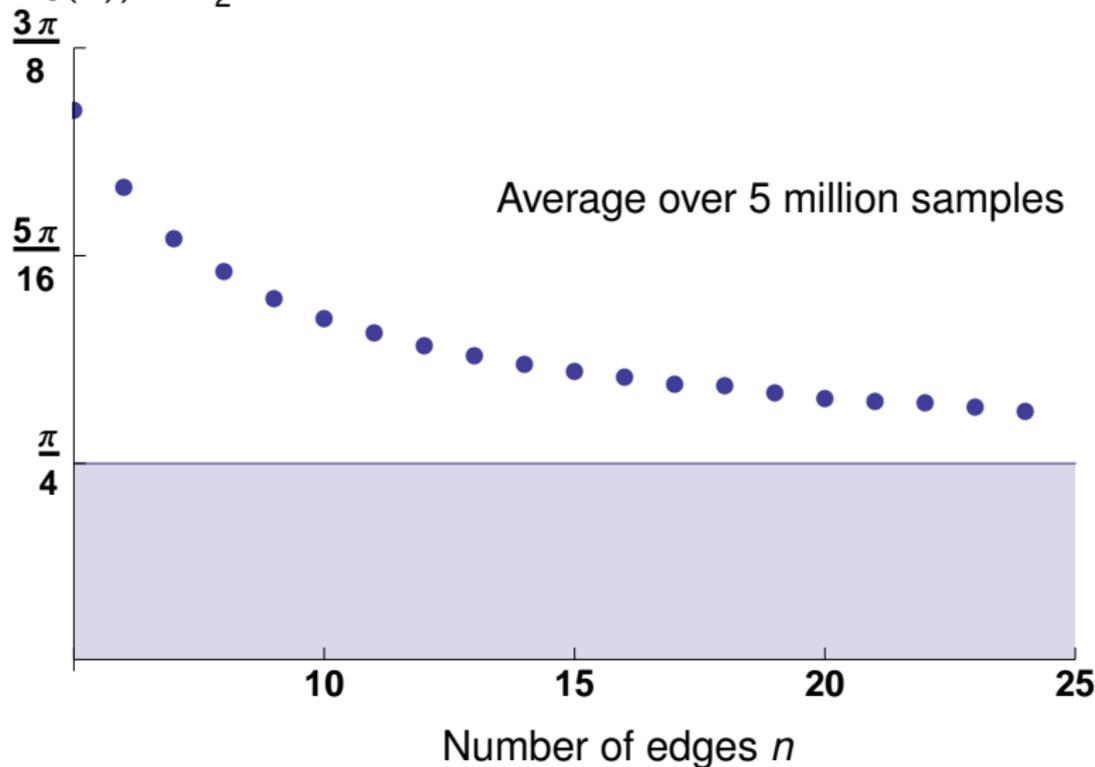
In 2007, Plunkett et. al. sampled random equilateral closed polygons and noticed that

$$E(\kappa, \text{Pol}_3(n; 1, \dots, 1)) \rightarrow \frac{\pi}{2}n + \alpha$$

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<sup>26</sup> 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.

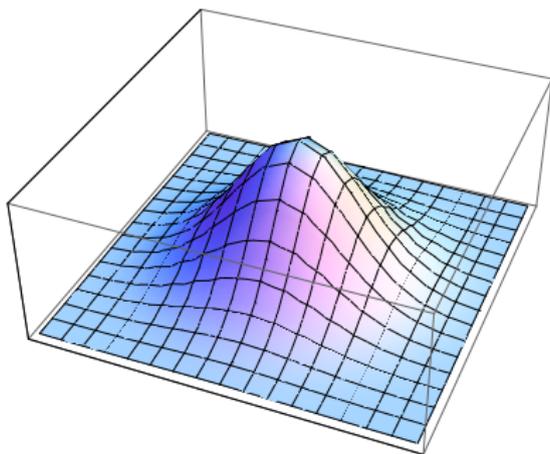
# Total curvature surplus in our measure on $\text{Pol}_3(n)$

$$E(\kappa, \text{Pol}_3(n)) - n\frac{\pi}{2}$$



## Definition

Let  $\mathcal{A}_3(n)$  be the space of open  $n$ -gons in  $\mathbb{R}^3$ , and  $\mathcal{P}_3(n) \subset \mathcal{A}_3(n)$  be the space of closed  $n$ -gons in  $\mathbb{R}^3$ .

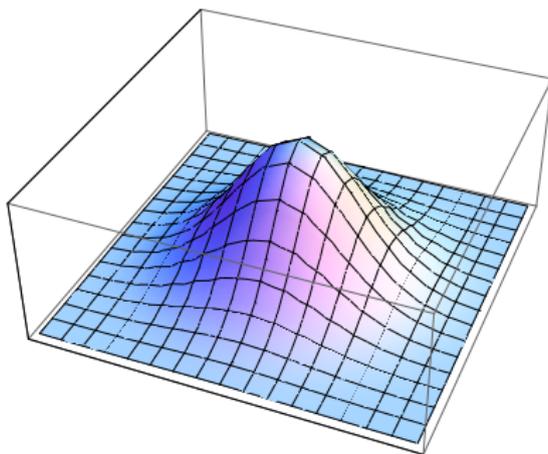


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## Definition

The *Hopf-Gaussian measure* on  $\mathcal{A}_3(n)$  is the pushforward of a multivariate Gaussian measure on  $\mathbb{H}^n$  by the Hopf map. The Hopf-Gaussian measure on  $\mathcal{P}_3(n)$  is the subspace measure.



Proposition (with Cantarella, Grosberg, Kusner)

*For any scale invariant function  $F$  on space polygons,*

$$E(F, \mathcal{A}_3(n)) = E(F, \text{Arm}_3(n)), E(F, \mathcal{P}_3(n)) = E(F, \text{Pol}_3(n)).$$

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## Proof.

The idea is that the Gaussian measure on  $\mathbb{H}^n$  is spherically symmetric, so the subspace measure on each  $S^{4n-1}$  is the standard one. Since the average over each sphere is the average over the whole space (by scale invariance), this is enough. □

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## Corollary

$$E(\kappa, \mathcal{P}_3(n)) = E(\kappa, \text{Pol}_3(n)).$$

# The pdf of the failure to close of an arm

If we write the Hopf map in coordinates, we see if

$$q = q_0 + q_1 \mathbf{i} + q_2 \mathbf{j} + q_3 \mathbf{k},$$

$$\text{Hopf}(q) = (q_0^2 + q_1^2 - q_2^2 - q_3^2, 2q_1 q_2 - 2q_0 q_3, 2q_0 q_2 + 2q_1 q_3).$$

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## Proposition (with Cantarella, Grosberg, Kusner)

*The first coordinate of the sum of  $k$  edges in  $\mathcal{A}_n$  is distributed as a difference of  $\chi^2(2k)$  variables. The pdf of this coordinate is*

$$f(y) = \frac{|y|^{k-1/2}}{4^k \sqrt{\pi} \Gamma(k)} K_{k-1/2}(|y|/2).$$

# The pdf of the failure to close of an arm

If we write the Hopf map in coordinates, we see if

$$q = q_0 + q_1 \mathbf{i} + q_2 \mathbf{j} + q_3 \mathbf{k},$$

$$\text{Hopf}(q) = (q_0^2 + q_1^2 - q_2^2 - q_3^2, 2q_1 q_2 - 2q_0 q_3, 2q_0 q_2 + 2q_1 q_3).$$

**Proposition (with Cantarella, Grosberg, Kusner)**

*The pdf  $G_k(\vec{r})$  of the vector joining the ends of  $k$  edges from a Hopf-Gaussian arm is spherically symmetric in  $\mathbb{R}^3$  and given by:*

$$G_k(\vec{r}) = \frac{r^{k-3/2}}{2^{2k+2} \pi^{3/2} \Gamma(k)} K_{k-3/2}(r/2),$$

where  $r = |\vec{r}|$ .

# The pdf of a pair of edges in $\mathcal{P}_3(n)$

Proposition (with Cantarella, Grosberg, Kusner)

The pdf of a pair of edges  $\vec{e}_1, \vec{e}_2$  in  $\mathcal{P}_3(n)$  is

$$P(\vec{e}_1, \vec{e}_2) = \frac{G_1(\vec{e}_1)G_1(\vec{e}_2)G_{n-2}(-\vec{e}_1 - \vec{e}_2)}{G_n(\vec{0})}.$$

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Proposition (with Cantarella, Grosberg, Kusner)

If  $x = (|\vec{e}_1| + |\vec{e}_2|)/2$ ,  $y = (|\vec{e}_1| - |\vec{e}_2|)/2$  and  $z = |\vec{e}_1 + \vec{e}_2|$ , this pairwise pdf is

$$P(\vec{e}_1, \vec{e}_2) = \frac{\Gamma(n)}{2\sqrt{\pi}\Gamma(2n-4)} e^{-x} z^{n-\frac{5}{2}} K_{n-\frac{7}{2}}\left(\frac{z}{2}\right)$$

# The curvature surplus explained

## Proposition (with Cantarella, Grosberg, Kusner)

*The expected value of the turning angle  $\theta$  for a single pair of edges in  $\mathcal{P}_3(n)$  is given by the formula*

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

so

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

## Proof.

Write

$$\theta(x, y, z) = \arccos \frac{z^2 - 2(x^2 + y^2)}{2x^2 - 2y^2}$$

and integrate this against the pairwise pdf for edges in  $\mathcal{P}_3$ . □

# Checking against the numerical data

$$E(\kappa, \text{Pol}_3(n)) - n\frac{\pi}{2}$$

$$\frac{3\pi}{8}$$

$$\frac{5\pi}{16}$$

$$\frac{\pi}{4}$$

Average over 5 million samples

10

15

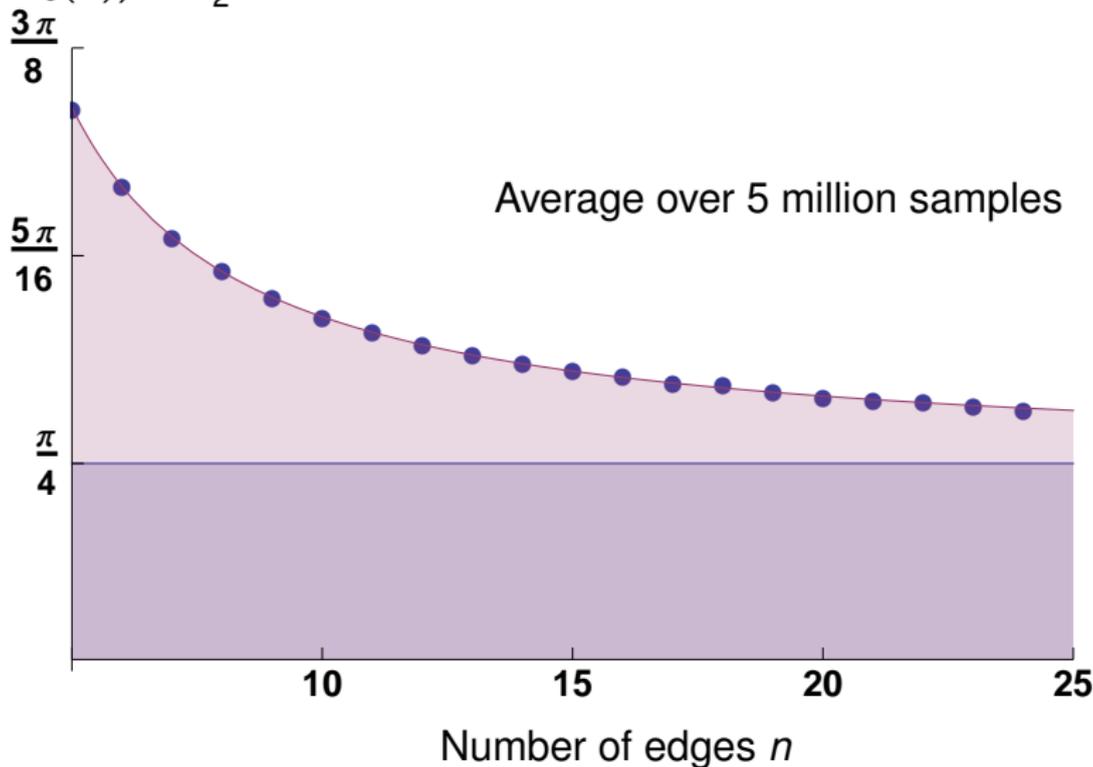
20

25

Number of edges  $n$

# Checking against the numerical data

$$E(\kappa, \text{Pol}_3(n)) - n\frac{\pi}{2}$$



# A consequence: topology at last!

Proposition (with Cantarella, Grosberg, Kusner)

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

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### Proof.

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

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

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

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



# New Results: Expected Total Curvature for Equilateral Random Polygons

A similar analysis can be used to get results about equilateral polygons. Here we don't have a closed form (yet), but we can express the results as a sum.

## Theorem (with Cantarella)

*The (exact) expectation for the total curvature of an equilateral random  $n$ -gon (in the standard measure) is*

$n$	$E(\kappa, \text{ePol}_3(n))$	(decimal)
4	8	8.
6	$6\pi - 8$	10.8496
8	$\frac{15}{4}\pi + \frac{32}{15}$	13.9143
10	$\frac{11}{2}\pi - \frac{64}{245}$	17.0175
12	$\frac{331,545}{51,776}\pi + \frac{512}{28,315}$	20.1351

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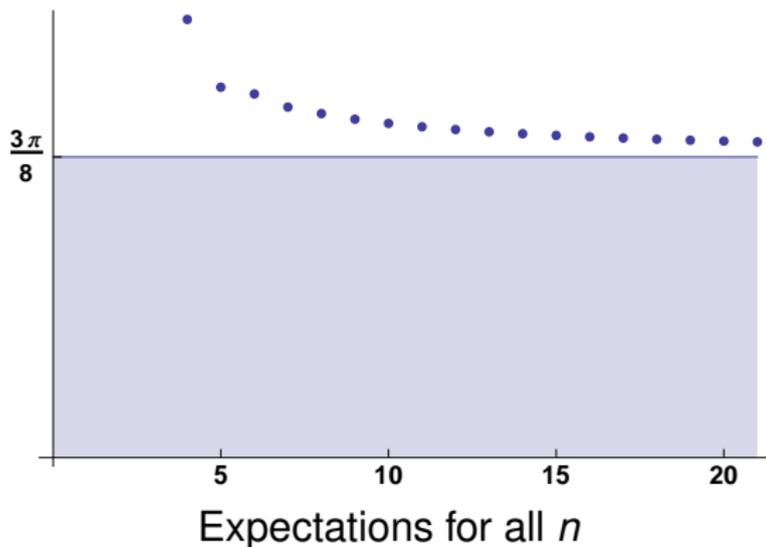
$n$	$E(\kappa, \text{ePol}_3(n))$	(decimal)
5	$-2\pi + 9\sqrt{3}$	9.30527
7	$\frac{316}{33}\pi - \frac{225}{22}\sqrt{3}$	12.369
9	$\frac{766}{289}\pi + \frac{11907}{2890}\sqrt{3}$	15.463
11	$\frac{90712}{14219}\pi - \frac{1686177}{1990660}\sqrt{3}$	18.5751
13	$\frac{23336570}{3407523}\pi + \frac{2381643}{22716820}\sqrt{3}$	21.6969

# Comparison with Asymptotic Results

## Theorem (Grosberg)

*We have*

$$E(\kappa, \text{ePol}_3(n)) - \frac{\pi}{2}n \rightarrow \frac{3}{8}\pi \text{ as } n \rightarrow \infty.$$

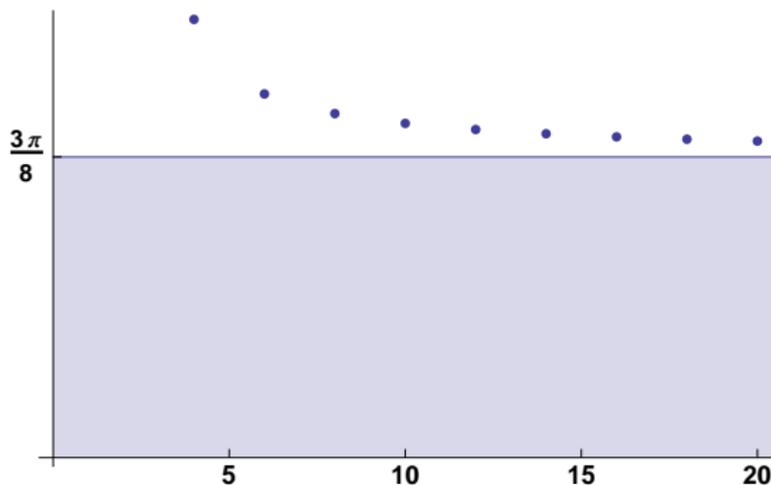


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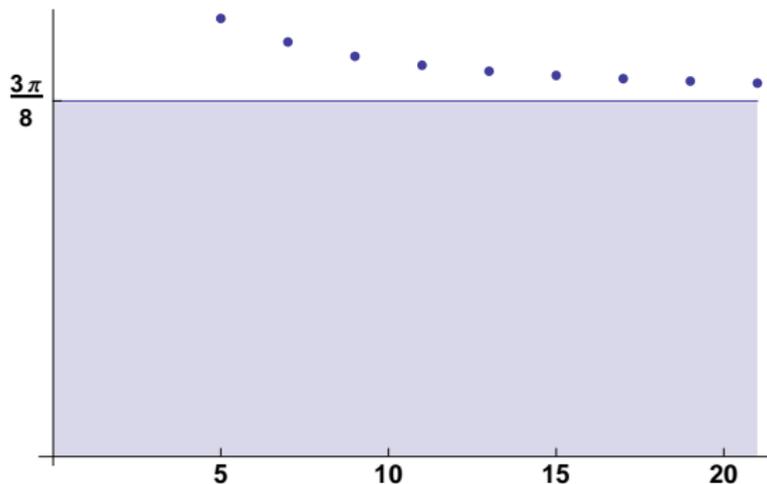


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## Some open questions

- 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?
- Geodesics in the Stiefel manifold are “optimal” reconfigurations of framed curves or polygons. Given a framed  $n$ -gon, there are  $2^n$  lifts to “spin-framed”  $n$ -gons. So given  $n$ -gons  $P_a$  and  $P_b$ , which pair of lifts is closest?

- *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!