A New Algorithm for Sampling Closed Equilateral Random Walks

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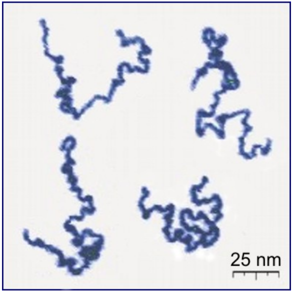
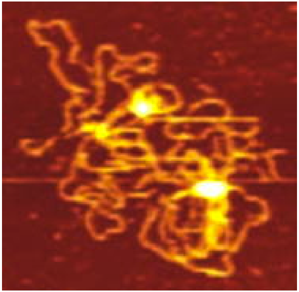
AMS Southeastern Sectional Meeting
November 9, 2014

Physics Question

What is the average shape of a polymer in solution or in melt?





Protonated P2VP
Roiter/Minko
Clarkson University

Plasmid DNA
Alonso-Sarduy, Dietler Lab
EPF Lausanne

Let $\mathrm{Arm}(n)$ be the moduli space of random walks in $\mathbb{R}^3$ consisting of n unit-length steps up to translation.

Then $\mathrm{Arm}(n) \cong \underbrace{S^2(1) \times \ldots \times S^2(1)}_{n}$.

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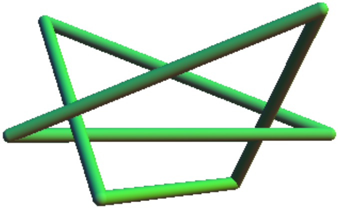
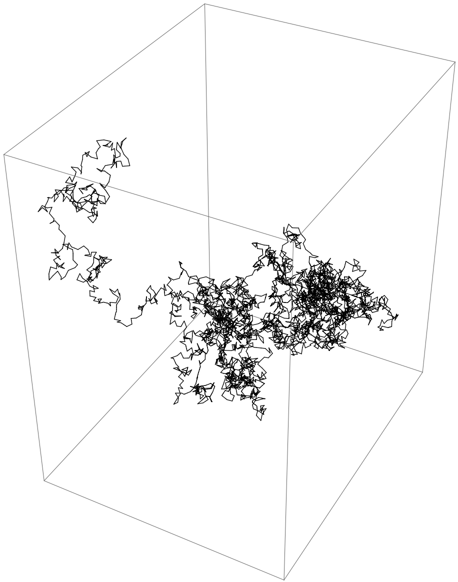
Let $\mathrm{Pol}(n) \subset \mathrm{Arm}(n)$ be the submanifold of closed random walks (or *random polygons*); i.e., those walks which satisfy

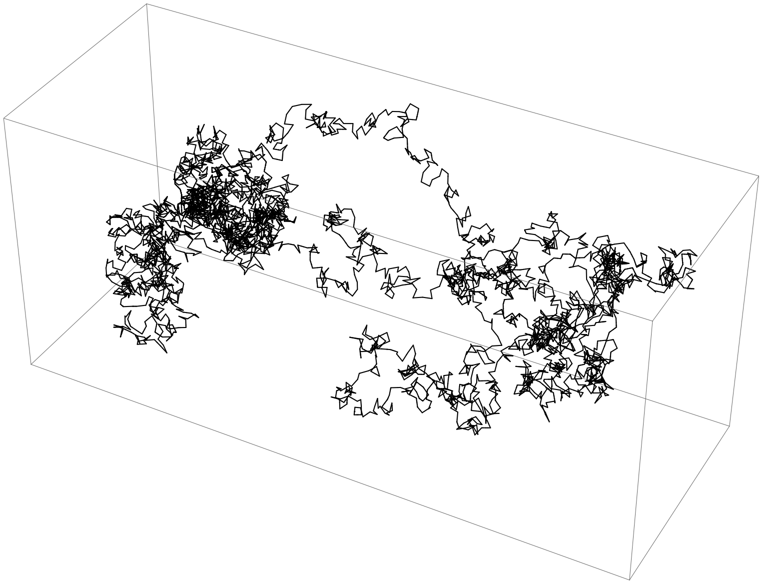
$$\sum_{i=1}^{n} \vec{e}_i = \vec{0}.$$



A Random Walk with 3,500 Steps



A Closed Random Walk with 3,500 Steps



Main Question

How can we sample closed equilateral random walks according to the codimension-3 Hausdorff measure on $\mathrm{Pol}(n) \subset \mathrm{Arm}(n)$*?*

Motivating Question

How do we understand $\mathrm{Pol}(n)$*? What is this space?*

Point of Talk

New direct sampling algorithms backed by symplectic geometry. Sample ensembles are guaranteed to be perfect. $O(n^3)$ *complexity, but reasonably fast in practice.*

(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)

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    - convergence to correct distribution unproved
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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 distribution
  - sinc integral method (Moore et al. 2005, Diao et al. 2011)
    - requires sampling complicated 1-d polynomial densities

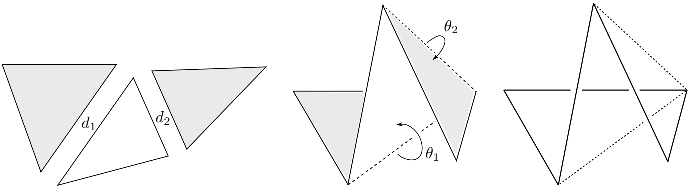
Definition

A triangulation T of the n-gon has $n-3$ nonintersecting chords. The lengths of these chords obey triangle inequalities, so they lie in a convex polytope in $\mathbb{R}^{n-3}$ called the *moment polytope* $\mathcal{P}$.

Definition

If $T^{n-3} = (S^1)^{n-3}$, there are *action-angle coordinates*:

$$\alpha\colon\ \mathcal{P} \times T^{n-3} \to \mathrm{Pol}(n)/\,\mathrm{SO}(3)$$



Theorem (with Cantarella, arXiv:1310.5924)

α *pushes the* ***standard probability measure*** *on* $\mathcal{P} \times T^{n-3}$ *forward to the* ***correct probability measure*** *on* $\mathrm{Pol}(n)/\,\mathrm{SO}(3)$.

Corollary

Sampling $\mathcal{P}$ *and* T^{n-3} *independently is a perfect sampling algorithm for* $\mathrm{Pol}(n)$.

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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. $\square$

Corollary

Sampling $\mathcal{P}$ and T^{n-3} independently is a perfect sampling algorithm for $\mathrm{Pol}(n)$.

Understanding the Triangulation Polytope

If the chord lengths are d_i then the triangle inequalities are

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

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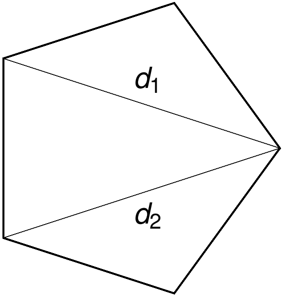

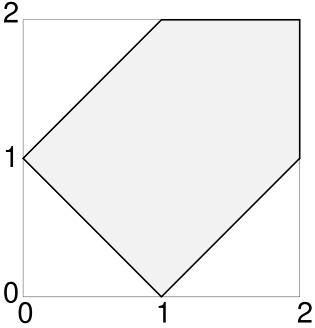

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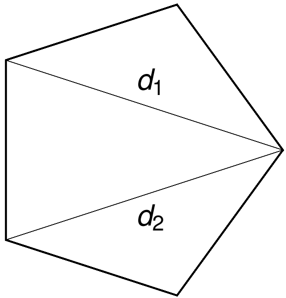

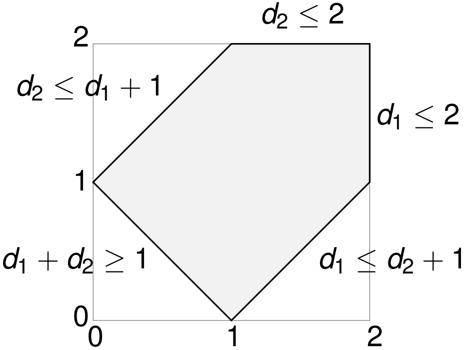

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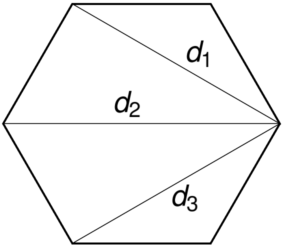

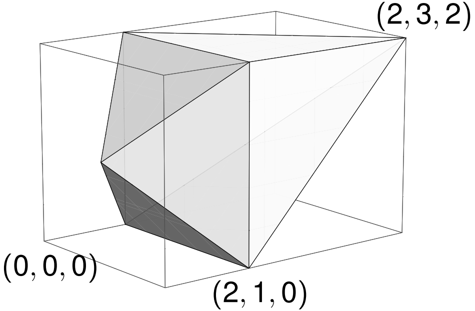

A change of coordinates

If we introduce a fake chordlength $d_0 = 1$, and make the linear transformation

$$a_i = d_i - d_{i+1},\ \text{for } 0 \leq i \leq n-4, \quad a_{n-3} = d_{n-3} - d_0$$

then our 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

$$\underbrace{-1 \leq a_i \leq 1, \quad \sum a_i = 0,}_{|d_i - d_{i+1}| \leq 1} \quad \underbrace{2\sum_{j=0}^{i-1} a_j + a_i \leq 1}_{d_i + d_{i+1} \geq 1}$$

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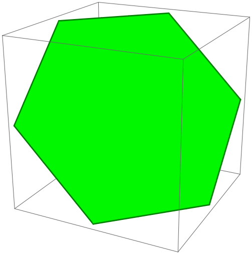
become

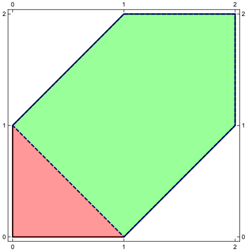
$$\underbrace{-1 \leq a_i \leq 1, \quad \sum a_i = 0,}_{\text{easy conditions}} \quad \underbrace{2\sum_{j=0}^{i-1} a_j + a_i \leq 1}_{\text{hard conditions}}$$

Definition

The n-dimensional cross-polytope $\mathcal{C}$ is the slice of the hypercube $[-1,1]^{n+1}$ by the plane $x_1 + \cdots + x_{n+1} = 0$.



$\rightarrow$



Idea

Sample points in the cross polytope, which all obey the “easy conditions”, and reject any samples which fail to obey the “hard conditions”.

Theorem (Marichal-Mossinghoff)

For even n, the volume of the projection of the $(n-3)$-dimensional cross-polytope $\mathcal{C}$ is

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

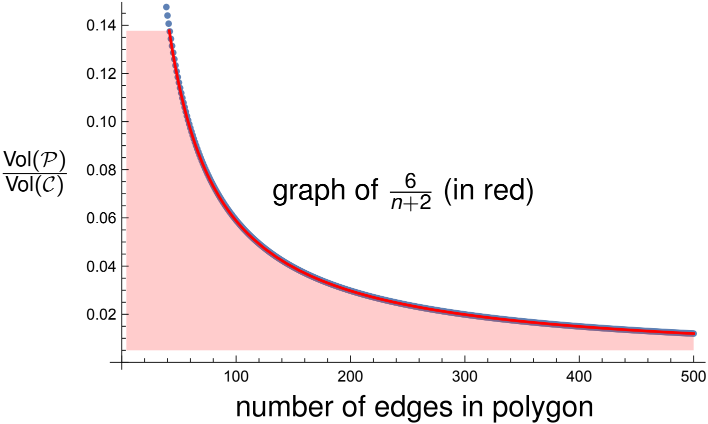
Theorem (Khoi, Takakura, Mandini)

The volume of the $(n-3)$-dimensional moment polytope for n-edge equilateral polygons $\mathcal{P}$ is

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

Runtime of algorithm depends on acceptance ratio

Acceptance ratio $= \frac{\mathrm{Vol}(\mathcal{P})}{\mathrm{Vol}(\mathcal{C})}$ is conjectured $\sim \frac{6}{n+2}$. It is certainly bounded below by $\frac{1}{n}$.

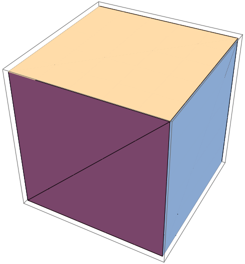


Definition

The hypersimplex $\Delta_{k,n}$ is the slice of the cube $[0,1]^n$ with $\sum_{i=1}^{n} x_i = k$ or the slab of $[0,1]^{n-1}$ with $k-1 \leq \sum_{i=1}^{n-1} x_i \leq k$.

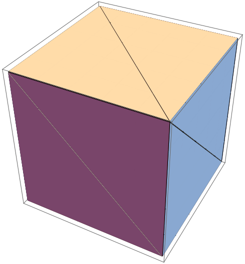
Theorem (Stanley)

There is a unimodular triangulation[1] *of* $\Delta_{k,n}$ *in* $[0,1]^{n-1}$ *indexed by permutations of* $(1,\ldots,n-1)$ *with* $k-1$ *descents.*



Standard triangulation

$\xrightarrow{\psi^{-1}}$



Stanley triangulation

[1] a decomposition into disjoint simplices of equal volume

Sampling the Cross Polytope

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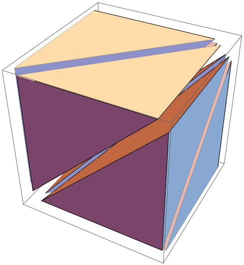

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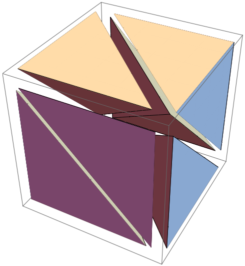

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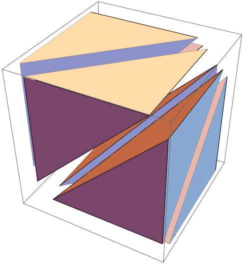

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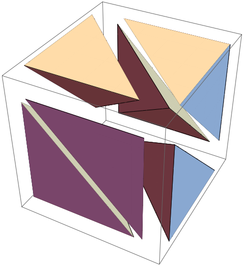

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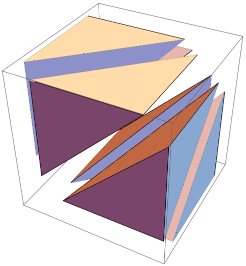

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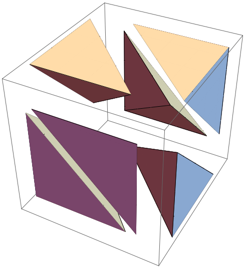

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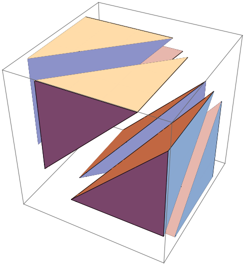

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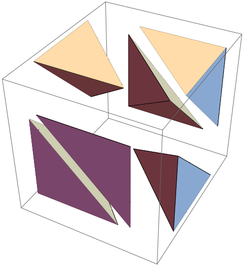

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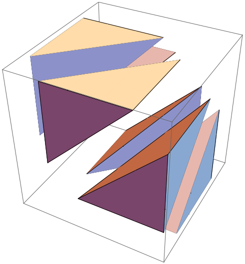

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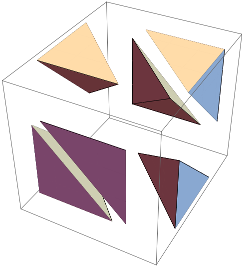

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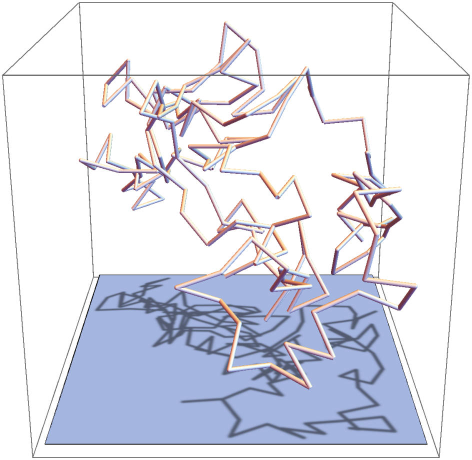
Moment Polytope Sampling Algorithm (for n even)

1. Generate a permutation of n numbers with $n/2 - 1$ descents. $O(n^2)$ time.
2. Generate a point in the corresponding simplex of the Stanley triangulation for $\Delta_{n/2,n}$.
3. Project up to the cross polytope in $[0, 1]^n$, over to the cross polytope in $[-1, 1]^n$ and down to a set of diagonals.
4. Test the proposed set of diagonals against the "hard" conditions. acceptance ratio $> 1/n$
5. Generate dihedral angles from T^{n-3}.
6. Build sample polygon in action-angle coordinates.

Example MPSA 160-gon



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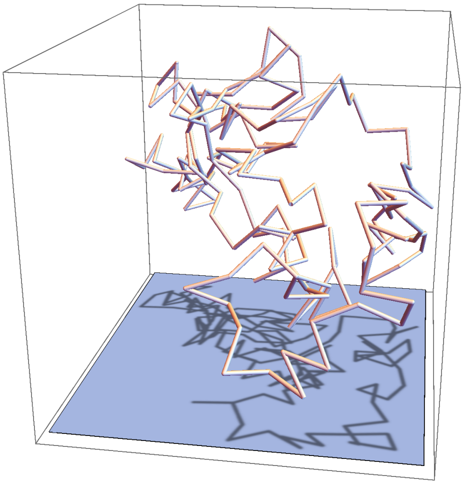

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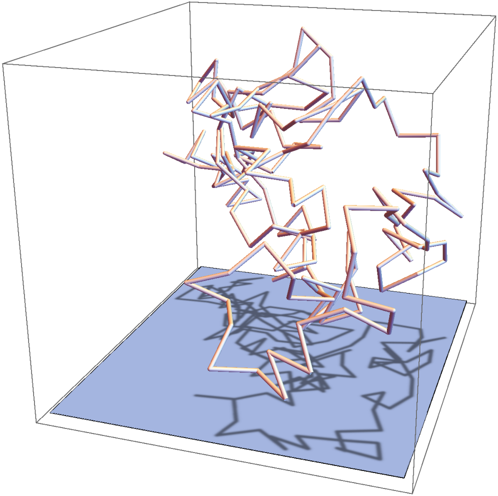

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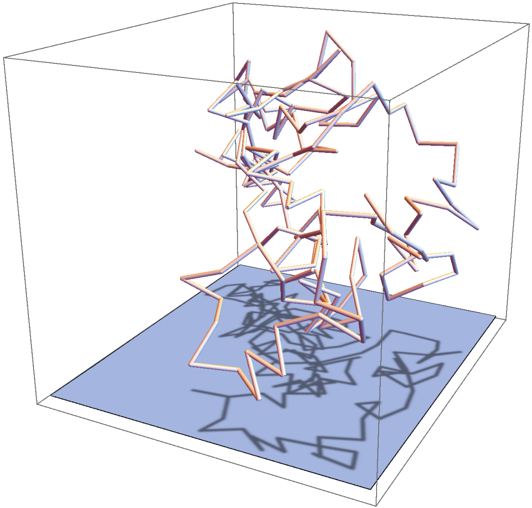

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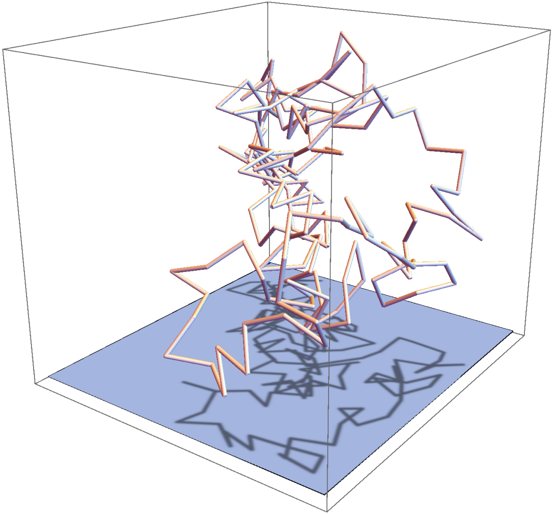

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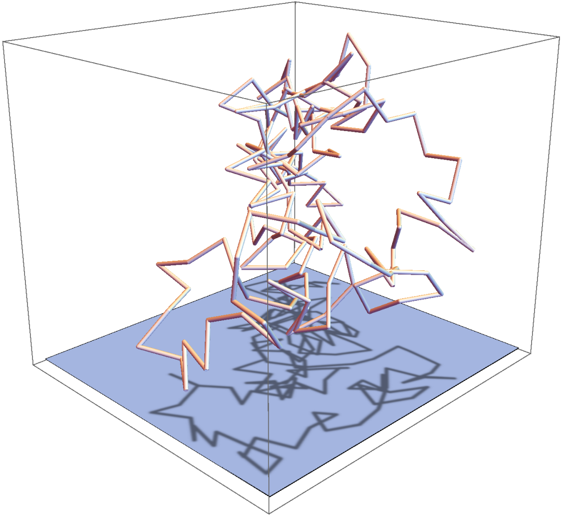

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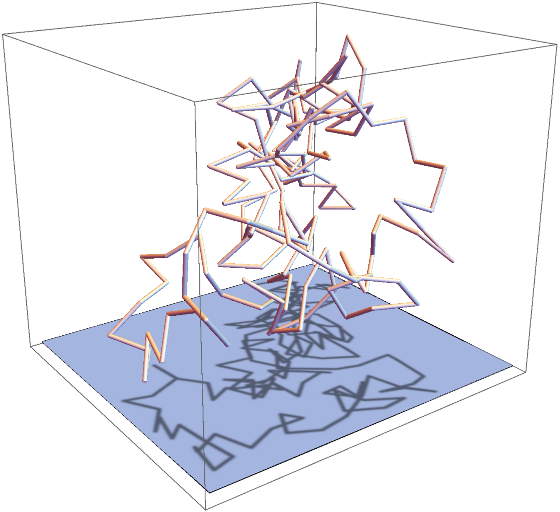

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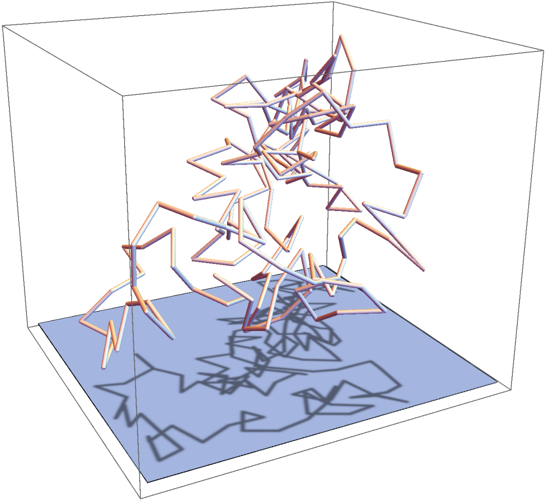

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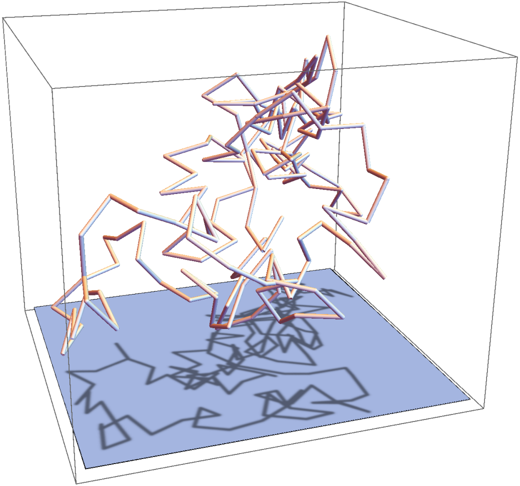

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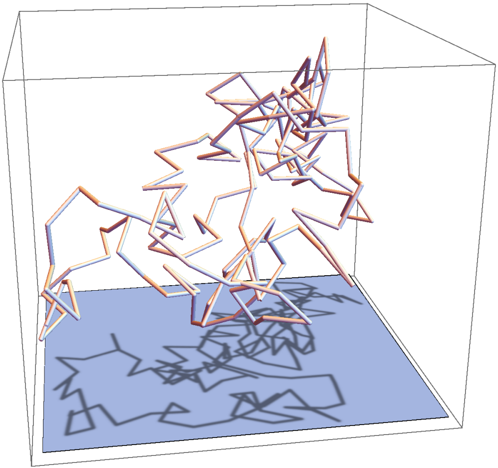

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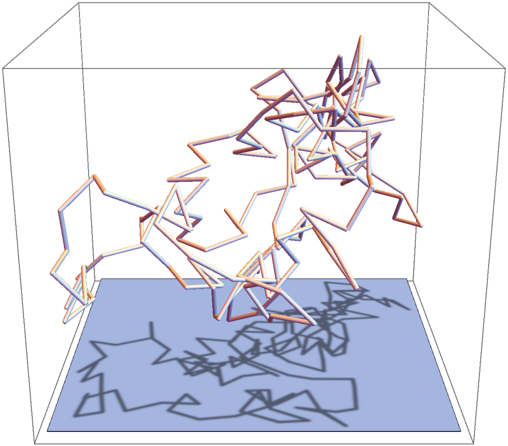

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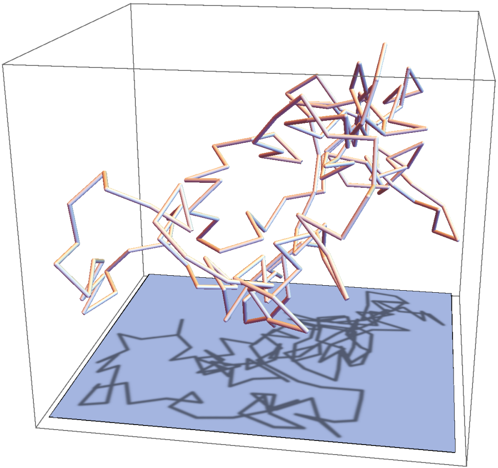

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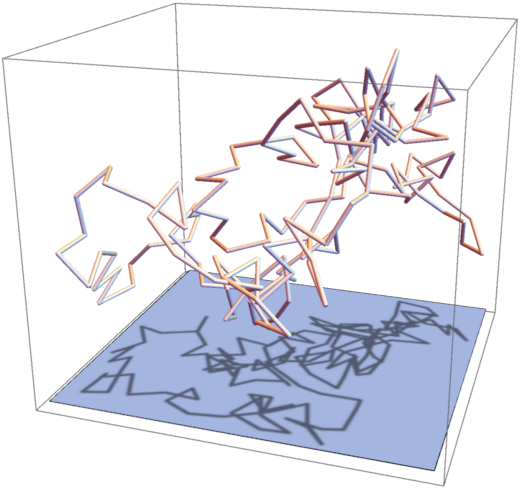

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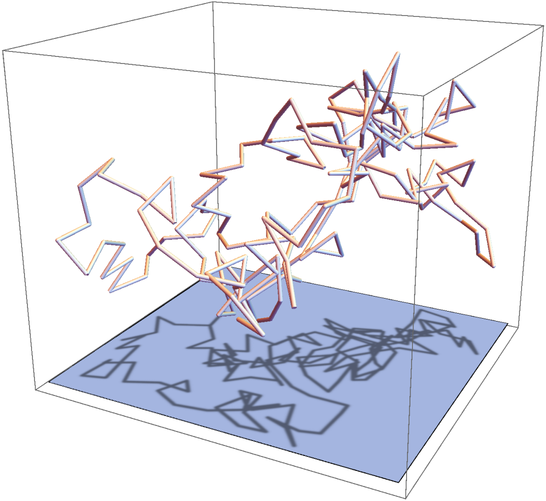

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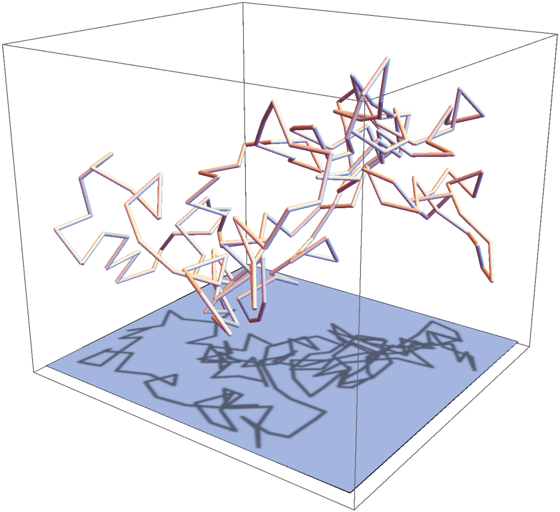
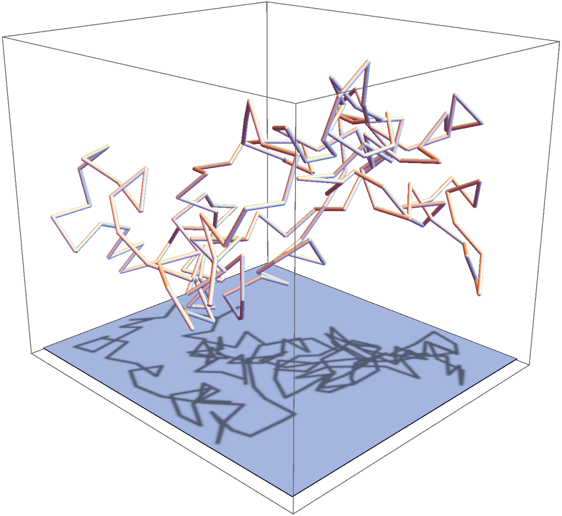
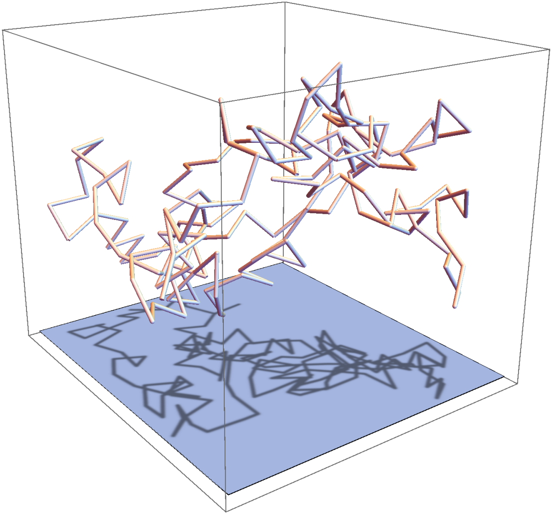


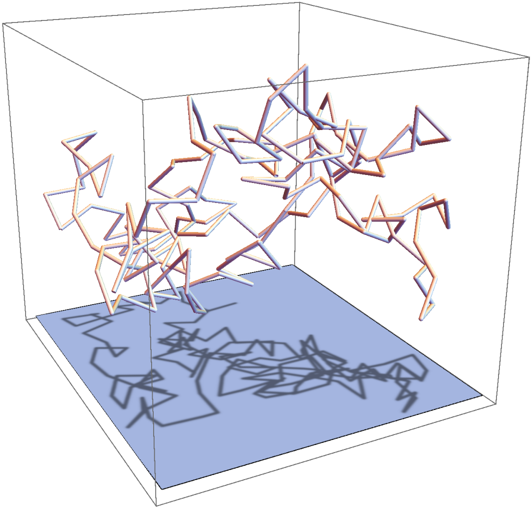
Example MPSA 160-gon



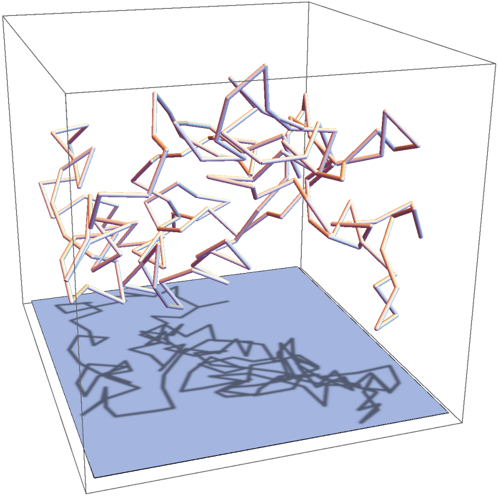
Example MPSA 160-gon



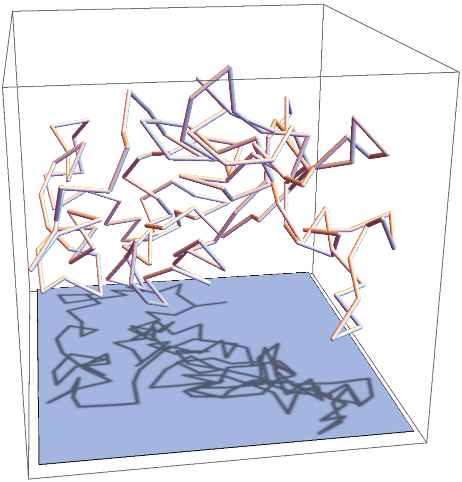
Example MPSA 160-gon



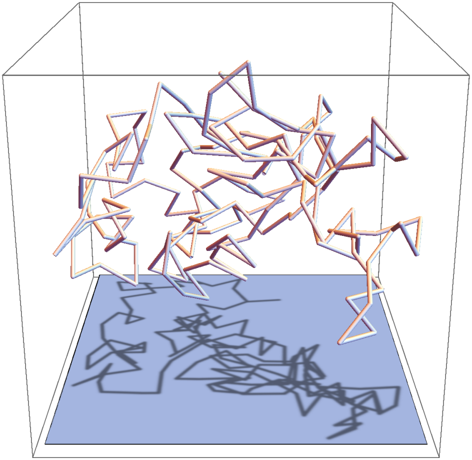
Example MPSA 160-gon



Example MPSA 160-gon



Example MPSA 160-gon



We ran 10,000 samples of 48-gons using MPSA and 10,000 samples of 48-gons using TSMCMC and computed total curvature:

Algorithm	Result	95% confidence interval
MPSA	76.5568	(76.4763, 76.6572)
TSMCMC(β)	78.0419	(76.4848, 79.545)
TSMCMC(β, δ)	76.6142945311	(76.5163, 76.7122)
Exact Value	76.6014	

TSMCMC(β) (no permutations) used lagged autocovariances up to lag 2018 in computing the error estimate, while TSMCMC(β, δ) (90% permutations) used up to lag 4. MPSA doesn't need to compute any lagged autocovariances and just uses the sample variance to find the confidence interval.

Future Directions

- Prove conjectured volume ratio $\operatorname{Vol}(\mathcal{P}) / \operatorname{Vol}(\mathcal{C}) \simeq 6/(n+2)$.
- Extend technique to odd numbers of edges. (Requires a new method for sampling the cross-polytope.)
- Improve runtime to $O(n^2)$ using a reordering method.
- Improve algorithm for generating random k-descent permutations.
- Reference implementation and reference ensembles of polygons.

Thank you for listening!

Supported by:

Simons Foundation NSF DMS–1105699

- *Probability Theory of Random Polygons from the Quaternionic Viewpoint*
  Jason Cantarella, Tetsuo Deguchi, and Clayton Shonkwiler
  Communications on Pure and Applied Mathematics **67** (2014), no. 10, 1658–1699.

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

- *The Symplectic Geometry of Closed Equilateral Random Walks in 3-space*
  Jason Cantarella and Clayton Shonkwiler
  arXiv:1310.5924.