The Symplectic Geometry of Polygon Space and How to Use It

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Geometry, Groups, and Dynamics
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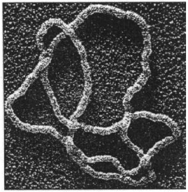
Idea

A theory of random knots requires a theory of random curves.



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

This curve is a point in what space?
What is the geometry of that space?

Goals

Basic Idea: model space curves by equilateral polygons.

Three main goals for this talk:

1. Describe how the moduli spaces of equilateral 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.

Definition

A random flight of n steps is a collection of n edges $\vec{e}_i$ distributed uniformly on the sphere. The vertices are partial sums of $\vec{e}_i$.

The space of possible random flights (up to translation) is $(S^2)^n$, which is a $2n$-dimensional symplectic (Kähler) manifold.

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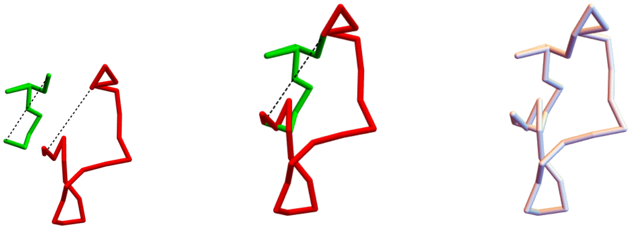
Definition

A random equilateral n-gon is an n-edge random flight conditioned on $\sum \vec{e}_i = 0$.

This is a $(2n-3)$-dimensional Riemannian manifold.

Idea

A random closed n-edge polygon is a k-edge random flight and an $n - k$-edge random flight, conditioned on having the same end-to-end distance.



Let $\phi_n(\ell)$ be the probability density function of the end to end distance in a random flight of n unit length steps. It's classical that (where $\operatorname{sinc} x = \frac{\sin x}{x}$):

$$\phi_n(\ell) = \frac{2\ell}{\pi}\int_0^\infty x \sin \ell x \operatorname{sinc}^n x \,\mathrm{d}x = \frac{2^{-n-1}}{\pi\,\ell\,(n-2)!}\times$$

$$\times \sum_{k=0}^{n-1} (-1)^k \binom{n-1}{k} \left([-2k+\ell+n-2]_+^{n-2} - [-2k+\ell+n]_+^{n-2} \right)$$

This is piecewise polynomial in ℓ of degree $n-3$.

Proof.

Fourier transform. (sinc is the transform of the 'boxcar function'.) □

Proposition (with Cantarella)

The probability density of the length of the chord connecting v_1 and v_k in an n-gon is given by

$$\frac{4\pi\ell^2}{C_n}\phi_k(\ell)\phi_{n-k}(\ell)$$

where

$$C_n = 2^{n-5}\pi^{n-4}\int_{-\infty}^{\infty} x^2 \operatorname{sinc}^n x \, \mathrm{d}x.$$

Fact

The whole pdf is piecewise-polynomial of degree $n-4$.

We can use this to compute some expected chordlengths exactly:

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

We can use this to compute some expected chordlengths exactly:

$$E(\text{chord}(37,112)) = \frac{\begin{array}{l}2586147629602481872372707134354784581828166239735638\\0021498840205773666873699649081859732772942937 51533\\82121765570397854911152980222231191532164599823 8455\\1958079667505955874840298583338222480954393259 65569\end{array}}{\begin{array}{l}5610189772922960964198156790682037660099932612 68626\\7074180822756774956691532447066775506907079371 36027\\4245191177865555750482138291702645696286373154 77158\\3073686410450971033104968203234573182439923950 55104\end{array}} \approx 4.60973$$

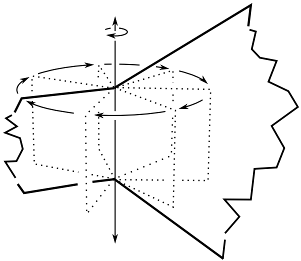
You can get any sum of functions of single chordlengths this way (but we don't understand the structure of the answers yet):

$$E(\text{HydrodynamicRadius}(15)) = \frac{4}{3883074281625}(427763619147 + 11873777090560 \log\left(\frac{7}{6}\right) - 11591065307360 \log\left(\frac{6}{5}\right) + 2915195692640 \log\left(\frac{5}{4}\right) - 173574718240 \log\left(\frac{4}{3}\right) + 1072203440 \log\left(\frac{3}{2}\right) - 10010 \log(2)) \approx 0.768279$$

Question

Why are expectations rational? *Why degree $n-4$?*

We can rotate the k-edge flight and the $n-k$ edge flight with respect to each other



This is a continuous symmetry of the polygon space.

Theorem (Duistermaat-Heckmann, stated informally)

On a $2m$-dimensional symplectic manifold,

d continuous, commuting Hamiltonian symmetries (i.e., a Hamiltonian T^d-action) $\rightarrow$ d conserved quantities (momenta)

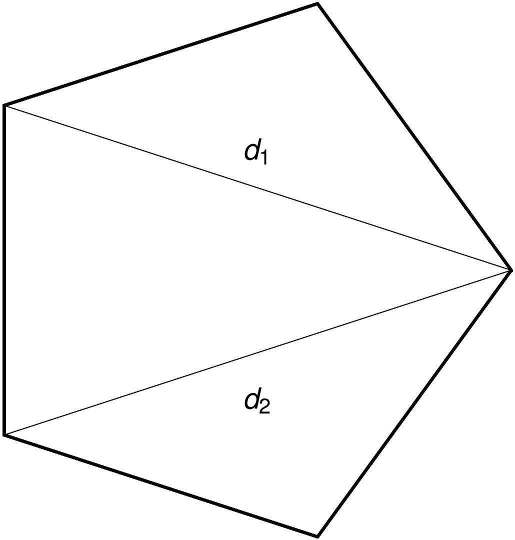
joint distribution is cts, piecewise-polynomial, degree $\leq m - d$.

Polygons (up to rotation) are $2n - 6 = 2m$ dimensional. We have 1 symmetry, so momentum is p.p. of degree $\leq$

$$m - 1 = (n - 3) - 1 = n - 4.$$

But we have more commuting symmetries than this!

Rotations around $n-3$ chords d_i by $n-3$ angles θ_i commute.



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$$S^2 \times \ldots \times S^2$$

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Symplectic details

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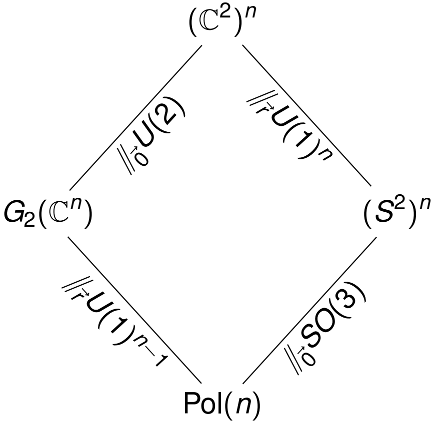
$$\mu(\vec{e}_1, \ldots, \vec{e}_n) = \sum \vec{e}_i.$$

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

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

The big symplectic picture (via Hausmann–Knutson)



Theorem (with Cantarella)

The joint distribution of $d_1, \ldots, d_{n-3}$ and $\theta_1, \ldots, \theta_{n-3}$ are all uniform (on their domains).

Proof.

Check D–H theorem applies (not entirely trivial, since Pol(n) can be singular and the torus action is only defined on an open dense subset; cf. Kapovich–Millson).

Then count: $m = n - 3$ and we have $n - 3$ symmetries, so the pdf of the momenta d_i is piecewise polynomial of degree $\leq$

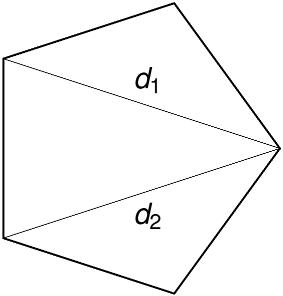
$$m - (n - 3) = (n - 3) - (n - 3) = 0.$$

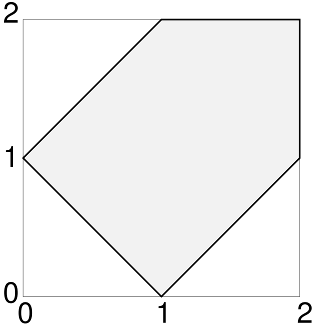
The pdf is continuous, so this means it's constant. □

What is the domain of the d_i?

Definition

The momenta $d_1, \ldots, d_{n-3}$ obey triangle inequalities which determine an $n-3$ dimensional polytope $\mathcal{P}_n \subset \mathbb{R}^{n-3}$. This is called the **moment polytope**.





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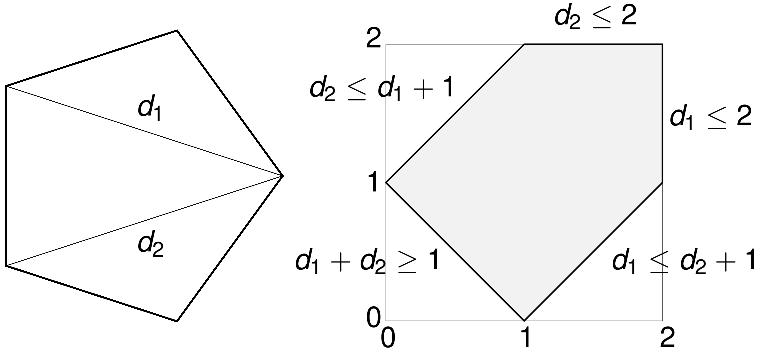


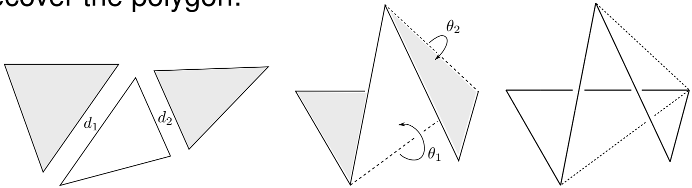
Action-angle coordinates

Definition

The d_i and θ_i are *action-angle coordinates* on polygon space. In these coordinates, the volume form is simple:

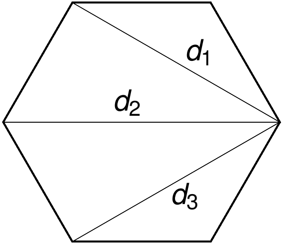
$$\mathrm{dVol} = \mathrm{d}d_1 \wedge \dots \mathrm{d}d_{n-3} \wedge \mathrm{d}\theta_1 \wedge \dots \mathrm{d}\theta_{n-3}.$$

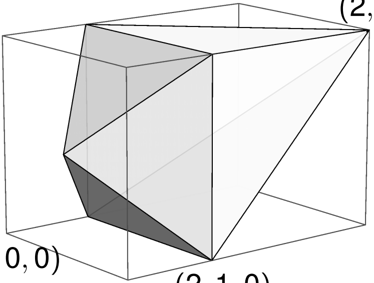
To recover the polygon:



- Build the triangles from the edgelengths.
- Put the first one in a standard position.
- Place the rest using the dihedral angles.

Structure of the moment polytope





The polytope $\mathcal{P}_n$ is defined by the triangle inequalities:

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

Theorem (with Cantarella, Duplantier, Uehara)

A direct sampling algorithm for equilateral closed polygons with expected performance $O(n^{5/2})$ per sample.

If we let

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

and $s_i \in [-1, 1]$, then d_i automatically have $|d_i - d_{i-1}| \leq 1$.

Proposition (with Cantarella, Duplantier, Uehara)

If we build d_i from s_i sampled uniformly in $[-1, 1]^n$, the d_i obey all triangle inequalities with probability $\sim 6\sqrt{6/\pi}\, n^{-3/2}$.

So rejection sample to build d_i, sample θ_i directly, and reassemble the polygon as above.

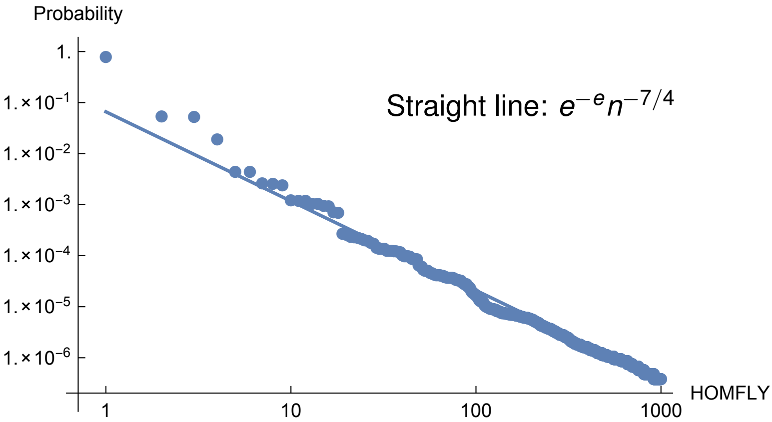
Diagonal sampling in 3 lines of code

```
RandomDiagonals[n_] :=
  Accumulate[
   Join[{1}, RandomVariate[UniformDistribution[{-1, 1}],
     n]]];

InMomentPolytopeQ[d_] :=
  And[Last[d] ≥ 0, Last[d] ≤ 2,
   And @@ (Total[#] ≥ 1 & /@ Partition[d, 2, 1])];

DiagonalSample[n_] := Module[{d},
   For[d = RandomDiagonals[n], ! InMomentPolytopeQ[d], ,
    d = RandomDiagonals[n]];
   d[[2 ;;]]
  ];
```

Experimental result: Knots in 60-gons



Log-log plot of ranked knot types $\sim$ linear (Zipf law?).

First observed by Baiesi-Orlandini-Stella.

Key question: Partition function (or total volume)

Question

How do we know that rejection sampling is expected to work after $\sim \sqrt{\pi/6^3}\, n^{3/2}$ *tries?*

Proposition

The $(n-3)$*-dimensional moment polytope* $\mathcal{P}_n$ *has volume*

$$-\frac{1}{2(n-3)!}\sum_{k=0}^{\lfloor n/2 \rfloor}(-1)^k\binom{n}{k}(n-2k)^{n-3} = \frac{2^{n-1}}{2\pi}\int_{-\infty}^{\infty} x^2 \operatorname{sinc}^n x \, \mathrm{d}x.$$

To estimate this for large n, observe that $\operatorname{sinc}^n x = (\sin x/x)^n$ approaches 0 quickly away from $x = 0$, so we can expand $\operatorname{sinc} x$ around 0.

We can make the substitution $x = y/\sqrt{n}$, and observe

$$x^2\,\mathrm{d}x \to \frac{y^2}{n^{3/2}}\,\mathrm{d}y$$

Expanding $\operatorname{sinc} y/\sqrt{n}$ around 0, we get

$$\operatorname{sinc} y/\sqrt{n} = 1 - {}^{y^2}\!/_{6n} + o({}^1\!/_n)$$

In the limit,

$$\lim_{n\to\infty}(1 - {}^{y^2}\!/_{6n} + o({}^1\!/_n))^n = e^{-y^2/6}.$$

So we have

$$\frac{2^{n-1}}{2\pi}\frac{1}{n^{3/2}}\int_{-\infty}^{\infty} e^{-y^2/6}y^2\,\mathrm{d}y = 3\sqrt{\frac{3}{\pi}}\,2^{n-\frac{3}{2}}\,\frac{1}{n^{3/2}}.$$

But how do we know the sinc formula?

Symplectic geometers (Takakura, Khoi, Mandini) have computed the symplectic volume of this space and found:

$$\operatorname{Vol}\mathcal{P}_n = -\frac{1}{2(n-3)!}\sum_{k=0}^{\lfloor n/2 \rfloor}(-1)^k\binom{n}{k}(n-2k)^{n-3}.$$

and we have the general integral formula

$$\frac{(-1)^p}{(n-2p-1)!}\sum_{k=0}^{\lfloor n/2 \rfloor}(-1)^k\binom{n}{k}(n-2k)^{n-2p-1} = \frac{2^n}{2\pi}\int_{-\infty}^{\infty}\frac{\sin^n x}{x^{n-2p}}\,\mathrm{d}x.$$

Why is this interesting?

Closed polygon space is a symplectic reduction of $(S^2)^n$: a toric symplectic manifold with action-angle coordinates given by rotating each edge around the z-axis and moment polytope $[-1, 1]^n$ given by the z coordinates of edges.

The volume of the central slab $\mathcal{S}_a$ of this hypercube where $-a \leq \sum x_i \leq a$ is given by Pólya's formula:

$$\mathrm{Vol}(\mathcal{S}_a) = \frac{2^{n-1} a}{\pi} \int_{-\infty}^{\infty} \mathrm{sinc}(ax)\ \mathrm{sinc}^{n-1} x \,\mathrm{d}x,$$

roughly because the slab area is the convolution of a collection of boxcar functions, each of which has Fourier transform $\mathrm{sinc}\, x$, so we should think of the right-hand integral in Fourier space.

$$\mathrm{Vol}(\mathcal{S}_a) = \frac{2^{n-1}a}{\pi} \int_{-\infty}^{\infty} \mathrm{sinc}(ax)\, \mathrm{sinc}^{n-1} x \, \mathrm{d}x.$$

When $a = 1$, this reduces to

$$\mathrm{Vol}(\mathcal{S}_1) = \frac{2^{n-1}}{\pi} \int_{-\infty}^{\infty} \mathrm{sinc}^{n} x \, \mathrm{d}x.$$

Compare to

$$\mathrm{Vol}(\mathcal{P}_n) = \frac{2^{n-1}}{2\pi} \int_{-\infty}^{\infty} x^2\, \mathrm{sinc}^{n} x \, \mathrm{d}x.$$

Question

Why does the symplectic volume of the reduction look like the Fourier transform of the 2nd derivative of the convolution of functions giving the area of a slice of a hypercube?

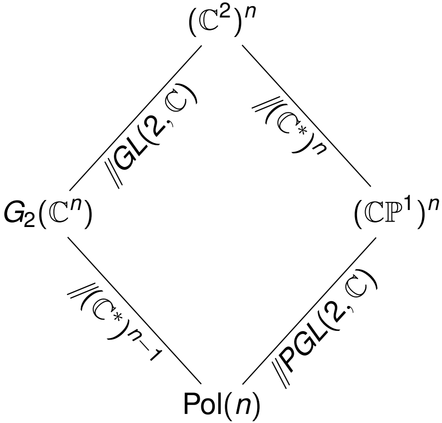
Question

Derivatives of hypercube slice volumes are lower-dimensional volumes of their boundaries (which are also hypercube slices). Does this mean that the volume of the moment polytope is a sum of volumes of hypercube slices?

Question

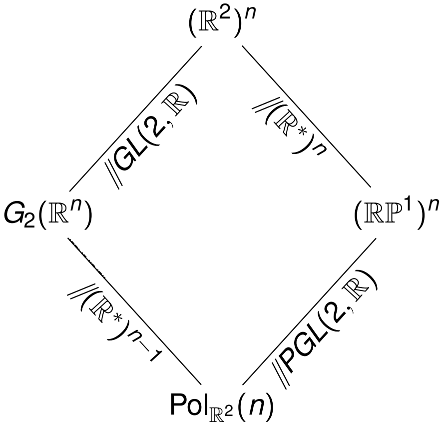
Does this mean that the moment polytope is a union of hypercube slices?

Broader Questions



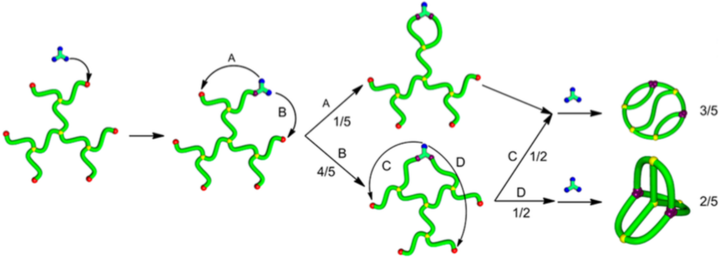
Question

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



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 conformation space of random polygonal graphs?

Thank you for listening!

- *The Symplectic Geometry of Closed Equilateral Random Walks in 3-Space*
  Jason Cantarella and Clayton Shonkwiler
  Annals of Applied Probability **26** (2016), 549–596.

- *A Fast Direct Sampling Algorithm for Equilateral Closed Polygons*
  Jason Cantarella, Bertrand Duplantier, Clayton Shonkwiler, and Erica Uehara
  Journal of Physics A **49** (2016), 275202.

`http://shonkwiler.org`