Closed Random Walks and Symplectic Geometry

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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.
Open Equilateral Random Polygon with 3,500 edges
Closed Equilateral Random Polygon with 3,500 edges
• What is the joint pdf of edge vectors in a closed walk?
Classical Problems

- What is the joint pdf of edge vectors in a closed walk?
- What can we prove about closed random walks?
  - What is the marginal distribution of a single chord length?
  - What is the joint distribution of several chord lengths?
  - What is the expectation of radius of gyration?
  - What is the expectation of total curvature?

- How do we sample closed equilateral random walks?
- What if the walk is confined to a sphere? (Confined DNA)
- What if the edge lengths vary? (Loop closures)
- Can we get error bars?

Point of Talk
New sampling algorithms backed by deep and robust mathematical framework. Guaranteed to converge, relatively easy to code.
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Point of Talk

*New sampling algorithms backed by deep and robust mathematical framework. Guaranteed to converge, relatively easy to code.*
(Incomplete?) History of Sampling Algorithms

- 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)
Markov Chain Algorithms
- crankshaft (Vologoskii et al. 1979, Klenin et al. 1988)
  - convergence to correct pdf unproved
- 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 pdf
  - requires sampling from complicated 1-d polynomial pdfs
Let $\text{Arm}(n; \vec{1})$ be the moduli space of random walks in $\mathbb{R}^3$ consisting of $n$ unit-length steps up to translation.

Then $\text{Arm}(n; \vec{1}) \cong S^2(1) \times \ldots \times S^2(1)$. 
Let \( \text{Arm}(n; \vec{1}) \) be the moduli space of random walks in \( \mathbb{R}^3 \) consisting of \( n \) unit-length steps up to translation.

Then \( \text{Arm}(n; \vec{1}) \cong S^2(1) \times \ldots \times S^2(1) \).

This space is easy to sample uniformly: choose \( \vec{w}_1, \ldots, \vec{w}_n \) independently from a spherically-symmetric distribution on \( \mathbb{R}^3 \) and let

\[
\vec{e}_i = \frac{\vec{w}_i}{\|\vec{w}_i\|}.
\]
Theorem (Archimedes)

Let \( f : S^2 \rightarrow \mathbb{R} \) be given by \((x, y, z) \mapsto z\). Then the pushforward of the standard measure on the sphere to the interval is \( 2\pi \) times Lebesgue measure.

Illustration by Kuperberg.
Theorem (Archimedes)

Let \( f : S^2 \to \mathbb{R} \) be given by \((x, y, z) \mapsto z\). Then the pushforward of the standard measure on the sphere to the interval is \(2\pi\) times Lebesgue measure.

Therefore, we can sample uniformly on (a full-measure subset of) \( S^2 \) by choosing a \( z \)-coordinate uniformly from \([-1, 1]\) and a \( \theta \)-coordinate uniformly from \( S^1 \).
Theorem (Archimedes)

Let \( f : S^2 \to \mathbb{R} \) be given by \((x, y, z) \mapsto z\). Then the pushforward of the standard measure on the sphere to the interval is \( 2\pi \) times Lebesgue measure.

[Diagram showing the pushforward of the standard measure on the sphere to the interval.]

Illustration by Kuperberg.

Thus, we can sample uniformly on (a full-measure subset of) \( \text{Arm}(n; \vec{1}) \) by choosing \((z_1, \ldots, z_n)\) uniformly from the cube \([-1, 1]^n\) and \((\theta_1, \ldots, \theta_n)\) uniformly from the \(n\)-torus \( T^n\).
Theorem (Rayleigh, 1919)

The length $\ell$ of the end-to-end vector of an $n$-step random walk has the probability density function

$$\phi_n(\ell) = \frac{2\ell}{\pi} \int_0^\infty y \sin \ell y \text{sinc}^n y \, dy.$$
Theorem (Rayleigh, 1919)

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$$
\phi_n(\ell) = \frac{2\ell}{\pi} \int_0^\infty y \sin \ell y \operatorname{sinc}^n y \, dy.
$$

Therefore, the expected end-to-end distance of an $n$-step random walk is

$$
E(\ell; \text{Arm}(n; \vec{1})) = \int_0^n \ell \phi_n(\ell) \, d\ell
$$
$E(\ell; \text{Arm}(n; \vec{1}))$ for small $n$

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Let $\text{Pol}(n; \vec{1}) \subset \text{Arm}(n; \vec{1})$ be the codimension-3 submanifold of closed random walks; i.e., those walks which satisfy

$$\sum_{i=1}^{n} \vec{e}_i = \vec{0}.$$ 

Individual edges are no longer independent!
A symplectic manifold \((M^{2n}, \omega)\) is a smooth \(2n\)-dimensional manifold \(M\) with a closed, non-degenerate 2-form \(\omega\) called the \textit{symplectic form}. The \(n\)th power of this form \(\omega^n\) is a volume form on \(M^{2n}\).

The circle \textit{acts by symplectomorphisms} on \(M^{2n}\) if the action preserves \(\omega\). A circle action generates a vector field \(X\) on \(M^{2n}\). We can contract the vector field \(X\) with \(\omega\) to generate a one-form:

\[
\iota_X \omega(\vec{v}) = \omega(X, \vec{v})
\]

If \(\iota_X \omega\) is exact, the map is called \textit{Hamiltonian} and it is \(dH\) for some smooth function \(H\) on \(M^{2n}\). The function \(H\) is called the \textit{momentum} associated to the action, or the \textit{moment map}.
A torus $T^k$ which acts by symplectomorphisms on $M$ so that the 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 $\mu$ is a convex polytope in $\mathbb{R}^k$ called the moment polytope.

**Theorem (Duistermaat–Heckman, 1982)**

The pushforward of the symplectic (or Liouville) measure to the moment polytope is piecewise polynomial. If $k = n$ the manifold is called a toric symplectic manifold and the pushforward measure is **Lebesgue measure** on the polytope.
A Down-to-Earth Example

Let \((M, \omega)\) be the 2-sphere with the standard area form. Let \(T^1 = S^1\) 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 \(2\pi\) times Lebesgue measure.*
If $M^{2n}$ is a toric symplectic manifold with moment polytope $P \subset \mathbb{R}^n$, then the inverse image of each point in the interior of $P$ is an $n$-torus. This yields

$$\alpha : P \times T^n \to M$$

which parametrizes a full-measure subset of $M$ by “action-angle coordinates”.

**Proposition**

*The map $\alpha : P \times T^n \to M$ is measure-preserving.*

Therefore, we can integrate over $M$ with respect to the symplectic measure by integrating over $P \times T^n$ and we can sample $M$ by sampling $P$ and $T^n$ independently and uniformly. For example, we can sample $S^2$ uniformly by choosing $z$ and $\theta$ independently and uniformly.
An Extended Example: Equilaterial Arm Space

- Toric symplectic manifold $\rightarrow$
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- Toric symplectic manifold $\rightarrow$ equilateral random walks
  $\text{Arm}(n; \vec{1}) = \prod S^2$. 
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An Extended Example: Equilateral Arm Space

- Toric symplectic manifold → equilateral random walks \( \text{Arm}(n; \vec{1}) = \Pi S^2 \).
- Torus action → spin each edge around \( z \) axis
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- Moment map $\mu$ →
An Extended Example: Equilateral Arm Space

- Toric symplectic manifold $\rightarrow$ equilateral random walks $\text{Arm}(n; \vec{1}) = \prod S^2$.
- Torus action $\rightarrow$ spin each edge around $z$ axis
- Moment map $\mu \rightarrow \mu(\vec{e}_1, \ldots, \vec{e}_n) = (z_1, \ldots, z_n)$, $z$-coordinates of $\vec{e}_i$. 
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An Extended Example: Equilaterial Arm Space

- Toric symplectic manifold → equilateral random walks $\text{Arm}(n; \vec{1}) = \prod S^2$.
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- Moment map $\mu \mapsto \mu(\vec{e}_1, \ldots, \vec{e}_n) = (z_1, \ldots, z_n)$, $z$-coordinates of $\vec{e}_i$.
- Moment polytope $P \mapsto$ hypercube $[-1, 1]^n$. 
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  $$\alpha(z_i, \theta_i) = (\sqrt{1 - z_i^2} \cos \theta_i, \sqrt{1 - z_i^2} \sin \theta_i, z_i).$$
An Extended Example: Equilateral Arm Space

- Toric symplectic manifold $\to$ equilateral random walks $\text{Arm}(n; \vec{T}) = \prod S^2$.
- Torus action $\to$ spin each edge around $z$ axis
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Definition
Given an (abstract) triangulation of the $n$-gon, the folds on any two chords commute. A *dihedral angle* move rotates around all of these chords by independently selected angles.
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The Triangulation Polytope

**Definition**

A abstract triangulation $T$ of the $n$-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* $\mathcal{P}$. 

![Diagram of a triangulation polytope](image)

![Diagram of a 3-dimensional space with a shaded polytope](image)
Definition
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Definition
If $\mathcal{P}$ is the triangulation polytope and $T^{n-3}$ is the torus of $n - 3$ dihedral angles, then there are action-angle coordinates:

$$\alpha : \mathcal{P} \times T^{n-3} \rightarrow \text{Pol}(n)/\text{SO}(3)$$
Main Theorem

Theorem (with Cantarella)

\( \alpha \) pushes the **standard probability measure** on \( \mathcal{P} \times T^{n-3} \)
forward to the **correct probability measure** on \( \text{Pol}(n)/\text{SO}(3) \).
Theorem (with Cantarella)

\( \alpha \) pushes the **standard probability measure** on \( P \times T^{n-3} \) forward to the **correct probability measure** on \( \text{Pol}(n)/\text{SO}(3) \).

**Proof.**

Millson-Kapovich toric symplectic structure on polygon space + Duistermaat-Heckmann theorem + Hitchin’s theorem on compatibility of Riemannian and symplectic volume on symplectic reductions of Kähler manifolds + Howard-Manon-Millson analysis of polygon space.
Theorem (with Cantarella)
\[ \alpha \text{ pushes the standard probability measure on } \mathcal{P} \times T^{n-3} \text{ forward to the correct probability measure on } \text{Pol}(n)/\text{SO}(3). \]

Proof.
Millson-Kapovich toric symplectic structure on polygon space + Duistermaat-Heckmann 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 convex polytopes is a sampling algorithm for closed equilateral polygons.
Proposition (with Cantarella)

The joint pdf of the $n - 3$ chord lengths in an abstract triangulation of the $n$-gon in a closed random equilateral polygon is Lesbesgue measure on the triangulation polytope.
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The joint pdf of the $n - 3$ chord lengths in an abstract triangulation of the $n$-gon in a closed random equilateral polygon is Lebesgue measure on the triangulation polytope.

The marginal pdf of a single chordlength is a piecewise-polynomial function given by the volume of a slice of the triangulation polytope in a coordinate direction.

These marginals derived by Moore/Grosberg 2004 and Diao/Ernst/Montemayor/Ziegler 2011.
Proposition (with Cantarella)

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Corollary (with Cantarella)

The expectation of any function of a collection of non-intersecting chordlengths can be computed by integrating over the triangulation polytope.
Theorem (with Cantarella)

The expected length of a chord skipping $k$ edges in an $n$-edge closed equilateral random walk is the $(k - 1)$st coordinate of the center of mass of the moment polytope for $\text{Pol}(n; \vec{1})$.

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Theorem (with Cantarella)

At least $\frac{1}{2}$ of equilateral hexagons are unknotted.
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At least $\frac{1}{2}$ of equilateral hexagons are unknotted.

Proof.
Consider the triangulation of the hexagon given by joining vertices 1, 3, and 5 by diagonals and its corresponding action-angle coordinates.
Using a result of Calvo, in either this triangulation or the 2–4–6 triangulation, the dihedral angles $\theta_1, \theta_2, \theta_3$ of a hexagonal trefoil must all be either between 0 and $\pi$ or between $\pi$ and $2\pi$.
Therefore, the fraction of knots is no bigger than

$$2 \frac{\text{Vol}([0, \pi]^3) + \text{Vol}([\pi, 2\pi]^3)}{\text{Vol}(T^3)} = \frac{4\pi^3}{8\pi^3} = \frac{1}{2}$$
Theorem (with Cantarella)

At least $\frac{1}{2}$ of equilateral hexagons are unknotted.
Recall

*Action-angle coordinates reduce sampling equilateral polygon space to the (solved) problem of sampling a convex polytope.*
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Definition (Hit-and-run Sampling Markov Chain)
Given $\bar{p}_k \in \mathcal{P} \subset \mathbb{R}^n$, 

...
Recall

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Definition (Hit-and-run Sampling Markov Chain)

Given $\vec{p}_k \in \mathcal{P} \subset \mathbb{R}^n$,

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1. Choose a random direction $\vec{v}$ uniformly on $S^{n-1}$.
2. Let $\ell$ be the line through $\vec{p}_k$ in direction $\vec{v}$.

Theorem (Smith, 1984)
The m-step transition probability of hit-and-run starting at any point $\vec{p}$ in the interior of $\mathcal{P}$ converges geometrically to Lebesgue measure on $\mathcal{P}$ as $m \to \infty$. 
Recall

*Action-angle coordinates reduce sampling equilateral polygon space to the (solved) problem of sampling a convex polytope.*

**Definition (Hit-and-run Sampling Markov Chain)**

Given $\mathbf{p}_k \in \mathcal{P} \subset \mathbb{R}^n$,

1. Choose a random direction $\mathbf{v}$ uniformly on $S^{n-1}$.
2. Let $\ell$ be the line through $\mathbf{p}_k$ in direction $\mathbf{v}$.
3. Choose $\mathbf{p}_{k+1}$ uniformly on $\ell \cap \mathcal{P}$.

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The $m$-step transition probability of hit-and-run starting at any point $\vec{p}$ in the interior of $P$ converges geometrically to Lesbegue measure on $P$ as $m \to \infty$. 
Definition (TSMCMC(β))

Given a triangulation $T$ of the $n$-gon and associated polytope $\mathcal{P}$. If $x_k = (\vec{p}_k, \vec{\theta}_k) \in \mathcal{P} \times T^{n-3}$, define $x_{k+1}$ by

- Update $\vec{p}_k$ by a hit-and-run step on $\mathcal{P}$ with probability $\beta$.
- Replace $\vec{\theta}_k$ with a new uniformly sampled point in $T^{n-3}$ with probability $1 - \beta$.

At each step, construct the corresponding polygon $\alpha(x_k)$ using action-angle coordinates.
A (new) Markov Chain for Polygon Spaces

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At each step, construct the corresponding polygon $\alpha(x_k)$ using action-angle coordinates.

Proposition (with Cantarella)

Starting at any polygon, the $m$-step transition probability of $\text{TSMCMC}(\beta)$ converges geometrically to the standard probability measure on $\text{Pol}(n)/\text{SO}(3)$. 
Suppose $f$ is a function on polygons. If a run $R$ of TSMCMC($\beta$) produces $x_1, \ldots, x_m$, let

$$\text{SampleMean}(f; R, m) := \frac{1}{m} \sum_{k=1}^{m} f(\alpha(x_k))$$

be the sample average of the values of $f$ over the run.

Because TSMCMC($\beta$) converges geometrically, we have

\[ \frac{1}{\sqrt{m}} \left( \text{SampleMean}(f; R, m) - E(f) \right) \xrightarrow{w} \mathcal{N}(0, \sigma(f)^2), \]

where $w$ denotes weak convergence, $E(f)$ is the expectation of $f.$
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**Because TSMCMC($\beta$) converges geometrically, we have**

**Theorem (Markov Chain Central Limit Theorem)**

*If $f$ is square-integrable, there exists a real number $\sigma(f)$ so that*\(^1\)

$$\sqrt{m}(\text{SampleMean}(f; R, m) - E(f)) \xrightarrow{w} \mathcal{N}(0, \sigma(f)^2),$$

*the Gaussian with mean 0 and standard deviation $\sigma(f)^2$.*

\(^1\) $w$ denotes weak convergence, $E(f)$ is the expectation of $f$
Given a length-$m$ run $R$ of TSMCMC and a square integrable function $f$, we can compute $\text{SampleMean}(f; R, m)$. There is a statistically consistent estimator called the Geyer IPS Estimator $\bar{\sigma}_m(f)$ for $\sigma(f)$.

According to the estimator, a 95% confidence interval for the expectation of $f$ is given by

$$E(f) \in \text{SampleMean}(f; R, m) \pm 1.96\bar{\sigma}_m(f)/\sqrt{m}.$$
Given a length-\(m\) run \(R\) of TSMCMC and a square integrable function \(f\), we can compute \(\text{SampleMean}(f; R, m)\). There is a statistically consistent estimator called the \textbf{Geyer IPS Estimator} \(\bar{\sigma}_m(f)\) for \(\sigma(f)\).

According to the estimator, a 95% confidence interval for the expectation of \(f\) is given by

\[
E(f) \in \text{SampleMean}(f; R, m) \pm 1.96 \bar{\sigma}_m(f)/\sqrt{m}.
\]

\textbf{Experimental Observation}

With 95\% confidence, we can say that the fraction of knotted equilateral hexagons is between 1.1 and 1.5 in 10,000.
Definition

A polygon $p \in \text{Pol}(n; \vec{1})$ is in *rooted spherical confinement* of radius $R$ if each diagonal length $d_i \leq R$. Such a polygon is contained in a sphere of radius $R$ centered at the first vertex.
Proposition (with Cantarella)

Polygons in $\text{Pol}(n; \vec{1})$ in rooted spherical confinement in a sphere of radius $R$ are a toric symplectic manifold with moment polytope determined by the fan triangulation inequalities

\[
0 \leq d_1 \leq 2 \quad 1 \leq d_i + d_{i+1} \quad 0 \leq d_{n-3} \leq 2
\]

\[
|d_i - d_{i+1}| \leq 1
\]

together with the additional linear inequalities

\[
d_i \leq R.
\]

These polytopes are simply subpolytopes of the fan triangulation polytopes. Many other confinement models are possible!
Confinement radii are 1.25, 1.5, 1.75, 2, 2.5, 3, 4, and 5.
Unconfined 100-gons
Unconfined 100-gons
Unconfined 100-gons
Unconfined 100-gons
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1.1-confined 100-gons
1.1-confined 100-gons
1.1-confined 100-gons
1.1-confined 100-gons
Thank you for listening!
• *Probability Theory of Random Polygons from the Quaternionic Viewpoint*
  Jason Cantarella, Tetsuo Deguchi, and Clayton Shonkwiler
  arXiv:1206.3161

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

• *The symplectic geometry of closed equilateral random walks in 3-space*
  Jason Cantarella and Clayton Shonkwiler