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

Clayton Shonkwiler

Colorado State University

Simons Center for Geometry and Physics
October 12, 2015

From Variable Edgelengths to Fixed Edgelengths

In his talk, Jason described a model for closed, relatively framed polygons in $\mathbb{R}^3$ of *total length* 2 based on the Grassmannian $G_2(\mathbb{C}^n)$.

From Variable Edgelengths to Fixed Edgelengths

In his talk, Jason described a model for closed, relatively framed polygons in $\mathbb{R}^3$ of *total length* 2 based on the Grassmannian $G_2(\mathbb{C}^n)$.

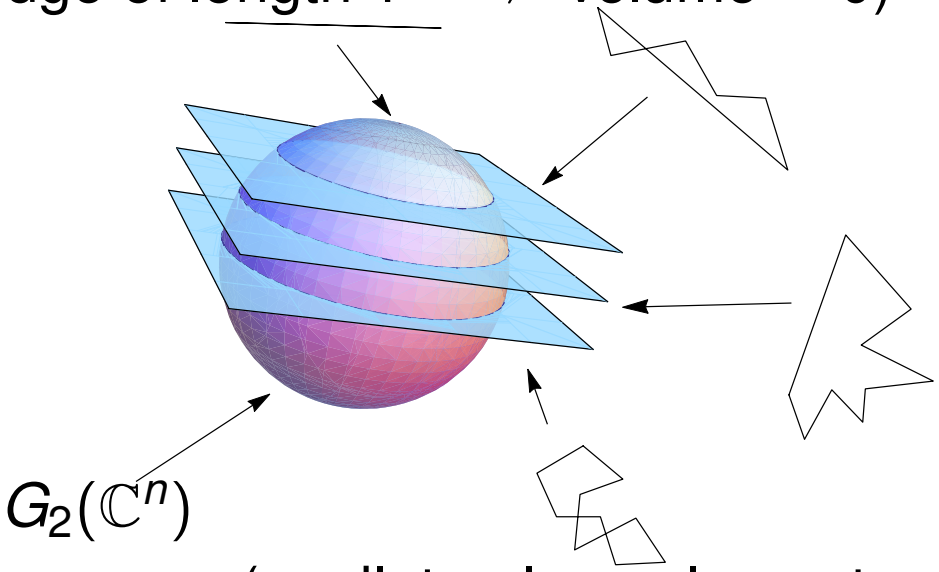
How to specialize to *unframed* polygons with *fixed* edgelengths (for example, equilateral polygons)?

From Variable Edgelengths to Fixed Edgelengths

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)?

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

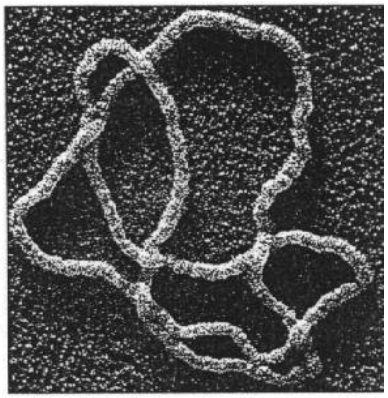


(equilaterals are largest volume)

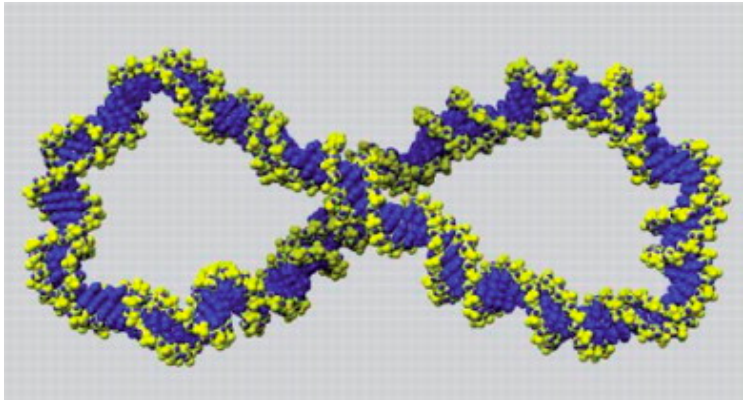
$G_2(\mathbb{C}^n)$ is an assembly of fixed edge length spaces

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

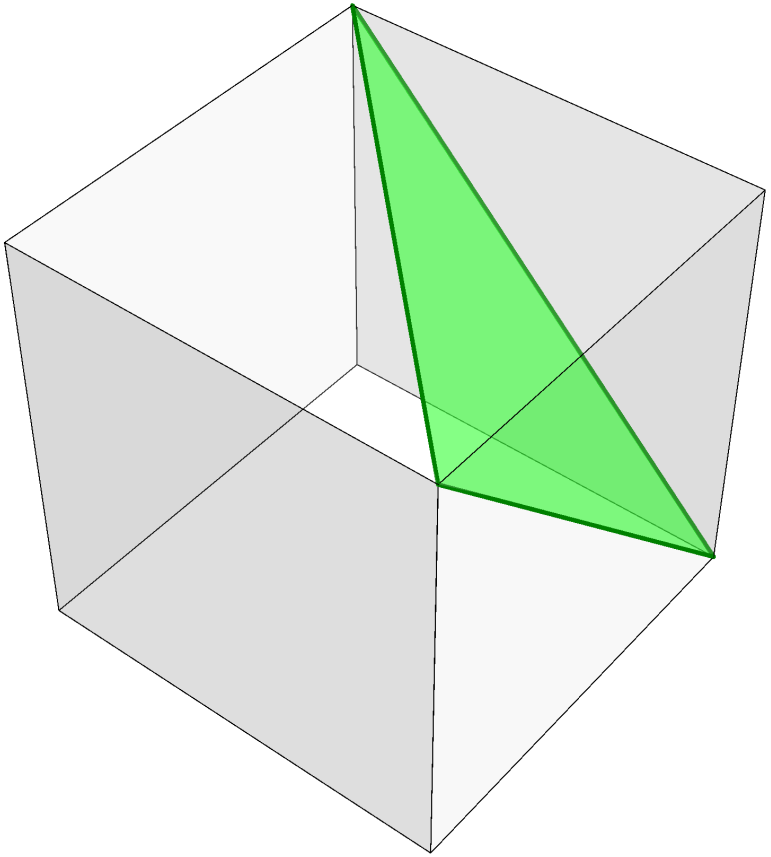
Three main goals for this talk:

1. Describe how the moduli spaces of fixed edgelength polygons 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

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



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

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

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:

$$\mathcal{E} : \begin{pmatrix} a_1 & b_1 \\ a_2 & b_2 \\ \vdots & \vdots \\ a_n & b_n \end{pmatrix} \mapsto \begin{pmatrix} |a_1|^2 + |b_1|^2 \\ |a_2|^2 + |b_2|^2 \\ \vdots \\ |a_n|^2 + |b_n|^2 \end{pmatrix}$$

Fixed Edgelength Spaces

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

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

Fixed Edgelength Spaces

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

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

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

$$\widehat{\mathrm{Pol}}(n; \vec{r}) = \mathcal{E}^{-1}(\vec{r})/U(1)^n.$$

Fixed Edgelength Spaces

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

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

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

$$\widehat{\mathrm{Pol}}(n; \vec{r}) = \mathcal{E}^{-1}(\vec{r})/U(1)^n.$$

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 $U(1)^n/\mathcal{D} \simeq U(1)^{n-1}$.

Fixed Edgelength Spaces

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

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

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

$$\widehat{\mathrm{Pol}}(n; \vec{r}) = \mathcal{E}^{-1}(\vec{r})/U(1)^{n-1}.$$

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 $U(1)^n/\mathcal{D} \simeq U(1)^{n-1}$.

The Big Picture (via Hausmann–Knutson)

$$\begin{tikzcd}
G_2(\mathbb{C}^n) & \\
\mathcal{E}^{-1}(\vec{r}) \arrow[u, hook] \arrow[dr, "/U(1)^{n-1}"'] & \\
& \widehat{\mathrm{Pol}}(n;\vec{r})
\end{tikzcd}$$

The Big Picture (via Hausmann–Knutson)

$$
\begin{tikzcd}
 & (\mathbb{C}^2)^n \\
V_2(\mathbb{C}^n) \arrow[ur, hook] \arrow[d, "/U(2)"'] & \\
G_2(\mathbb{C}^n) & \\
\mathcal{E}^{-1}(\vec{r}) \arrow[u, hook] \arrow[dr, "/U(1)^{n-1}"'] & \\
 & \widehat{\mathrm{Pol}}(n;\vec{r})
\end{tikzcd}
$$

The Big Picture (via Hausmann–Knutson)

$$
\begin{tikzcd}
 & (\mathbb{C}^2)^n & \\
V_2(\mathbb{C}^n) \arrow[ur, hook] \arrow[d, "/U(2)"'] & & \mathcal{E}^{-1}(\vec{r}) = \prod S^3(r_i) \arrow[ul, hook'] \arrow[d, "/U(1)^n"] \\
G_2(\mathbb{C}^n) & & \prod S^2(r_i) \\
\mathcal{E}^{-1}(\vec{r}) \arrow[u, hook] \arrow[dr, "/U(1)^{n-1}"'] & & \mathrm{Pol}(n;\vec{r}) \arrow[u, hook'] \arrow[dl, "/SO(3)"] \\
 & \widehat{\mathrm{Pol}}(n;\vec{r}) &
\end{tikzcd}
$$

The Big Symplectic Picture

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

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.

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.

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.

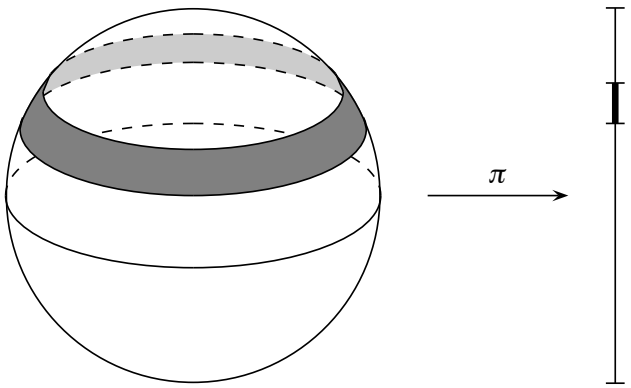
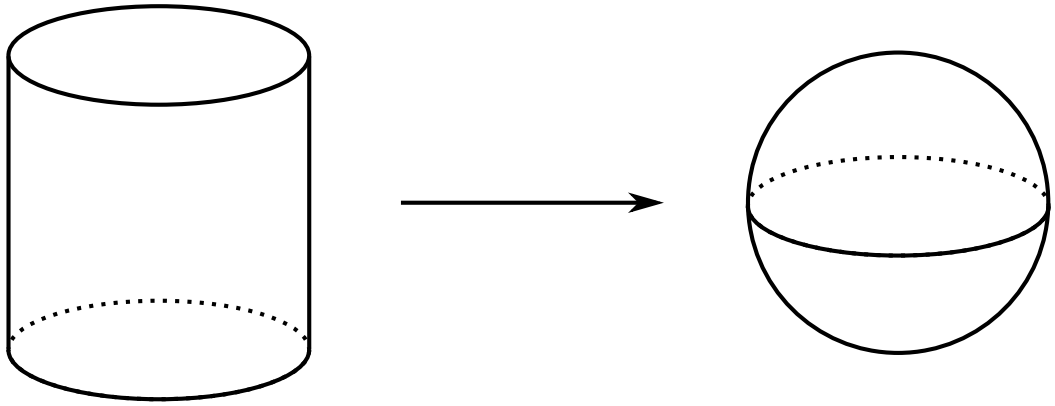


Illustration by Kuperberg.

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)

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

The Big Algebraic Geometry Picture

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

The Big Algebraic Geometry Picture

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

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

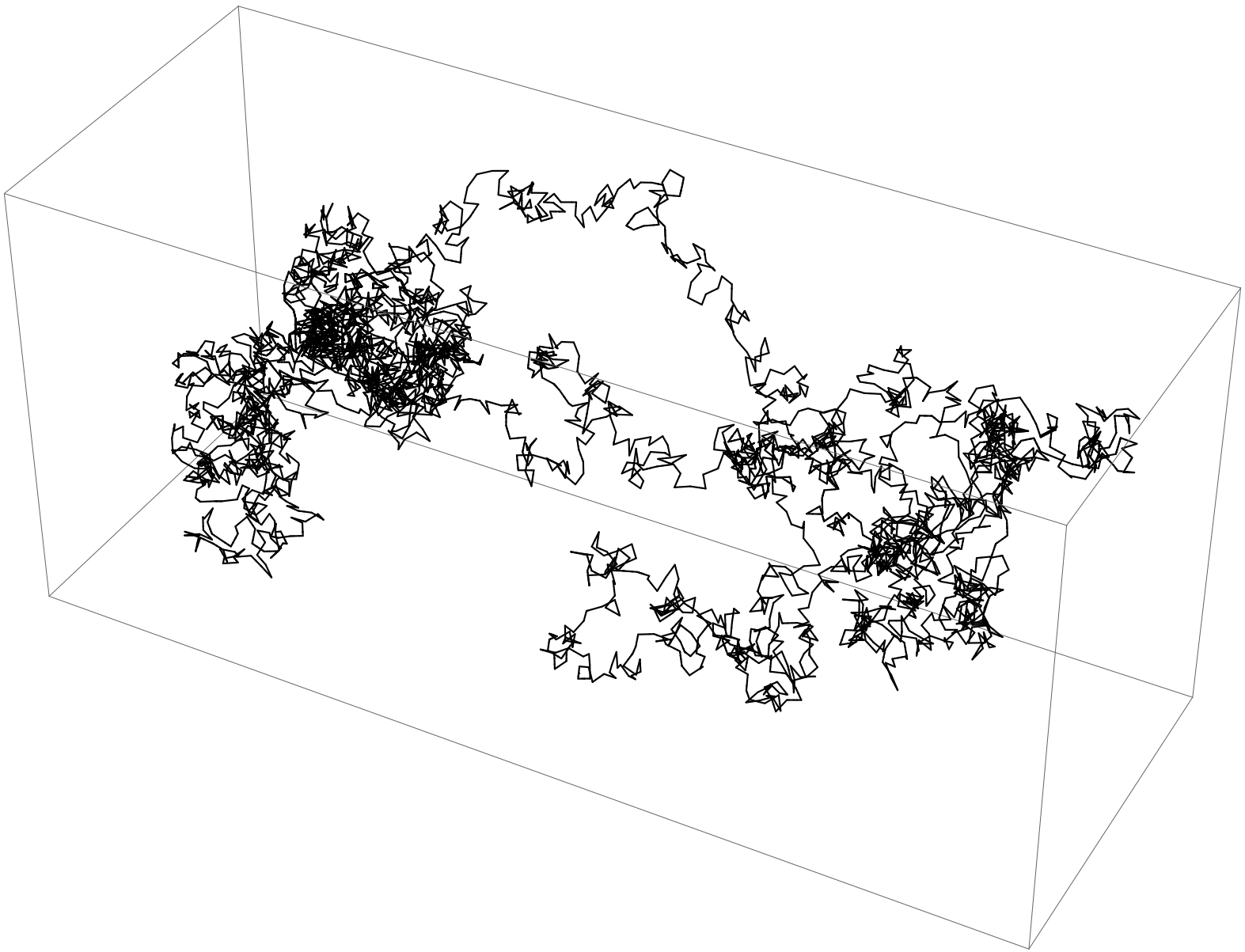
$$\begin{tikzcd}
 & (\mathbb{C}^2)^n \arrow[dl, dash, "/\!/GL(2,\mathbb{C})"'] \arrow[dr, dash, "/\!/(\mathbb{C}^*)^n"] & \\
G_2(\mathbb{C}^n) \arrow[dr, dash, "/\!/(\mathbb{C}^*)^{n-1}"'] & & \prod(\mathbb{CP}^1)^n \arrow[dl, dash, "/\!/PGL(2,\mathbb{C})"] \\
 & \widehat{\mathrm{Pol}}(n;\vec{r}) &
\end{tikzcd}$$

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 $\widehat{\mathrm{Pol}}(n;\vec{r})$?

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

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 *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 *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

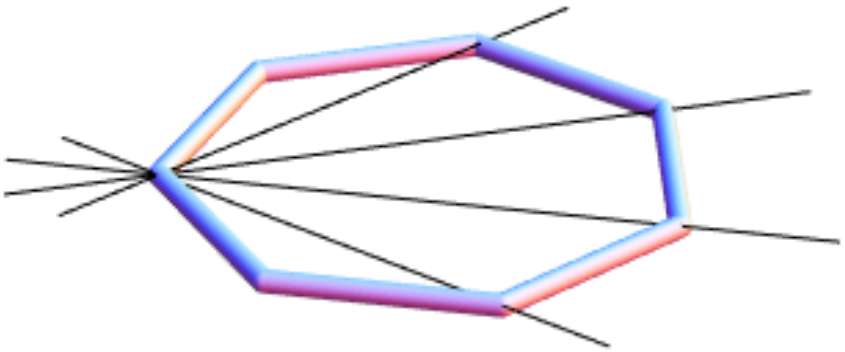
$$\mu(\vec{e}_1, \ldots, \vec{e}_n) = \sum \vec{e}_i.$$

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

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

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



$\widehat{\mathrm{Pol}}(n;\vec{r})$ is Toric

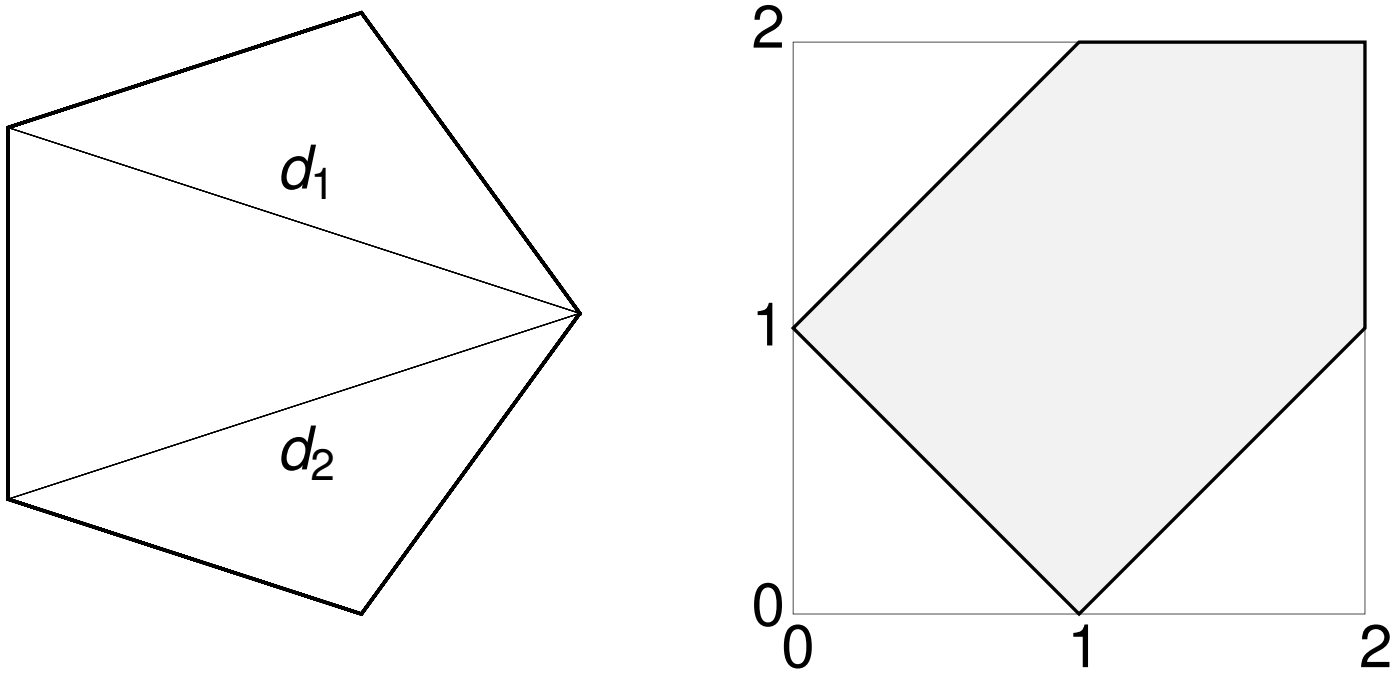
Given an (abstract) triangulation of the n-gon, the folds on any two chords commute. Thus, rotating around all $n-3$ of these chords by independently selected angles defines a T^{n-3} action on $\widehat{\mathrm{Pol}}(n;\vec{r})$ which preserves the chord lengths.

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

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

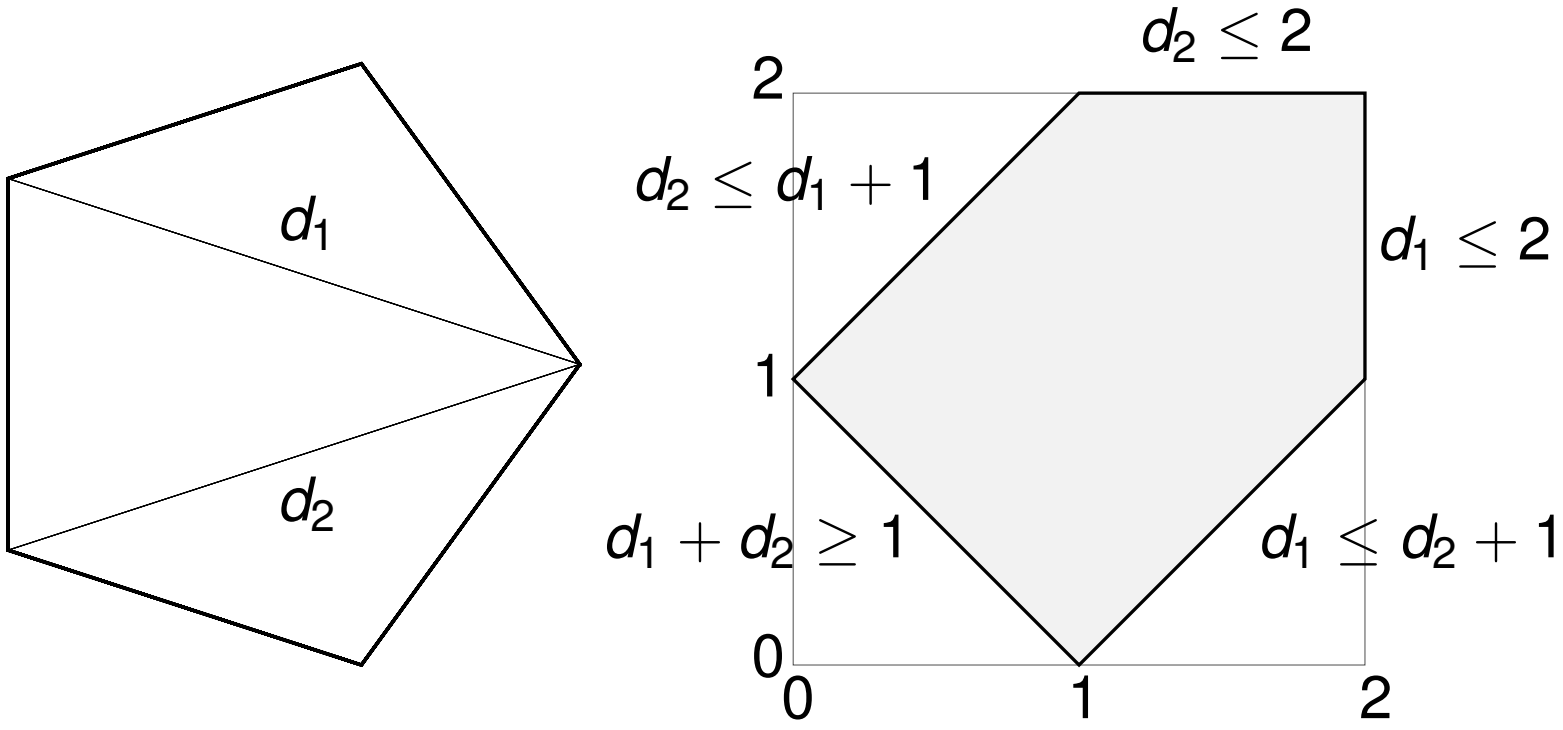
Definition

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* $\mathcal{P}_n(\vec{r})$.



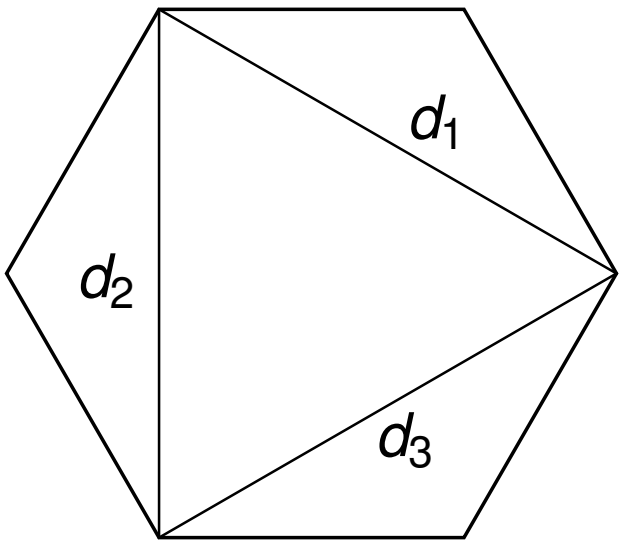
Definition

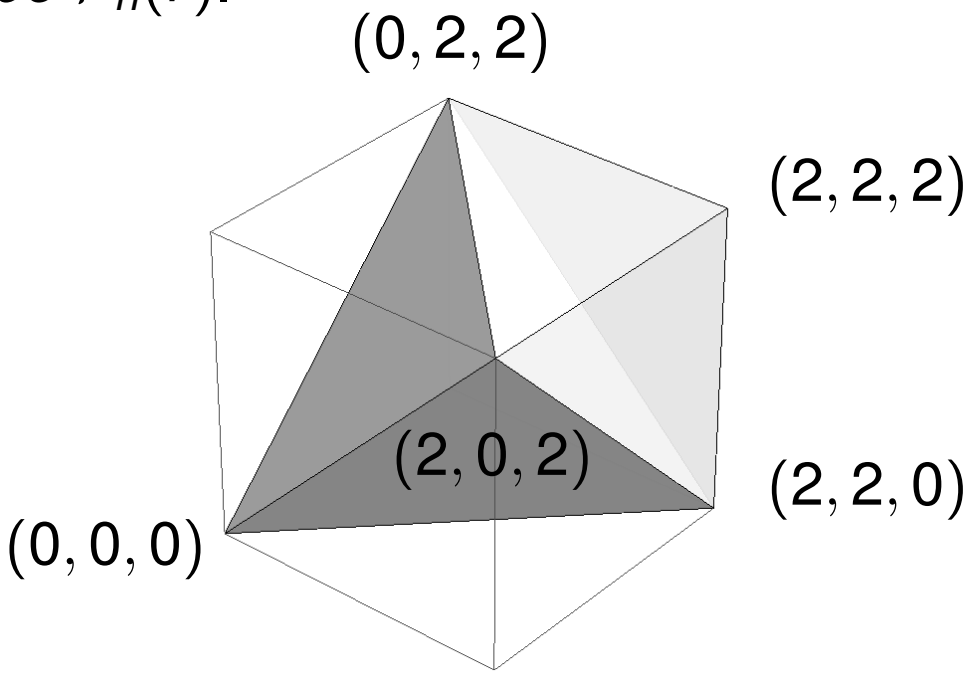
An abstract triangulation T of an n-gon picks out $n-3$ nonintersecting chords. The lengths of these chords obey triangle inequalities, so they lie in a convex polytope in $\mathbb{R}^{n-3}$ called the *triangulation polytope* $\mathcal{P}_n(\vec{r})$.



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* $\mathcal{P}_n(\vec{r})$.

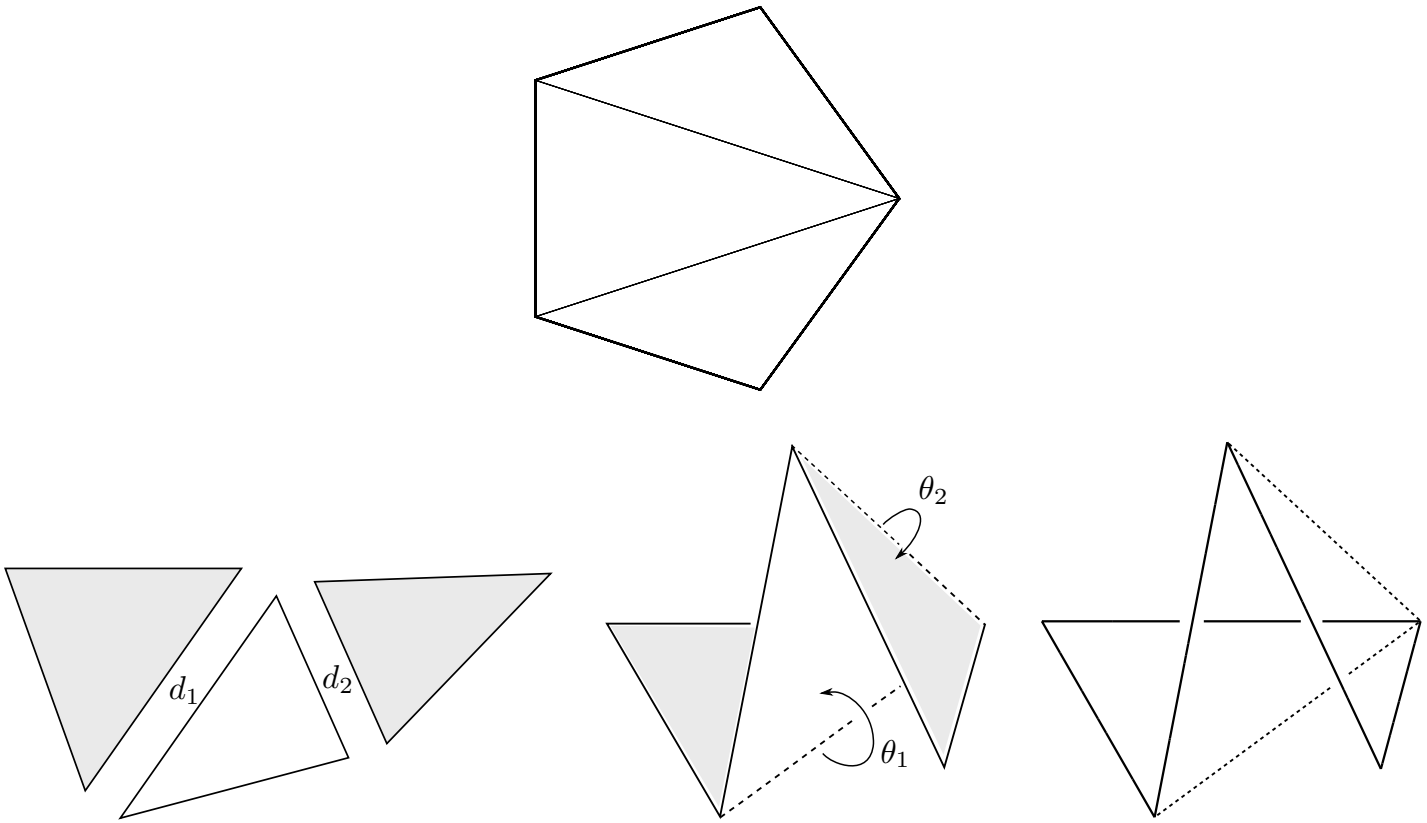




Definition

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*:

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



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 $\widehat{\mathrm{Pol}}(n; \vec{r})$.*

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 $\widehat{\mathrm{Pol}}(n; \vec{r})$.*

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. $\square$

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 $\widehat{\mathrm{Pol}}(n; \vec{r})$.*

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

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

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	$\frac{97,456}{78,400}$	$\frac{111,499}{78,400}$	$\frac{118,608}{78,400}$	$\frac{120,985}{78,400}$	$\frac{118,608}{78,400}$	$\frac{111,499}{78,400}$	$\frac{97,456}{78,400}$

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

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

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

$$\approx 4.60973$$

Excluded Volume?

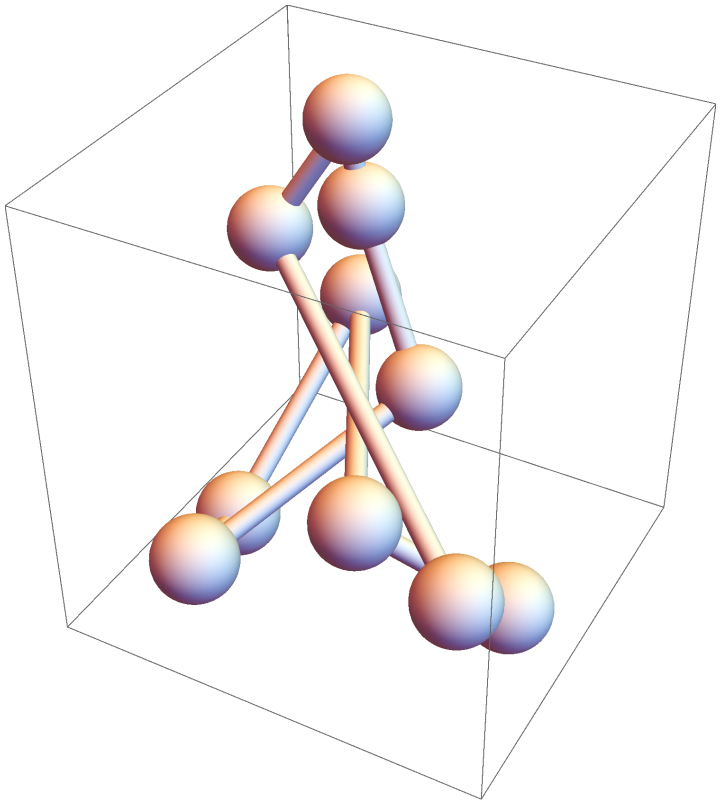
Question

How to incorporate excluded volume into the model?

Excluded Volume?

Question

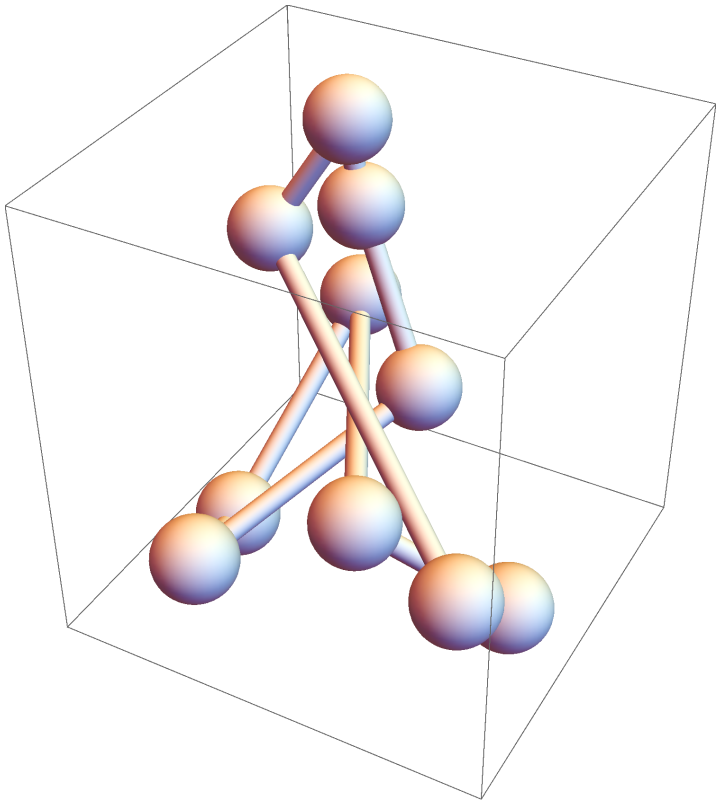
How to incorporate excluded volume into the model?



Excluded Volume?

Question

How to incorporate excluded volume into the model?



$$\left| \sum_{i=j}^{k} \vec{e}_i \right|^2 \geq \epsilon.$$

Proposition (with Cantarella)

At least $1/2$ of the space of equilateral 6-edge polygons consists of unknots.

Proposition (with Cantarella)

At least $1/2$ 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 $1/2$ 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?

An (Incomplete?) History

Sampling Algorithms for Equilateral Polygons:

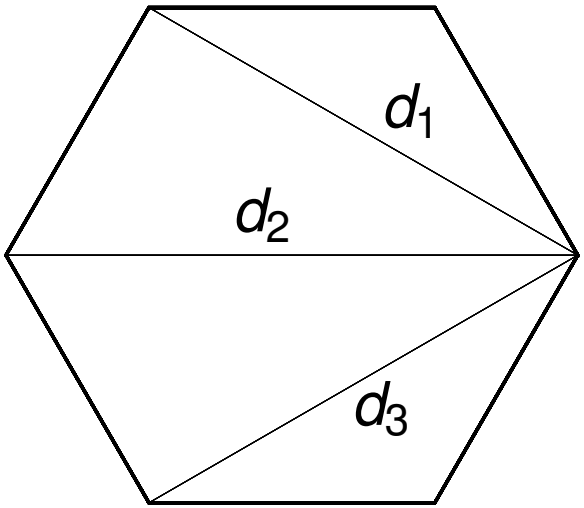
- Markov Chain Algorithms
  - crankshaft (Vologoskii 1979, Klenin 1988)
  - polygonal fold (Millett 1994)
- Direct Sampling Algorithms
  - triangle method (Moore 2004)
  - generalized hedgehog method (Varela 2009)
  - sinc integral method (Moore 2005, Diao 2011)

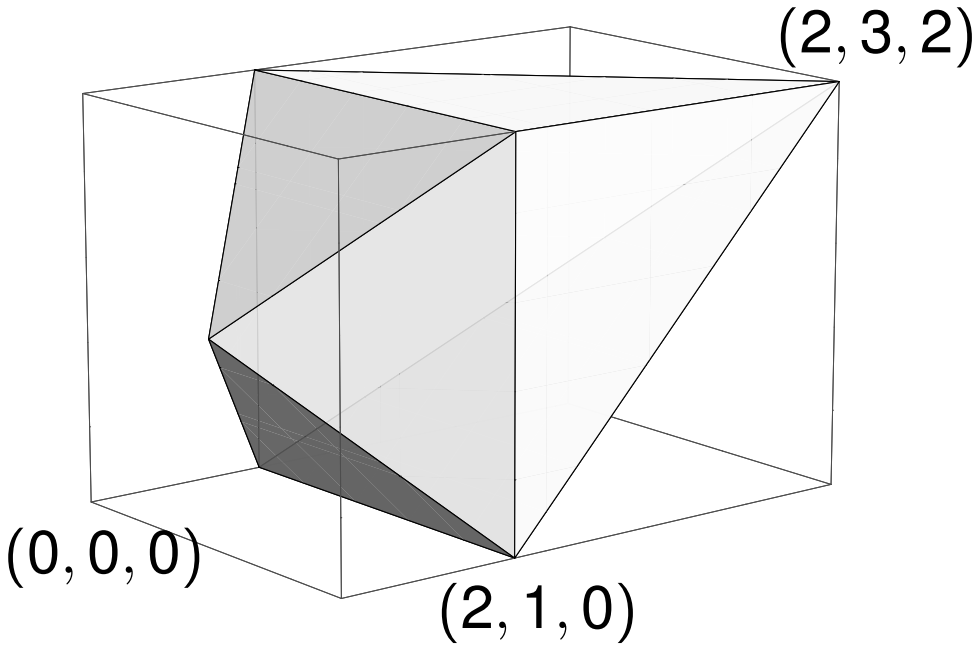
An (Incomplete?) History

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
  - 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

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

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

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 $s_1, \ldots, s_{n-3}$ and the inequalities

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

become

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

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 $s_1, \ldots, s_{n-3}$ and the inequalities

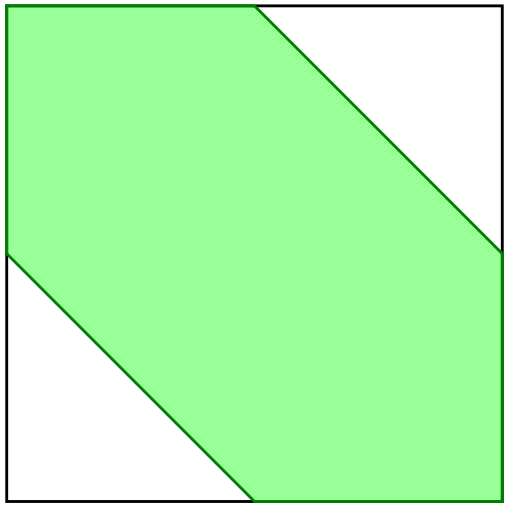
$$0 \leq d_1 \leq 2 \qquad \begin{array}{c} 1 \leq d_i + d_{i+1} \\ |d_i - d_{i+1}| \leq 1 \end{array} \qquad 0 \leq d_{n-3} \leq 2$$

become

$$\underbrace{-1 \leq s_i \leq 1, \quad -1 \leq \sum_{i=1}^{n-3} s_i \leq 1,}_{\text{easy conditions}} \quad \underbrace{\sum_{j=1}^{i} s_j + \sum_{j=1}^{i+1} s_j \geq -1}_{\text{hard conditions}}$$

Definition

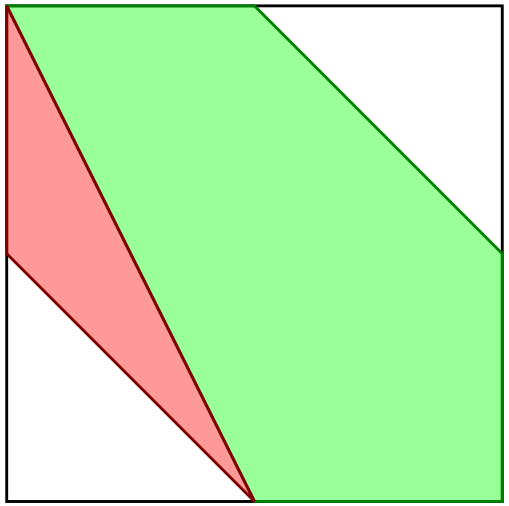
The $(n-3)$-dimensional polytope $\mathcal{Q}_n$ is the slab of the hypercube $[-1,1]^{n-3}$ determined by $-1 \leq s_1 + \ldots + s_{n-3} \leq 1$.



$\mathcal{Q}_5$

Definition

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



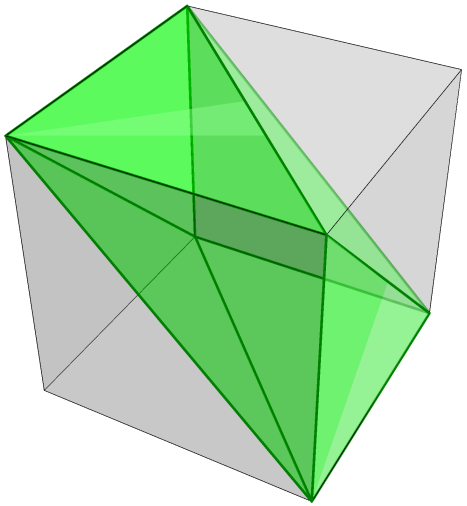
$\mathcal{C}_5$

Idea

Sample points in $\mathcal{Q}_n$, which all obey the "easy conditions", and reject any samples which fail to obey the "hard conditions".

Definition

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



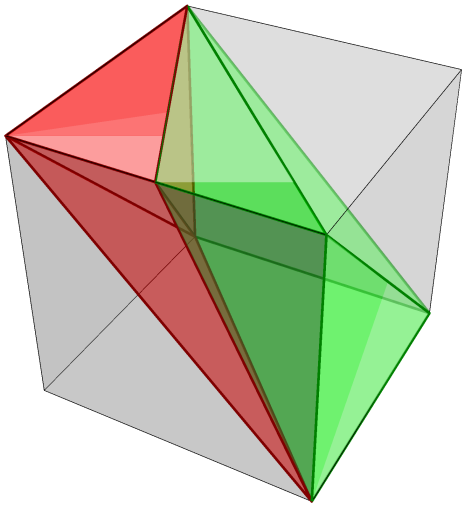
$\mathcal{Q}_6$

Idea

Sample points in $\mathcal{Q}_n$, which all obey the "easy conditions", and reject any samples which fail to obey the "hard conditions".

Definition

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



$\mathcal{C}_6$

Idea

Sample points in $\mathcal{Q}_n$, which all obey the "easy conditions", and reject any samples which fail to obey the "hard conditions".

Theorem (Marichal–Mossinghoff)

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

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

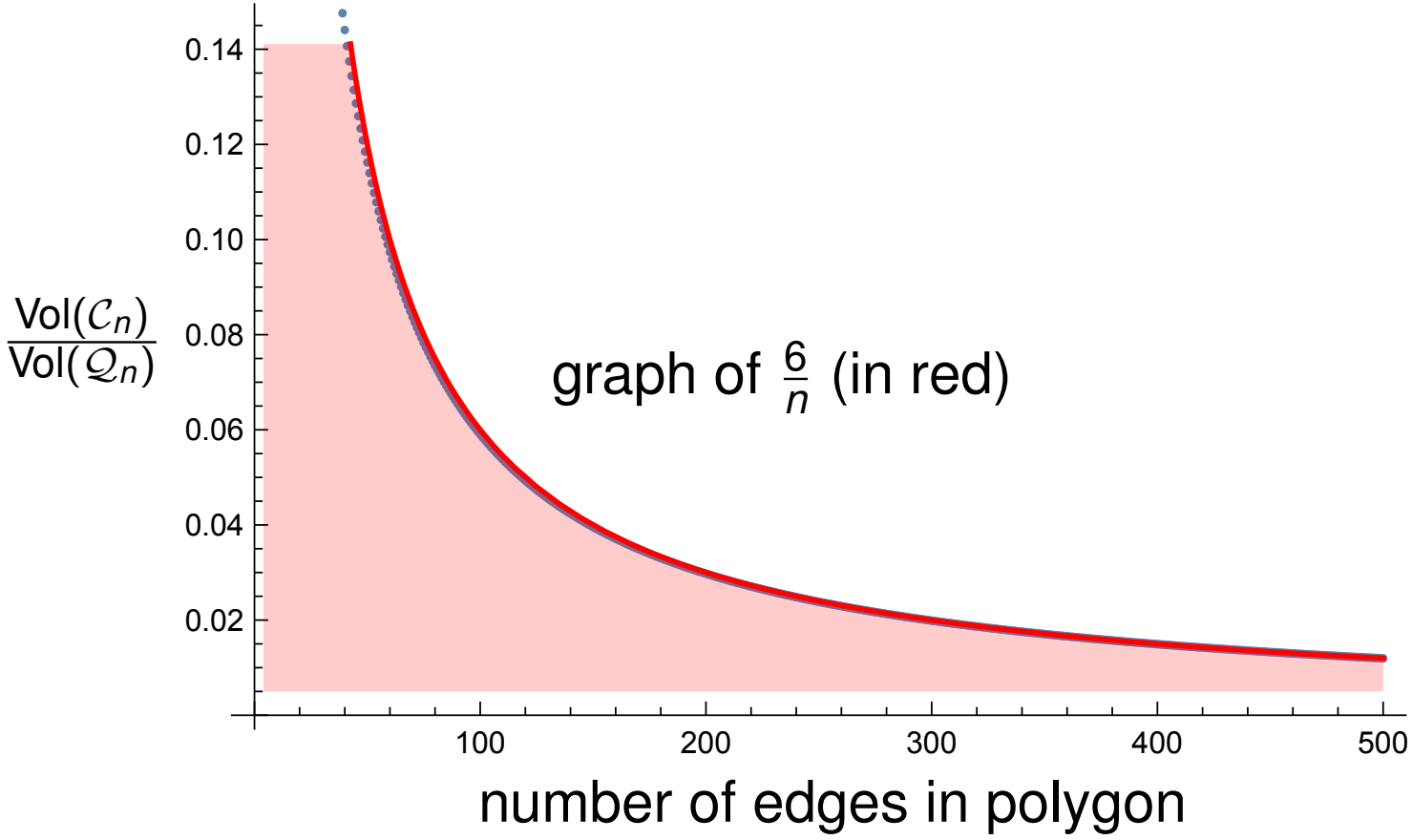
Theorem (Khoi, Takakura, Mandini)

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

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

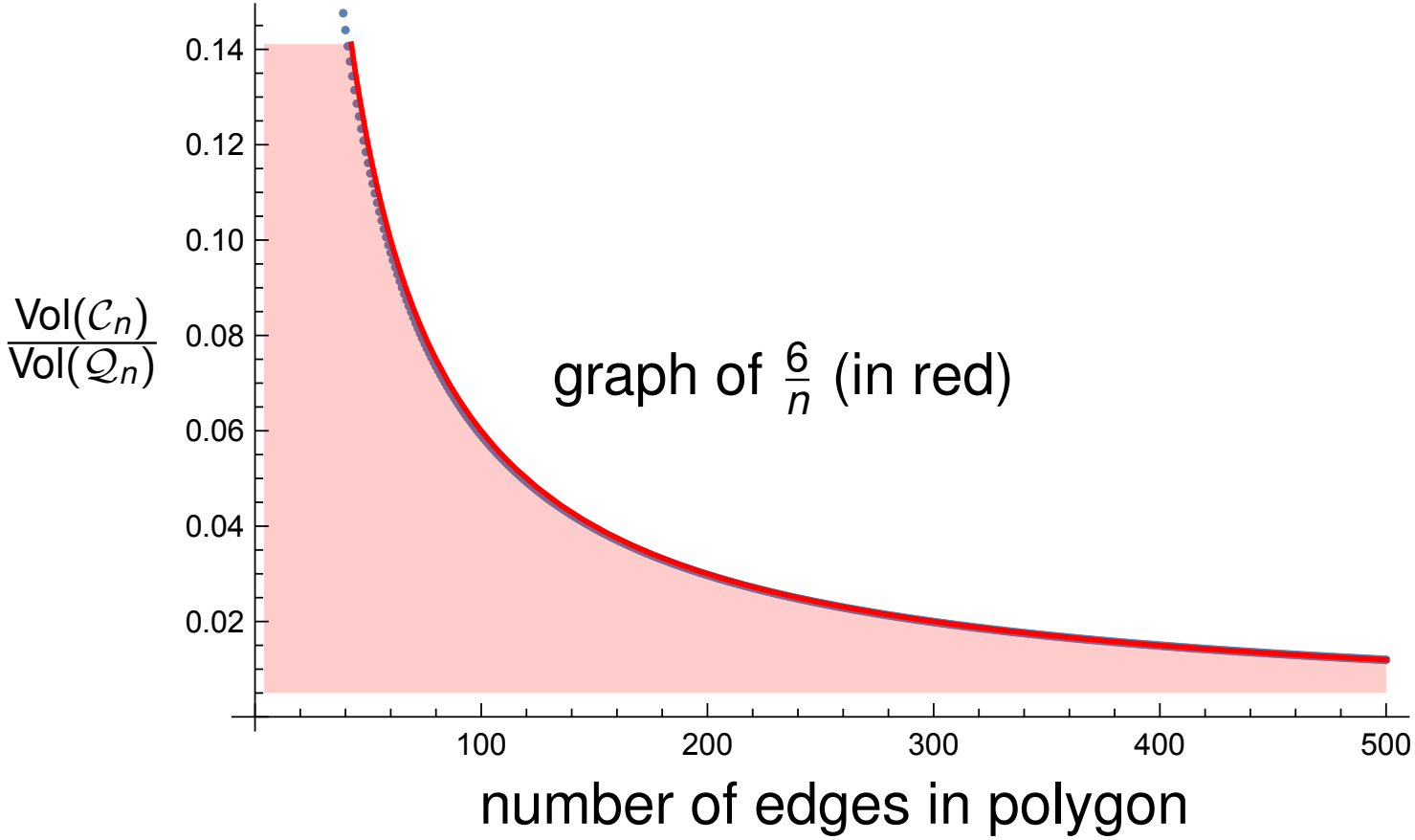
Runtime of algorithm depends on acceptance ratio

Acceptance ratio $= \frac{\mathrm{Vol}(\mathcal{C}_n)}{\mathrm{Vol}(\mathcal{Q}_n)}$ is conjectured $\simeq \frac{6}{n}$. It is certainly bounded below by $\frac{1}{n}$.



Runtime of algorithm depends on acceptance ratio

Acceptance ratio $= \frac{\mathrm{Vol}(\mathcal{C}_n)}{\mathrm{Vol}(\mathcal{Q}_n)}$ is conjectured $\simeq \frac{6}{n}$. It is certainly bounded below by $\frac{1}{n}$.



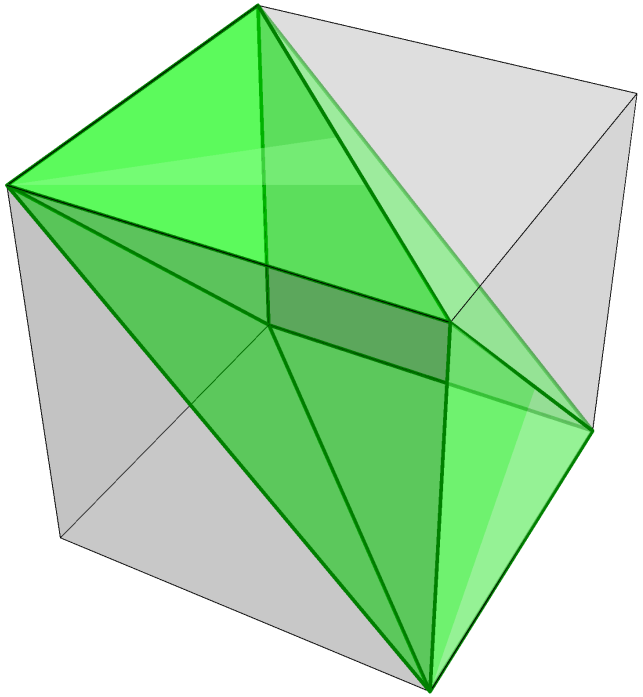
Moral

This approach is reasonable if we can sample $\mathcal{Q}_n$ efficiently.

Sampling $\mathcal{Q}_n$

We can sample $\mathcal{Q}_n$ by rejection sampling $[-1,1]^{n-3}$. The acceptance probability is

$$\frac{\mathrm{Vol}\,\mathcal{Q}_n}{\mathrm{Vol}[-1,1]^{n-3}}.$$



$\mathcal{Q}_6$

Sampling $\mathcal{Q}_n$

We can sample $\mathcal{Q}_n$ by rejection sampling $[-1,1]^{n-3}$. The acceptance probability is

$$\frac{\mathrm{Vol}\,\mathcal{Q}_n}{\mathrm{Vol}[-1,1]^{n-3}}.$$

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

Sampling $\mathcal{Q}_n$

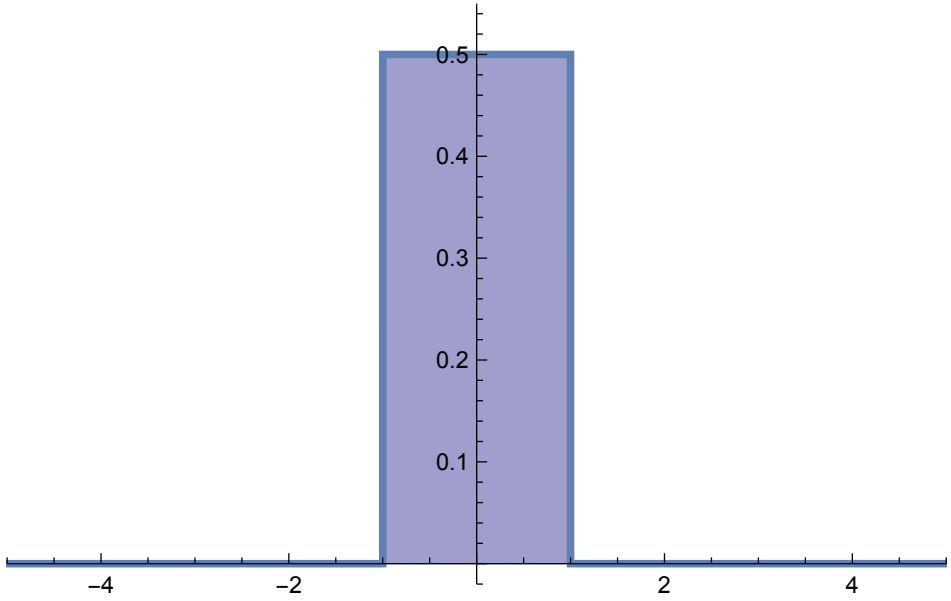
We can sample $\mathcal{Q}_n$ by rejection sampling $[-1,1]^{n-3}$. The acceptance probability is

$$\frac{\mathrm{Vol}\,\mathcal{Q}_n}{\mathrm{Vol}[-1,1]^{n-3}}.$$

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

$n = 4$

$\mathbb{P}(-1 \leq \sum s_i \leq 1) = 1$



Sampling $\mathcal{Q}_n$

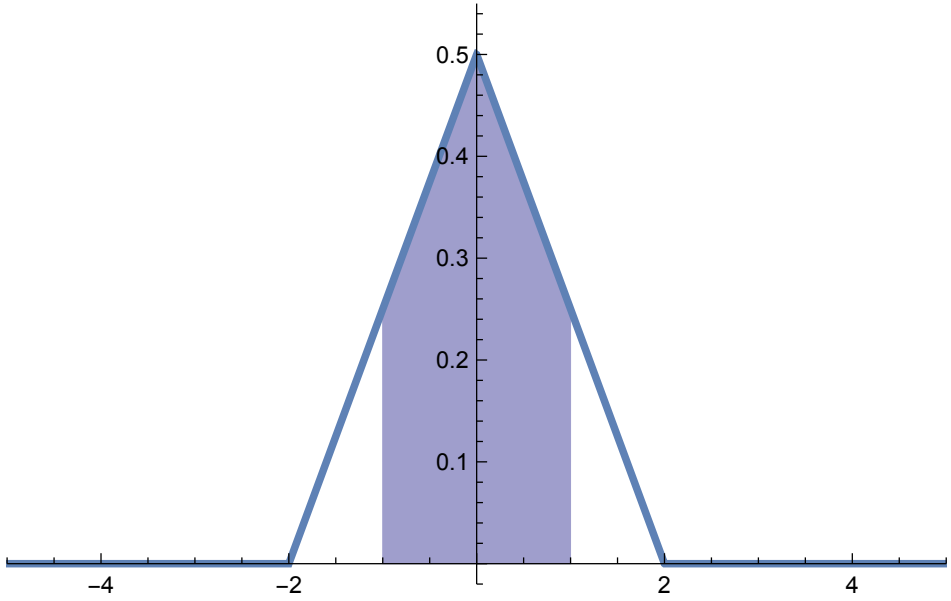
We can sample $\mathcal{Q}_n$ by rejection sampling $[-1,1]^{n-3}$. The acceptance probability is

$$\frac{\mathrm{Vol}\,\mathcal{Q}_n}{\mathrm{Vol}[-1,1]^{n-3}}.$$

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

$n = 5$

$\mathbb{P}(-1 \leq \sum s_i \leq 1) = \frac{3}{4}$



Sampling $\mathcal{Q}_n$

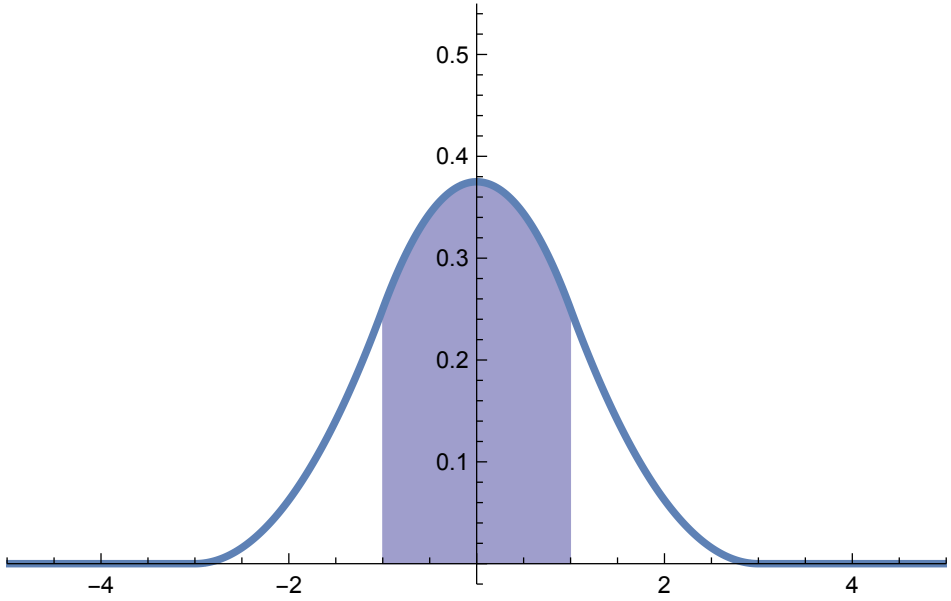
We can sample $\mathcal{Q}_n$ by rejection sampling $[-1,1]^{n-3}$. The acceptance probability is

$$\frac{\mathrm{Vol}\,\mathcal{Q}_n}{\mathrm{Vol}[-1,1]^{n-3}}.$$

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

$n = 6$

$\mathbb{P}(-1 \leq \sum s_i \leq 1) = \frac{2}{3}$



Sampling $\mathcal{Q}_n$

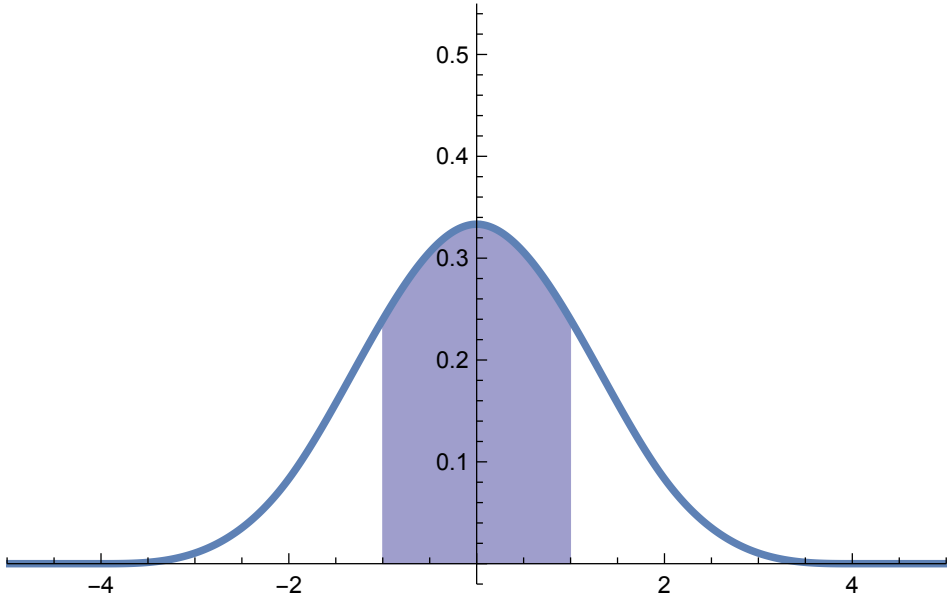
We can sample $\mathcal{Q}_n$ by rejection sampling $[-1,1]^{n-3}$. The acceptance probability is

$$\frac{\mathrm{Vol}\,\mathcal{Q}_n}{\mathrm{Vol}[-1,1]^{n-3}}.$$

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

$n = 7$

$\mathbb{P}(-1 \leq \sum s_i \leq 1) = \frac{115}{192}$



Sampling $\mathcal{Q}_n$

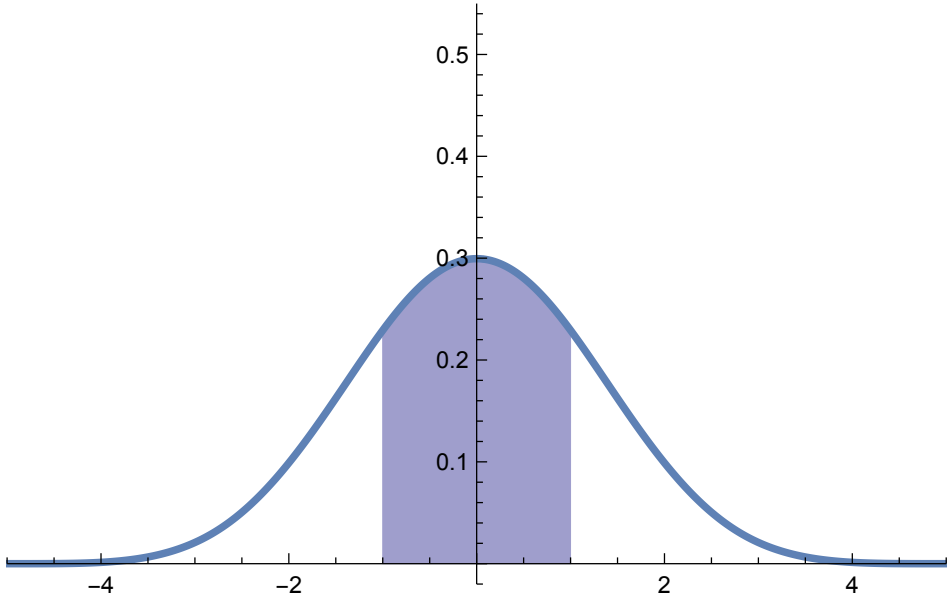
We can sample $\mathcal{Q}_n$ by rejection sampling $[-1,1]^{n-3}$. The acceptance probability is

$$\frac{\mathrm{Vol}\,\mathcal{Q}_n}{\mathrm{Vol}[-1,1]^{n-3}}.$$

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

$n = 8$

$\mathbb{P}(-1 \leq \sum s_i \leq 1) = \frac{11}{20}$



Sampling $\mathcal{Q}_n$

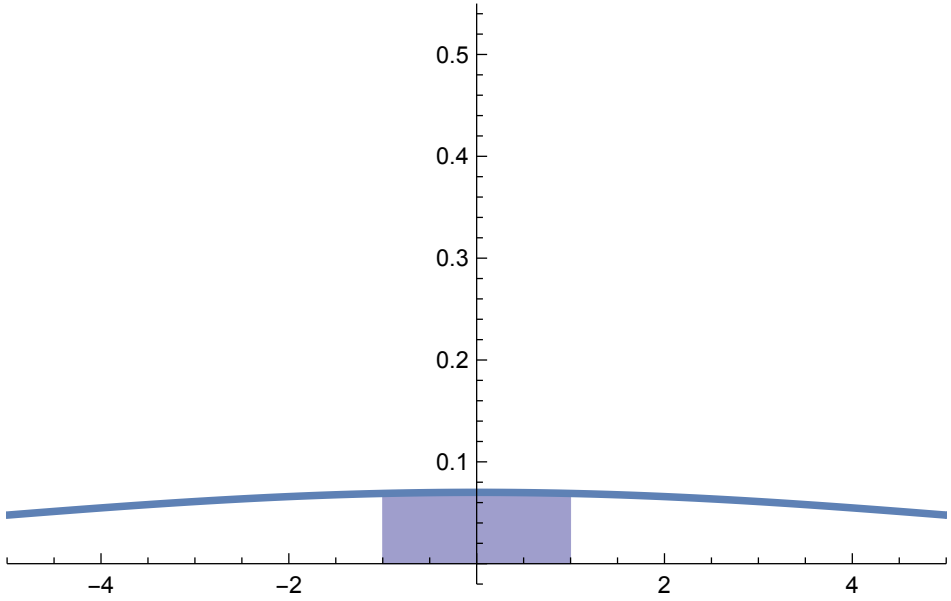
We can sample $\mathcal{Q}_n$ by rejection sampling $[-1,1]^{n-3}$. The acceptance probability is

$$\frac{\mathrm{Vol}\,\mathcal{Q}_n}{\mathrm{Vol}[-1,1]^{n-3}}.$$

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

$n = 100$

$\mathbb{P}(-1 \leq \sum s_i \leq 1) \approx 0.13938$



Sampling $\mathcal{Q}_n$

We can sample $\mathcal{Q}_n$ by rejection sampling $[-1,1]^{n-3}$. The acceptance probability is

$$\frac{\mathrm{Vol}\,\mathcal{Q}_n}{\mathrm{Vol}[-1,1]^{n-3}}.$$

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**,

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

Sampling $\mathcal{Q}_n$

We can sample $\mathcal{Q}_n$ by rejection sampling $[-1,1]^{n-3}$. The acceptance probability is

$$\frac{\operatorname{Vol} \mathcal{Q}_n}{\operatorname{Vol}[-1,1]^{n-3}}.$$

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**,

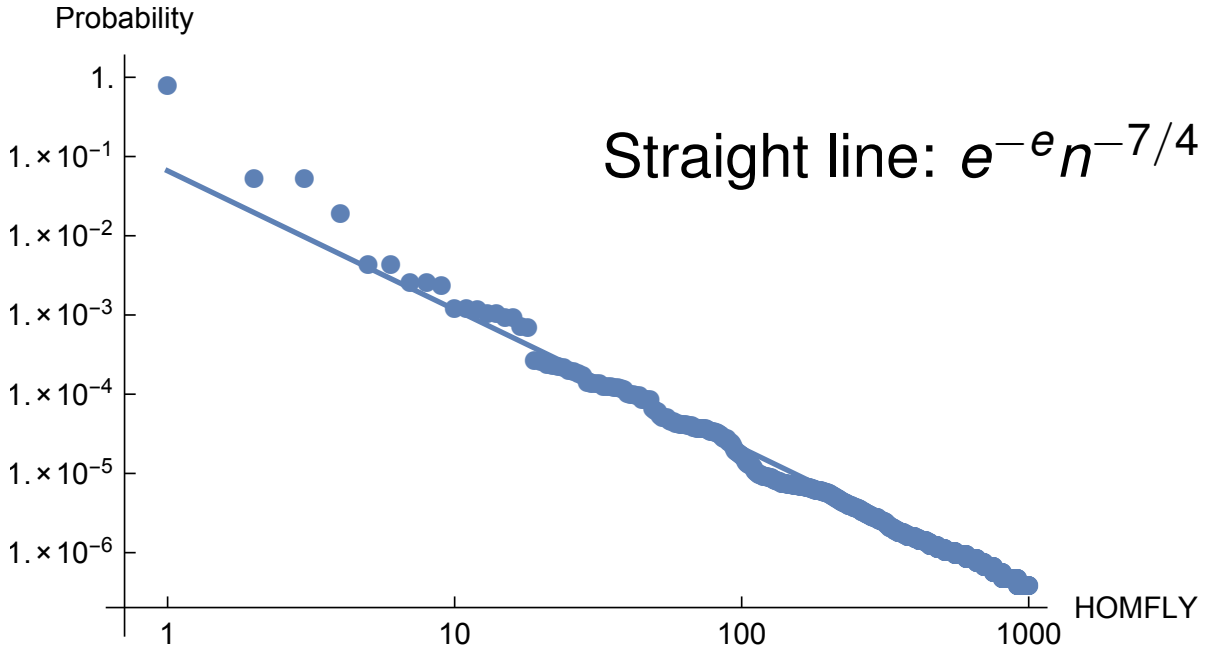
$$\mathbb{P}\left(-1 \leq \sum_{i=0}^{n-4} s_i \leq 1\right) \simeq \mathbb{P}\left(-1 \leq \mathcal{N}\left(0, \sqrt{\frac{n-3}{3}}\right) \leq 1\right)$$

$$= \operatorname{erf}\left(\sqrt{\frac{3}{2(n-3)}}\right) \simeq \sqrt{\frac{6}{\pi n}}.$$

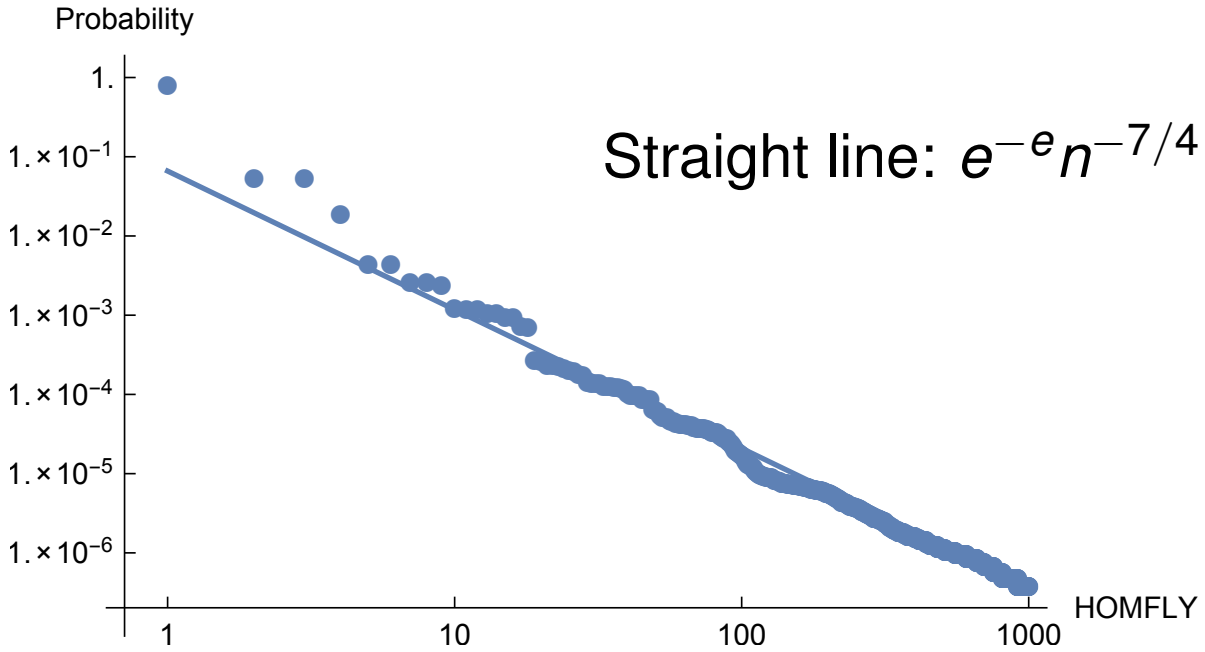
Action-Angle Method (with Cantarella and Uehara, 2015)

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



Knot Types of 10 Million 60-gons



Algorithm	distinct HOMFLYs
Polygonal Folds[1]	2219
Crankshaft Moves	6110
Hedgehog Method	1111
Triangle Method	3505
Action-Angle Method	$\geq$ 6371

[1] 100 million samples, instead of 10 million.

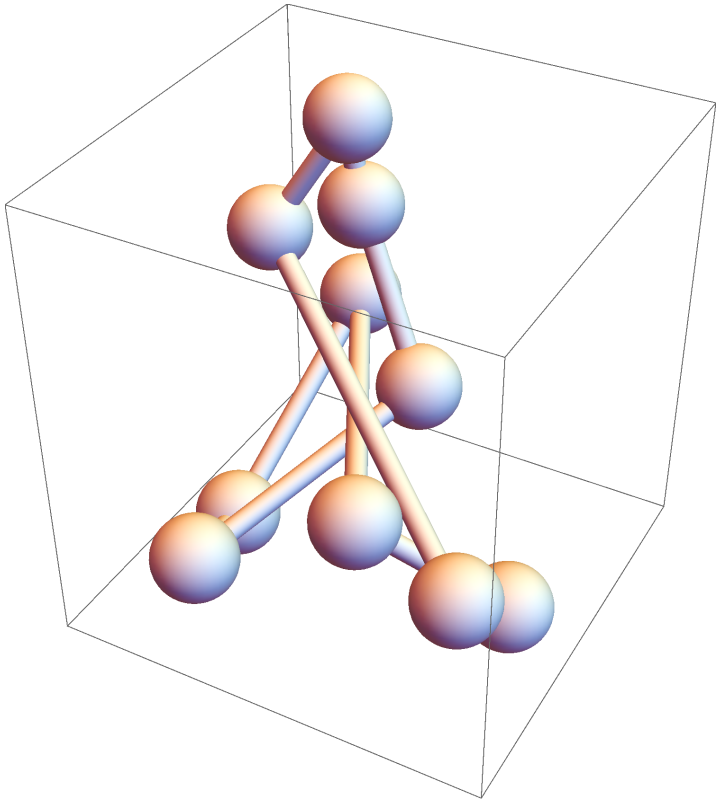
Questions

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

Question

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

Symplectic Geometry and Excluded Volume



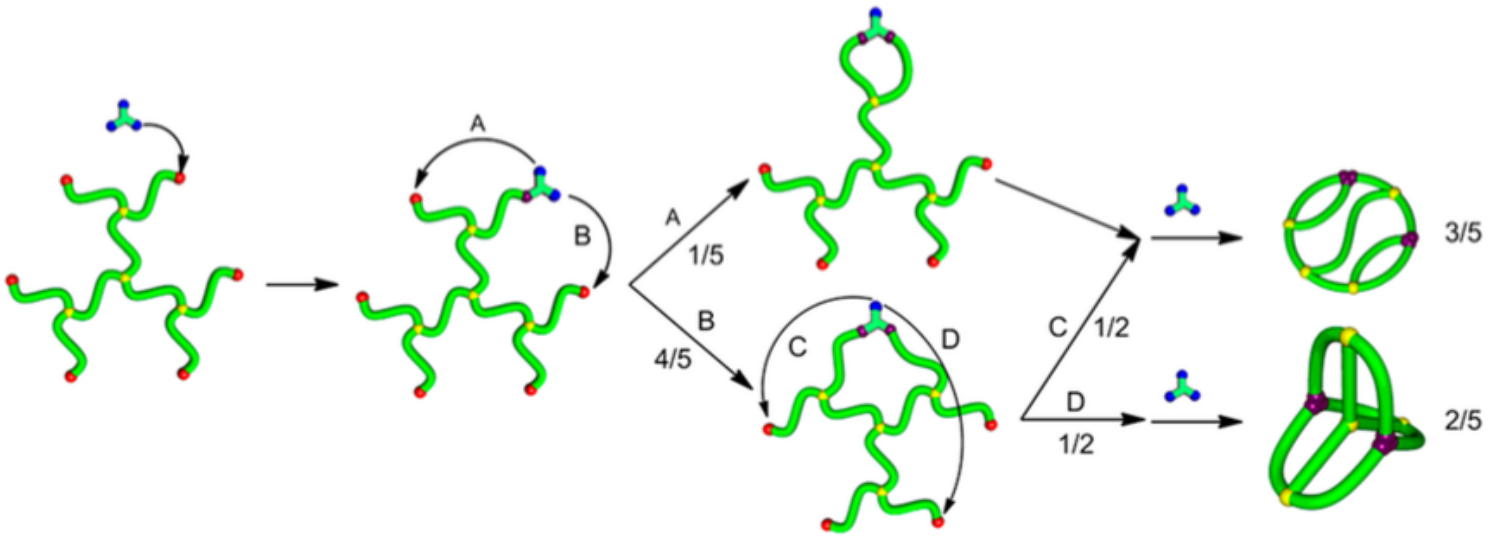
Question

How to incorporate excluded volume into the model?

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

Question

What is the analog of the symplectic story for n-gons in the plane?



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, Clayton Shonkwiler, and Erica Uehara
  `arXiv:1510.02466`

`http://shonkwiler.org`