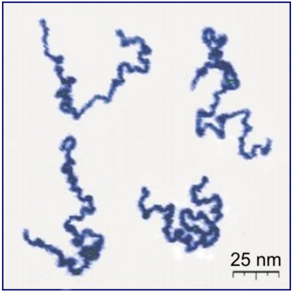
Grassmannians and Random Polygons

Jason Cantarella Alexander Grosberg Tetsuo Deguchi
Robert B. Kusner Clayton Shonkwiler

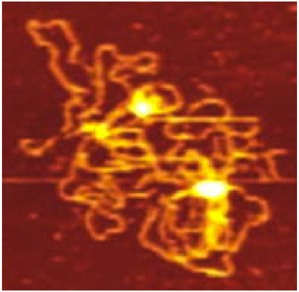
PAL
November 6, 2014

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.*

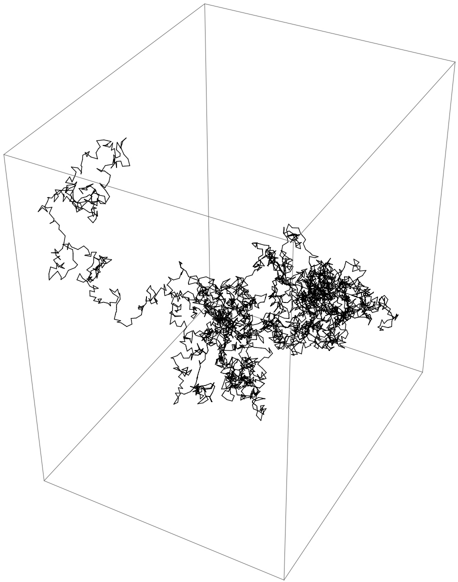
The Moral of the Story

Equilateral polygons are the most physically interesting, but the moduli spaces of equilateral n-gons are tricky beasts.

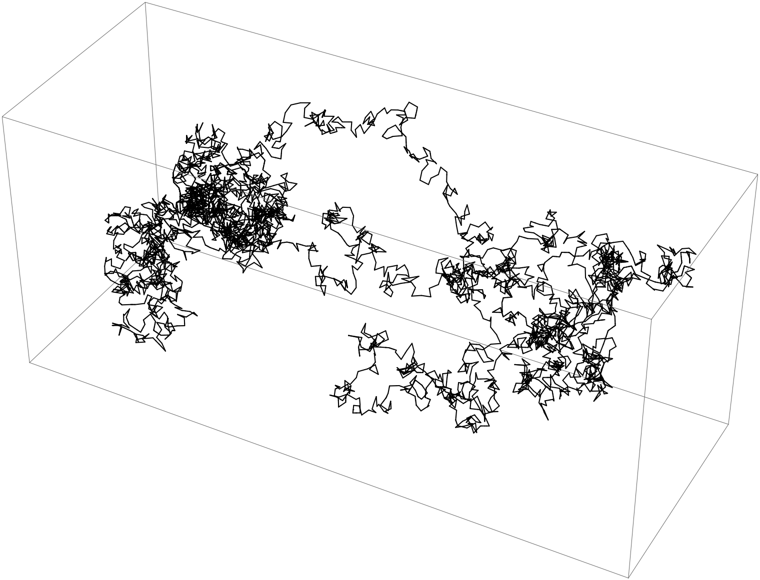
However, if we allow ourselves to consider polygons of fixed total length, then the moduli spaces are Stiefel and Grassmann manifolds and we can use knowledge of the Riemannian geometry of these spaces to find fast sampling algorithms and to prove surprising theorems.

In fact, this is a reduction of unified theory of *framed* n-gons of fixed total length.

A Random Walk with 3,500 Steps



A Closed Random Walk with 3,500 Steps

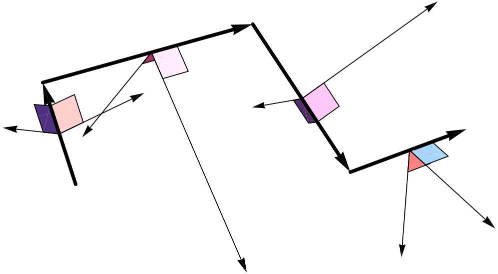


Definition

Let $\widetilde{\text{FArm}}(n)$ be the space of framed n-gons of total length 2 (up to translation) in $\mathbb{R}^3$. In other words,

$$\widetilde{\text{FArm}}(n) = \{((e_1, f_1, g_1), \ldots, (e_n, f_n, g_n))\} \subset (\mathrm{Mat}_{3\times 3}(\mathbb{R}))^n$$

such that $|e_i| = |f_i| = |g_i|$ and e_i, f_i, and g_i are mutually orthogonal for all i.

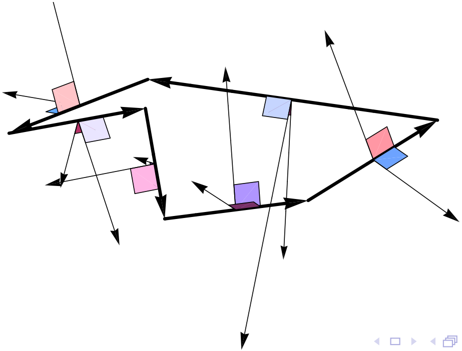


Definition

Let $\widetilde{\mathrm{FPol}}(n)$ be the space of closed, framed n-gons of total length 2 (up to translation) in $\mathbb{R}^3$. In other words,

$$\widetilde{\mathrm{FPol}}(n) = \{((e_1, f_1, g_1), \ldots, (e_n, f_n, g_n)) : \sum e_i = 0\} \subset \widetilde{\mathrm{FArm}}(n).$$

Let $\mathrm{FArm}(n) = \widetilde{\mathrm{FArm}}(n)/SO(3)$ and $\mathrm{FPol}(n) = \widetilde{\mathrm{FPol}}(n)/SO(3)$.



Note that

$$\widetilde{\mathrm{FArm}}(n) = \bigcup_{\vec{r} \in \Delta} \widetilde{\mathrm{FArm}}(n; \vec{r})$$

and

$$\widetilde{\mathrm{FPol}}(n) = \bigcup_{\vec{r} \in \Xi} \widetilde{\mathrm{FPol}}(n; \vec{r}),$$

where for example $\widetilde{\mathrm{FPol}}(n; \vec{r})$ is the collection of closed, framed n-gons with edgelength vector $\vec{r}$, and likewise for $\mathrm{FArm}(n)$ and $\mathrm{FPol}(n)$.

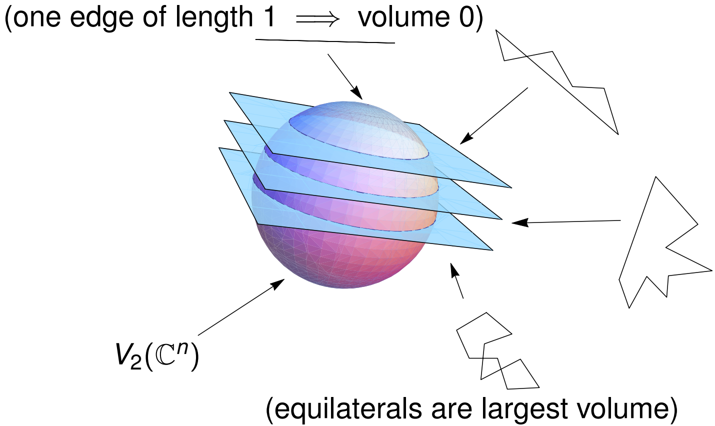
These spaces turn out to be extremely nice.

Proposition (Hausmann–Knutson '97, Howard–Manon–Millson '11)

We have the following commutative diagram, where the center and right vertical arrows are 2^n-fold coverings over proper framed polygons:

$$\begin{tikzcd} U(2) \arrow[r] \arrow[d] & V_2(\mathbb{C}^n) \arrow[r, two heads] \arrow[d] & Gr_2(\mathbb{C}^n) \arrow[d] \\ SO(3) \times U(1) \arrow[r] & \widetilde{\mathrm{FPol}}(n) \arrow[r, two heads] & \mathrm{FPol}(n)/U(1) \end{tikzcd}$$

Big picture (Cartoon, not entirely proved)



$V_2(\mathbb{C}^n)$ is an assembly of fixed edge length spaces
with their proper (different) relative volumes

Quaternions: natural coordinates for frames

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

$$\begin{aligned} \mathsf{FrHopf} : \mathbb{H} &\to \mathrm{Mat}_{3\times 3}(\mathbb{R}) \\ q &\mapsto (\bar{q}\mathbf{i}q, \bar{q}\mathbf{j}q, \bar{q}\mathbf{k}q). \end{aligned}$$

The columns are mutually orthogonal and have the same norm. Moreover,

$$\mathsf{FrHopf}(q) = \mathsf{FrHopf}(q') \Leftrightarrow q' = \pm q.$$

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Corollary

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

Framed Arms Via the Frame Hopf Map

As a consequence,

$$\begin{aligned} \text{FrHopf} : \mathbb{H}^n &\to \{\text{Framed arms of any total length}\} \\ (q_1, \ldots, q_n) &\mapsto (\text{FrHopf}(q_1), \ldots, \text{FrHopf}(q_n)) \end{aligned}$$

This map is 2^n-to-1 away from the coordinate planes.

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This map is 2^n-to-1 away from the coordinate planes.

Lemma

$$\begin{aligned}\mathrm{FrHopf}^{-1}(\widetilde{\mathrm{FArm}}(n)) &= \{(q_1, \ldots, q_n) : \sum |\,\mathrm{FrHopf}(q_i)| = \sum |q_i|^2 = 2\}\\ &= S^{4n-1}(\sqrt{2}).\end{aligned}$$

Proposition (with Cantarella and Deguchi)

The following diagram commutes, the vertical maps are smooth submersions, and the center and right arrows are 2^n-fold coverings over proper arms:

$$
\begin{tikzcd}
SU(2) = Sp(1) \arrow[r] \arrow[d, "\mathrm{FrHopf}"'] & S^{4n-1} \arrow[r, two heads] \arrow[d, "\mathrm{FrHopf}"'] & S^{4n-1}/Sp(1) = \mathbb{H}P^{n-1} \arrow[d] \\
SO(3) \arrow[r] & \widetilde{\mathrm{FArm}(n)} \arrow[r, two heads] & \mathrm{FArm}(n)
\end{tikzcd}
$$

Define the *symmetric measures* on $\widetilde{\mathrm{FArm}(n)}$ and $\mathrm{FArm}(n)$ by pushing forward Haar measure on S^{4n-1} and $\mathbb{H}P^{n-1}$, respectively.

The Symmetric Measure for Unframed Arms

$$
\begin{tikzcd}
SU(2) = Sp(1) \arrow[r] \arrow[d, two heads, "\mathrm{FrHopf}"'] & S^{4n-1} \arrow[r, two heads] \arrow[d, two heads, "\mathrm{FrHopf}"'] & S^{4n-1}/Sp(1) = \mathbb{H}P^{n-1} \arrow[d, two heads] \\
SO(3) \arrow[r] \arrow[d, equal] & \widetilde{\mathrm{FArm}}(n) \arrow[r, two heads] \arrow[d, two heads, "\pi"'] & \mathrm{FArm}(n) \arrow[d, two heads, "\pi"'] \\
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\end{tikzcd}$$

Define the *symmetric measures* on $\widetilde{\mathrm{Arm}}(n)$ and $\mathrm{Arm}(n)$ to be the pushforwards of Haar measure on S^{4n-1} and $\mathbb{H}P^{n-1}$, respectively.

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SU(2) = Sp(1) \arrow[r] \arrow[d, two heads, "\mathrm{FrHopf}"'] & S^{4n-1} \arrow[r, two heads] \arrow[d, two heads, "\mathrm{FrHopf}"'] & S^{4n-1}/Sp(1) = \mathbb{H}P^{n-1} \arrow[d, two heads] \\
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Declaring the vertical maps to be Riemannian submersions, $\widetilde{\mathrm{FArm}}(n)$, $\mathrm{FArm}(n)$, $\widetilde{\mathrm{Arm}}(n)$, and $\mathrm{Arm}(n)$ become Riemannian orbifolds.

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

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

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Proposition (Hausmann–Knutson '97)

$\operatorname{FrHopf}^{-1}(\widetilde{\operatorname{FPol}}(n)) = V_2(\mathbb{C}^n)$.

The proof is (a computation) worth doing!

In complex form, the map $\pi \circ \mathrm{FrHopf}(q)$ can be written as

$$\pi \circ \mathrm{FrHopf}(a + b\mathbf{j}) = (\overline{a + b\mathbf{j}})\mathbf{i}(a + b\mathbf{j}) = \mathbf{i}(|a|^2 - |b|^2 + 2\bar{a}b\mathbf{j})$$

Thus the polygon closes $\iff$

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

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

The Model Space for Closed Polygons

$$
\begin{tikzcd}
U(2) \arrow[r] \arrow[d, two heads, "\mathrm{FrHopf}"'] & V_2(\mathbb{C}^n) \arrow[r, two heads] \arrow[d, two heads, "\mathrm{FrHopf}"'] & Gr_2(\mathbb{C}^n) \arrow[d, two heads] \\
SO(3) \times U(1) \arrow[r] \arrow[d, two heads] & \widetilde{\mathrm{FPol}}(n) \arrow[r, two heads] \arrow[d, two heads, "\pi"'] & \mathrm{FPol}(n)/U(1) \arrow[d, two heads, "\pi"'] \\
SO(3) \arrow[r] & \widetilde{\mathrm{Pol}}(n) \arrow[r, two heads] & \mathrm{Pol}(n)
\end{tikzcd}
$$

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Define the *symmetric measures* on $\widetilde{\mathrm{FPol}}(n)$, $\mathrm{FPol}(n)$, $\widetilde{\mathrm{Pol}}(n)$, and $\mathrm{Pol}(n)$ to be the pushforwards of Haar measure on $V_2(\mathbb{C}^n)$ and $V_2(\mathbb{C}^n)/SU(2)$, respectively.

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Declaring the vertical maps to be Riemannian submersions, $\widetilde{\mathrm{FPol}}(n)$, $\mathrm{FPol}(n)$, $\widetilde{\mathrm{Pol}}(n)$, and $\mathrm{Pol}(n)$ become Riemannian orbifolds.

Proposition (with Cantarella and Deguchi)

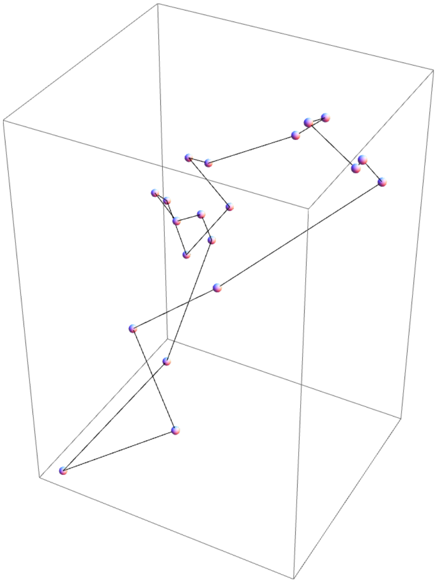
The natural (Haar) measure on $V_2(\mathbb{C}^n)$ (and hence the symmetric measure on $\widetilde{\mathrm{FPol}}(n)$ or $\widetilde{\mathrm{Pol}}(n)$) is obtained by generating random complex n-vectors with independent Gaussian coordinates and applying (complex) Gram-Schmidt.

```
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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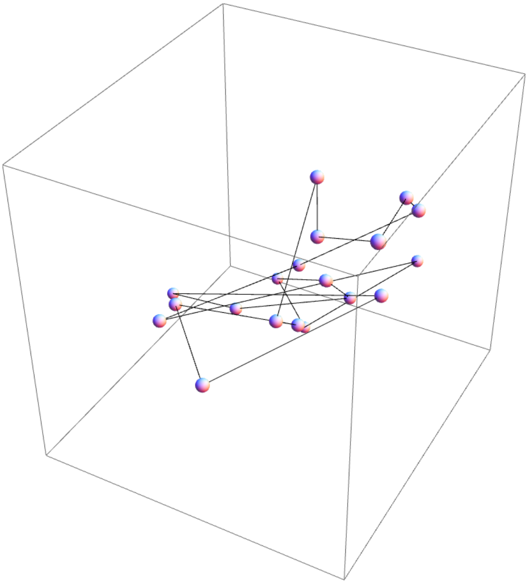

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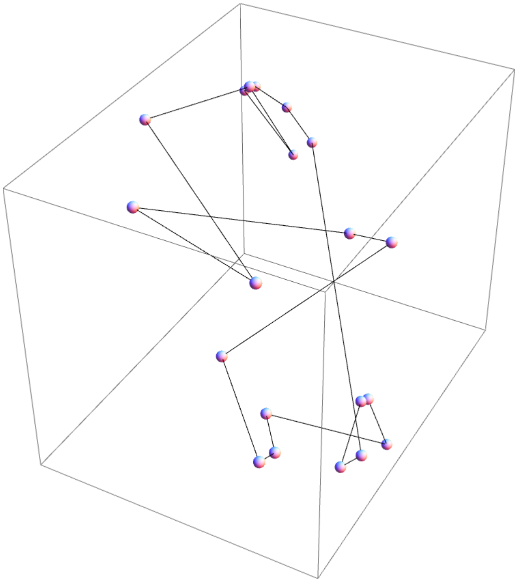

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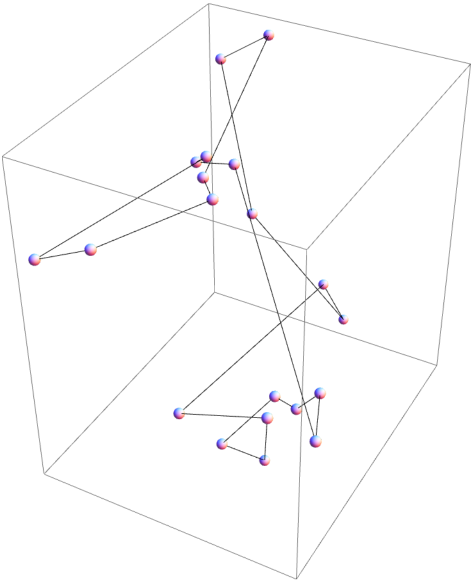

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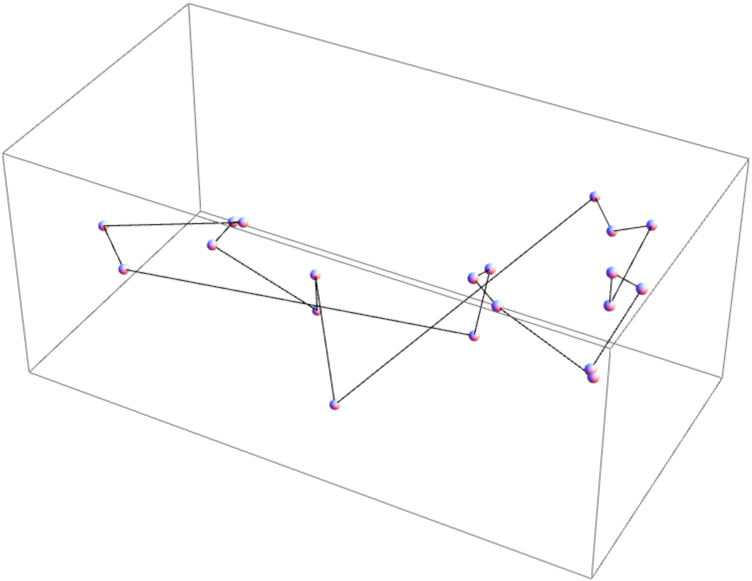
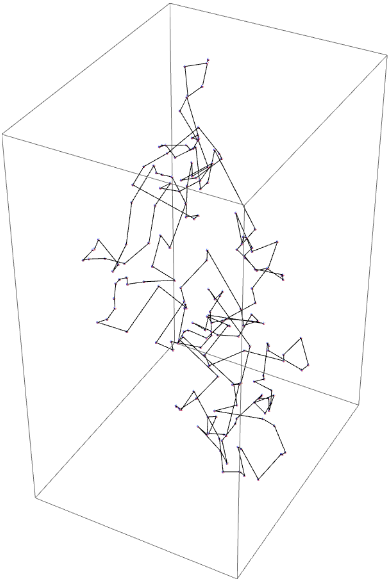
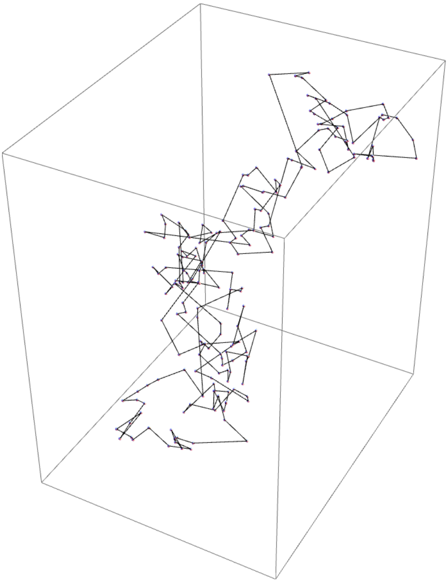


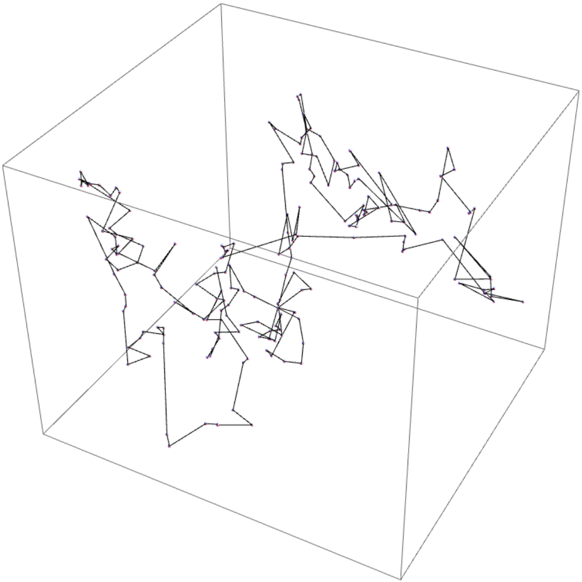
Examples of 200-gons



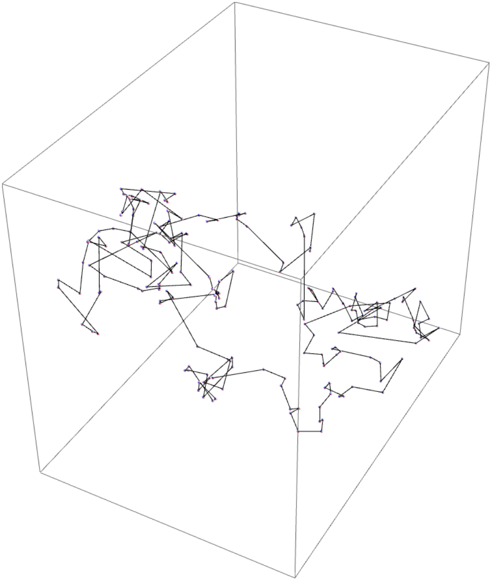
Examples of 200-gons

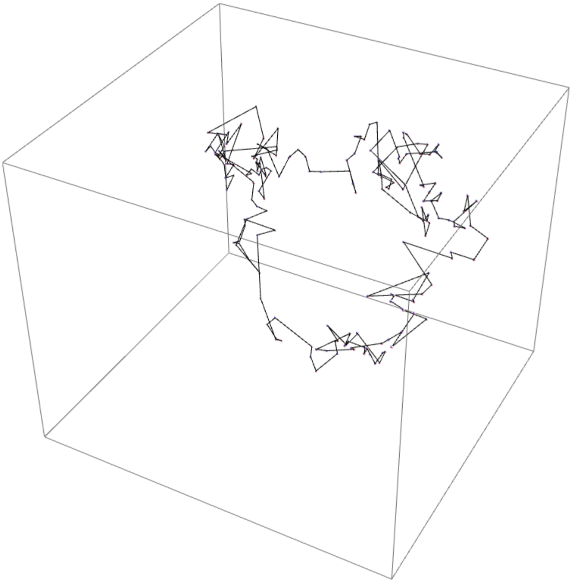


Examples of 200-gons

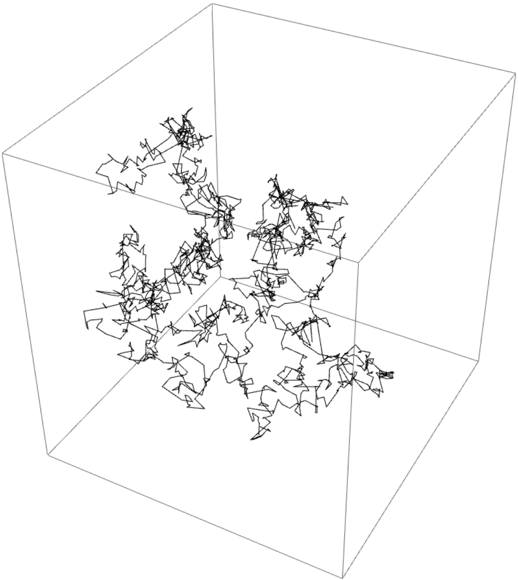


Examples of 200-gons

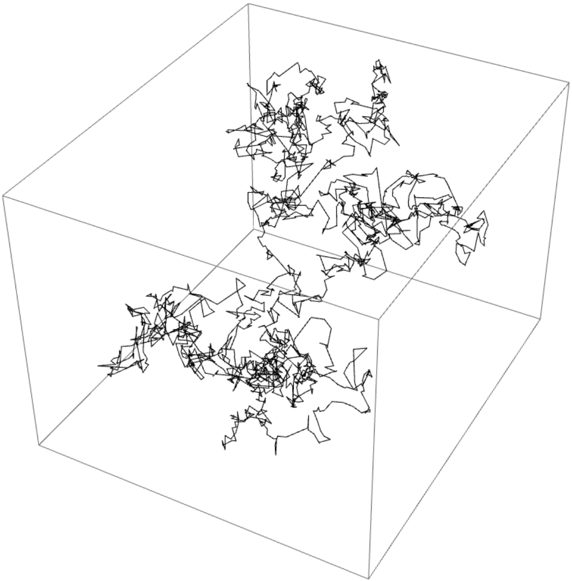




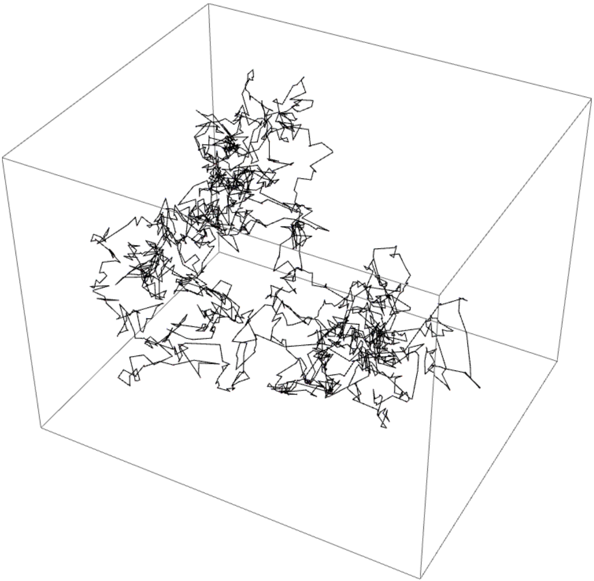
Examples of 2,000-gons



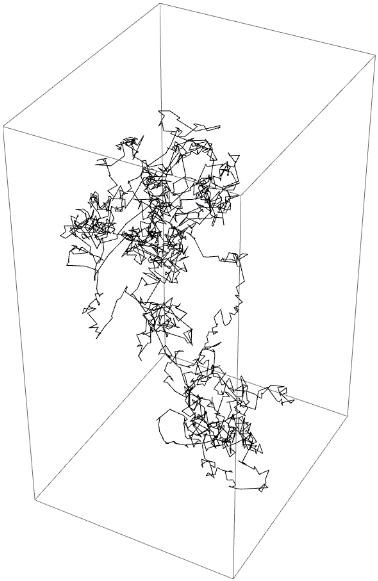
Examples of 2,000-gons



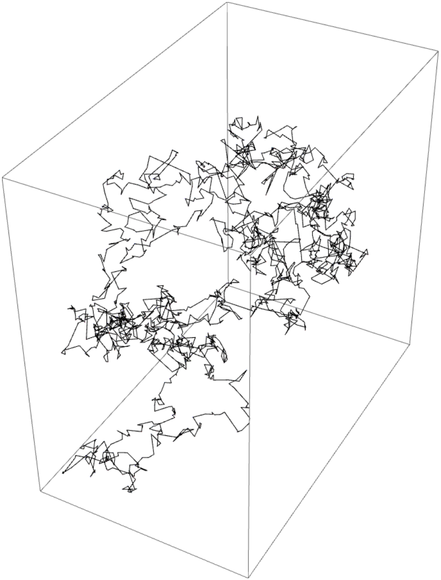
Examples of 2,000-gons



Examples of 2,000-gons



Examples of 2,000-gons



Expected Value of Radius of Gyration

Definition

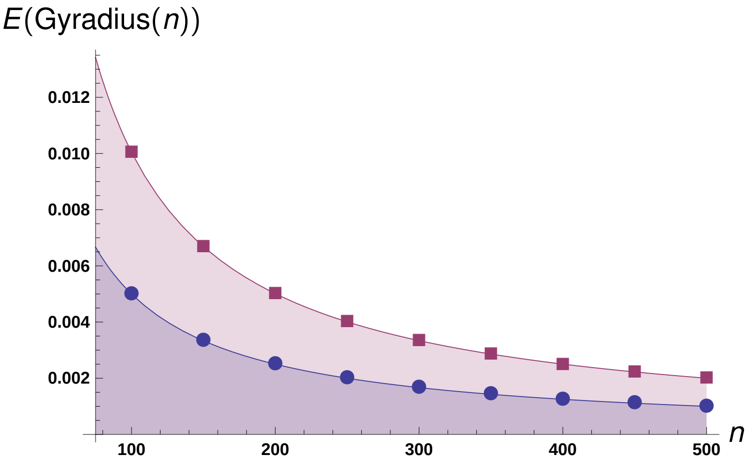
The squared radius of gyration $\operatorname{Gyradius}(P)$ is the average squared distance between any two vertices of P.

Theorem (with Cantarella and Deguchi)

The expected values of Gyradius *are*

$$E(\operatorname{Gyradius}, \operatorname{Arm}(n)) = \frac{n+2}{(n+1)(n+{}^1\!/\!_2)},$$
$$E(\operatorname{Gyradius}, \operatorname{Pol}(n)) = \frac{1}{2}\frac{1}{n},$$

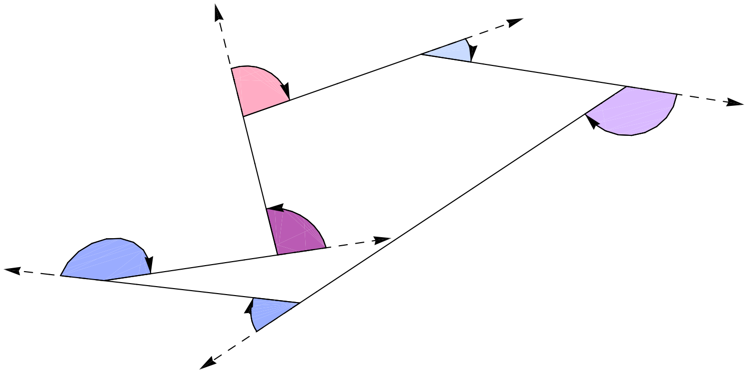
Checking Gyradius against Experiment



Pol(n) and Arm(n)

Definition

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



Lemma

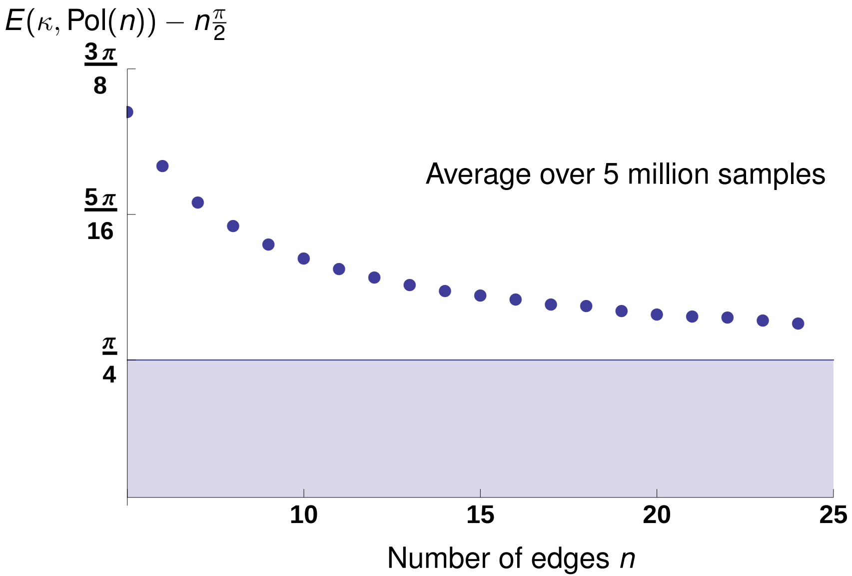
The expected total curvature of a polygon in $\mathrm{Arm}(n)$ *(or any* $\mathrm{Arm}(n;\vec{r})$*) is* $(n-1)\pi/2$*.*

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

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

> 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 on Pol(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:

Theorem (with Cantarella, Grosberg, Kusner)

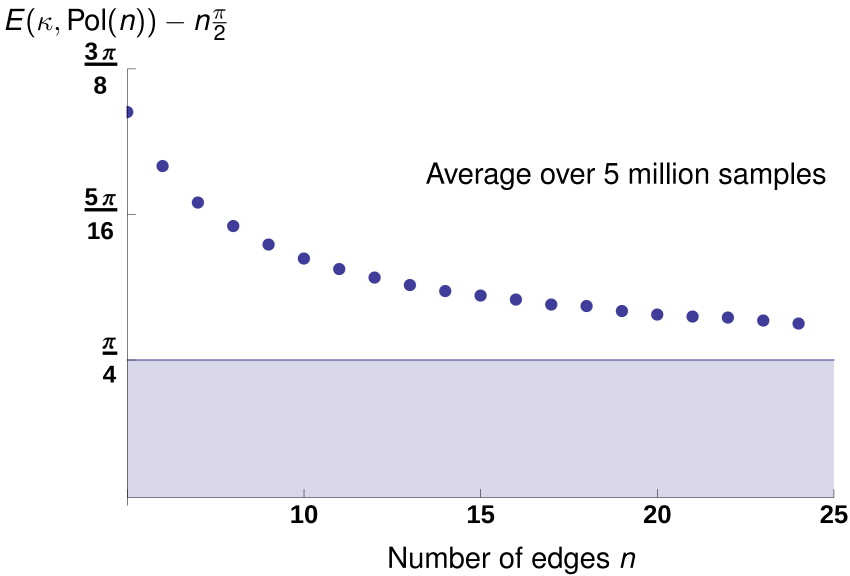
The expected value of the turning angle θ for a single pair of edges in $\mathrm{Pol}_3(n)$ is given by the formula

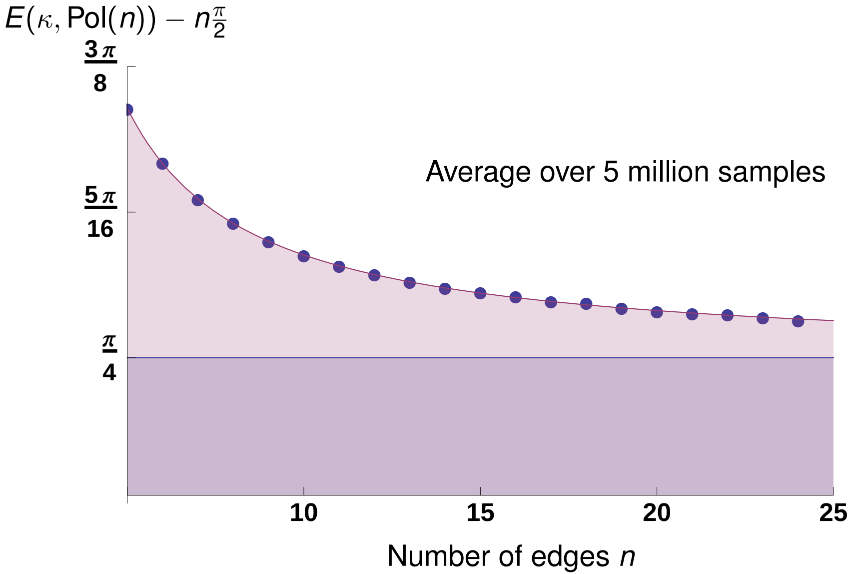
$$E(\theta) = \frac{\pi}{2} + \frac{\pi}{4}\frac{2}{2n-3}$$

so

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

Checking against the numerical data




$E(\kappa, \mathrm{Pol}(n)) - n\frac{\pi}{2}$
$\frac{3\pi}{8}$
$\frac{5\pi}{16}$
$\frac{\pi}{4}$
Average over 5 million samples
10
15
20
25
Number of edges n

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?

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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*.*

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Conjecture

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

Theorem (with Cantarella, Grosberg, Kusner)

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

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Proof.

Let x be the fraction of polygons in $\mathrm{Pol}(n)$ 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

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

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

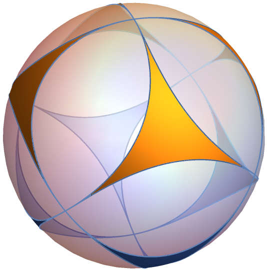
$$x < \frac{(n-2)(n-3)}{2(2n-3)}.$$

$\square$

Theorem (with Cantarella)

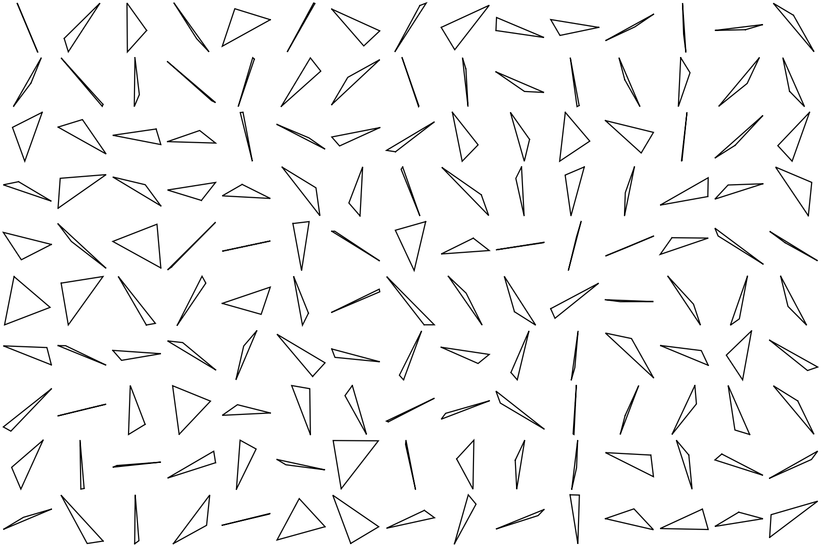
With respect to the symmetric measure on planar triangles, the fraction of acute triangles is exactly

$$\frac{\ln 8}{\pi} - \frac{1}{2} \simeq 0.161907$$



The acute triangles inside $G_2(\mathbb{R}^3)$.

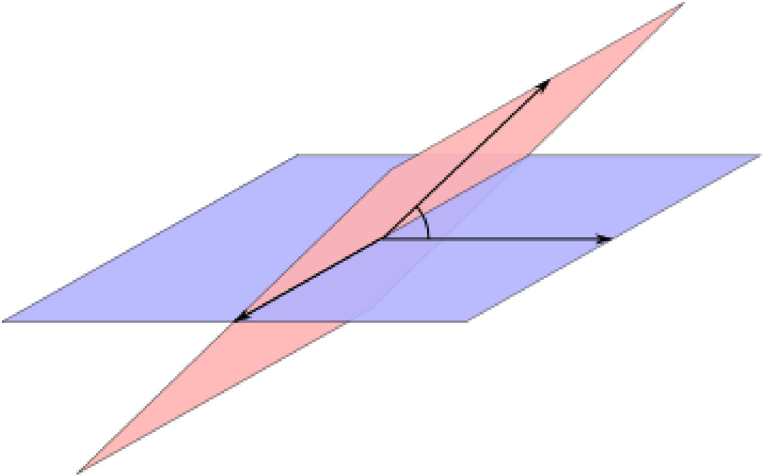
150 Random Triangles



The (Riemannian) Geometry of the Grassmannian

Question

How far apart are two points in $Gr_2(\mathbb{C}^n)$?



Jordan Angles and the Distance Between Planes

Theorem (Jordan)

Any two planes in $\mathbb{C}^n$ have a pair of orthonormal bases $\vec{v}_1, \vec{w}_1$ and $\vec{v}_2, \vec{w}_2$ so that

1. *$\vec{v}_2$ minimizes the angle between $\vec{v}_1$ and any vector on plane P_2. $\vec{w}_2$ minimizes the angle between the vector $\vec{w}_1$ perpendicular to $\vec{v}_1$ in P_1 and any vector in P_2.*
2. *(vice versa)*

*The angles between $\vec{v}_1$ and $\vec{v}_2$ and $\vec{w}_1$ and $\vec{w}_2$ are called the **Jordan angles** between the two planes. The rotation carrying $\vec{v}_1 \to \vec{v}_2$ and $\vec{w}_1 \to \vec{w}_2$ is called the **direct rotation** from P_1 to P_2 and it is the shortest path from P_1 to P_2 in the Grassmann manifold $Gr_2(\mathbb{C}^n)$.*

Theorem (Jordan)

- *Let Π_1 be the map $P_1 \to P_1$ given by orthogonal projection $P_1 \to P_2$ followed by orthogonal projection $P_2 \to P_1$. The basis $\vec{v}_1, \vec{w}_1$ is given by the eigenvectors of Π_1.*
- *Let Π_2 be the map $P_2 \to P_2$ given by orthogonal projection $P_2 \to P_1$ followed by orthogonal projection $P_1 \to P_2$. The basis $\vec{v}_2, \vec{w}_2$ is given by the eigenvectors of Π_2.*

Conclusion

The bases $\vec{v}_1, \vec{w}_1$ and $\vec{v}_2, \vec{w}_2$ give the rotations of polygons P_1 and P_2 that are closest to one another in the Stiefel manifold $V_2(\mathbb{C}^n)$. This is how we should align polygons.

- 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?

- Can this procedure be generalized to give sampling algorithms (and computations) for *confined* or *thick* polygons (this would be much more biologically realistic)?

A question you are uniquely suited to answer:

- What is the polygon interpretation of living on a Schubert variety in $G_2(\mathbb{R}^n)$ or $G_2(\mathbb{C}^n)$?

- *Probability Theory of Random Polygons from the Quaternionic Viewpoint*
  Jason Cantarella, Tetsuo Deguchi, and Clayton Shonkwiler
  Communications on Pure and Applied Mathematics **67** (2014), no. 10, 1658–1699.

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

Thank you!