The Symplectic Geometry of Polygon Space and How to Use It

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Fragment
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From Variable Edgelengths to Fixed Edgelengths

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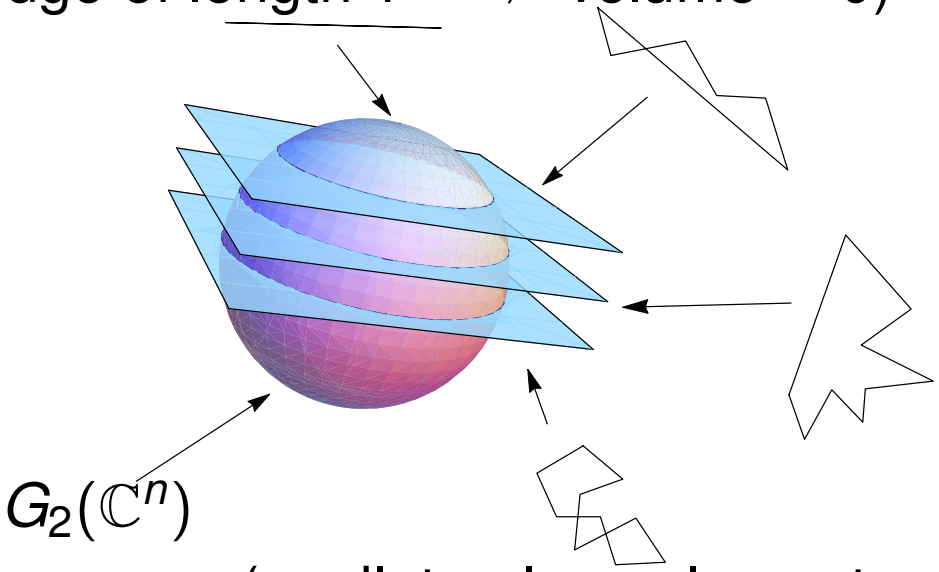
(one edge of length 1 $\implies$ volume $= 0$)

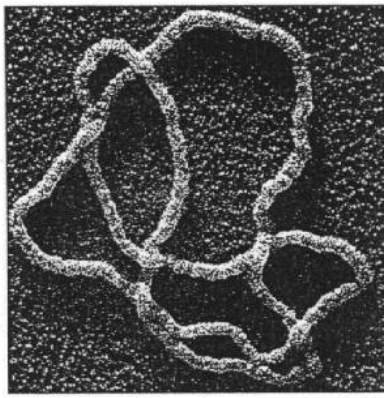


(equilaterals are largest volume)

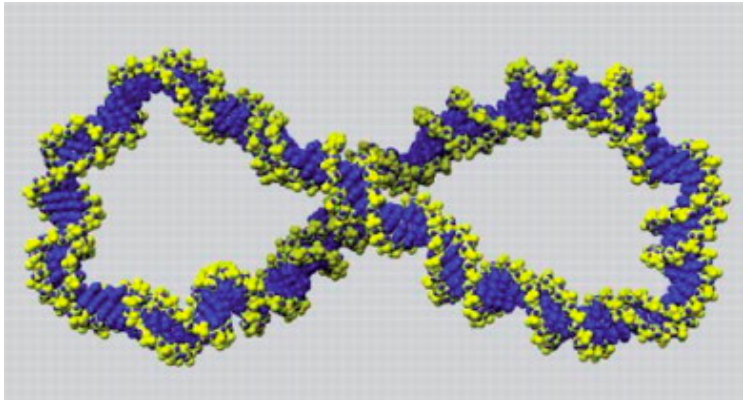
$G_2(\mathbb{C}^n)$ is an assembly of fixed edge length spaces

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.

Goals

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.

Random Walks

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

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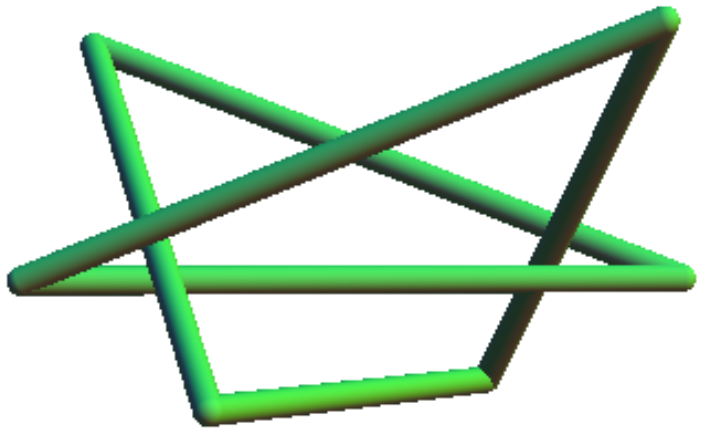
Let $\mathrm{Pol}(n; \vec{r}) \subset \mathrm{Arm}(n; \vec{r})$ be the submanifold of closed random walks (or *random polygons*); i.e., those walks which satisfy

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



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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, $\mathrm{Pol}(n; \vec{r}) = \mu^{-1}(\vec{0})$

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

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

$$\widehat{\mathrm{Pol}}(n; \vec{r}) = \mu^{-1}(\vec{0})/SO(3) = \left(S^2(r_1) \times \ldots \times S^2(r_n)\right) /\!\!/_{\vec{0}} SO(3).$$

The Big Symplectic Picture (via Hausmann–Knutson)

$$
\begin{tikzcd}
 & (\mathbb{C}^2)^n \arrow[dl, dash, "/\!/_{\vec{0}} U(2)"'] \arrow[dr, dash, "/\!/_{\vec{r}} U(1)^n"] & \\
G_2(\mathbb{C}^n) \arrow[dr, dash, "/\!/_{\vec{r}} U(1)^{n-1}"'] & & \prod S^2(r_i) \arrow[dl, dash, "/\!/_{\vec{0}} SO(3)"] \\
 & \widehat{\mathrm{Pol}}(n; \vec{r}) &
\end{tikzcd}
$$

Some Details

A symplectic manifold (M, ω) is a smooth $2n$-dimensional manifold M with a closed, non-degenerate 2-form ω called the *symplectic form*. The nth power of this form $\omega^n = \underbrace{\omega \wedge \ldots \wedge \omega}_{n}$ is a volume form on M.

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The circle $U(1)$ *acts by symplectomorphisms* on M if the action preserves ω. A circle action generates a vector field X on M. We can contract the vector field X with ω 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 *Hamiltonian*. The function H is called the *momentum* associated to the action, or the *moment map*.

Some More Details

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 μ 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.*

A Down-to-Earth Example

Let (M, ω) 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 2π times Lebesgue measure.

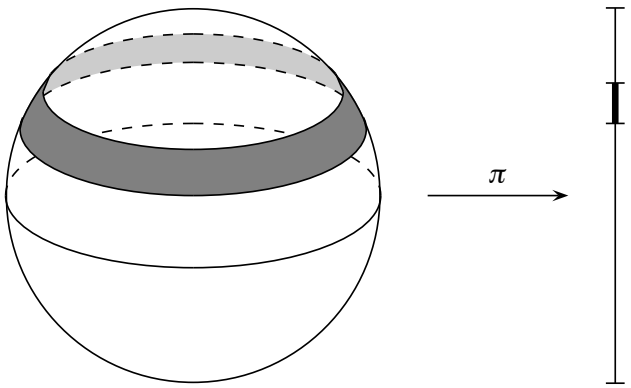
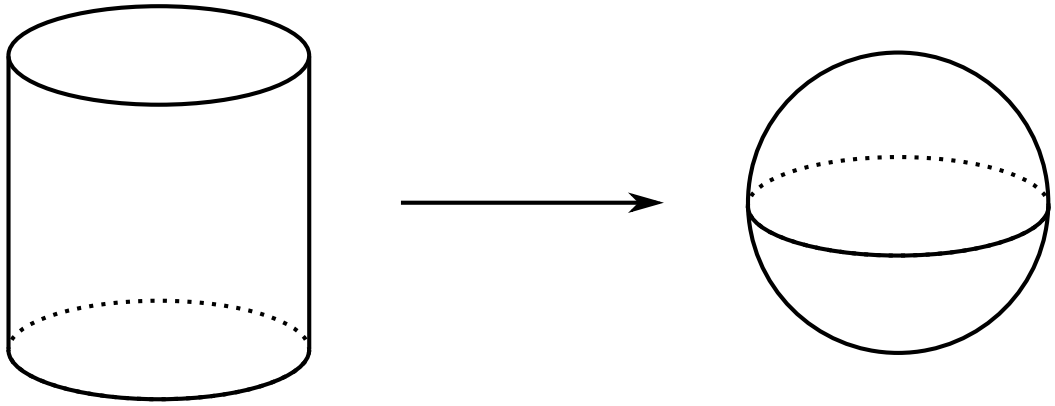


Illustration by Kuperberg.

Action-Angle Coordinates are Cylindrical Coordinates



(z, θ) $\qquad$ $(\sqrt{1-z^2}\cos\theta, \sqrt{1-z^2}\sin\theta, z)$

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, ω) 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 ω. The manifold $M /\!\!/_{\vec{v}} G$ is called the symplectic reduction of M by G (over $\vec{v}$).

The Big Symplectic Picture (repeated)

$$
\begin{tikzcd}
 & (\mathbb{C}^2)^n \arrow[dl, dash, "/\!/_{\vec{0}} U(2)"'] \arrow[dr, dash, "/\!/_{\vec{r}} U(1)^n"] & \\
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 & \widehat{\mathrm{Pol}}(n; \vec{r}) &
\end{tikzcd}
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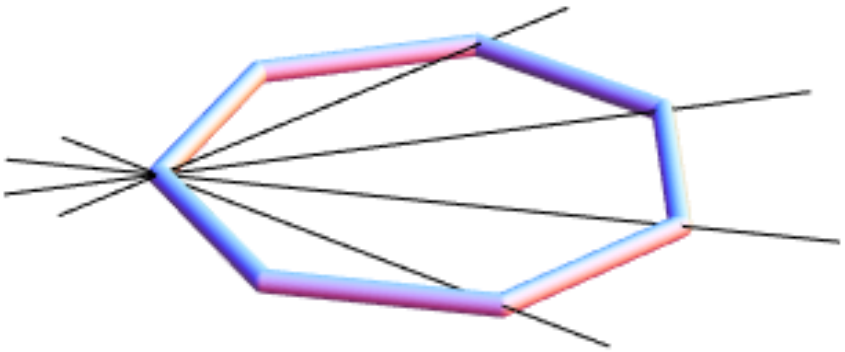
$\widehat{\mathrm{Pol}}(n;\vec{r})$ is Toric

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 $\widehat{\mathrm{Pol}}(n;\vec{r})$ which preserves the chord lengths.



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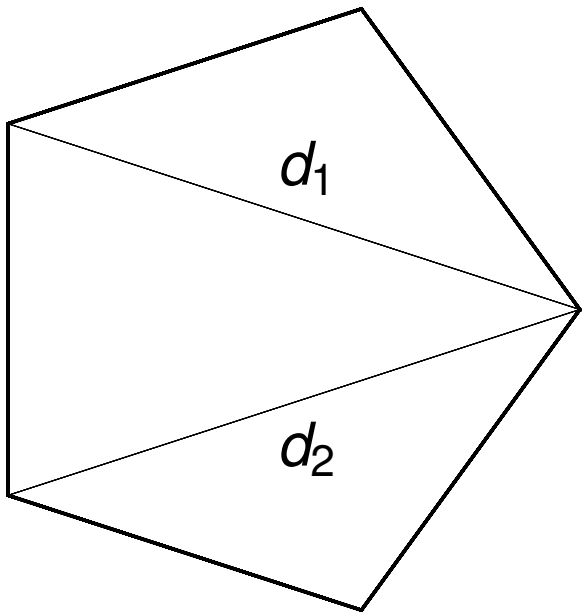
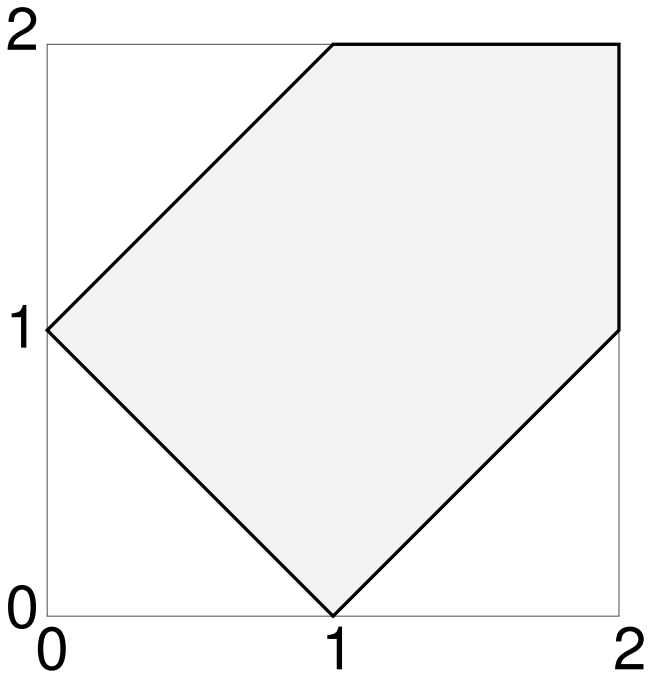
This action turns out to be Hamiltonian. Since the chordlengths $d_1, \ldots, d_{n-3}$ are the conserved quantities, the corresponding moment map is $\delta : \widehat{\mathrm{Pol}}(n;\vec{r}) \to \mathbb{R}^{n-3}$ given by

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

Definition

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





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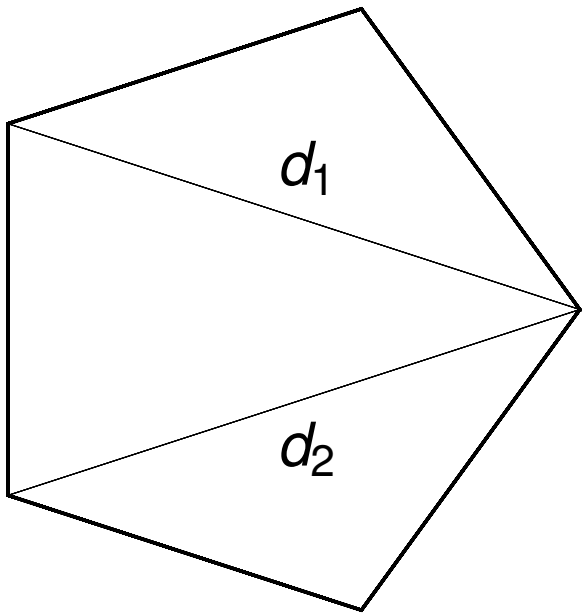

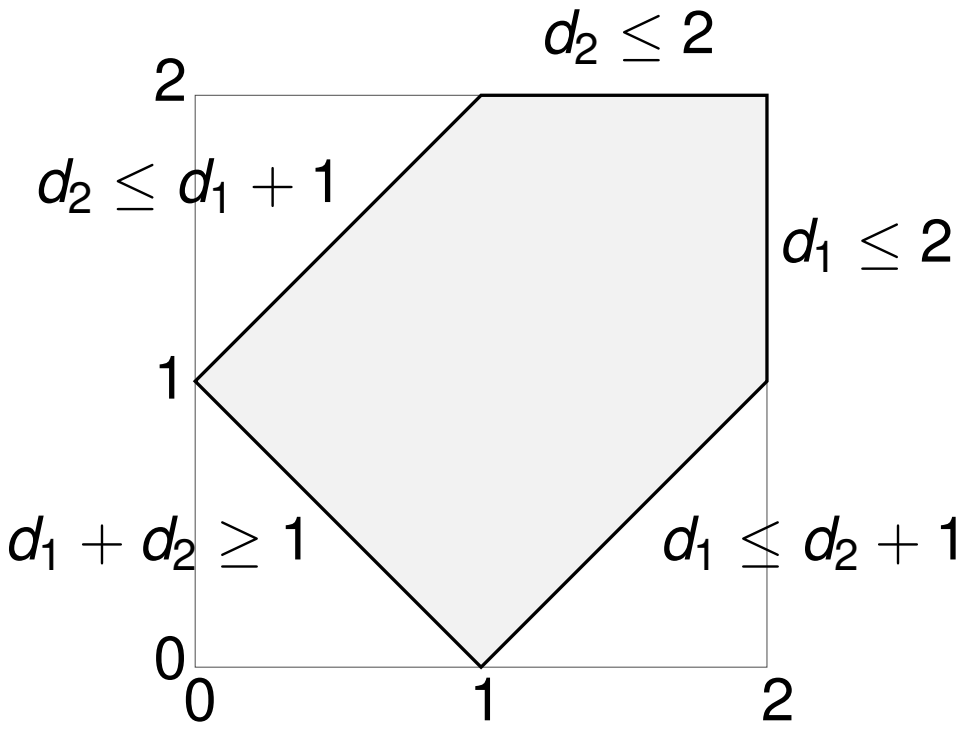

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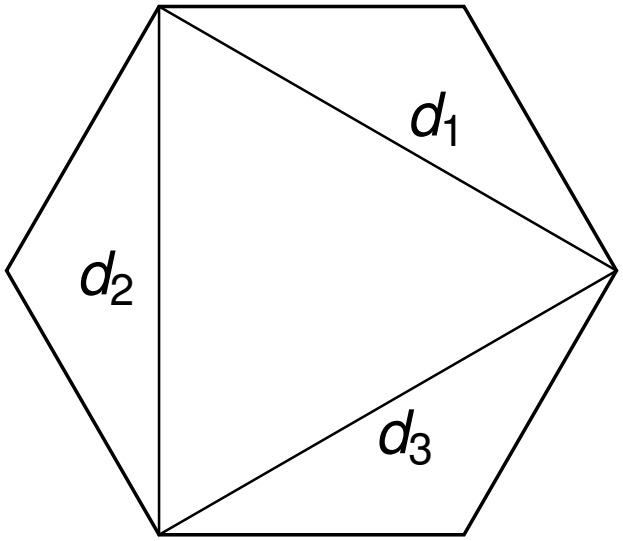
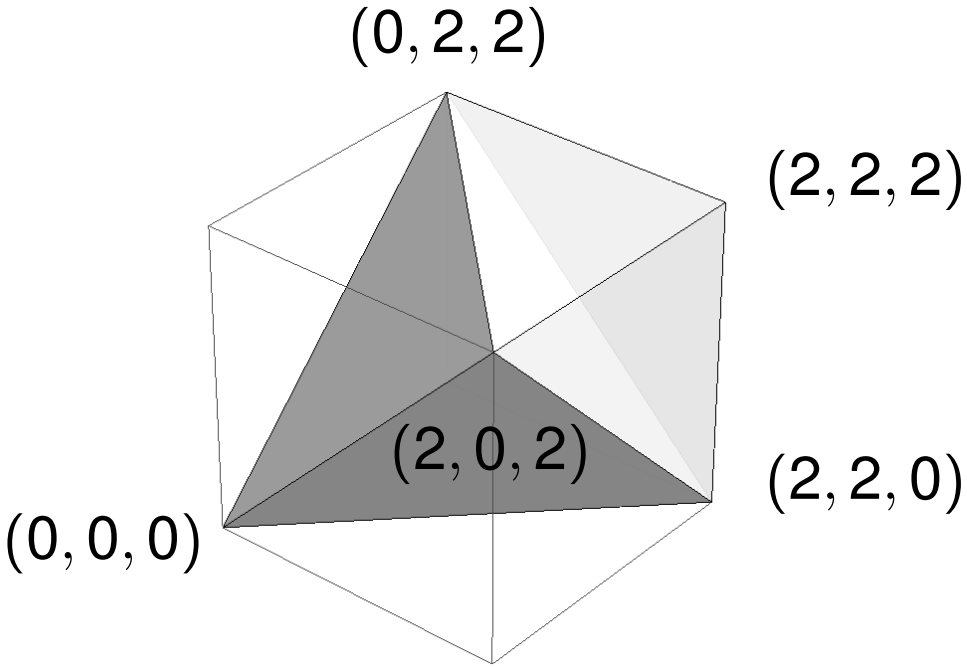
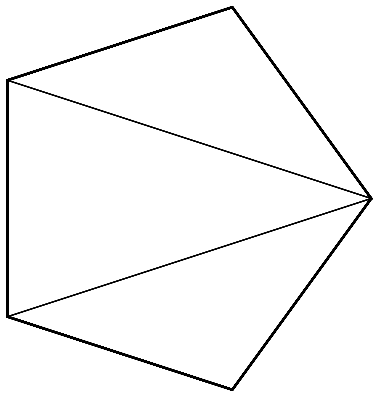


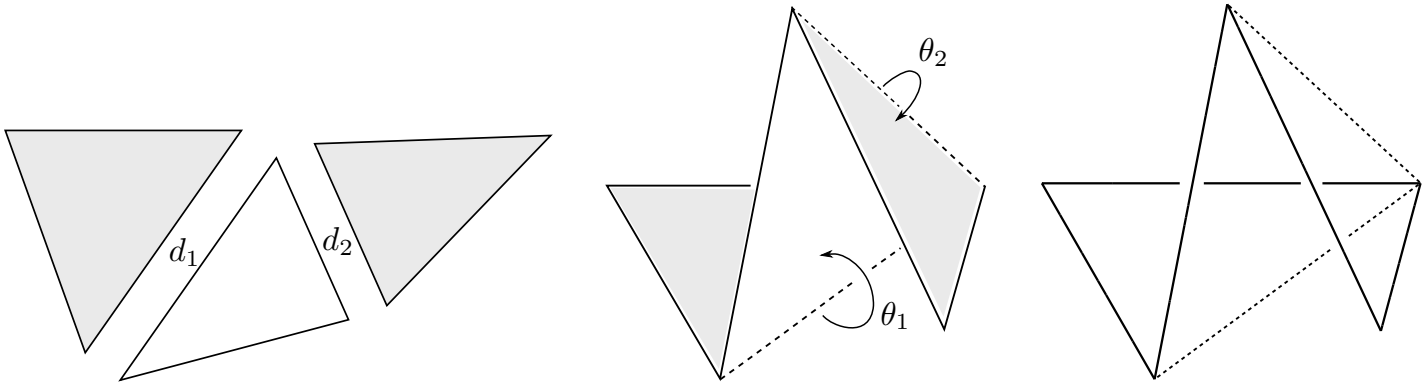


Definition

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*:

$$\alpha\colon\ \mathcal{P}_n(\vec{r}) \times T^{n-3} \to \widehat{\mathrm{Pol}}(n;\vec{r})$$





Theorem (with Cantarella)

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

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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 $\mathrm{Pol}(n; \vec{1})$.

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n	$k=2$	3	4	5	6	7	8
4	1						
5	$\frac{17}{15}$	$\frac{17}{15}$					
6	$\frac{14}{12}$	$\frac{15}{12}$	$\frac{14}{12}$				
7	$\frac{461}{385}$	$\frac{506}{385}$	$\frac{506}{385}$	$\frac{461}{385}$			
8	$\frac{1,168}{960}$	$\frac{1,307}{960}$	$\frac{1,344}{960}$	$\frac{1,307}{960}$	$\frac{1,168}{960}$		
9	$\frac{112,121}{91,035}$	$\frac{127,059}{91,035}$	$\frac{133,337}{91,035}$	$\frac{133,337}{91,035}$	$\frac{127,059}{91,035}$	$\frac{112,121}{91,035}$	
10	$\frac{97,456}{78,400}$	$\frac{111,499}{78,400}$	$\frac{118,608}{78,400}$	$\frac{120,985}{78,400}$	$\frac{118,608}{78,400}$	$\frac{111,499}{78,400}$	$\frac{97,456}{78,400}$

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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 $\mathrm{Pol}(n; \vec{1})$.

$$E(\mathrm{chord}(37, 112)) =$$

$$\frac{2586147629602481872372707134354784581828166239735638002149884020577366687369964908185973277294293751533821217655703978549111529802222311915321645998238455195807966750595587484029858333822248095439325965569}{5610189772922960964198156790682037660099932612686267074180822756774956691532447066775506907079371360274245191177865555750482138291702645696286373154771583073686410450971033104968203234573182439923950551040}$$

$$\approx 4.60973$$

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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)

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    - convergence to correct distribution unproved
  - polygonal fold (Millett 1994)
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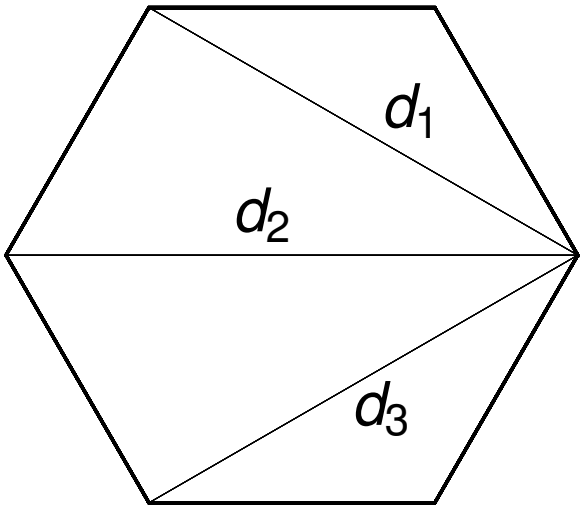
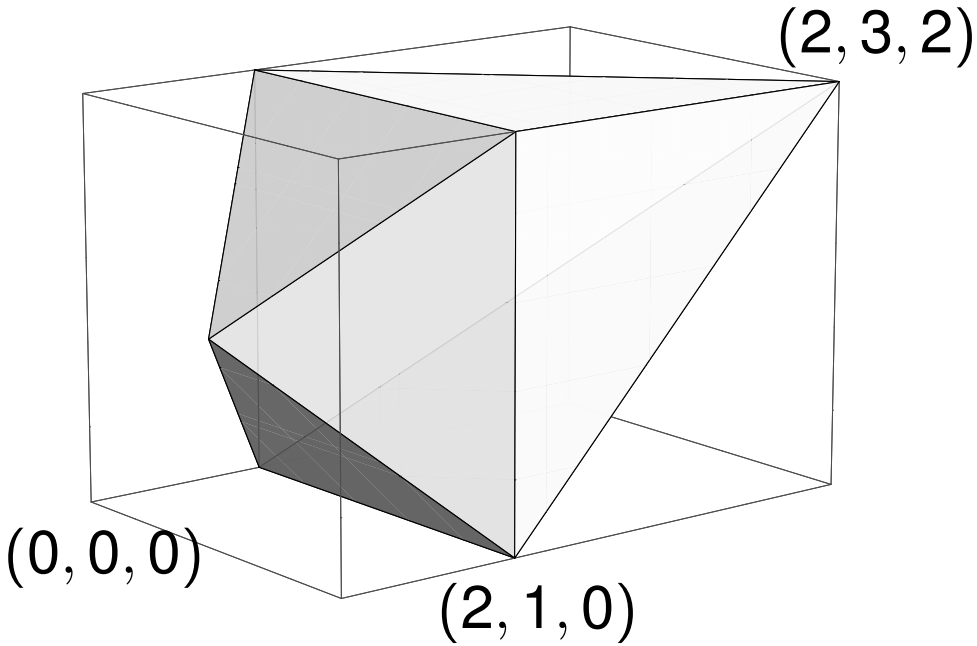
- Direct Sampling Algorithms
  - triangle method (Moore et al. 2004)
    - samples a subset of closed polygons
  - generalized hedgehog method (Varela et al. 2009)
    - unproved whether this is correct distribution
  - sinc integral method (Moore et al. 2005, Diao et al. 2011)
    - requires sampling complicated 1-d polynomial densities

The Fan Triangulation Polytope





The polytope $\mathcal{P}_n = \mathcal{P}_n(\vec{1})$ corresponding to the "fan triangulation" is defined by the triangle inequalities:

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

A Change of Coordinates

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

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

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

become

$$\underbrace{-1 \leq s_i \leq 1, \quad -1 \leq \sum_{i=1}^{n-3} s_i \leq 1,}_{|d_i - d_{i+1}| \leq 1} \quad \underbrace{\sum_{j=1}^{i} s_j + \sum_{j=1}^{i+1} s_j \geq -1}_{d_i + d_{i+1} \geq 1}$$

The Key Result

Let $\mathcal{C}_n \subset [-1, 1]^{n-3}$ be determined by the inequalities on the previous slide.

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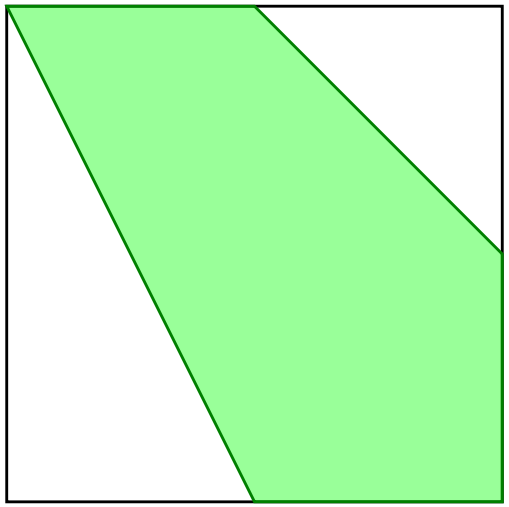

$\mathcal{C}_5$

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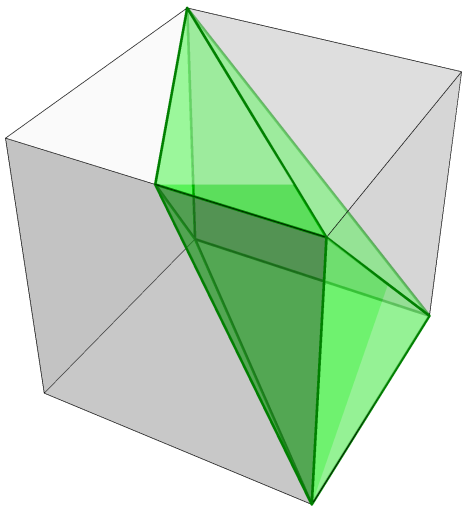

$\mathcal{C}_6$

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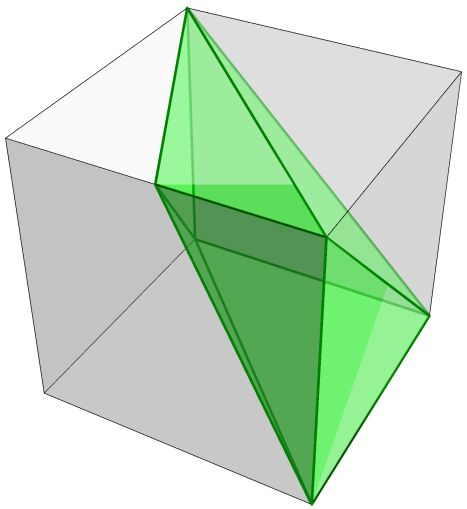

$\mathcal{C}_6$

Theorem (with Cantarella, Duplantier, Uehara)

The probability that a point in the hypercube lies in $\mathcal{C}_n$ is asymptotic to

$$\frac{6\sqrt{6}}{\sqrt{\pi}} \frac{1}{n^{3/2}}.$$

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)

$$\operatorname{Vol}\mathcal{C}_n = \frac{2^{n-1}}{2\pi}\int_{-\infty}^{\infty}\frac{\sin^n x}{x^{n-2}}\,\mathrm{d}x$$

[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

Theorem (Khoi, Takakura, Mandini)

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

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

Observation (Edwards, 1922)

$$\operatorname{Vol}\mathcal{C}_n = \frac{2^{n-1}}{2\pi}\int_{-\infty}^{\infty}\frac{\sin^n x}{x^{n-2}}\,\mathrm{d}x$$

Making the substitution $x = y/\sqrt{n}$ gives

$$\begin{aligned}
\operatorname{Vol}\mathcal{C}_n &= \frac{2^{n-1}}{2\pi}\int_{-\infty}^{\infty}\left(\frac{\sin\left(y/\sqrt{n}\right)}{y/\sqrt{n}}\right)^n \frac{y^2\,\mathrm{d}y}{n^{3/2}} \\
&\sim \frac{2^{n-1}}{2\pi}\frac{1}{n^{3/2}}\int_{-\infty}^{\infty}\left(e^{-y^2/6n}\right)^n y^2\,\mathrm{d}y \\
&= \frac{2^{n-1}}{2\pi}\frac{1}{n^{3/2}}\int_{-\infty}^{\infty} e^{-y^2/6}y^2\,\mathrm{d}y \\
&= 3\sqrt{\frac{3}{\pi}}\,2^{n-\frac{3}{2}}\,\frac{1}{n^{3/2}}.
\end{aligned}$$

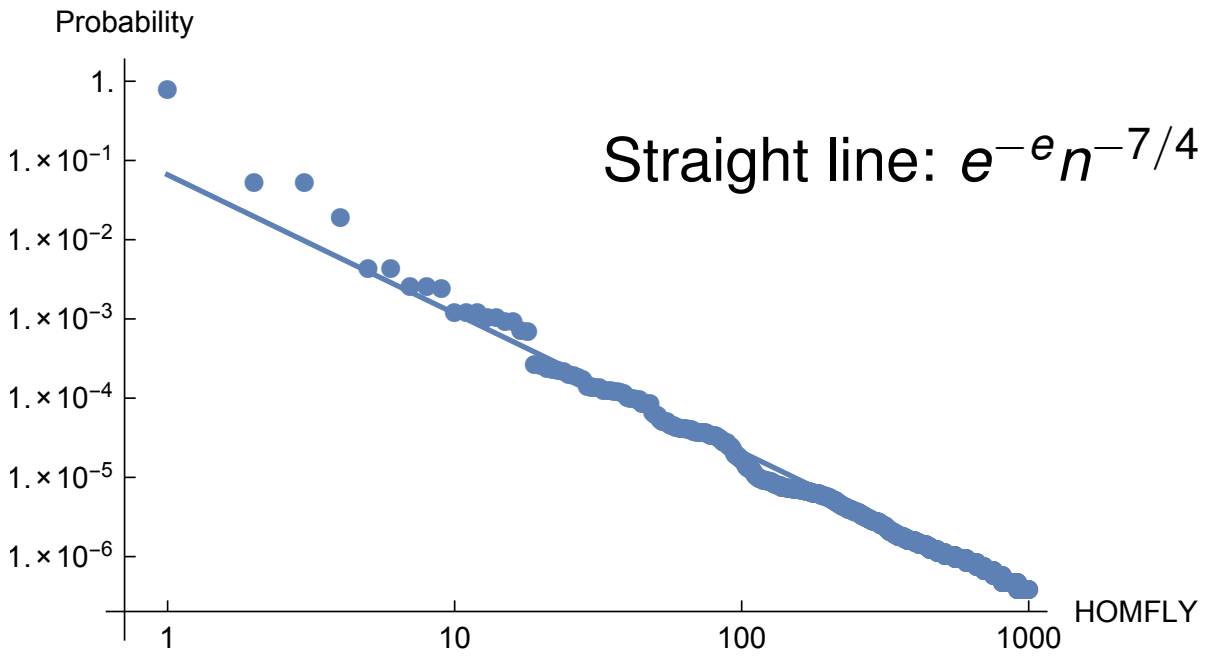
Therefore,

$$\frac{\operatorname{Vol}\mathcal{C}_n}{\operatorname{Vol}[-1,1]^{n-3}} \sim \frac{3\sqrt{\frac{3}{\pi}}\,2^{n-\frac{3}{2}}\,\frac{1}{n^{3/2}}}{2^{n-3}} = \frac{6\sqrt{6}}{\sqrt{\pi}}\frac{1}{n^{3/2}}.$$

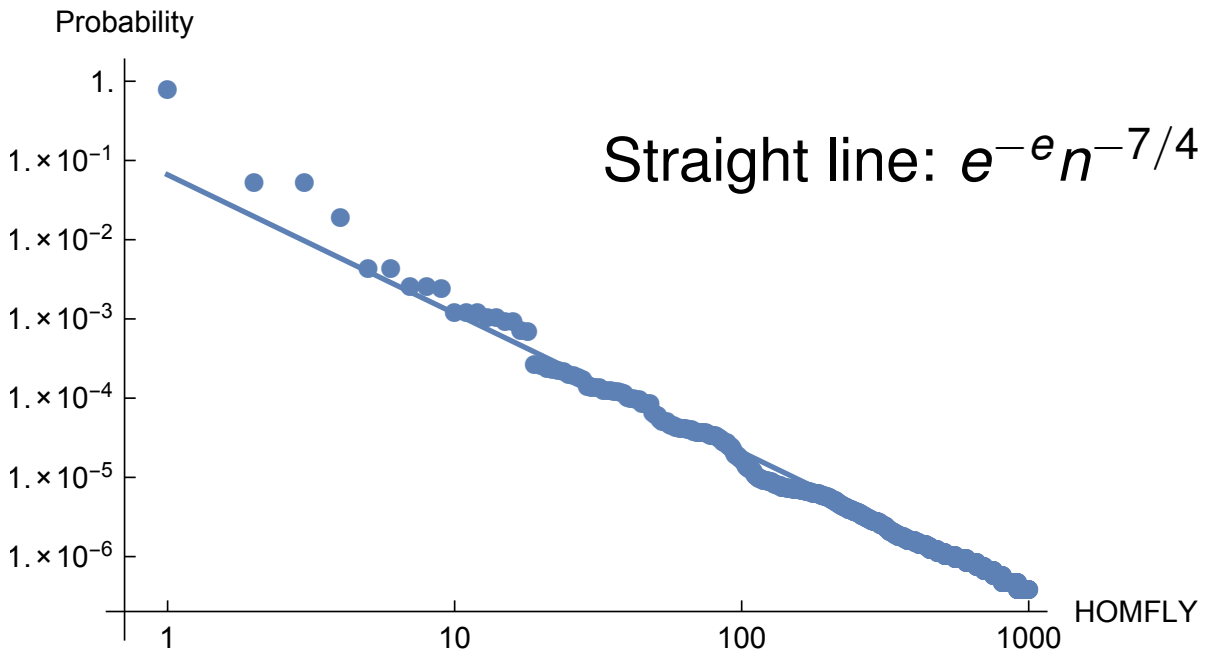
Action-Angle Method (with Cantarella, Duplantier, Uehara)

1. *Generate* $(s_1, \ldots, s_{n-3})$ *uniformly on* $[-1, 1]^{n-3}$ $O(n)$ *time*
2. *Test whether* $(s_1, \ldots, s_{n-3}) \in \mathcal{C}_n$ *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*

Knot Types of 10 Million 60-gons



Knot Types of 10 Million 60-gons



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.

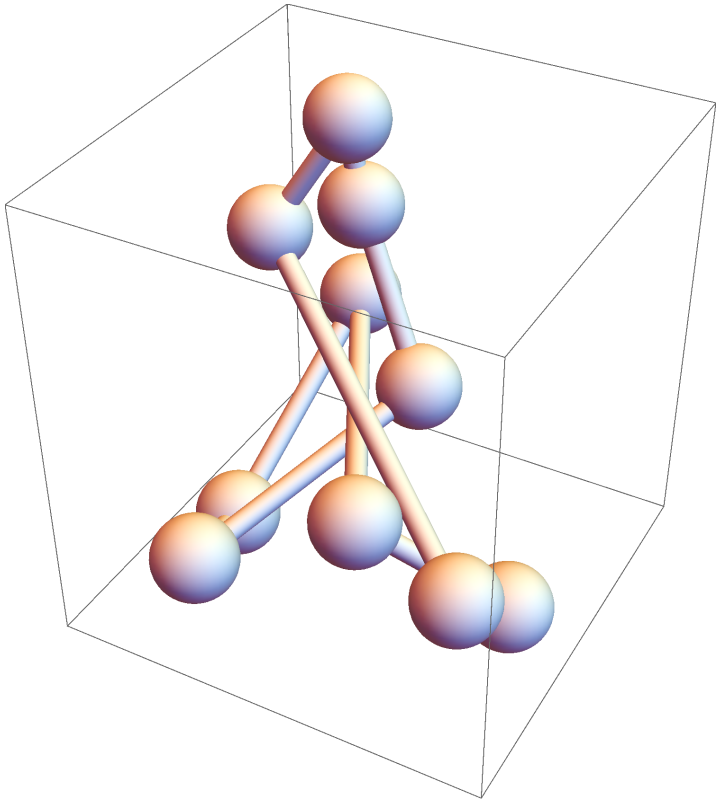
Questions

$$\begin{tikzcd}
 & (\mathbb{C}^2)^n \arrow[dl, dash, "/\!/GL(2,\mathbb{C})"'] \arrow[dr, dash, "/\!/(\mathbb{C}^*)^n"] & \\
G_2(\mathbb{C}^n) \arrow[dr, dash, "/\!/(\mathbb{C}^*)^{n-1}"'] & & \prod(\mathbb{CP}^1)^n \arrow[dl, dash, "/\!/PGL(2,\mathbb{C})"] \\
 & \widehat{\mathrm{Pol}}(n;\vec{r}) &
\end{tikzcd}$$

Question

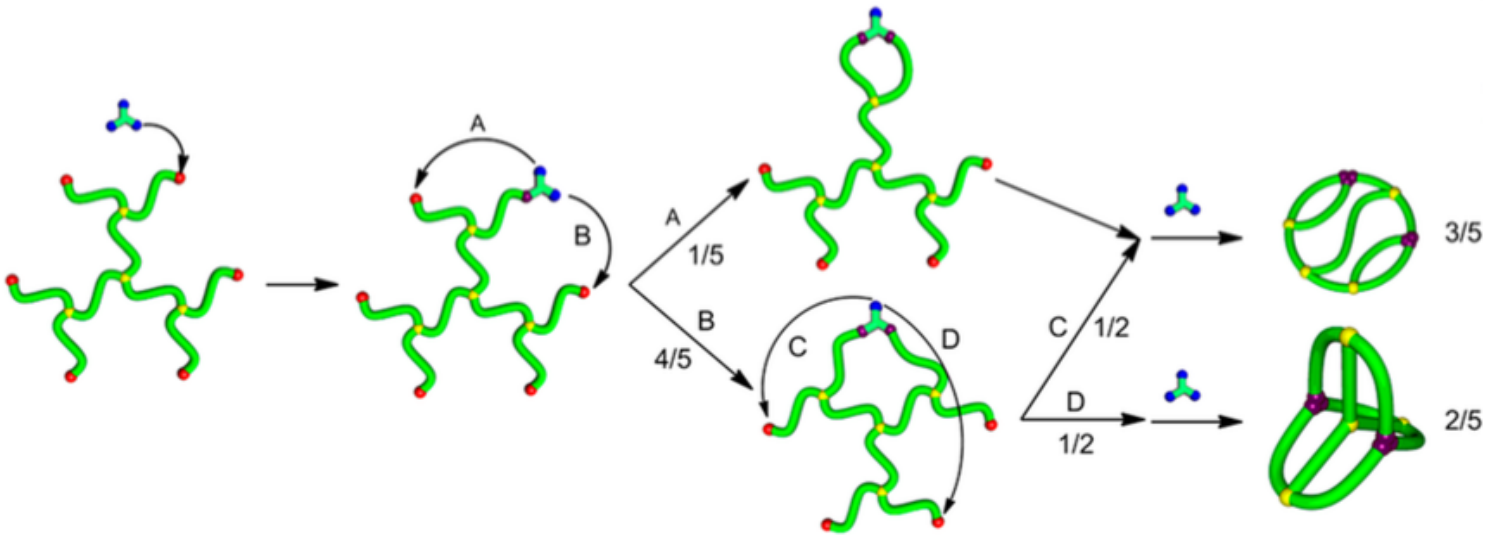
How to use algebraic geometry to understand $\widehat{\mathrm{Pol}}(n;\vec{r})$*?*

Symplectic Geometry and Excluded Volume



Question

How to incorporate excluded volume into the model?



Tezuka Lab, Tokyo Institute of Technology

Question

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

A Theory of Piecewise-Linear Submanifolds

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!

References

- *The Symplectic Geometry of Closed Equilateral Random Walks in 3-Space*
  Jason Cantarella and Clayton Shonkwiler
  Annals of Applied Probability, to appear.

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

`http://shonkwiler.org`