The Geometry of Random Polygons

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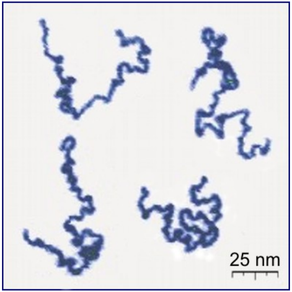
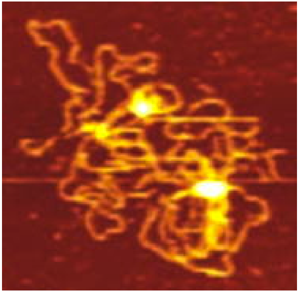
Physics Question

What is the average shape of a polymer in solution?



Protonated P2VP
Roiter/Minko
Clarkson University



Plasmid DNA
Alonso-Sarduy, Dietler Lab
EPF Lausanne

Physics Question

What is the average shape of a polymer in solution?

Physics Answer

> *Modern polymer physics is based on the analogy between a polymer chain and a random walk.*
>
> —*Alexander Grosberg, NYU.*

Math Question

With respect to a given probability measure on closed polygons, what is the expected value of radius of gyration or total curvature?

Topology of cyclo-octane energy landscape
Martin, Thompson, Coutsias, Watson

Numerical Analysis Question

How can we construct random samples drawn from the space of closed space n-gons? More generally, how should we numerically integrate over the space of closed polygons?

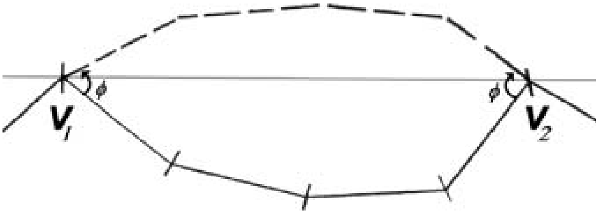


Illustration of crankshaft algorithm of Vologoskii et. al.
Benham/Mielke

Definition

The space $\mathrm{Arm}_3(n)$ is the space of n-edge polygonal arms of length 2 in $\mathbb{R}^3$ (up to translation), thought of as an n-tuple of edge vectors $(\vec{e}_1, \ldots, \vec{e}_n)$.

Let $\mathbb{H}$ be the space of quaternions. The Hopf map applied to $q = q_0 + q_1\mathbf{i} + q_2\mathbf{j} + q_3\mathbf{k}$ is

$$\begin{aligned}\mathrm{Hopf}(q) &= \bar{q}\mathbf{i}q \\ &= (q_0^2 + q_1^2 - q_2^2 - q_3^2, 2q_1q_2 - 2q_0q_3, 2q_0q_2 + 2q_1q_3).\end{aligned}$$

takes quaternions to imaginary quaternions (a copy of $\mathbb{R}^3$) and has $|\,\mathrm{Hopf}(q)| = |q|^2$.

Proposition

Hopf *extends coordinatewise to a smooth, surjective map from the round sphere of radius* $\sqrt{2}$ *in* $\mathbb{H}^n$ *to* $\mathrm{Arm}_3(n)$*.*

Definition

The *symmetric measure* on $\mathrm{Arm}_3(n)$ is the pushforward of the standard measure on the $\sqrt{2}$-sphere in $\mathbb{H}^n$.

Definition

The space $\mathrm{Pol}_3(n)$ is the space of n-edge closed polygons of length 2 in $\mathbb{R}^3$ (up to translation).

The quaternionic n-sphere $S^{4n-1}(\sqrt{2})$ is the join $S^{2n-1} \star S^{2n-1}$ of complex n-spheres:

$$(\vec{a}, \vec{b}, \theta) \mapsto \sqrt{2}(\cos\theta\vec{a} + \sin\theta\vec{b}\,\mathbf{j}) \tag{1}$$

where $\vec{a}$, $\vec{b} \in \mathbb{C}^n$ lie in the unit sphere and $\theta \in [0, \pi/2]$. We focus on

$$S^{4n-1}(\sqrt{2}) \supset \{(\vec{a}, \vec{b}, \pi/4) \mid \langle \vec{a}, \vec{b} \rangle = 0\} = V_2(\mathbb{C}^n)$$

Proposition (Hausmann and Knutson)

$\mathrm{Hopf}^{-1}(\mathrm{Pol}_3(n)) = V_2(\mathbb{C}^n)$.

Sampling random polygons (directly!)

Proposition (with Cantarella and Deguchi)

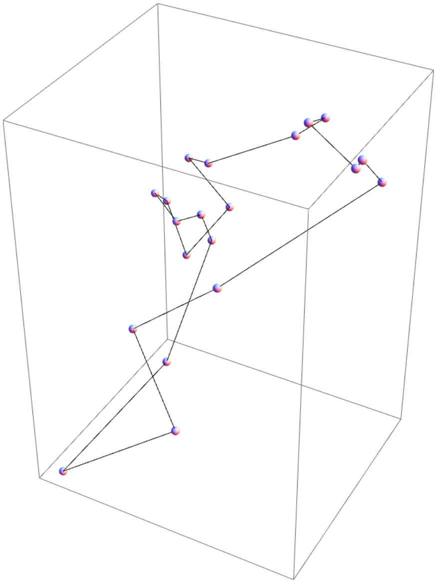
The natural (Haar) measure on $V_2(\mathbb{C}^n)$ is obtained by generating random complex n-vectors with independent Gaussian coordinates and applying (complex) Gram-Schmidt.

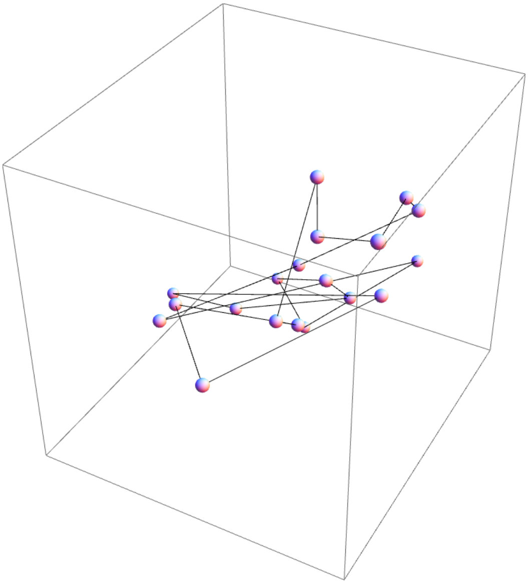
```
In[9]:= RandomComplexVector[n_] := Apply[Complex,
          Partition[#, 2] & /@ RandomVariate[NormalDistribution[], {1, 2 n}], {2}][[1]];

        ComplexDot[A_, B_] := Dot[A, Conjugate[B]];
        ComplexNormalize[A_] := (1 / Sqrt[Re[ComplexDot[A, A]]]) A;

        RandomComplexFrame[n_] := Module[{a, b, A, B},
          {a, b} = {RandomComplexVector[n], RandomComplexVector[n]};
           A = ComplexNormalize[a];
           B = ComplexNormalize[b - Conjugate[ComplexDot[A, b]] A];
          {A, B}
         ];
```

Now we need only apply the Hopf map to generate an edge set:

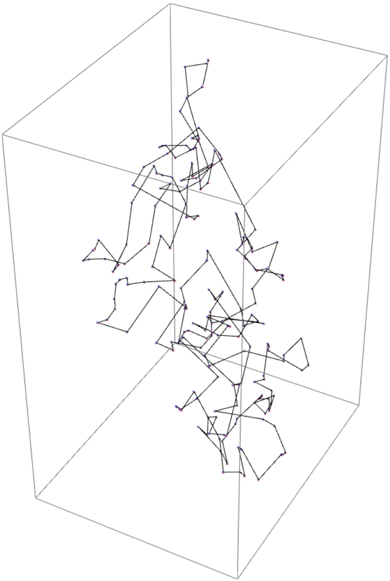
```
In[6]:= ToEdges[{A_, B_}] := {#[[2]], #[[3]], #[[4]]} & /@ (HopfMap /@ Transpose[{A, B}]);
```

Examples of 20-gons

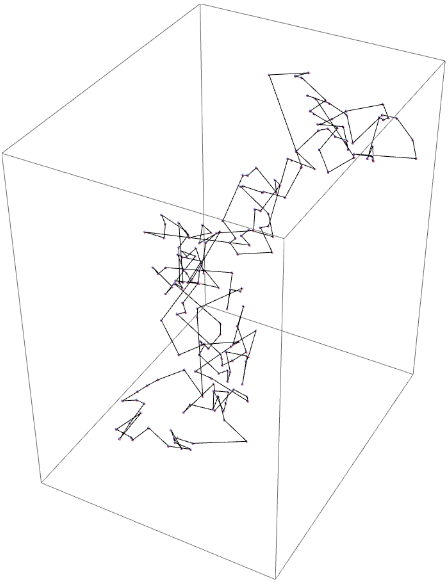




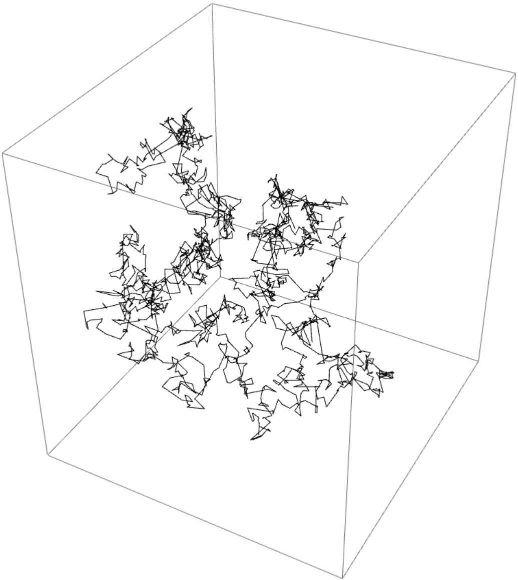
Examples of 200-gons



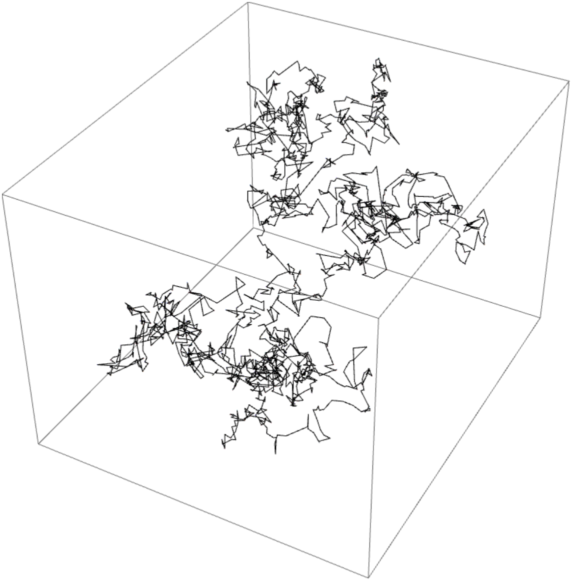
Examples of 200-gons



Examples of 2,000-gons



Examples of 2,000-gons



Key Idea

We can now compute expected values of geometric quantities for random polygons by integrating over the Stiefel manifold.

Definition

The square of the radius of gyration $\mathrm{Gyradius}(P)$ is half the average squared distance between any two vertices of P:

$$\mathrm{Gyradius}(P) = \frac{1}{2n^2} \sum_{i,j} |v_i - v_j|^2.$$

In principle

$$E(\mathrm{Gyradius}(P), \mathrm{Pol}_3(n)) = \frac{1}{\mathrm{Vol}(V_2(\mathbb{C}^n))} \int_{V_2(\mathbb{C}^n)} \mathrm{Gyradius}(P).$$

Definition

The **edge set ensemble** $\mathcal{P}$ of polygons corresponding to a given set of edges $\vec{e}_i$ is the set of polygons formed by all rearrangements of the $\vec{e}_i$.

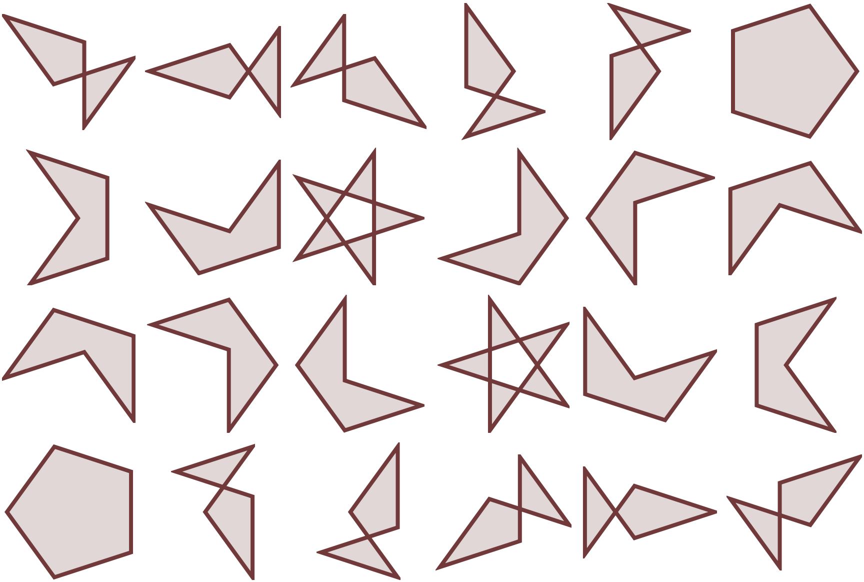
Proposition

If $\text{sGyradius}(\mathcal{P})$ *is the mean of* $\text{Gyradius}(P)$ *for* $P \in \mathcal{P}$*,*

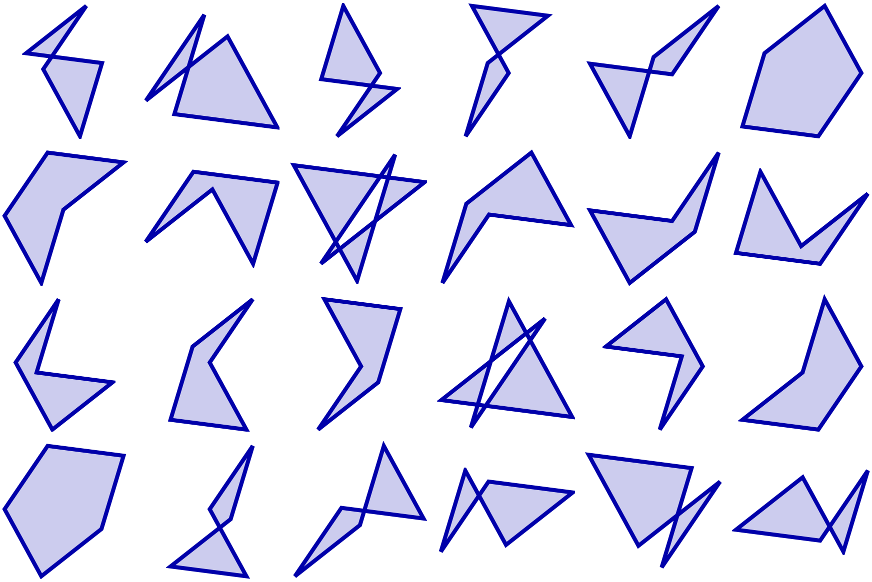
$$\begin{aligned}\text{sGyradius}(\mathcal{P}) &= \frac{n+1}{12n}\sum_{j=1}^{n}|e_j|^2\\ &= \frac{n+1}{12n}\sum_{j=1}^{n}(a_j\bar{a}_j + b_j\bar{b}_j)^2,\end{aligned}$$

where $e_j = \text{Hopf}(a_j + b_j\mathbf{j})$

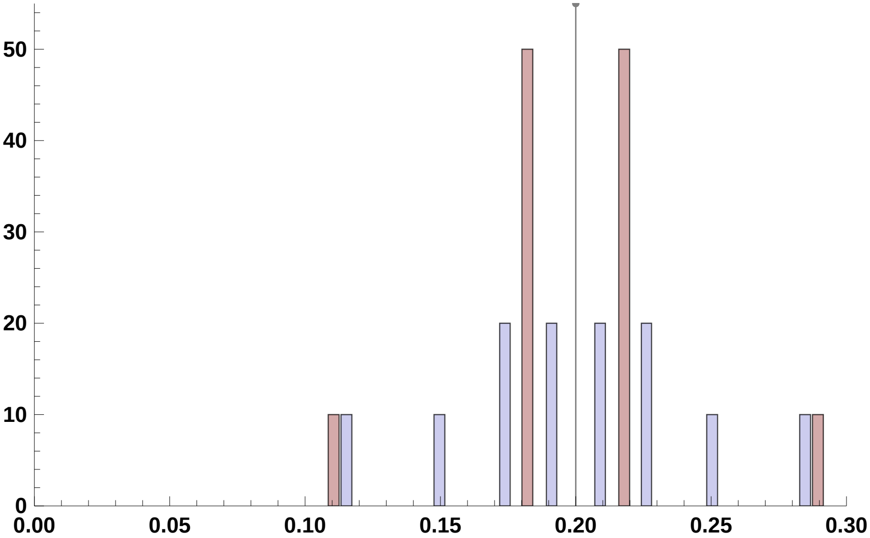
The Edge Set Ensemble Including a Regular Pentagon



The Edge Set Ensemble of another 5-edge set



A Histogram of Squared Gyradii



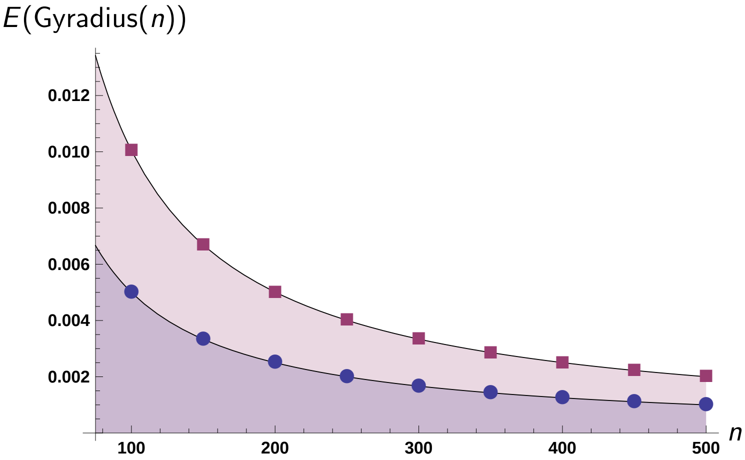
Expected Value of Radius of Gyration

Theorem (with Cantarella and Deguchi)

The expected values of Gyradius *are*

$$E(\text{Gyradius}, \text{Arm}_3(n)) = \frac{n+2}{(n+1)(n+1/2)},$$
$$E(\text{Gyradius}, \text{Pol}_3(n)) = \frac{1}{2n}.$$

Checking Gyradius Against Experiment



$\text{Arm}_3(n)$ and $\text{Pol}_3(n)$

Thank you!

- *Probability Theory of Random Polygons from the Quaternionic Viewpoint*
  Jason Cantarella, Tetsuo Deguchi, and Clayton Shonkwiler
  arXiv:1206.3161
  To appear in *Communications on Pure and Applied Mathematics*.

- *The Expected Total Curvature of Random Polygons*
  Jason Cantarella, Alexander Y. Grosberg, Robert Kusner, and Clayton Shonkwiler
  arXiv:1210.6537.

Thank you for your attention!