The differential geometry of spaces of polygons and polymers

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Geometry and Shape Analysis in Biological Sciences
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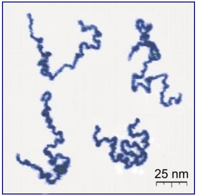
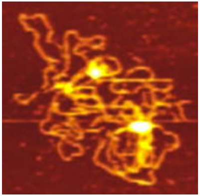
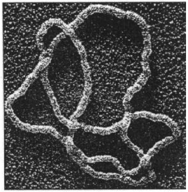
Space curves model useful biological shapes



Protonated P2VP

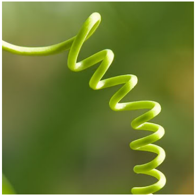


Plasmid DNA



Knotted DNA

Elafin



Plant tendril

Cowpea root

Main Ideas

- Replace curves with polygons.
- Use the (differential, symplectic, algebraic) geometry of polygon space.
- Add constraints (closed, fixed edgelength, confined, different topology) as needed.
- Geometric structure $\rightarrow$ efficient algorithms.

Definition

The quaternions $\mathbb{H}$ are the skew-algebra over $\mathbb{R}$ defined by adding **i**, **j**, and **k** so that

$$\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = -1, \quad \mathbf{ijk} = -1$$

Proposition

Unit quaternions (S^3) double-cover SO(3) *(orthonormal frames for 3-space) via the Hopf map.*

$$\text{Hopf}(q) = (\bar{q}\mathbf{i}q, \bar{q}\mathbf{j}q, \bar{q}\mathbf{k}q),$$

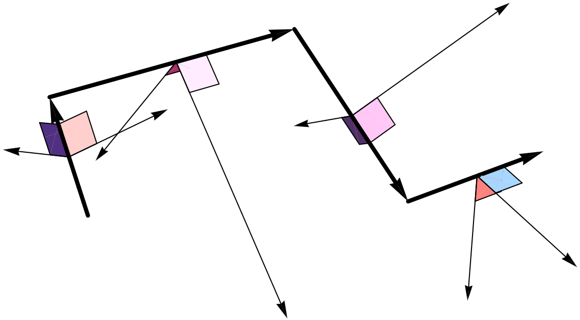
where the entries turn out to be purely imaginary quaternions, and hence vectors in $\mathbb{R}^3$.

Constructing polygons from quaternions: Arms

Given a vector $\vec{q} \in \mathbb{H}^n$, we can construct a polygon:

$$\underbrace{(q_1, \ldots, q_n)}_{\text{vector of quaternions}} \rightarrow \underbrace{(\mathrm{Hopf}(q_1), \ldots, \mathrm{Hopf}(q_n))}_{\text{vector of frames}} \rightarrow \underbrace{(\bar{q}_1 \mathbf{i} q_1, \ldots, \bar{q}_n \mathbf{i} q_n)}_{\text{vector of edges}}$$

We call the polygon $\mathrm{Hopf}(\vec{q})$.

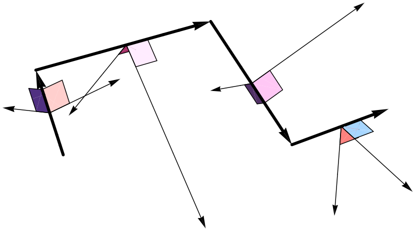


Proposition

$$\textit{framed n-gons of total length 1} \iff S^{4n-1} \subset \mathbb{H}^n$$

Proof.

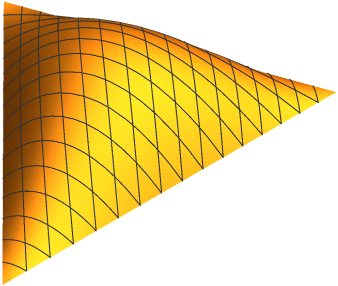
The length of i-th edge is $|\bar{q}_i \mathbf{i} q_i| = |q_i|^2$. □



Proposition (with Shonkwiler)

The distribution of edges in the quaternionic model is:

- *directions are sampled independently, uniformly on* $(S^2)^n$.
- *lengths are sampled by the Dirichlet* $(2, \ldots, 2)$ *distribution on the simplex* $\{\vec{x} | x_i \geq 0, \sum x_i = 1\}$.



$\iff$ pdf is $\sim x_1 x_2 \cdots x_n$

Alignment is an irritating problem in shape comparison: this geometric structure makes it easy.

Proposition

Multiplying $\vec{q}$ by w rotates polygon by matrix $\mathrm{Hopf}(w) \in \mathrm{SO}(3)$.

Conclusion

Framed, length 1, space polygons (up to trans/rot) $\iff$

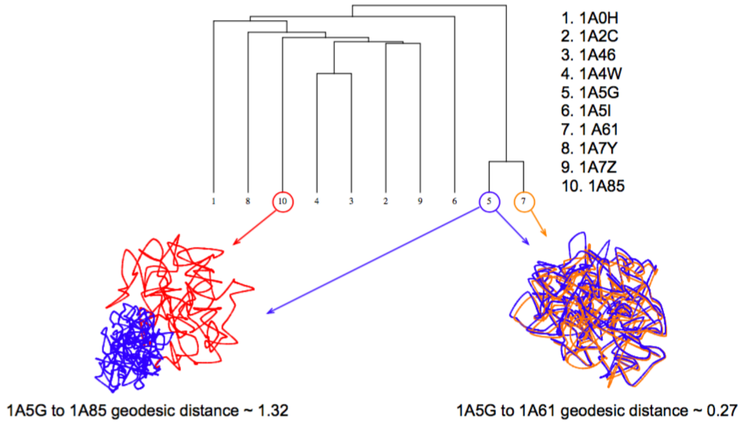
$$\mathbb{H}P^n = S^{4n-1}/(\vec{q} \simeq w\vec{q}, w \in \mathbb{H})$$

The metric on $\mathbb{H}P^n$ then gives a translation and rotation invariant distance function for space polygons:

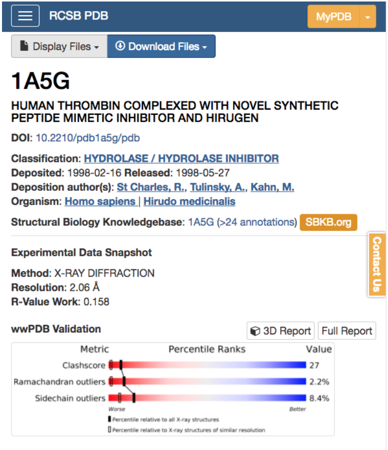
$$\mathrm{dist}(P, Q) = \mathrm{acos}\sqrt{\frac{\langle P, Q\rangle \langle Q, P\rangle}{\langle P, P\rangle \langle Q, Q\rangle}}$$

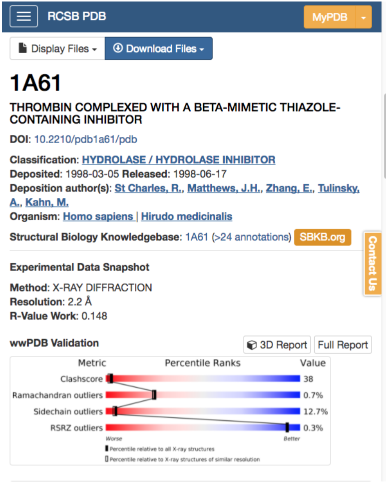
Shape comparison of proteins from PDB

We can use the $\mathbb{H}P^n$ distance to cluster protein shapes. Here is a proof-of-concept experiment with 10 proteins done by Tom Needham (Ohio State).



1A5G and 1A61 in the PDB





A natural question is: how statistically significant is a distance of 0.27? In this setting, the answer is classical:

Proposition (based on Skriganov)

The probability that two random open polygons of n edges are within distance d of one another is given by

$$\sin^{4n} \frac{d}{2}$$

So we expect most completely unrelated polygons to be at distances which are very close to π.

Every quaternion $q = a + b\mathbf{j}$, where $a, b \in \mathbb{C}$. This means that we can take *complex* vectors $(\vec{a}, \vec{b})$ corresponding to a quaternionic vector $\vec{q}$.

Proposition (Hausmann/Knutson)

P is closed, length 2 $\iff$ *the vectors* $(\vec{a}, \vec{b})$ *are Hermitian orthonormal.*

Proof.

$$\mathrm{Hopf}(a + b\mathbf{j}) = (\overline{a + b\mathbf{j}})\mathbf{i}(a + b\mathbf{j}) = \mathbf{i}(|a|^2 - |b|^2 + 2\bar{a}b\mathbf{j})$$

so we have

$$\sum \mathrm{Hopf}(a + b\mathbf{j}) = 0 \iff \sum |a|^2 = \sum |b^2|, \sum \bar{a}b = 0.$$

□

Conclusion (Hausmann/Knutson)

Closed, framed space polygons $\Longleftrightarrow$ *Stiefel manifold* $V_2(\mathbb{C}^n)$*.*

Proposition (Hausmann/Knutson)

The action of the matrix group $\mathrm{U}(2)$ *on* $V_2(C^n)$

- *rotates the polygon in space (*$\mathrm{SU}(2)$ *action)* ***and***
- *spins all vectors of the frame (*$\mathrm{U}(1)$ *action).*

Conclusion (Hausmann/Knutson)

Closed, rel. framed space polygons of length 2 $\Longleftrightarrow$
Grassmannian of 2-planes in complex n-space $G_2(\mathbb{C}^n)$*.*

An invariant distance between closed polygons is easy to compute in linear time:

Proposition

Given two closed, (relatively) framed polygons as $n \times 2$ complex matrices $Y_1 = (\vec{a}_1, \vec{b}_1)$ and $Y_2 = (\vec{a}_2, \vec{b}_2)$, let $\cos\theta_1, \cos\theta_2$ be the singular values of $Y_1^T Y_2$.

The singular values are invariant under translation and rotation and allow us to construct several metrics on polygon space:

$$d_{geo}(Y_1, Y_2) = \sqrt{\theta_1^2 + \theta_2^2}, \quad d_{chord}(Y_1, Y_2) = \sqrt{\sin^2\theta_1 + \sin^2\theta_2}$$

This provides a space curve version of well-known construction for plane curves:

Theorem (Younes–Michor–Shah–Mumford)

Roughly speaking,

$$\left\{\begin{array}{c}\textit{Contours in}\\ \mathbb{R}^2\ \textit{modulo}\\ \textit{similarities}\end{array}\right\} \longleftrightarrow Gr(2, C^\infty(S^1, \mathbb{R})),$$

where $Gr(k, V)$ is the Grassmannian of k-dimensional linear subspaces of the vector space V.

Proposition (with Grosberg, Kusner, Shonkwiler)

The expected value of total turning angle for an n-turn

- *open polygon is*
$$\frac{\pi}{2}n$$
- *closed polygon is*
$$\frac{\pi}{2}n + \frac{\pi}{4}\frac{2n}{2n-3}.$$

Proposition (with Grosberg, Kusner,Shonkwiler)

At least $1/3$ *of rel. framed hexagons and* $1/11$ *of rel. framed heptagons are unknots.*

To describe the space of equilateral polygons, we first recall that $G_2(\mathbb{C}^n)$ is a symplectic space; in fact it is the symplectic reduction of $\mathbb{C}^{2n}$ by $U(2)$.

$$G_2(\mathbb{C}^n) = \underbrace{\mathbb{C}^{2n} /\!\!/ U(2)}_{U(2) \text{ acts on vectors } \vec{a},\vec{b}}$$

Proposition (Knutson-Hausmann, Millson-Kapovich)

(Unframed) equilateral polygon space is a symplectic space; it is the symplectic reduction of $G_2(\mathbb{C}^n)$ by $U(1)^{n-1}$:

$$\mathrm{ePol}_n = \underbrace{G_2(\mathbb{C}^n) /\!\!/ U(1)^{n-1}}_{U(1)^{n-1} \text{ rotates each frame around edge}}$$

Symplectic spaces are the right setting for classical mechanics:

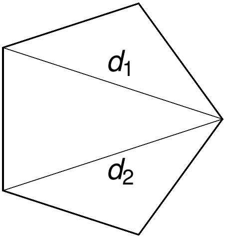
Theorem (Duistermaat-Heckmann, stated informally)

On a $2m$-dimensional (symplectic) space,

d continuous, commuting (Hamiltonian) symmetries $\rightarrow$
d conserved quantities (momenta)

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

Polygons (up to rotation) are $2n-6 = 2(n-3)$ dimensional. Rotations around $n-3$ chords d_i by $n-3$ angles θ_i commute.



Theorem (with Shonkwiler)

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 (hard part).

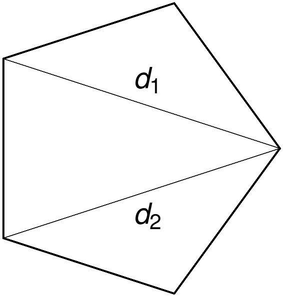
Then count: $m = n - 3$ and we have $n - 3$ symmetries, so the pdf of the momenta d_i is piecewise polynomial of degree $\leq$

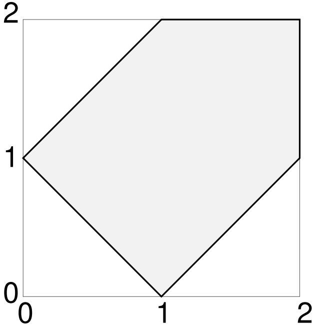
m - (n-3) = (n-3) - (n-3) = 0 .

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

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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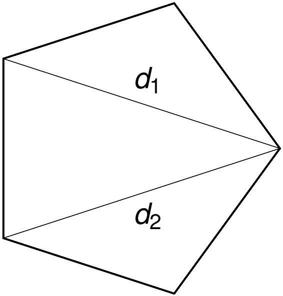
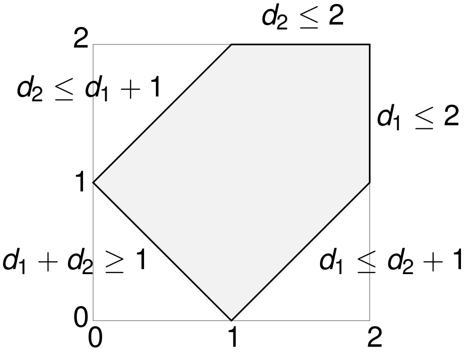


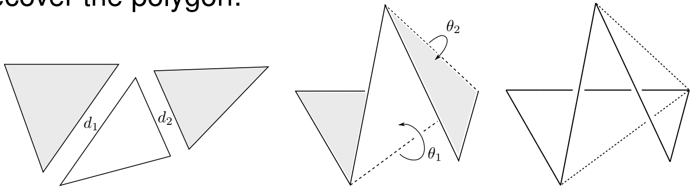


Definition

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

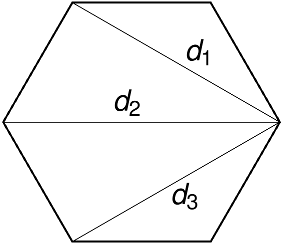
$$\mathrm{dVol} = \mathrm{d}d_1 \wedge \ldots \mathrm{d}d_{n-3} \wedge \mathrm{d}\theta_1 \wedge \ldots \mathrm{d}\theta_{n-3}.$$

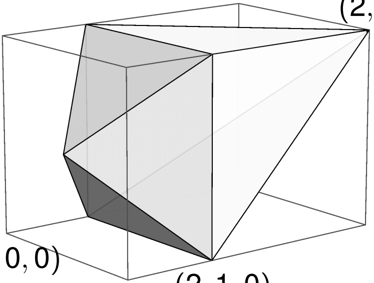
To recover the polygon:



- 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:

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

Theorem (with Duplantier, Shonkwiler, 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 Duplantier, Shonkwiler, 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 ;;]]
  ];
```

Not first direct sampling algorithm (Grosberg-Moore, Diao-Ernst-Montemayor-Ziegler), but numerically stable, simple and fast.

Proposition (with Shonkwiler)

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.

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 Shonkwiler)

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$$E(\text{chord}(37,112)) = \frac{\begin{array}{l}2586147629602481872372707134354784581828166239735638\\0021498840205773666873699649081859732772942937515 33\\8212176557039785491115298022223119153216459982384 55\\1958079667505955874840298583338222480954393259655 69\end{array}}{\begin{array}{l}5610189772922960964198156790682037660099932612686 26\\7074180822756774956691532447066775506907079371360 27\\4245191177865555750482138291702645696286373154771 58\\3073686410450971033104968203234573182439923950551 04\end{array}} \approx 4.60973$$

Current: Equilateral polygons in other dimensions

Proposition

The space of closed equilateral polygons in $\mathbb{R}^k$ is the quotient of (almost all) of the space $(S^{k-1})^n$ by the (diagonal) action of the Möbius group on S^{k-1}.

Proof.

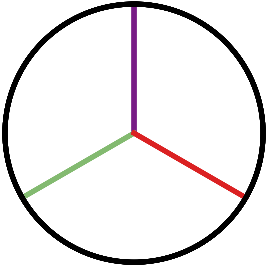
For each n point cloud on S^{k-1} (where fewer than $n/2$ points coincide) there is a unique (rotation-free) Möbius transformation which takes the center of mass to the origin. This associates a unique closed equilateral polygon with almost every polygonal arm. □

Current Project

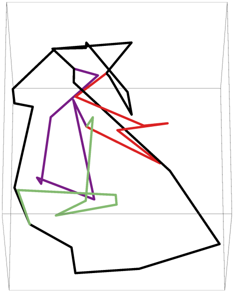
Use this structure to provide robust coordinates for equilateral polygons in all dimensions.

Current: Topologically Constrained Random Walks

A **topologically constrained random walk** (TCRW) is a collection of random walks in $\mathbb{R}^3$ whose components are required to realize the edges of some fixed multigraph.

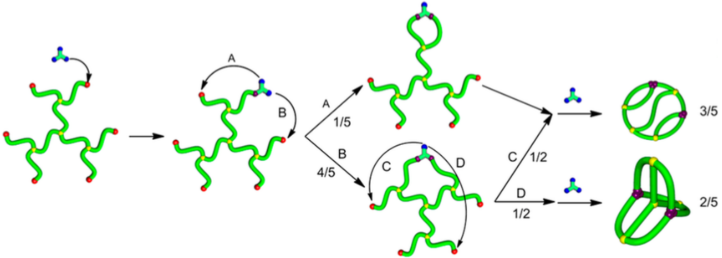


Abstract graph



TCRW

Current: Topologically Constrained Random Walks



Tezuka Lab, Tokyo Institute of Technology

A synthetic $K_{3,3}$!

Thank you!

Funding from Simons Foundation, NSF, Issac Newton Institute,

- *Probability Theory of Random Polygons from the Quaternionic Viewpoint* with T. Deguchi, and C. Shonkwiler *Comm. on Pure & Applied Mathematics* **67** (2014)
- *The Expected Total Curvature of Random Polygons* with A. Y. Grosberg, R. Kusner, and C. Shonkwiler *American Journal of Mathematics* **137** (2015)
- *The Symplectic Geometry of Closed Equilateral Random Walks in 3-space* with C. Shonkwiler *Annals of Applied Probability* **26** (2016).
- *A Fast Direct Sampling Algorithm for Equilateral Closed Polygons* with B. Duplantier, C. Shonkwiler, and E. Uehara. *Journal of Physics A* **49** (2016).