The Geometric Structure of the Space of Stick Knots

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A Natural Question

What is the minimum number of sticks needed to build a 9_{47} knot in $\mathbb{R}^3$? In other words, what is the *stick number* of the 9_{47}?

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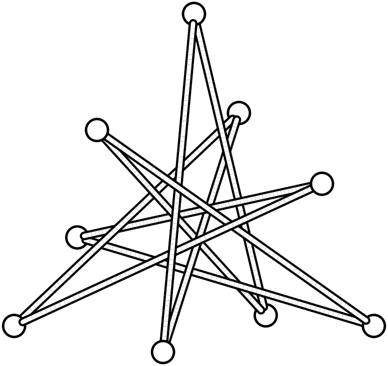
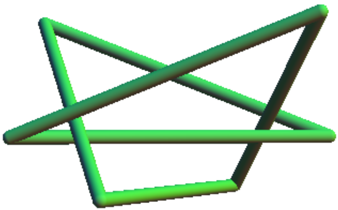


Answer: 9.

(Very Few) Facts About Stick Numbers



- [Calvo, Huh–Oh] $\frac{7+\sqrt{8c(K)+1}}{2} \leq s(K) \leq \frac{3(c(K)+1)}{2}$, where $c(K)$ is the crossing number of K.
- [Jin] $s(T_{p,q}) = 2q$ if $2 \leq p < q < 2p$.
- [Huh-No-Oh] $s(K) \leq c(K) + 2$ for 2-bridge knots with $c(K) \geq 6$.
- No known examples for which the equilateral stick number is different from the stick number, though Rawdon–Scharein conjecture this happens for 8_{19}, 9_{29}, $10_{16}, \ldots$

Point of Talk

It is in some ways easier to address the related questions:

- *Given n, what knot types is it possible to realize with n sticks?*
- *With what frequencies do the different knot types arise?*
- *More generally, what is the structure of the moduli space of n-stick knots?*

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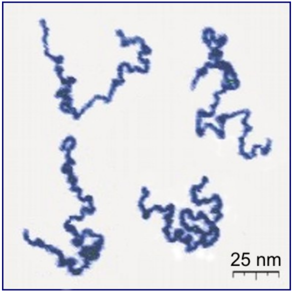
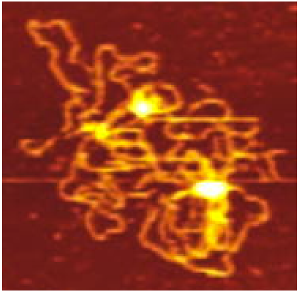
...but how big are these components?

Statistical Physics Point of View

A polymer in solution takes on an ensemble of random shapes, with topology (knot type!) as the unique conserved quantity.



Protonated P2VP
Roiter/Minko
Clarkson University



Plasmid DNA
Alonso-Sarduy, Dietler Lab
EPF Lausanne

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Physics Setup

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Our (geometers and topologists) job

Understand the probability that a closed random walk (a.k.a., random stick knot) is knotted and the distribution of knot types that result from different conditions on the walk (walk model, number of segments, confinement, self-avoidance, fixed bond angles, etc).

Theorem (Hausmann–Knutson)

The moduli space of all (non-equilateral) knots made from n sticks up to scaling, translation, and rotation is the base space of an (almost) torus bundle whose total space is $G_2(\mathbb{C}^n)$.

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In preparation for the (surprisingly simple) proof:

Notation

Let $\mathrm{Pol}(n)$ *be the space of n-stick knots (or n-edge closed polygons) of total perimeter 2 in* $\mathbb{R}^3$ *up to translation.*

Let $\mathrm{Arm}(n)$ *be the space of open n-edge polygonal arms of total perimeter 2 in* $\mathbb{R}^3$ *up to translation.*

Let $\mathbb{H}$ *be the space of quaternions.*

Definition

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Proposition (Hausmann-Knutson)

Applying Hopf *coordinatewise yields a map* $\mathrm{Hopf} : S^{4n-1}(\sqrt{2}) \subset \mathbb{H}^n \to \mathrm{Arm}_3(n)$. *The fibers are generically* $(S^1)^n$.

Recall that $\mathrm{Hopf}(a + b\mathbf{j}) = \mathbf{i}(|a|^2 - |b|^2 + 2a\bar{b}\mathbf{j})$ and write $\vec{q} \in \mathbb{H}^n$ as

$$\vec{q} = \vec{a} + \vec{b}\mathbf{j}.$$

Closure Conditions

Recall that $\mathrm{Hopf}(a + b\mathbf{j}) = \mathbf{i}(|a|^2 - |b|^2 + 2a\bar{b}\mathbf{j})$ and write $\vec{q} \in \mathbb{H}^n$ as

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Then $\mathrm{Hopf}(q)$ forms a closed polygon (a.k.a. stick knot) iff

$$\begin{aligned}\vec{0} = \sum \mathrm{Hopf}(q_\ell) &= \sum \mathbf{i}\left(|a_\ell|^2 - |b_\ell|^2 + 2a_\ell\bar{b}_\ell\mathbf{j}\right) \\ &= \mathbf{i}\left(\|\vec{a}\|^2 - \|\vec{b}\|^2 + 2\langle \vec{a}, \vec{b}\rangle\mathbf{j}\right) \\ &\Leftrightarrow \|\vec{a}\| = \|\vec{b}\| \text{ and } \langle \vec{a}, \vec{b}\rangle = 0.\end{aligned}$$

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\end{aligned}$$

Hence, $\mathrm{Hopf}^{-1}(\mathrm{Pol}(n)) = V_2(\mathbb{C}^n) \subset \mathbb{H}^n$, the Stiefel manifold of orthonormal 2-frames in $\mathbb{C}^n$.

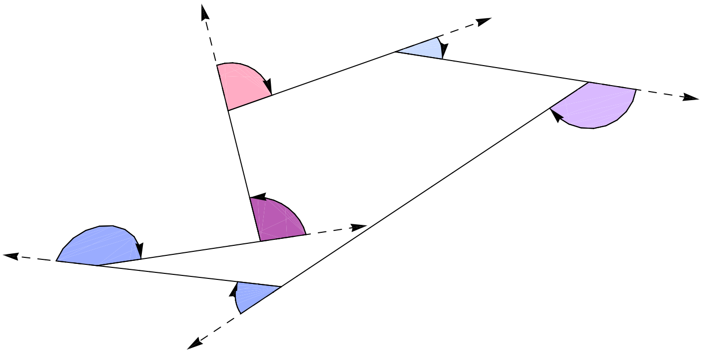
$$
\begin{tikzcd}
U(2) \arrow[r] \arrow[d] & V_2(\mathbb{C}^n) \subset \mathbb{H}^n \arrow[r, two heads] \arrow[d, "\text{Hopf}"'] & G_2(\mathbb{C}^n) \arrow[d] \\
SO(3) \arrow[r] & \mathrm{Pol}(n) \arrow[r, two heads] & \mathrm{Pol}(n)/SO(3) = \widehat{\mathrm{Pol}}(n)
\end{tikzcd}
$$

Theorem (with Cantarella and Deguchi)

The volume form of the standard Riemannian metric on $G_2(\mathbb{C}^n)$ *defines the natural probability measure on n-stick knots of total length 2 up to translation and rotation. It has a (transitive) action by isometries given by the action of* $U(n)$ *on* $G_2(\mathbb{C}^n)$*.*

Definition

The total curvature of a stick knot is the sum of its turning angles.



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The expected total curvature of an n-stick knot of length 2 sampled according to the measure on $G_2(\mathbb{C}^n)$ *is*

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Proof.

Since the expected total curvature of 6- and 7-stick knots is $< 4\pi$, this follows from a direct application of Fáry–Milnor. $\square$

Theoretical results are challenging, but we can supplement with experiments. How?

Proposition (classical?)

The natural measure on $G_2(\mathbb{C}^n)$ is obtained by generating two random complex n-vectors with independent Gaussian coordinates and their span.

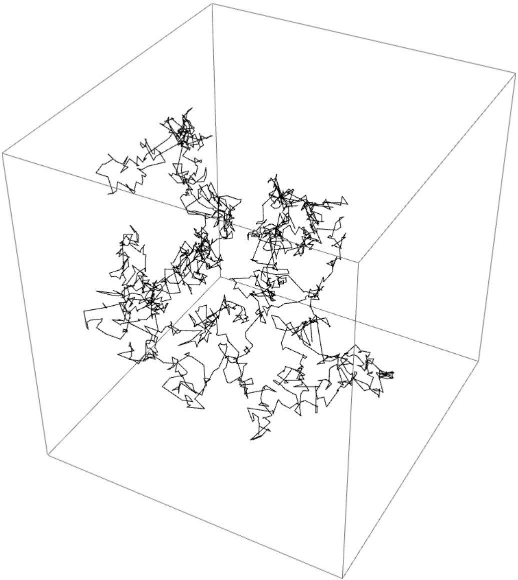
```
In[9]:= RandomComplexVector[n_] := Apply[Complex,
            Partition[#, 2] & /@ RandomVariate[NormalDistribution[], {1, 2 n}], {2}][[1]];

        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}
         ];
```

Using this, we can generate ensembles of random n-stick knots and distributions of knot types . . .

Random 2,000-gons



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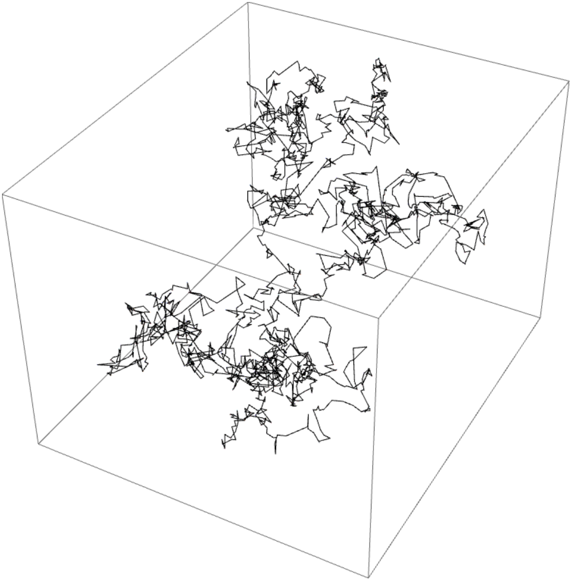

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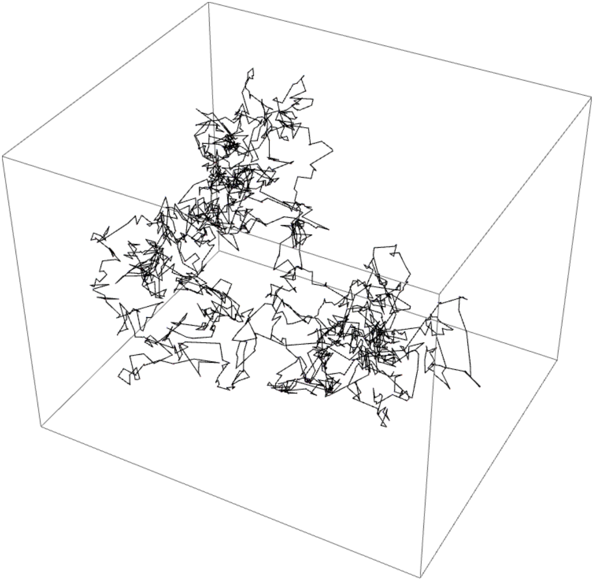

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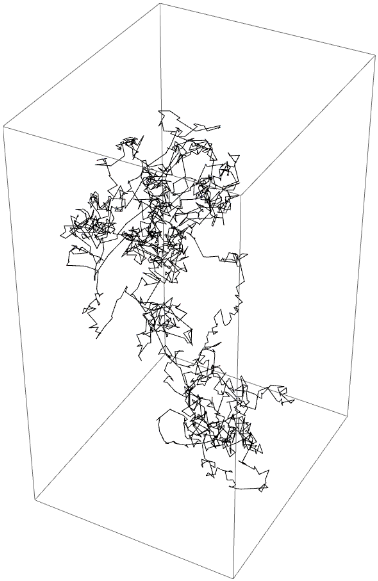

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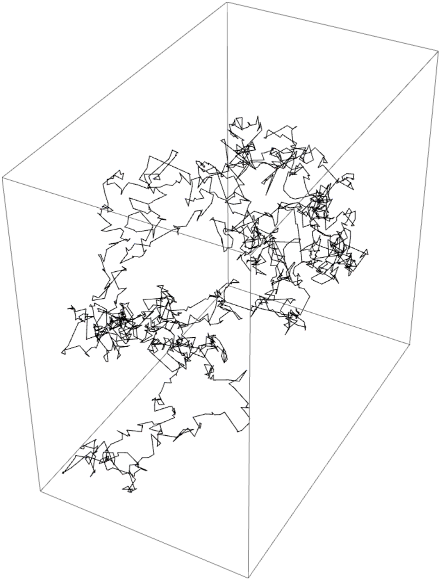

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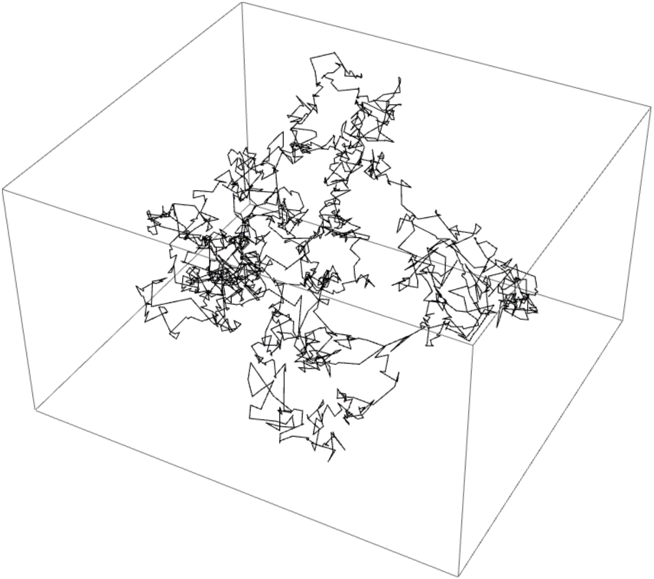

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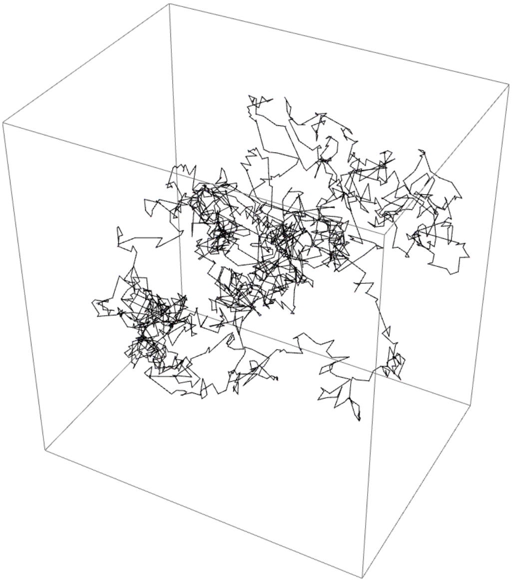

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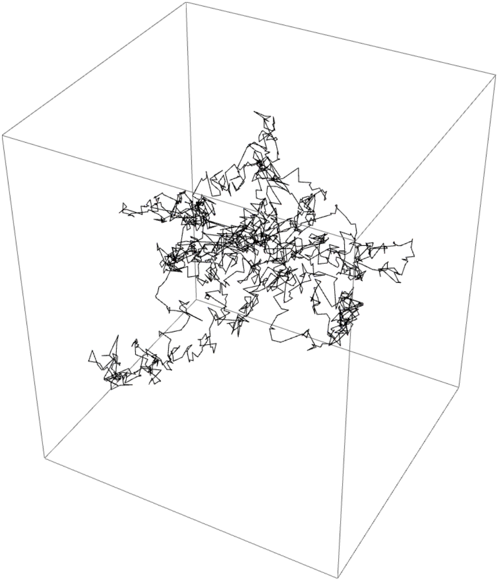

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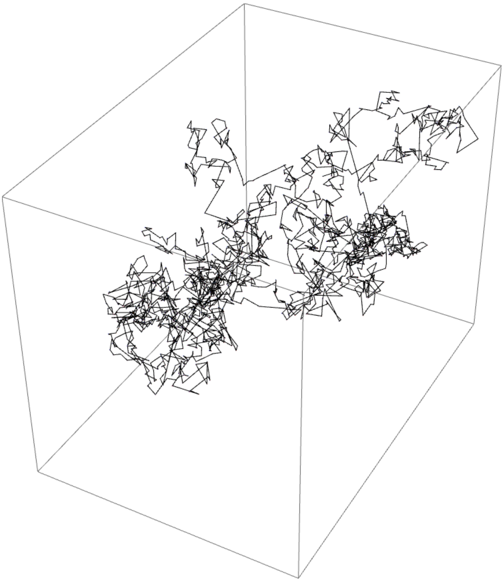

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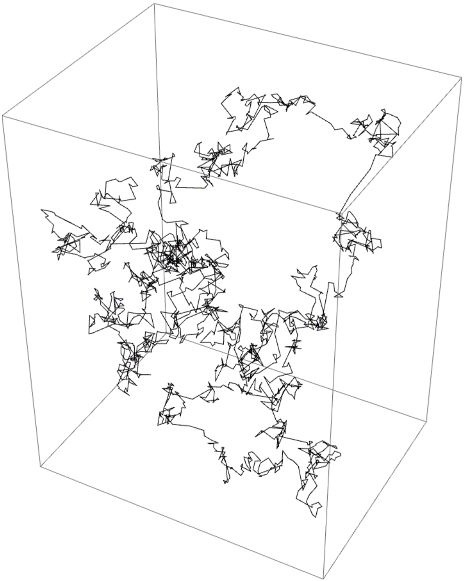

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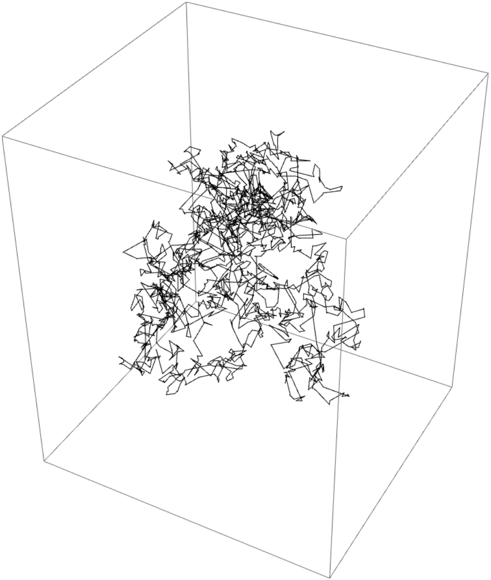

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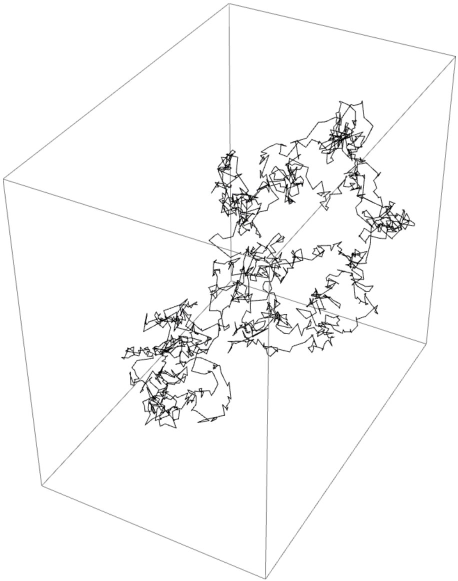

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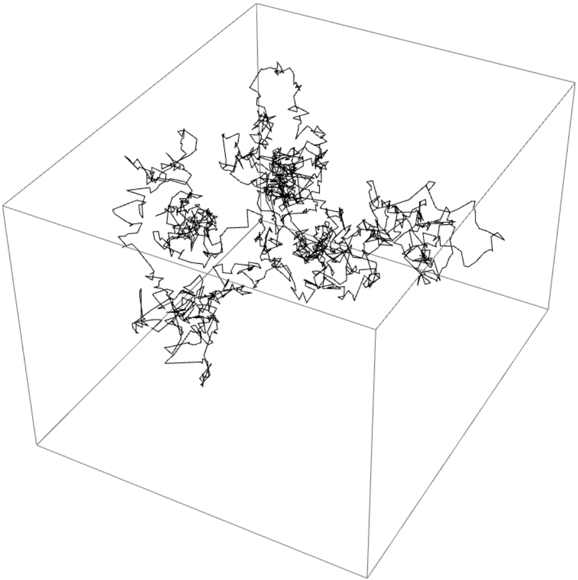

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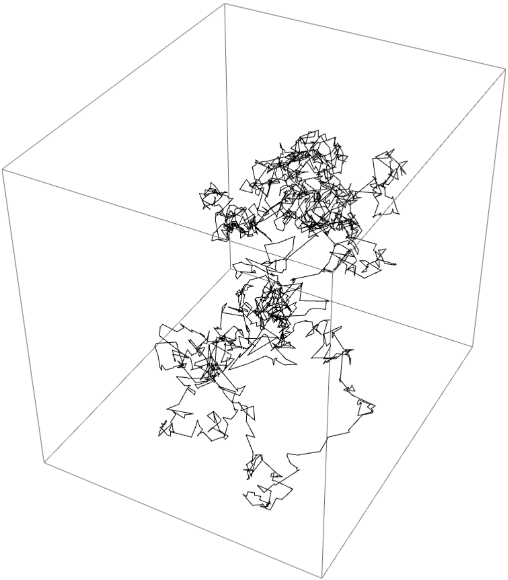

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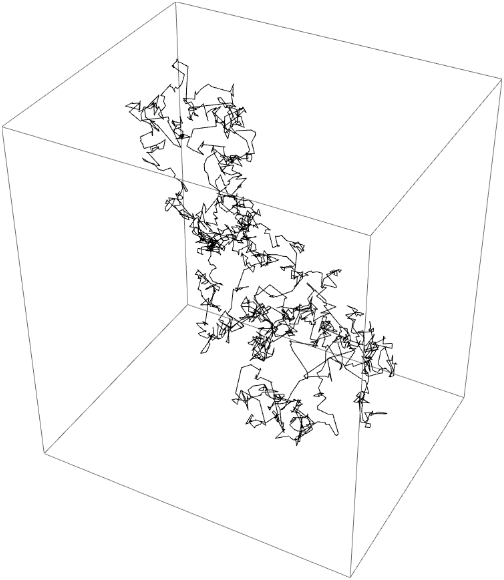

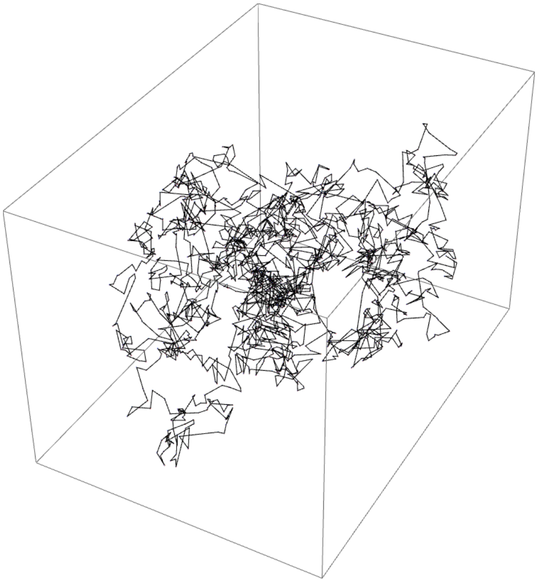

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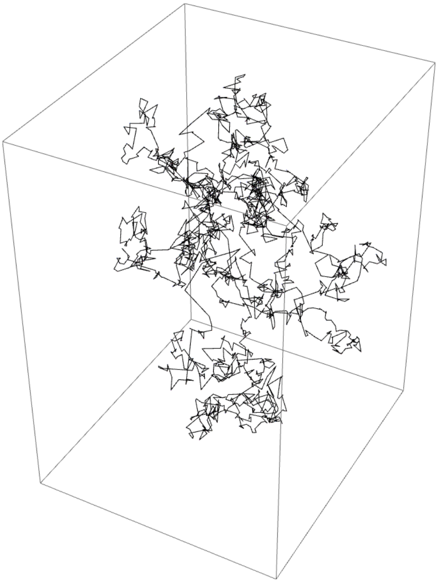

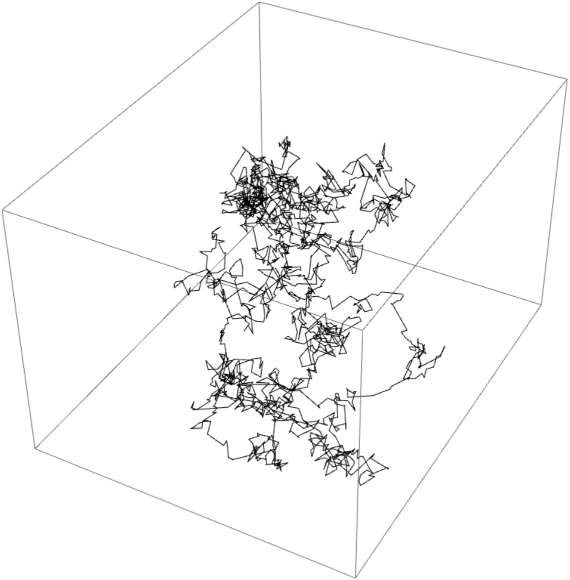

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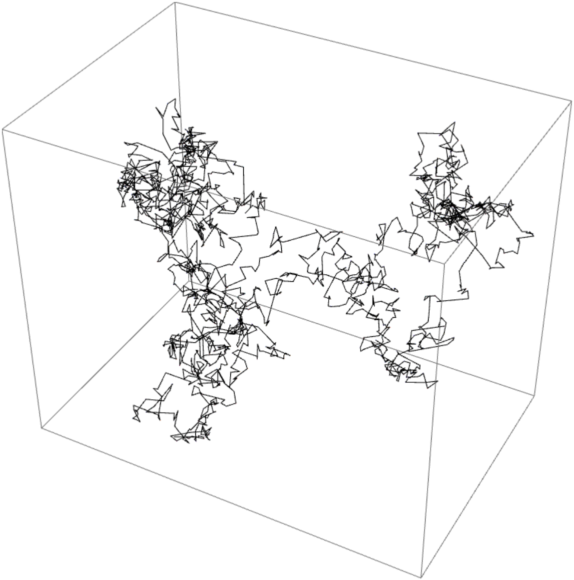

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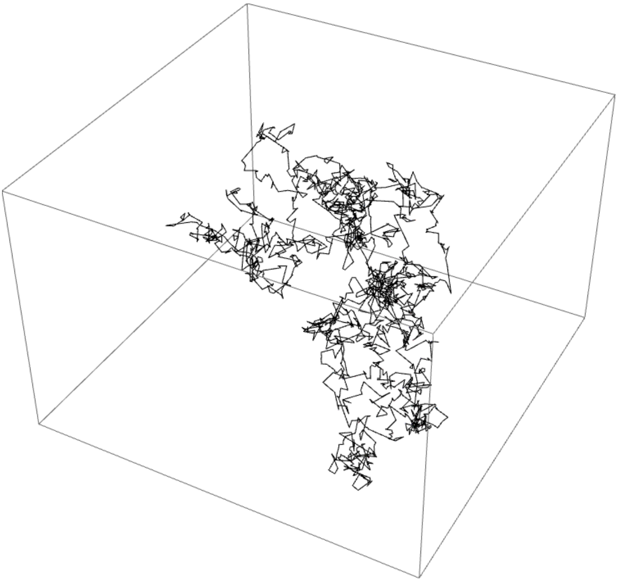

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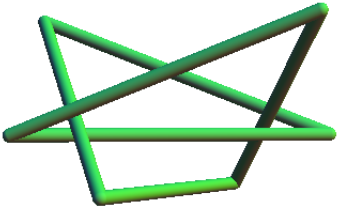
The moduli space of *equilateral* n-edge polygonal arms up to translation is just $\underbrace{S^2(1) \times \ldots \times S^2(1)}_{n}$.

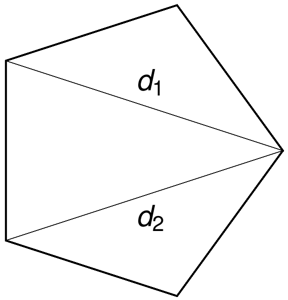
Let ePol(n) be the submanifold of equilateral n-stick knots; i.e., those elements of $(S^2)^n$ which satisfy

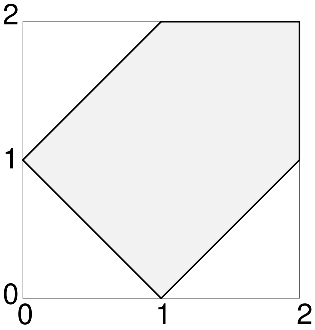
$$\sum_{i=1}^{n} \vec{e}_i = \vec{0}.$$



Definition

An abstract triangulation T of the n-gon picks out $n-3$ nonintersecting chords. The lengths of these chords obey triangle inequalities, so they lie in a convex polytope in $\mathbb{R}^{n-3}$ called the *triangulation polytope* $\mathcal{P}_n$.





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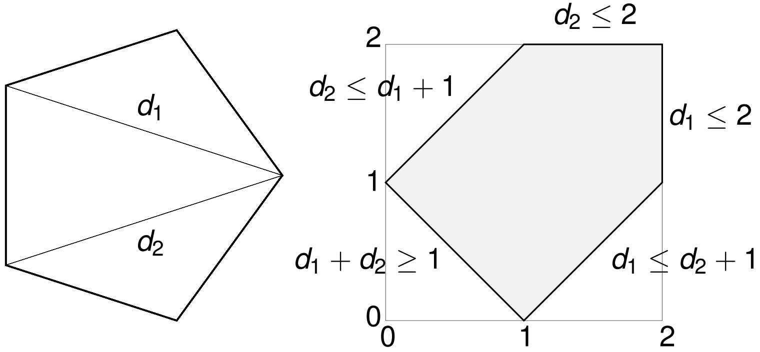

The Triangulation Polytope

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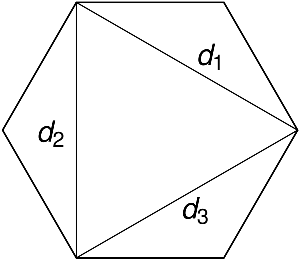
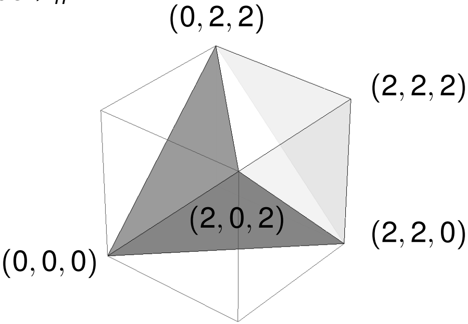
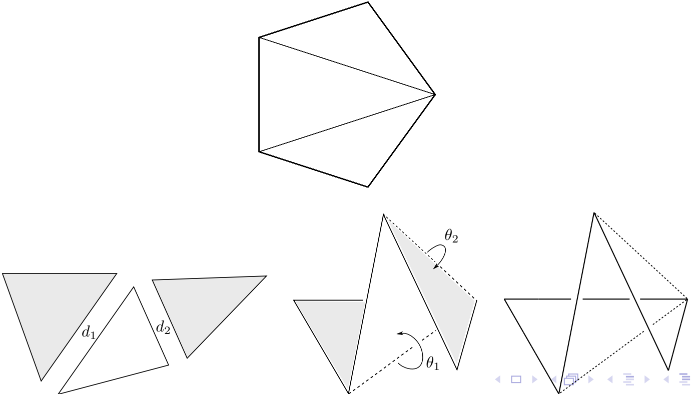




Definition

If $\mathcal{P}_n$ is the triangulation polytope and $T^{n-3} = (S^1)^{n-3}$ is the torus of $n-3$ dihedral angles, then there are *action-angle coordinates*:

$$\alpha\colon\ \mathcal{P}_n \times T^{n-3} \to \mathrm{Pol}(n)/\,\mathrm{SO}(3)$$



Theorem (with Cantarella)

*α pushes the **standard probability measure** on $\mathcal{P}_n \times T^{n-3}$ forward to the **correct probability measure** on $\operatorname{ePol}(n)/\operatorname{SO}(3)$.*

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Ingredients of the Proof.

Kapovich–Millson toric symplectic structure on polygon space + Duistermaat–Heckman theorem + Hitchin's theorem on compatibility of Riemannian and symplectic volume on symplectic reductions of Kähler manifolds + Howard–Manon–Millson analysis of polygon space. $\square$

Corollary (with Cantarella)

At least $^1/_2$ *of the space of equilateral 6-stick knots consists of unknots.*

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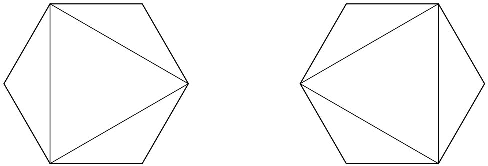
At least $1/2$ of the space of equilateral 6-stick knots consists of unknots.

Proof.

Translating a theorem of Calvo to action-angle coordinates, the dihedral angles $\theta_1, \theta_2, \theta_3$ in at least one of the following triangulations of a nontrivial 6-stick knot must satisfy either $\theta_i \in [0, \pi]$ for all *i* or $\theta_i \in [\pi, 2\pi]$ for all *i*.



□

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Algorithm (with Cantarella)

A Markov chain which converges to the correct measure on $\mathrm{ePol}(n)/\mathrm{SO}(3)$*. Steps in the chain are generated in* $O(n^2)$ *time. This generalizes to other fixed edgelength polygon spaces as well as to polygons in various confinement regimes.*

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Algorithm (with Cantarella and Uehara)

An unbiased sampling algorithm which generates a uniform point on $\mathrm{ePol}(n)/\mathrm{SO}(3)$ *in* $O(n^3)$ *time.*

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How can we be so sure?

Algorithm (with Cantarella)

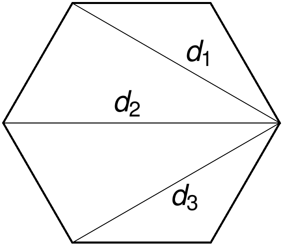
A Markov chain which converges to the correct measure on $\mathrm{ePol}(n)/\mathrm{SO}(3)$. *Steps in the chain are generated in* $O(n^2)$ *time. This generalizes to other fixed edgelength polygon spaces as well as to polygons in various confinement regimes.*

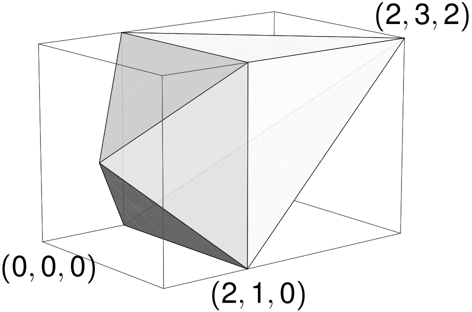
Algorithm (with Cantarella and Uehara)

An unbiased sampling algorithm which generates a uniform point on $\mathrm{ePol}(n)/\mathrm{SO}(3)$ *in* $O(n^3)$ *time.*

The hard part is sampling the convex polytope $\mathcal{P}_n$.

The Fan Triangulation Polytope





The polytope $\mathcal{F}_n$ corresponding to the “fan triangulation” is defined by the triangle inequalities:

$$0 \leq d_1 \leq 2 \qquad \begin{array}{c} 1 \leq d_i + d_{i+1} \\ |d_i - d_{i+1}| \leq 1 \end{array} \qquad 0 \leq d_{n-3} \leq 2$$

If we introduce a fake chordlength $d_0 = 1$, and make the linear transformation

$$s_i = d_i - d_{i+1}, \text{ for } 0 \le i \le n-4, \quad s_{n-3} = d_{n-3} - d_0$$

then our inequalities

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become

$$\underbrace{-1 \le s_i \le 1, \quad \sum s_i = 0,}_{|d_i - d_{i+1}| \le 1} \quad \underbrace{2\sum_{j=0}^{i-1} s_j + s_i \le 1}_{d_i + d_{i+1} \ge 1}$$

A change of coordinates

If we introduce a fake chordlength $d_0 = 1$, and make the linear transformation

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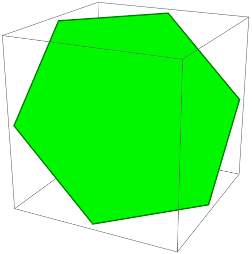
become

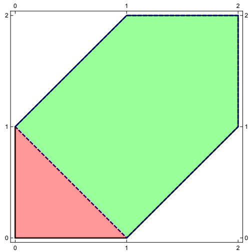
$$\underbrace{-1 \le s_i \le 1, \quad \sum s_i = 0,}_{\text{easy conditions}} \quad \underbrace{2\sum_{j=0}^{i-1} s_j + s_i \le 1}_{\text{hard conditions}}$$

Definition

The n-dimensional cross-polytope $\mathcal{C}_n$ is the slice of the hypercube $[-1, 1]^{n+1}$ by the plane $x_1 + \cdots + x_{n+1} = 0$.



$\rightarrow$



Idea

Sample points in the cross polytope, which all obey the "easy conditions", and reject any samples which fail to obey the "hard conditions".

Theorem (Marichal-Mossinghoff)

The volume of the projection of the $(n-3)$-dimensional cross-polytope $\mathcal{C}_{n-3}$ is

$$\frac{\sum_{j=0}^{\lfloor \frac{n-2}{2} \rfloor} (-1)^j (n-2j-2)^{n-3} \binom{n-2}{j}}{(n-3)!}$$

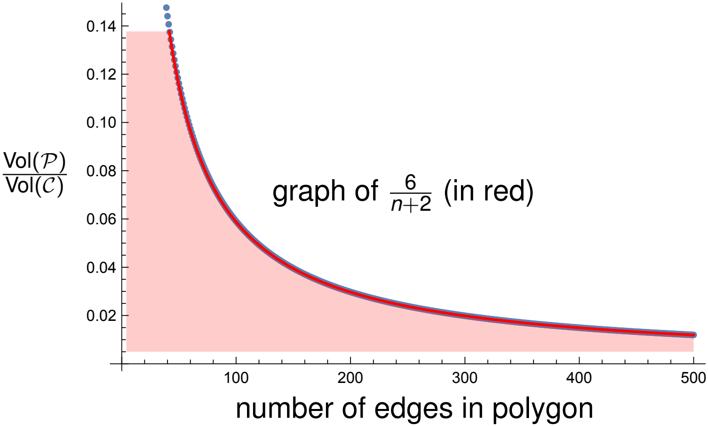
Theorem (Khoi, Takakura, Mandini)

The volume of the $(n-3)$-dimensional fan triangulation polytope for n-edge equilateral polygons $\mathcal{F}_n$ is

$$-\frac{\sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^j (n-2j)^{n-3} \binom{n}{j}}{2(n-3)!}$$

Runtime of algorithm depends on acceptance ratio

Acceptance ratio $= \frac{\mathrm{Vol}(\mathcal{F}_n)}{\mathrm{Vol}(\mathcal{C}_{n-3})}$ is conjectured $\sim \frac{6}{n+2}$. It is certainly bounded below by $\frac{1}{n}$.



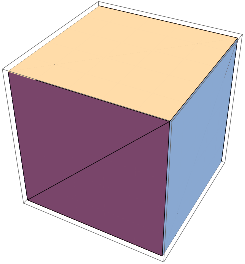
Sampling the Cross Polytope

Definition

The hypersimplex $\Delta_{k,n}$ is the slab of the cube $[0,1]^{n-1}$ with $k-1 \leq \sum_{i=1}^{n-1} x_i \leq k$.

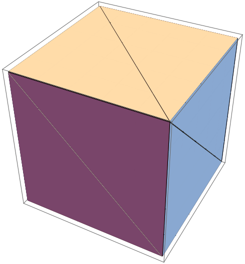
Theorem (Stanley)

There is a unimodular triangulation[1] *of* $\Delta_{k,n}$ *in* $[0,1]^{n-1}$ *indexed by permutations of* $(1,\ldots,n-1)$ *with* $k-1$ *descents.*



Standard triangulation

$\xrightarrow{\psi^{-1}}$



Stanley triangulation

[1] a decomposition into disjoint simplices of equal volume

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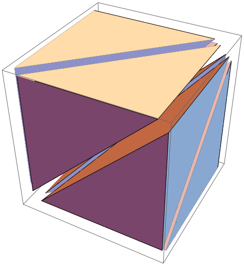

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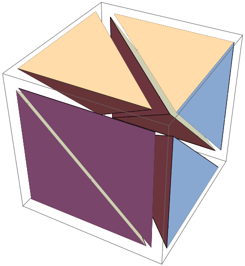

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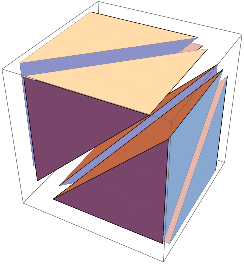

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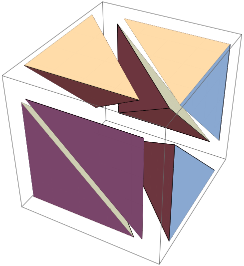

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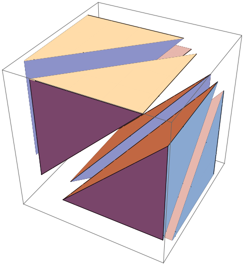

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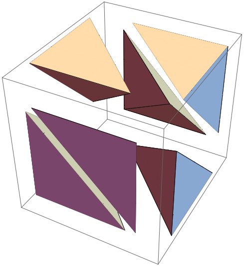

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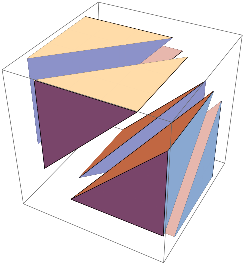

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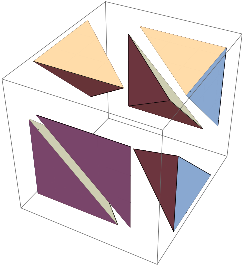

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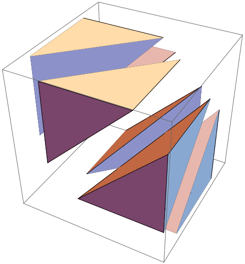

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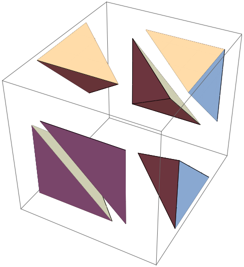

Standard triangulation

Stanley triangulation

[1] a decomposition into disjoint simplices of equal volume

Recall that we're interested in the cross polytope determined by

$$s_0 + s_1 + \ldots + s_{n-3} = 0$$

in the cube $[-1, 1]^{n-2}$. After translation, scaling, and dropping the last coordinate, this corresponds to the slab

$$\frac{n-2}{2} - 1 \leq x_0 + x_1 + \ldots + x_{n-3} \leq \frac{n-2}{2}$$

in the cube $[0, 1]^{n-3}$.

For even n this is just the hypersimplex $\Delta_{(n-2)/2, n-2}$ and Stanley's triangulation applies.

For odd n this is covered by the union $\Delta_{\frac{n-2}{2}-\frac{1}{2}, n-2} \cup \Delta_{\frac{n-2}{2}+\frac{1}{2}, n-2}$, which we can rejection sample.

Moment Polytope Sampling Algorithm (with Cantarella and Uehara, 2015)

1. *Generate a permutation of* $n-3$ *numbers with* $n/2-2$ *descents.* $\boxed{O(n^2)\ \textit{time}}$.
2. *Generate a point in the corresponding simplex of the Stanley triangulation for* $\Delta_{(n-2)/2,n-2}$.
3. *Project up to the cross polytope in* $[0,1]^{n-2}$*, over to the cross polytope in* $[-1,1]^{n-2}$ *and down to a set of diagonals.*
4. *Test the proposed set of diagonals against the "hard" conditions.* $\boxed{\textit{acceptance ratio} > 1/n}$
5. *Generate dihedral angles from* T^{n-3}.
6. *Build sample polygon in action-angle coordinates.*

- Enriched sampling for low stick numbers from tightly confined knots.
- Other topological constraints on random walks (e.g., specify a graph).
- Compare distributions of knot types obtained by different models for random knots. Is there evidence for universal properties of random knot distributions?
- Stronger theoretical bounds on knot probabilities, average knot invariants, etc.
- Generalize to moduli spaces of other piecewise-linear submanifolds (polyhedral surfaces, planar polygons, . . .).

Thank you!

Thank you for listening!

Supported by:

Simons Foundation   NSF DMS–1105699

- *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, 658–1699.
- *The Expected Total Curvature of Random Polygons*
  Jason Cantarella, Alexander Y Grosberg, Robert Kusner, and Clayton Shonkwiler
  American Journal of Mathematics **137** (2015), no. 2, 411–438
- *The Symplectic Geometry of Closed Equilateral Random Walks in 3-Space*
  Jason Cantarella and Clayton Shonkwiler
  Annals of Applied Probability, to appear.

`http://arxiv.org/a/shonkwiler_c_1`

Recall the volumes of the cross polytope and moment polytope:

$$\mathrm{Vol}(\mathcal{C}_{n-3}) = \frac{\sum_{j=0}^{\left\lfloor \frac{n-2}{2} \right\rfloor} (-1)^j (n-2j-2)^{n-3} \binom{n-2}{j}}{(n-3)!}$$

$$\mathrm{Vol}(\mathcal{F}_n) = -\frac{\sum_{j=0}^{\left\lfloor \frac{n}{2} \right\rfloor} (-1)^j (n-2j)^{n-3} \binom{n}{j}}{2(n-3)!}$$

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$$= \frac{2^{n-3}}{(n-3)!} \left\langle {n-3 \atop n/2-2} \right\rangle,$$

where $\left\langle {m \atop k} \right\rangle$ is the Eulerian number which gives the number of permutations of $\{1, \ldots, m\}$ with exactly k descents. The Eulerian numbers satisfy the recurrence relation

$$\left\langle {m \atop k} \right\rangle = (k+1) \left\langle {m-1 \atop k} \right\rangle + (m-k) \left\langle {m-1 \atop k-1} \right\rangle$$

Eulerian Numbers

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$\left\langle {m \atop k} \right\rangle$	k								
	1								
	1	1							
	1	4	1						
	1	11	11	1					
m	1	26	66	26	1				
	1	57	302	302	57	1			
	1	120	1191	2416	1191	120	1		
	1	247	4293	15619	15619	4293	247	1	
	1	502	14608	88234	156190	88234	14608	502	1

Recall the volumes of the cross polytope and moment polytope:

$$\mathrm{Vol}(\mathcal{C}_{n-3}) = \frac{\sum_{j=0}^{\left\lfloor \frac{n-2}{2} \right\rfloor} (-1)^j (n-2j-2)^{n-3} \binom{n-2}{j}}{(n-3)!}$$

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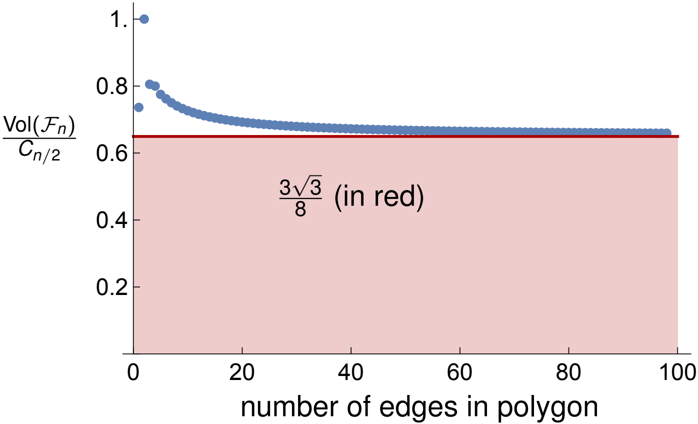
$$\mathrm{Vol}(\mathcal{F}_n) = -\frac{\sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^j (n-2j)^{n-3} \binom{n}{j}}{2(n-3)!}$$

$$\underset{\text{conj.}}{\simeq} \frac{3\sqrt{3}}{8} C_{n/2}$$

where C_m is the mth Catalan number

$$C_m = \frac{1}{m+1}\binom{2m}{m} = \frac{\Gamma(2m+1)}{\Gamma(m+2)\Gamma(m+1)}.$$

The ratio of $\mathrm{Vol}(\mathcal{F}_n)$ to $C_{n/2}$:



The normalized volume $(n-3)!\,\mathrm{Vol}(\mathcal{F}_n)$ of the moment polytope is the $k=1$ case of a two-parameter family $V(n,k)$ given by the recurrence relation

$$V(n,k) = (n-k-1)\,V(n-1,k-1) + (n+k-1)\,V(n-1,k+1)$$

subject to the boundary conditions

$$V(n,0)=0, \qquad V(3,1)=1, \qquad V(3,2)=\frac{1}{2}.$$

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0	1	$\frac{1}{2}$
0		
0		
0		
0		
0		
0		
0		

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0	1	$\frac{1}{2}$						
0	2	1						
0	5	4	1					
0	24	22	8	1				
0	154	160	75	16	1			
0	1280	1445	800	236	32	1		
0	13005	15680	9821	3584	721	64	1	
0	156800	199066	137088	58478	15232	2178	128	1

cf. OEIS A012249 “Volume of a certain rational polytope…”

Conjecture

$$\mathrm{Vol}(\mathcal{F}_n) \simeq \frac{3\sqrt{3}}{8} C_{n/2}.$$

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$$\mathrm{Vol}(\mathcal{F}_n) \simeq \frac{3\sqrt{3}}{8} C_{n/2}.$$

Combining the conjecture with $\mathrm{Vol}(\mathcal{C}_{n-3}) = \frac{2^{n-3}}{(n-3)!} \left\langle {n-3 \atop n/2-2} \right\rangle$, Stirling's approximation, and

Theorem (Giladi–Keller '94)

$$\left\langle {n-3 \atop n/2-2} \right\rangle \simeq \sqrt{\frac{6}{\pi(n-2)}}\,(n-3)!$$

would suffice to prove

$$\frac{\mathrm{Vol}(\mathcal{F}_n)}{\mathrm{Vol}(\mathcal{C}_{n-3})} \simeq \frac{6\sqrt{n-2}}{n^{3/2}}.$$

$\frac{6\sqrt{n-2}}{n^{3/2}}$ and $\frac{6}{n+2}$ are basically indistinguishable as asymptotic estimates for $\frac{\mathrm{Vol}(\mathcal{F}_n)}{\mathrm{Vol}(\mathcal{C}_{n-3})}$: