Introduction II: The Symplectic Geometry of Polygon Space and How to Use It

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In his talk, Jason described a model for closed, relatively framed polygons in $\mathbb{R}^3$ of total length 2 based on the Grassmannian $G_2(\mathbb{C}^n)$. How to specialize to unframed polygons with fixed edgelengths (for example, equilateral polygons)? $G_2(\mathbb{C}^n)$ is an assembly of fixed edge length spaces.
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How to specialize to unframed polygons with fixed edgelengths (for example, equilateral polygons)?

(one edge of length 1 $\implies$ volume = 0)

$G_2(\mathbb{C}^n)$ is an assembly of fixed edge length spaces

(equilaterals are largest volume)
Random Polygons and Ring Polymers

Statistical Physics Point of View

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

Knotted DNA
Wassermann et al.
*Science* 229, 171–174

DNA Minicircle simulation
Harris Lab
University of Leeds, UK

The basic paradigm is to model these by standard random walks conditioned on closure; i.e., equilateral random polygons.
Three main goals for this talk:

1. Describe how the moduli spaces of fixed edgelength polygons connects with the Grassmannian story.

2. Use symplectic geometry to find nice coordinates on equilateral polygon space.

3. Give a direct sampling algorithm which generates a random equilateral $n$-gon in $O(n^{5/2})$ time.
The Edgelength Map

We can define the *edgelength map* \( \mathcal{E} : G_2(\mathbb{C}^n) \to \Delta_{n,2} \) from the Grassmannian to the second hypersimplex

\[
\Delta_{n,2} = \left\{ (r_1, \ldots, r_n) \in [0, 1]^n : \sum r_i = 2 \right\}.
\]
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\]

Specifically, if we represent elements of \( G_2(\mathbb{C}^n) \) by \( n \times 2 \) complex matrices where the columns give an orthonormal basis for the 2-plane, then:

\[
\mathcal{E} : \begin{pmatrix} a_1 & b_1 \\ a_2 & b_2 \\ \vdots & \vdots \\ a_n & b_n \end{pmatrix} \mapsto \begin{pmatrix} |a_1|^2 + |b_1|^2 \\ |a_2|^2 + |b_2|^2 \\ \vdots \\ |a_n|^2 + |b_n|^2 \end{pmatrix}
\]
For any point $\vec{r} = (r_1, \ldots, r_n) \in \Delta_{n,2}$, the space of framed $n$-gons in $\mathbb{R}^3$ with edgelengths $r_1, \ldots, r_n$ up to translation and rotation is the inverse image

$$\mathcal{E}^{-1}(\vec{r}) \subset G_2(\mathbb{C}^n).$$
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\[ E^{-1}(\vec{r}) \subset G_2(\mathbb{C}^n). \]

If we want unframed polygons with fixed edgelengths, we should divide \( E^{-1}(\vec{r}) \) by the \( U(1)^n \) which spins the individual edge frames:

\[ \widehat{\text{Pol}}(n; \vec{r}) = E^{-1}(\vec{r})/U(1)^n. \]
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In fact, the diagonal subgroup $D \subset U(1)^n$ has no effect on relatively framed polygons, so we should really divide by the effective action of $U(1)^n/D \simeq U(1)^{n-1}$. 

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In fact, the diagonal subgroup $\mathcal{D} \subset U(1)^n$ has no effect on relatively framed polygons, so we should really divide by the effective action of $U(1)^n/\mathcal{D} \simeq U(1)^{n-1}$.
$G_2(\mathbb{C}^n)$

$\mathcal{E}^{-1}(\vec{r})$

$\left\lfloor U(1)^{n-1} \right\rfloor \rightarrow \text{Pol}(n; \vec{r})$
\( \mathbb{C}^2 \) \( n \) \( \mathbb{C}^n \) 

\( V_2(\mathbb{C}^n) \)/\( U(2) \) 

\( G_2(\mathbb{C}^n) \) 

\( \mathcal{E}^{-1}(\vec{r}) \)/\( U(1)^{n-1} \) \( \widehat{\text{Pol}}(n; \vec{r}) \)
\[(\mathbb{C}^2)^n \supseteq G_2(\mathbb{C}^n) \]

\[\mathcal{E}^{-1}(\vec{r}) = \prod S^3(r_i)\]

\[\mathcal{E}^{-1}(\vec{r}) \supseteq \text{Pol}(n; \vec{r})\]

\[G_2(\mathbb{C}^n) \lor U(2)\]

\[\text{Pol}(n; \vec{r}) \lor U(1)^n\]

\[\prod S^2(r_i)\]

\[\text{Pol}(n; \vec{r}) \lor \text{SO}(3)\]

\[\langle \rangle \lor \text{Pol}(n; \vec{r})\]
The Big Symplectic Picture

\[ \mathbb{C}^2 \times \mathbb{C}^n / / \mathbb{R} \mathbb{U}(1)^n \]

\[ G_2(\mathbb{C}^n) \]

\[ \mathbb{C}^2 \times \mathbb{C}^n / / \mathbb{R} \mathbb{U}(2) \]

\[ \mathbb{R} \mathbb{U}(1)^n \]

\[ \mathbb{R} \mathbb{U}(1)^n - 1 \]

\[ \mathbb{R} \mathbb{SO}(3) \]

\[ \Pi S^2(r_i) \]

\[ \mathbb{Sph}(n; \vec{r}) \]
A symplectic manifold \((M, \omega)\) is a smooth \(2n\)-dimensional manifold \(M\) with a closed, non-degenerate 2-form \(\omega\) called the \textit{symplectic form}. The \(n\)th power of this form \(\omega^n = \omega \wedge \ldots \wedge \omega\) is a volume form on \(M\).
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The circle \(U(1)\) \textit{acts by symplectomorphisms} on \(M\) if the action preserves \(\omega\). A circle action generates a vector field \(X\) on \(M\). We can contract the vector field \(X\) with \(\omega\) to generate a one-form:

\[
\iota_X \omega (\vec{v}) = \omega (X, \vec{v})
\]

If \(\iota_X \omega\) is exact, meaning it is \(dH\) for some smooth function \(H\) on \(M\), the action is called \textit{Hamiltonian}. The function \(H\) is called the \textit{momentum} associated to the action, or the \textit{moment map}.
A torus $T^k = U(1)^k$ which acts by symplectomorphisms on $M$ so that each circle action is Hamiltonian induces a moment map $\mu : M \to \mathbb{R}^k$ where the action preserves the fibers (inverse images of points).

**Theorem (Atiyah, Guillemin–Sternberg, 1982)**

The image of $\mu$ is a convex polytope in $\mathbb{R}^k$ called the moment polytope.

**Theorem (Duistermaat–Heckman, 1982)**

The pushforward of the symplectic measure to the moment polytope is piecewise polynomial. If $k = n = \frac{1}{2} \dim(M)$, then the manifold is called a toric symplectic manifold and the pushforward measure is Lebesgue measure on the polytope.
Let \((M, \omega)\) be the 2-sphere with the standard area form. Let \(U(1)\) act by rotation around the \(z\)-axis. Then the moment polytope is the interval \([-1, 1]\), and \(S^2\) is a toric symplectic manifold.

**Theorem (Archimedes, Duistermaat–Heckman)**

*The pushforward of the standard measure on the sphere to the interval is \(2\pi\) times Lebesgue measure.*

Illustration by Kuperberg.
Action-Angle Coordinates are Cylindrical Coordinates

\[(z, \theta) \rightarrow (\sqrt{1 - z^2} \cos \theta, \sqrt{1 - z^2} \sin \theta, z)\]

Corollary

This map pushes the standard probability measure on \([-1, 1] \times S^1\) forward to the correct probability measure on \(S^2\).
**Theorem (Marsden–Weinstein, Meyer)**

If \( G \) is a \( g \)-dimensional compact Lie group which acts in a Hamiltonian fashion on the symplectic manifold \((M, \omega)\) with associated moment map \( \mu : M \to \mathbb{R}^g \), then for any \( \vec{v} \) in the moment polytope so that the action of \( G \) preserves the fiber \( \mu^{-1}(\vec{v}) \subset M \), the quotient

\[
M \sslash _{\vec{v}} G := \frac{\mu^{-1}(\vec{v})}{G}
\]

has a natural symplectic structure induced by \( \omega \). The manifold \( M \sslash _{\vec{v}} G \) is called the symplectic reduction of \( M \) by \( G \) (over \( \vec{v} \)).
The Big Symplectic Picture (repeated)

\[
\begin{align*}
\mathbb{C}^2 \times G_2(\mathbb{C}^n) & \xrightarrow{\oplus \mathbb{U}(2)} (\mathbb{C}^2)^n \\
\mathbb{C}^n & \xrightarrow{\oplus \mathbb{U}(1)^n} (\mathbb{C}^2)^n \\
\prod S^2(r_i) & \xrightarrow{\oplus \mathbb{SO}(3)} \mathbb{U}(1)^{n-1} \\
\text{Pol}(n; \vec{r}) & \xrightarrow{\oplus \mathbb{U}(1)^{n-1}} G_2(\mathbb{C}^n)
\end{align*}
\]
The Big Algebraic Geometry Picture

The virtue of this view is that on open dense subsets you can traverse down the diagram by way of quotient maps.

Question: What is the pushforward measure from $G_2(\mathbb{C}^n)$ or $\prod (\mathbb{CP}^1)^n$ to $\hat{\text{Pol}}(n; \vec{r})$?
The virtue of this view is that on open dense subsets you can traverse down the diagram by way of quotient maps.

Question: What is the pushforward measure from $G_2(C^n)\prod (CP^1)^n$ to $\hat{\text{Pol}}(n; \vec{r})$?
The Big Algebraic Geometry Picture

The virtue of this view is that on open dense subsets you can traverse down the diagram by way of quotient maps.

**Question**

*What is the pushforward measure from $G_2(\mathbb{C}^n)$ or $\prod(\mathbb{CP}^1)^n$ to $\hat{\text{Pol}}(n; \vec{r})$?*
A Closed Random Walk with 3,500 Steps
Interpreting the Right Half of the Diagram

We can interpret $S^2(r_1) \times \ldots \times S^2(r_n)$ as the moduli space of random walks in $\mathbb{R}^3$ with fixed edgelengths $r_1, \ldots, r_n$ up to translation. This is a symplectic manifold.
Interpreting the Right Half of the Diagram

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The diagonal $SO(3)$ action is *area-preserving* on each factor, so this action is by symplectomorphisms. In fact, the action is Hamiltonian with corresponding moment map

$\mu : S^2(r_1) \times \ldots \times S^2(r_n) \to \mathbb{R}^3$ given by

$$\mu(\vec{e}_1, \ldots, \vec{e}_n) = \sum \vec{e}_i.$$
Interpreting the Right Half of the Diagram

We can interpret $S^2(r_1) \times \ldots \times S^2(r_n)$ as the moduli space of random walks in $\mathbb{R}^3$ with fixed edgelengths $r_1, \ldots, r_n$ up to translation. This is a symplectic manifold.

The diagonal $SO(3)$ action is \textit{area-preserving} on each factor, so this action is by symplectomorphisms. In fact, the action is Hamiltonian with corresponding moment map

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given by

\[ \mu(\vec{e}_1, \ldots, \vec{e}_n) = \sum \vec{e}_i. \]

Therefore, the space $\widehat{\text{Pol}}(n; \vec{r})$ of closed polygons up to translation and rotation is equal to

\[ \mu^{-1}(\vec{0})/SO(3) = \left( S^2(r_1) \times \ldots \times S^2(r_n) \right) \sslash_{\vec{0}} SO(3). \]
Given an (abstract) triangulation of the \( n \)-gon, the folds on any two chords commute. Thus, rotating around all \( n - 3 \) of these chords by independently selected angles defines a \( T^{n-3} \) action on \( \widehat{\text{Pol}}(n; \vec{r}) \) which preserves the chord lengths.
Given an (abstract) triangulation of the $n$-gon, the folds on any two chords commute. Thus, rotating around all $n - 3$ of these chords by independently selected angles defines a $T^{n-3}$ action on $\widehat{\text{Pol}}(n; \vec{r})$ which preserves the chord lengths.

This action turns out to be Hamiltonian. Since the chordlengths $d_1, \ldots, d_{n-3}$ are the conserved quantities, the corresponding moment map is $\delta : \widehat{\text{Pol}}(n; \vec{r}) \to \mathbb{R}^{n-3}$ given by

$$\delta(P) = (d_1, \ldots, d_{n-3}).$$
The Triangulation Polytope

Definition
An abstract triangulation $T$ of an $n$-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* $\mathcal{P}_n(\vec{r})$. 
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\begin{align*}
  d_1 + d_2 &\geq 1 \\
d_2 &\leq d_1 + 1 \\
d_1 &\leq 2 \\
d_2 &\leq 2 \\
d_1 &\leq d_2 + 1
\end{align*}
Definition
An abstract triangulation $T$ of an $n$-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 $\mathcal{P}_n(\vec{r})$. 

$\begin{align*}
(0, 2, 2) \\
(2, 0, 2) \\
(2, 2, 0) \\
(0, 0, 0)
\end{align*}$
Definition

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

$$\alpha: \mathcal{P}_n(\vec{r}) \times T^{n-3} \to \widehat{\text{Pol}}(n; \vec{r})$$
Theorem (with Cantarella)

$\alpha$ pushes the **standard probability measure** on $P_n(\vec{r}) \times T^{n-3}$ forward to the **correct probability measure** on $\hat{\text{Pol}}(n; \vec{r})$. 
Theorem (with Cantarella)

$\alpha$ pushes the **standard probability measure** on $\mathcal{P}_n(\vec{r}) \times T^{n-3}$ forward to the **correct probability measure** on $\hat{\text{Pol}}(n; \vec{r})$.

**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.
Theorem (with Cantarella)
\( \alpha \) pushes the \textbf{standard probability measure} on \( \mathcal{P}_n(\vec{r}) \times T^{n-3} \) forward to the \textbf{correct probability measure} on \( \hat{\text{Pol}}(n; \vec{r}) \).

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.

Corollary
Any sampling algorithm for \( \mathcal{P}_n(\vec{r}) \) is a sampling algorithm for closed polygons with edgelength vector \( \vec{r} \).
Proposition (with Cantarella)

The expected length of a chord skipping $k$ edges in an $n$-edge equilateral polygon is the $(k - 1)$st coordinate of the center of mass of the moment polytope for $\text{Pol}(n; \vec{1})$. 
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The expected length of a chord skipping \( k \) edges in an \( n \)-edge equilateral polygon is the \((k - 1)\)st coordinate of the center of mass of the moment polytope for \( \text{Pol}(n; \vec{1}) \).

<table>
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<tr>
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$$E(\text{chord}(37, 112)) =$$

2586147629602481872372707134354784581828166239735638
002149884020577366687369964908185973277294293751533
821217655703978549111529802222311915321645998238455
195807966750595587484029858333822248095439325965569
561018977292296096419815679068203766009993261268626
7074180822275677495669153244706677550690707937136027
424519117786555575048213829170264569628637315477158
307368641045097103310496820323457318243992395055104

$\approx 4.60973$
Question

How to incorporate excluded volume into the model?
Excluded Volume?

Question
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Excluded Volume?

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How to incorporate excluded volume into the model?

\[ \left| \sum_{i=j}^{k} \mathbf{e}_i \right|^2 \geq \epsilon. \]
Proposition (with Cantarella)

At least \( \frac{1}{2} \) of the space of equilateral 6-edge polygons consists of unknots.
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At least \( \frac{1}{2} \) of the space of equilateral 6-edge polygons consists of unknots.

Despite the proposition, we observe experimentally that (with 95% confidence) between 1.1 and 1.5 in 10,000 hexagons are knotted.
Proposition (with Cantarella)

At least $\frac{1}{2}$ of the space of equilateral 6-edge polygons consists of unknots.

Despite the proposition, we observe experimentally that (with 95% confidence) between 1.1 and 1.5 in 10,000 hexagons are knotted.

How can we be so sure?
Sampling Algorithms for Equilateral Polygons:

- **Markov Chain Algorithms**
  - crankshaft (Vologoskii 1979, Klenin 1988)
  - polygonal fold (Millett 1994)

- **Direct Sampling Algorithms**
  - triangle method (Moore 2004)
  - generalized hedgehog method (Varela 2009)
  - sinc integral method (Moore 2005, Diao 2011)
Sampling Algorithms for Equilateral Polygons:

- **Markov Chain Algorithms**
  - crankshaft (Vologoskii et al. 1979, Klenin et al. 1988)
    - convergence to correct distribution unproved
  - polygonal fold (Millett 1994)
    - convergence to correct distribution unproved

- **Direct Sampling Algorithms**
  - triangle method (Moore et al. 2004)
    - samples a subset of closed polygons
  - generalized hedgehog method (Varela et al. 2009)
    - unproved whether this is correct distribution
    - requires sampling complicated 1-d polynomial densities
The polytope $\mathcal{P}_n = \mathcal{P}_n(\vec{1})$ corresponding to the “fan triangulation” is defined by the triangle inequalities:

\[
0 \leq d_1 \leq 2 \quad \quad \quad \quad \quad \quad \quad 1 \leq d_i + d_{i+1} \quad \quad \quad \quad \quad \quad \quad 0 \leq d_{n-3} \leq 2
\]

\[
|d_i - d_{i+1}| \leq 1
\]
A Change of Coordinates

If we introduce fake chordlength $d_0 = 1 = d_{n-2}$, and make the linear transformation

$$ s_i = d_i - d_{i-1}, \text{ for } 1 \leq i \leq n - 2 $$

then $\sum s_i = d_{n-2} - d_0 = 0$, so $s_{n-2}$ is determined by $s_1, \ldots, s_{n-3}$
A Change of Coordinates

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then $\sum s_i = d_{n-2} - d_0 = 0$, so $s_{n-2}$ is determined by $s_1, \ldots, s_{n-3}$ and the inequalities

$$0 \leq d_1 \leq 2 \quad 1 \leq d_i + d_{i+1} \quad |d_i - d_{i+1}| \leq 1 \quad 0 \leq d_{n-3} \leq 2$$

become

$$-1 \leq s_i \leq 1, \quad -1 \leq \sum_{i=1}^{n-3} s_i \leq 1, \quad \sum_{i=1}^{n-3} s_i \leq -1$$

$$\sum_{j=1}^{i} s_j + \sum_{j=1}^{i+1} s_j \geq -1 \quad |d_i - d_{i+1}| \leq 1 \quad d_i + d_{i+1} \geq 1$$
If we introduce fake chordlength $d_0 = 1 = d_{n-2}$, and make the linear transformation

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then $\sum s_i = d_{n-2} - d_0 = 0$, so $s_{n-2}$ is determined by $s_1, \ldots, s_{n-3}$ and the inequalities

$$0 \leq d_1 \leq 2 \quad 1 \leq d_i + d_{i+1} \quad 0 \leq |d_i - d_{i+1}| \leq 1 \quad 0 \leq d_{n-3} \leq 2$$

become

$$-1 \leq s_i \leq 1, \quad -1 \leq \sum_{i=1}^{n-3} s_i \leq 1,$$

$$\sum_{j=1}^{i} s_j + \sum_{j=1}^{i+1} s_j \geq -1$$

\begin{itemize}
  \item easy conditions
  \item hard conditions
\end{itemize}
**Definition**

The \((n - 3)\)-dimensional polytope \(Q_n\) is the slab of the hypercube \([-1, 1]^{n-3}\) determined by \(-1 \leq s_1 + \ldots + s_{n-3} \leq 1\).
Basic Idea

Definition
The \((n - 3)\)-dimensional polytope \(Q_n\) is the slab of the hypercube \([-1, 1]^{n-3}\) determined by \(-1 \leq s_1 + \ldots + s_{n-3} \leq 1\).

\[ C_5 \]

Idea
Sample points in \(Q_n\), which all obey the “easy conditions”, and reject any samples which fail to obey the “hard conditions”. 
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\(Q_6\)
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**Idea**

Sample points in $Q_n$, which all obey the “easy conditions”, and reject any samples which fail to obey the “hard conditions”.
Relative volumes

Theorem (Marichal–Mossinghoff)

The volume of $Q_n$ is

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

Theorem (Khoi, Takakura, Mandini)

The volume of $C_n$ is

$$\frac{\sqrt{n-2}}{2(n-3)!} \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^{k+1} \binom{n}{k} (n-2k)^{n-3}$$
Runtime of algorithm depends on acceptance ratio

Acceptance ratio \( \frac{\text{Vol}(C_n)}{\text{Vol}(Q_n)} \) is conjectured \( \approx \frac{6}{n} \). It is certainly bounded below by \( \frac{1}{n} \).

graph of \( \frac{6}{n} \) (in red)
Acceptance ratio \( \frac{\text{Vol}(C_n)}{\text{Vol}(Q_n)} \) is conjectured \( \approx \frac{6}{n} \). It is certainly bounded below by \( \frac{1}{n} \).

\[ \text{graph of } \frac{6}{n} \text{ (in red)} \]

**Moral**

*This approach is reasonable if we can sample \( Q_n \) efficiently.*
We can sample $Q_n$ by rejection sampling $[-1, 1]^{n-3}$. The acceptance probability is

$$\frac{\text{Vol } Q_n}{\text{Vol}[-1, 1]^{n-3}}.$$
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But this is just the probability that a sum of $n - 3$ independent Uniform([-1, 1]) variates is between −1 and 1.
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But this is just the probability that a sum of $n - 3$ independent Uniform($[-1, 1]$) variates is between $-1$ and $1$.

\begin{align*}
n &= 4 \\
\mathbb{P}(−1 \leq \sum s_i \leq 1) &= 1
\end{align*}
We can sample $Q_n$ by rejection sampling $[-1, 1]^{n-3}$. The acceptance probability is

$$\frac{\text{Vol } Q_n}{\text{Vol}[-1, 1]^{n-3}}.$$ 

But this is just the probability that a sum of $n-3$ independent Uniform([-1, 1]) variates is between -1 and 1.

For $n = 5$,

$$P(-1 \leq \sum s_i \leq 1) = \frac{3}{4}$$
We can sample $Q_n$ by rejection sampling $[-1, 1]^{n-3}$. The acceptance probability is

$$\frac{\text{Vol } Q_n}{\text{Vol}[-1, 1]^{n-3}}.$$ 

But this is just the probability that a sum of $n - 3$ independent Uniform$([-1, 1])$ variates is between $-1$ and $1$.

$n = 6$

$$\mathbb{P}(-1 \leq \sum s_i \leq 1) = \frac{2}{3}$$
We can sample $Q_n$ by rejection sampling $[-1, 1]^{n-3}$. The acceptance probability is

$$\frac{\text{Vol } Q_n}{\text{Vol }[-1, 1]^{n-3}}.$$

But this is just the probability that a sum of $n - 3$ independent Uniform$([-1, 1])$ variates is between $-1$ and $1$.

\[ n = 7 \]

\[ \mathbb{P}(-1 \leq \sum s_i \leq 1) = \frac{115}{192} \]
We can sample $Q_n$ by rejection sampling $[-1, 1]^{n-3}$. The acceptance probability is

$$\frac{\text{Vol } Q_n}{\text{Vol } [-1, 1]^{n-3}}.$$

But this is just the probability that a sum of $n - 3$ independent Uniform([-1, 1]) variates is between $-1$ and 1.

\[ n = 8 \]

\[ P(-1 \leq \sum s_i \leq 1) = \frac{11}{20} \]
We can sample $Q_n$ by rejection sampling $[-1, 1]^{n-3}$. The acceptance probability is

$$\frac{\text{Vol } Q_n}{\text{Vol}[-1, 1]^{n-3}}.$$ 

But this is just the probability that a sum of $n - 3$ independent Uniform($[-1, 1]$) variates is between $-1$ and $1$.

$n = 100$

$$\mathbb{P}(-1 \leq \sum s_i \leq 1) \approx 0.13938$$
We can sample $Q_n$ by rejection sampling $[-1, 1]^{n-3}$. The acceptance probability is

$$\frac{\text{Vol } Q_n}{\text{Vol}[-1, 1]^{n-3}}.$$

But this is just the probability that a sum of $n - 3$ independent Uniform([-1, 1]) variates is between $-1$ and $1$.

By Shepp’s local limit theorem,

$$\mathbb{P}\left(-1 \leq \sum_{i=0}^{n-4} s_i \leq 1\right) \approx \mathbb{P}\left(-1 \leq \mathcal{N}\left(0, \sqrt{\frac{n-3}{3}}\right) \leq 1\right).$$
We can sample $Q_n$ by rejection sampling $[-1, 1]^{n-3}$. The acceptance probability is

\[
\frac{\text{Vol } Q_n}{\text{Vol}[-1, 1]^{n-3}}.
\]

But this is just the probability that a sum of $n - 3$ independent Uniform([-1, 1]) variates is between −1 and 1.

By Shepp’s **local limit theorem**,

\[
P\left(-1 \leq \sum_{i=0}^{n-4} s_i \leq 1\right) \sim P\left(-1 \leq \mathcal{N}\left(0, \sqrt{\frac{n-3}{3}}\right) \leq 1\right)
\]

\[
= \text{erf}\left(\sqrt{\frac{3}{2(n-3)}}\right) \approx \sqrt{\frac{6}{\pi n}}.
\]
The Action-Angle Method

Action-Angle Method (with Cantarella and Uehara, 2015)

1. Generate \((s_1, \ldots, s_{n-3})\) uniformly on \([-1, 1]^{n-3}\) \(O(n)\) time

2. Test whether \(-1 \leq \sum s_i \leq 1\) acceptance ratio \(\simeq 1/\sqrt{n}\)

3. Let \(s_{n-2} = -\sum s_i\) and test \((s_1, \ldots, s_{n-2})\) against the “hard” conditions acceptance ratio \(> 1/n\)

4. Change coordinates to get diagonal lengths

5. Generate dihedral angles from \(T^{n-3}\)

6. Build sample polygon in action-angle coordinates
Knot Types of 10 Million 60-gons

Straight line: $e^{-e n^{-7/4}}$
Knot Types of 10 Million 60-gons

Straight line: \( e^{-e} n^{-7/4} \)

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>distinct HOMFLYs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polygonal Folds(^1)</td>
<td>2219</td>
</tr>
<tr>
<td>Crankshaft Moves</td>
<td>6110</td>
</tr>
<tr>
<td>Hedgehog Method</td>
<td>1111</td>
</tr>
<tr>
<td>Triangle Method</td>
<td>3505</td>
</tr>
<tr>
<td>Action-Angle Method</td>
<td>( \geq 6371 )</td>
</tr>
</tbody>
</table>

\(^1\)100 million samples, instead of 10 million.
Questions
Question

How to use algebraic geometry to understand $\hat{\text{Pol}}(n; \vec{r})$?
Question

How to incorporate excluded volume into the model?
Geometry of the Space of Planar Polygons

Question

What is the analog of the symplectic story for n-gons in the plane?
Topologically Constrained Random Walks

Question
What special geometric structures exist on the moduli space of topologically-constrained random walks patterned on a given graph?

Tezuka Lab, Tokyo Institute of Technology
Question

Is there a generalization to a geometric theory of (immersed) closed piecewise-linear surfaces in $\mathbb{R}^3$? Or, more generally, closed PL $k$-manifolds in $\mathbb{R}^n$?
Thank you!

Thank you for listening!
• *The Symplectic Geometry of Closed Equilateral Random Walks in 3-Space*
  Jason Cantarella and Clayton Shonkwiler

• *A Fast Direct Sampling Algorithm for Equilateral Closed Polygons*
  Jason Cantarella, Clayton Shonkwiler, and Erica Uehara
  arXiv:1510.02466

http://shonkwiler.org