The Symplectic Geometry of Polygon Space and How to Use It

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From Variable Edgelengths to Fixed Edgelengths

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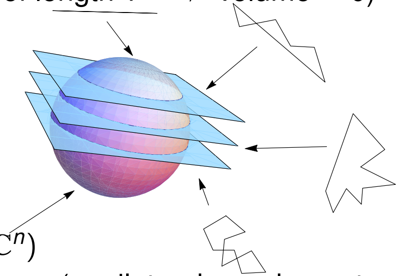
(one edge of length 1 $\implies$ volume $= 0$)



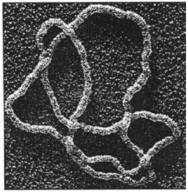
$G_2(\mathbb{C}^n)$

(equilaterals are largest volume)

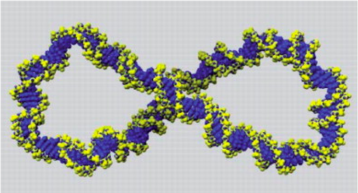
$G_2(\mathbb{C}^n)$ is an assembly of fixed edge length spaces

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.

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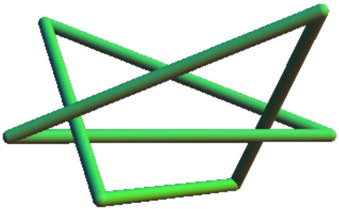
Then $\mathrm{Arm}(n;\vec{r}) \cong S^2(r_1) \times \ldots \times S^2(r_n)$.

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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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

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

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*.

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.*

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.*

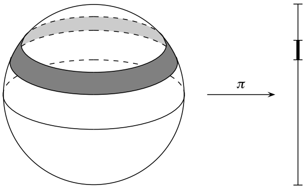
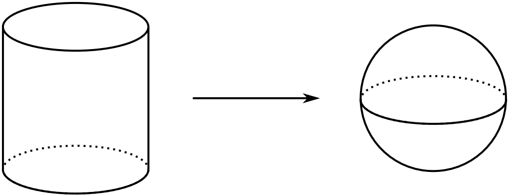


Illustration by Kuperberg.

Action-Angle Coordinates are Cylindrical Coordinates



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

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)

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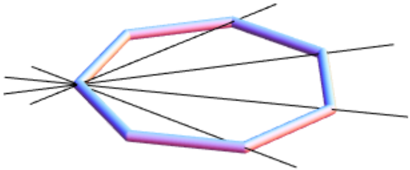
 & \widehat{\mathrm{Pol}}(n; \vec{r}) &
\end{tikzcd}
$$

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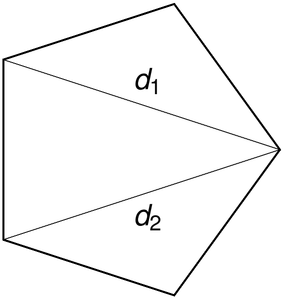
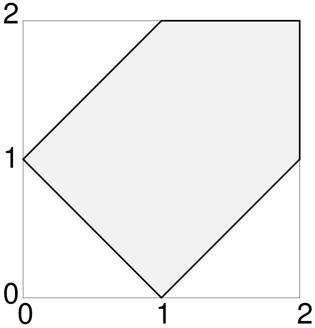
This action turns out to be Hamiltonian. Since the chordlengths $d_1, \ldots, d_{n-3}$ are the conserved quantities, the corresponding moment map is $\delta : \widehat{\text{Pol}}(n; \vec{r}) \to \mathbb{R}^{n-3}$ given by

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

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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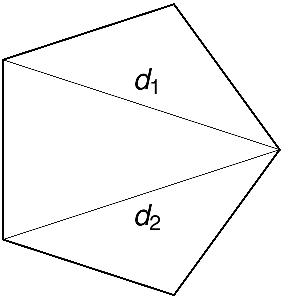

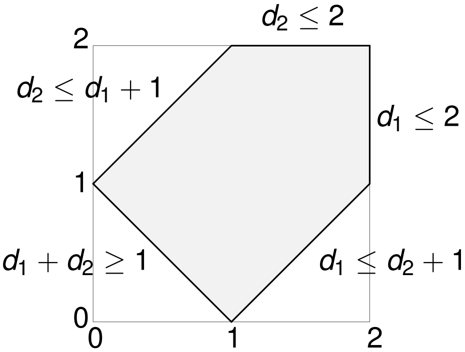

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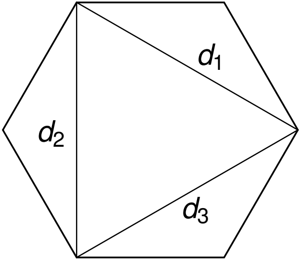
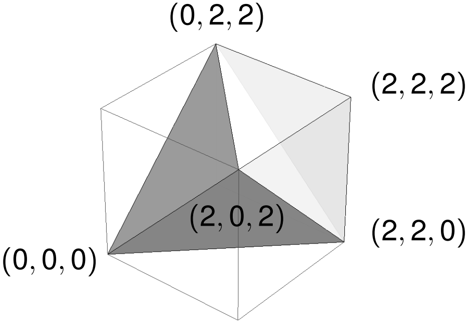
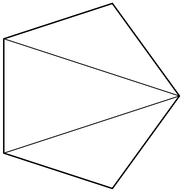


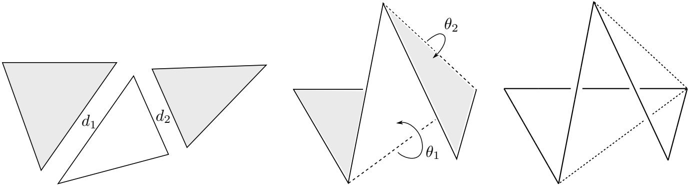


Definition

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

$$E(\mathrm{chord}(37,112)) = \frac{\begin{array}{l}25861476296024818723727071343547845818281662397356380\\0021498840205773666873699649081859732772942937515 33\\82121765570397854911152980222231191532164599823845 5\\19580796675059558748402985833382224809543932596556 9\end{array}}{\begin{array}{l}56101897729229609641981567906820376600999326126862 6\\70741808227567749566915324470667755069070793713602 7\\42451911778655557504821382917026456962863731547715 8\\30736864104509710331049682032345731824399239505510 4\end{array}} \approx 4.60973$$

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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)

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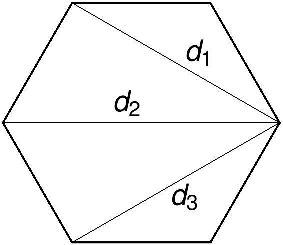
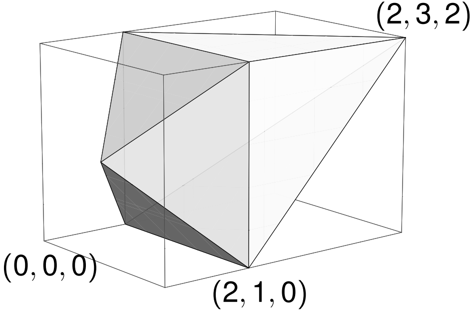
- Direct Sampling Algorithms
  - triangle method (Moore et al. 2004)
    - samples a subset of closed polygons
  - generalized hedgehog method (Varela et al. 2009)
    - unproved whether this is correct distribution
  - sinc integral method (Moore et al. 2005, Diao et al. 2011)
    - requires sampling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

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

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

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

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

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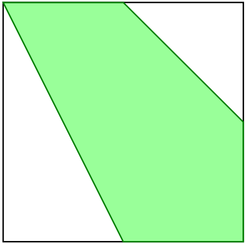

$\mathcal{C}_5$

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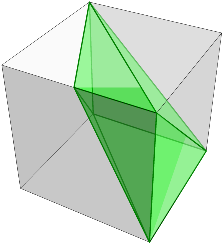
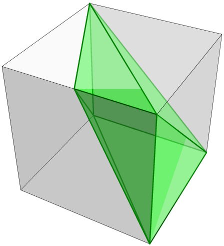


$\mathcal{C}_6$

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



$\mathcal{C}_6$

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)

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

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

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

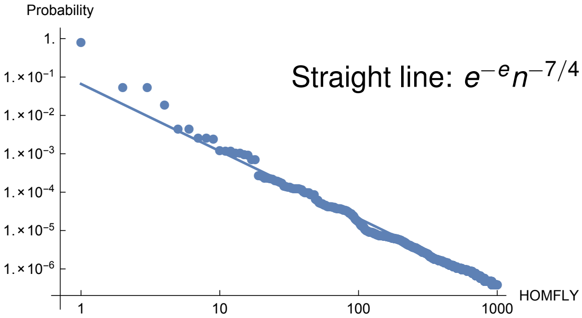
Therefore,

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

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

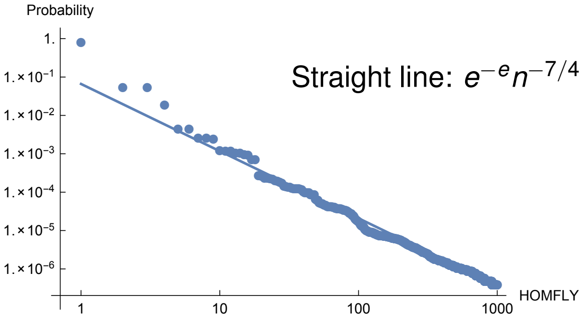
1. *Generate* $(s_1, \ldots, s_{n-3})$ *uniformly on* $[-1, 1]^{n-3}$ *$O(n)$ time*
2. *Test whether* $(s_1, \ldots, s_{n-3}) \in \mathcal{C}_n$ *acceptance ratio* $\sim 1/n^{3/2}$
3. *Let* $s_{n-2} = -\sum s_i$ *and change coordinates to get diagonal lengths*
4. *Generate dihedral angles from* T^{n-3}
5. *Build sample polygon in action-angle coordinates*

Knot Types of 10 Million 60-gons



Straight line: $e^{-e} n^{-7/4}$

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

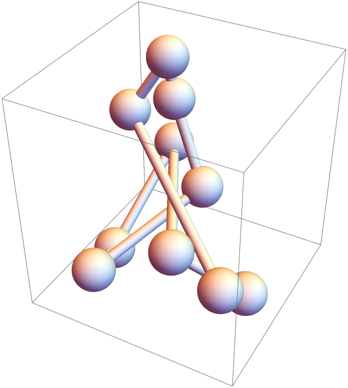
Algebraic Geometry and Measures

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

Question

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

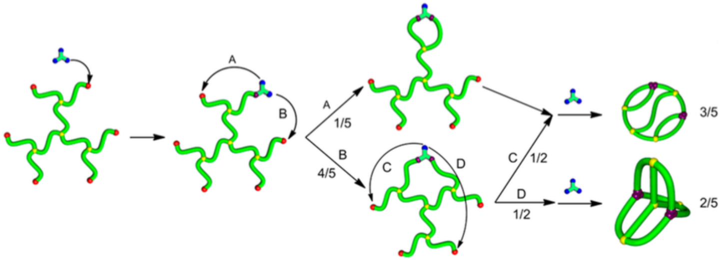
Symplectic Geometry and Excluded Volume



Question

How to incorporate excluded volume into the model?

Topologically Constrained Random Walks



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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 for listening!

- *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