The Symplectic Geometry of Polygon Space and How to Use It

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Fragment
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In Fragment last spring, Jason Cantarella described a model for closed, relatively framed polygons in $\mathbb{R}^3$ of \textit{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 (equilaterals are largest volume) $\text{one edge of length } 1 \Rightarrow \text{volume } = 0$.
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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)
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 connect with a larger symplectic geometry 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.
Let $\text{Arm}(n; \vec{r})$ be the moduli space of random walks in $\mathbb{R}^3$ consisting of $n$ steps up to translation of lengths $\vec{r} = (r_1, \ldots, r_n)$.

Then $\text{Arm}(n; \vec{r}) \cong S^2(r_1) \times \ldots \times S^2(r_n)$. 
Let $\text{Arm}(n; \vec{r})$ be the moduli space of random walks in $\mathbb{R}^3$ consisting of $n$ steps up to translation of lengths $\vec{r} = (r_1, \ldots, r_n)$.

Then $\text{Arm}(n; \vec{r}) \cong S^2(r_1) \times \ldots \times S^2(r_n)$.

Let $\text{Pol}(n; \vec{r}) \subset \text{Arm}(n; \vec{r})$ be the submanifold of closed random walks (or random polygons); i.e., those walks which satisfy

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

\[ S^2(r_1) \times \ldots \times S^2(r_n) \]

is a symplectic manifold and the diagonal \( SO(3) \) action is \textit{area-preserving} on each factor, so this action is by symplectomorphisms.
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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

\[ \mu(\vec{e}_1, \ldots, \vec{e}_n) = \sum \vec{e}_i. \]
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Therefore, \( \text{Pol}(n; \vec{r}) = \mu^{-1}(\vec{0}) \)
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$$
\mu(\vec{e}_1, \ldots, \vec{e}_n) = \sum \vec{e}_i.
$$

Therefore, $\text{Pol}(n; \vec{r}) = \mu^{-1}(\vec{0})$ and the space $\widehat{\text{Pol}}(n; \vec{r})$ of closed polygons up to translation and rotation is a symplectic reduction

$$
\widehat{\text{Pol}}(n; \vec{r}) = \mu^{-1}(\vec{0}) / SO(3) = \left( S^2(r_1) \times \ldots \times S^2(r_n) \right) \parallel_{\vec{0}} SO(3).
$$
The Big Symplectic Picture (via Hausmann–Knutson)

\[
\begin{array}{c}
(C^2)^n \\
\downarrow \text{G}_2(C^n) \\
\downarrow \text{Pol}(n; \vec{r}) \\
\downarrow \text{SO}(3)
\end{array}
\]

\[
\begin{array}{c}
\prod S^2(r_i) \\
\downarrow \text{U}(1)^n \\
\downarrow \text{U}(2) \\
\downarrow \text{U}(1)^{n-1}
\end{array}
\]
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

$$M//_{\vec{v}} G := \mu^{-1}(\vec{v})/G$$

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

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

\[ \mathbb{G}_2(\mathbb{C}^n) \]

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

\[ \hat{\text{Pol}}(n; \vec{r}) \]

\[ \mathbb{U}(2) \]

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

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

\[ \mathbb{U}(1)^{n-1} \]
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 $\hat{\text{Pol}}(n; \vec{r})$ 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
The lengths $d_1, \ldots, d_{n-3}$ obey triangle inequalities, and these inequalities turn out to exactly determine the moment polytope $\mathcal{P}_n(\vec{r}) \subset \mathbb{R}^{n-3}$. 

![Diagram of the Triangulation Polytope with lengths $d_1$ and $d_2$]
The Triangulation Polytope

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![Diagram of the triangulation polytope with labeled vertices](image)
Definition

If $\mathcal{P}_n(\vec{r})$ is the moment 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 $\mathcal{P}_n(\vec{r}) \times T^{n-3}$ forward to the correct probability measure on $\hat{\text{Pol}}(n; \vec{r})$. 
Theorem (with Cantarella)

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

Corollary

Any sampling algorithm for $P_n(\vec{r})$ 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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$$E(\text{chord}(37, 112)) =$$

2586147629602481872372707134354784581828166239735638
002149884020577366687369964908185973277294293751533
821217655703978549111529802222311915321645998238455
1958079667505955874840298583338222248095439325965569
561018977292296096419815679068203766009993261268626
7074180822275677495669153244706677550690707937136027
424519117786555575048213829170264569628637315477158
307368641045097103310496820323457318243992395055104
\approx 4.60973
Proposition (with Cantarella)

At least $\frac{1}{2}$ of the space of equilateral 6-edge polygons consists of unknots.
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Despite the proposition, we observe experimentally that (with 95% confidence) between 1.1 and 1.5 in 10,000 hexagons are knotted.
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How can we be so sure?
An (Incomplete?) History of Polygon Sampling

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)
An (Incomplete?) History of Polygon Sampling

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)
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- **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:

\[
0 \leq d_1 \leq 2 \quad 1 \leq d_i + d_{i+1} \quad |d_i - d_{i+1}| \leq 1 \quad 0 \leq d_{n-3} \leq 2
\]
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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$$s_i = d_i - d_{i-1}, \text{ for } 1 \leq i \leq n-2$$

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

$$-1 \leq s_i \leq 1, \quad -1 \leq \sum_{i=1}^{n-3} s_i \leq 1, \quad \sum_{j=1}^{i} s_j + \sum_{j=1}^{i+1} s_j \geq -1 \quad |d_i - d_{i+1}| \leq 1 \quad d_i + d_{i+1} \geq 1$$
Let $C_n \subset [-1, 1]^{n-3}$ be determined by the inequalities on the previous slide.
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**Theorem (with Cantarella, Duplantier, Uehara)**

The probability that a point in the hypercube lies in $C_n$ is asymptotic to

$$\frac{6\sqrt{6}}{\sqrt{\pi}} \frac{1}{n^{3/2}}.$$
The Volume of $\mathcal{C}_n$

**Theorem (Khoi, Takakura, Mandini)**

The volume of $\mathcal{C}_n$ is

$$\frac{1}{2(n-3)!} \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^{k+1} \binom{n}{k} (n-2k)^{n-3}$$
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Observation (Edwards, 1922)

$$\text{Vol } C_n = \frac{2^{n-1}}{2\pi} \int_{-\infty}^{\infty} \frac{\sin^n x}{x^{n-2}} \, dx$$
[T]here is in these days far too great a tendency on the part of teachers to push on their pupils so fast to the Higher Branches of Analysis or to Physical Mathematics that many have neither time nor opportunity for the cultivation of real personal proficiency, or for the acquirement of that individual manipulative skill which is essential to any real confidence of the student in his own power to conduct unaided investigation.

– Joseph Edwards, 1922
The Volume of $C_n$

**Theorem (Khoi, Takakura, Mandini)**

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**Observation (Edwards, 1922)**

$$\text{Vol } C_n = \frac{2^{n-1}}{2\pi} \int_{-\infty}^{\infty} \frac{\sin^n x}{x^{n-2}} \, dx$$
Making the substitution $x = y / \sqrt{n}$ gives

\[
\text{Vol } C_n = \frac{2^{n-1}}{2\pi} \int_{-\infty}^{\infty} \left( \frac{\sin (y/\sqrt{n})}{y/\sqrt{n}} \right)^n \frac{y^2 \, dy}{n^{3/2}}
\]
\[
\sim \frac{2^{n-1}}{2\pi} \frac{1}{n^{3/2}} \int_{-\infty}^{\infty} \left( e^{-y^2/6n} \right)^n y^2 \, dy
\]
\[
= \frac{2^{n-1}}{2\pi} \frac{1}{n^{3/2}} \int_{-\infty}^{\infty} e^{-y^2/6} y^2 \, dy
\]
\[
= 3 \sqrt{\frac{3}{\pi}} 2^{n-\frac{3}{2}} \frac{1}{n^{3/2}}.
\]

Therefore,

\[
\frac{\text{Vol } C_n}{\text{Vol } [-1, 1]^{n-3}} \sim \frac{3 \sqrt{\frac{3}{\pi}} 2^{n-\frac{3}{2}} \frac{1}{n^{3/2}}}{2^{n-3}} = \frac{6\sqrt{6}}{\sqrt{\pi}} \frac{1}{n^{3/2}}.
\]
Action-Angle Method (with Cantarella, Duplantier, Uehara)

1. Generate \((s_1, \ldots, s_{n-3})\) uniformly on \([-1, 1]^{n-3}\) \(O(n)\) time
2. Test whether \((s_1, \ldots, s_{n-3}) \in C_n\) acceptance ratio \(\sim 1/n^{3/2}\)
3. Let \(s_{n-2} = -\sum s_i\) and change coordinates to get diagonal lengths
4. Generate dihedral angles from \(T^{n-3}\)
5. Build sample polygon in action-angle coordinates
We sampled 10 million 60-gons and computed their HOMFLY polynomials. 42 of the 60-gons were numerically singular, but the rest yielded 6371 distinct HOMFLY polynomials.

Straight line: \( e^{-e \cdot n^{-7/4}} \)
We sampled 10 million 60-gons and computed their HOMFLY polynomials. 42 of the 60-gons were numerically singular, but the rest yielded 6371 distinct HOMFLY polynomials.
Questions
Question

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

*How to incorporate excluded volume into the model?*
Topologically Constrained Random Walks

Question
What special geometric structures exist on the moduli space of topologically-constrained random walks patterned on a given graph?
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 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, Bertrand Duplantier, Clayton Shonkwiler, and Erica Uehara
  arXiv:1510.02466

  http://shonkwiler.org