

# Grassmannians and Random Polygons

Clayton Shonkwiler

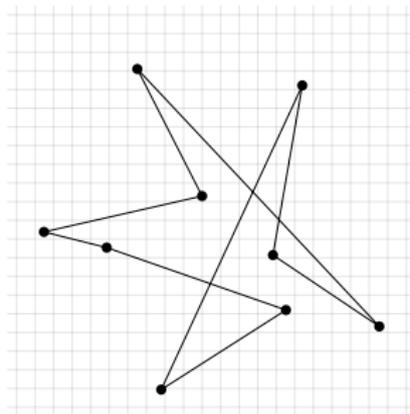
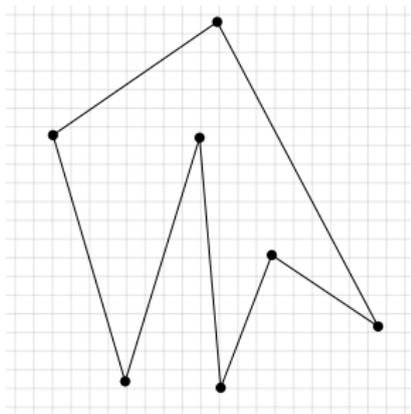
Colorado State University

April 17, 2015

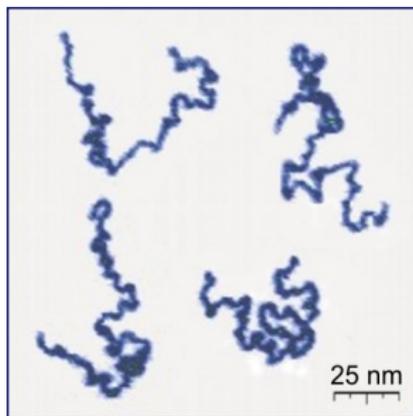
## Definition

A polygon given by vertices  $v_1, \dots, v_n$  is a collection of line segments in the plane or in  $\mathbb{R}^3$  joining each  $v_i$  to  $v_{i+1}$  (and  $v_n$  to  $v_1$ ). The *edge vectors*  $\vec{e}_i$  of the polygons are the differences between vertices:

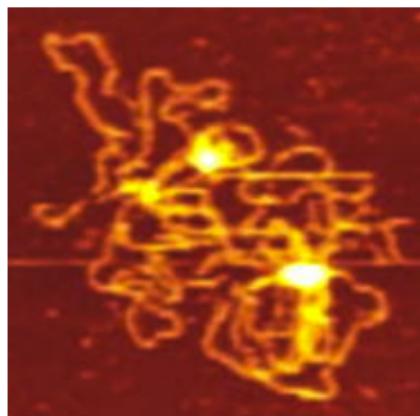
$$\vec{e}_i = v_{i+1} - v_i \quad (\text{and } \vec{e}_n = v_1 - v_n).$$



# Applications of Polygon Model

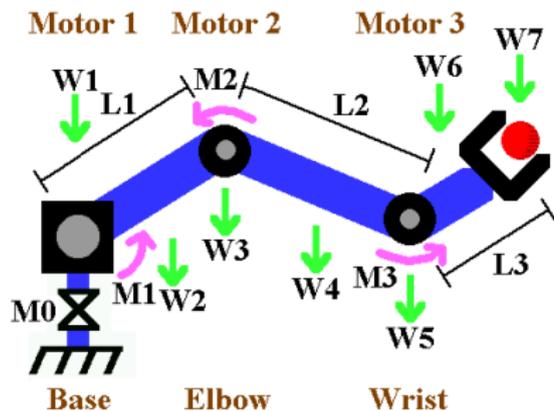


Protonated P2VP  
Roiter/Minko  
Clarkson University

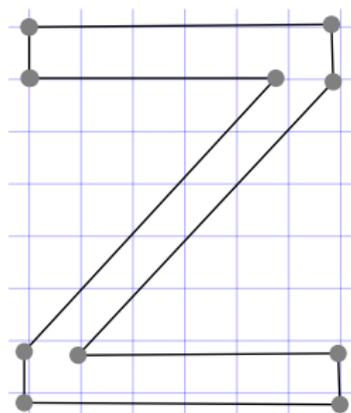


Plasmid DNA  
Alonso-Sarduy, Dietler Lab  
EPF Lausanne

# Applications of Polygon Model



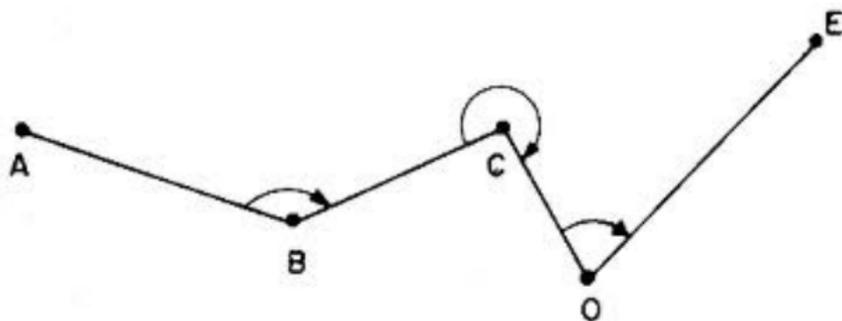
Robot Arm  
Society Of Robots



Polygonal Letter Z

## Definition

The space of possible shapes of a polygon (with a fixed number of edges) is called a *configuration space*.

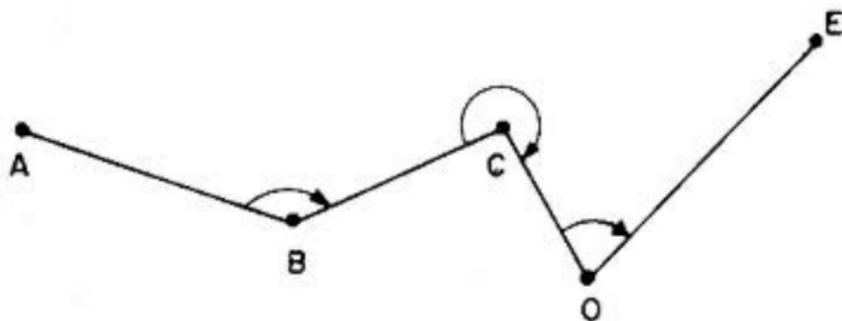


## Theorem

If we fix the lengths of the edges in advance, the configuration space of  $n$ -edge open polygons is the set of  $n - 1$  turning angles  $\theta_1, \dots, \theta_{n-1}$ . This space is called an  $(n - 1)$ -torus.

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## Question

*How can we describe closed plane polygons?*

- 1 Use turning angles. (But what condition on turning angles means the polygon closes?)
- 2 Use edge vectors. (What happens when you rotate the polygon?)
- 3 Use complex numbers.

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- 3 Use complex numbers.

# Complex Numbers and the Square Root of a Polygon

## Definition

An  $n$ -edge polygon could be given by a collection of edge vectors  $\vec{e}_1, \dots, \vec{e}_n$  of the polygon. The polygon closes  $\iff \vec{e}_1 + \dots + \vec{e}_n = \vec{0}$ .

## Definition

A complex number  $z$  is written  $z = a + bi$  where  $i^2 = -1$ . We can also write  $z = re^{i\theta} = (r \cos \theta) + i(r \sin \theta)$ .

## Definition

We will describe an  $n$ -edge polygon by complex numbers  $w_1, \dots, w_n$  so that the edge vectors obey

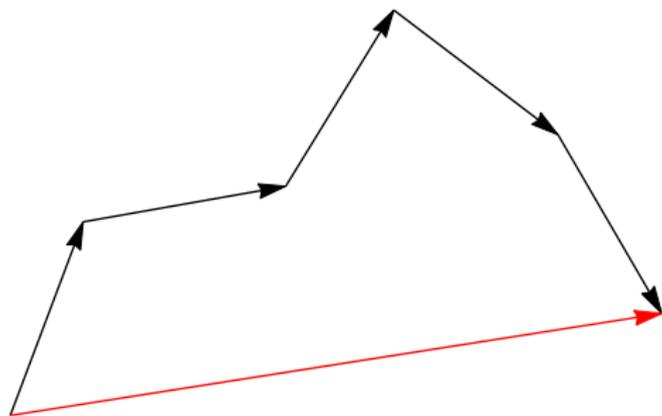
$$\vec{e}_k = w_k^2$$

The complex  $n$ -vector  $(w_1, \dots, w_n) \in \mathbb{C}^n$  is the square root of the polygon!

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# Closure and The Square Root Description

## Definition

If a polygon  $P$  is given by  $\vec{w} = (w_1, \dots, w_n) \in \mathbb{C}^n$ , we can also associate the polygon with two real  $n$ -vectors  $\vec{a} = (a_1, \dots, a_n)$  and  $\vec{b} = (b_1, \dots, b_n)$  where  $w_k = a_k + b_k i$ .

$$\vec{w} = \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{pmatrix} = \begin{pmatrix} a_1 + b_1 i \\ a_2 + b_2 i \\ \vdots \\ a_n + b_n i \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} + \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix} i = \vec{a} + \vec{b}i$$

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## Proposition (Hausmann and Knutson, 1997)

*The polygon  $P$  is closed  $\iff$  the vectors  $\vec{a}$  and  $\vec{b}$  are **orthogonal** and **have the same length**.*

## Proof.

We know  $w_k^2 = (a_k + b_k i) * (a_k + b_k i) = (a_k^2 - b_k^2) + 2a_k b_k i$ . So

$$\begin{aligned} 0 = \sum w_k^2 &\iff \sum (a_k^2 - b_k^2) = 0 \text{ and } \sum 2a_k b_k = 0 \\ &\iff \vec{a} \cdot \vec{a} - \vec{b} \cdot \vec{b} = 0 \text{ and } 2\vec{a} \cdot \vec{b} = 0. \end{aligned}$$



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*The length of the polygon is given by the sum of the squares of the norms of  $\vec{a}$  and  $\vec{b}$ .*

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We know that the length of  $P$  is the sum  $\sum |\vec{e}_i| = \sum |w_k|^2$ . But

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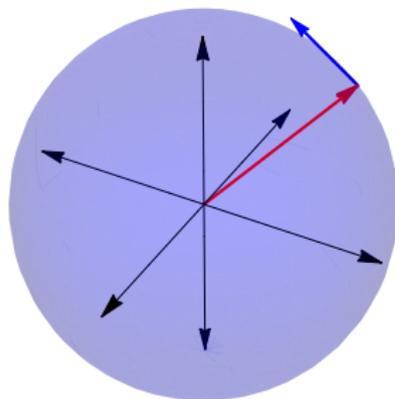
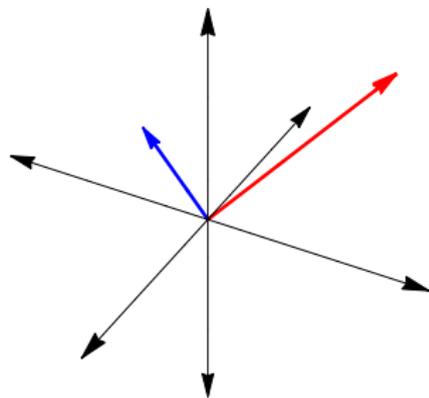


# Putting it all together

Since the Stiefel manifold  $V_2(\mathbb{R}^n)$  is the space of pairs of vectors in  $\mathbb{R}^n$  which are unit length and perpendicular, we see that closed polygons in the plane of total perimeter 2 are parametrized by  $V_2(\mathbb{R}^n)$ .

A sample element of  $V_2(\mathbb{R}^3)$ :

$$\begin{pmatrix} 0.535398 & -0.71878 \\ 0.678279 & 0.678818 \\ 0.503275 & -0.150204 \end{pmatrix}$$



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Theorem (Hausmann and Knutson, 1997)

*The space of length-2 closed polygons in the plane **up to translation** is double-covered by  $V_2(\mathbb{R}^n)$ .*

Conclusion

*The right way to compare shapes that have a preferred orientation (meaning you're not allowed to rotate them) is by computing distances in the Stiefel manifold.*

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# Rotation and the Square Root Description

## Proposition (Hausmann and Knutson, 1997)

The rotation by angle  $\phi$  of the polygon given by  $\vec{a}$ ,  $\vec{b}$  has square root description given by the vectors  $\cos(\phi/2)\vec{a} - \sin(\phi/2)\vec{b}$  and  $\sin(\phi/2)\vec{a} + \cos(\phi/2)\vec{b}$ .

### Proof.

We can write  $\vec{e}_k = w_k^2 = (r_k e^{i\theta_k})^2 = r_k^2 e^{i2\theta_k}$ . If we rotate the polygon by  $\phi$ , we rotate each  $\vec{e}_k$  by  $\phi$  and the new polygon is given by

$$u_k^2 = r_k^2 e^{i(2\theta_k + \phi)} = r_k^2 e^{i2(\theta_k + \frac{\phi}{2})}$$

So  $u_k = r_k e^{i(\theta_k + \frac{\phi}{2})}$

$$= r_k \cos(\theta_k + \frac{\phi}{2}) + r_k \sin(\theta_k + \frac{\phi}{2})i$$

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Since the Grassmannian  $G_2(\mathbb{R}^n)$  is the space of (2-dimensional) planes in  $\mathbb{R}^n$ , we have:

Theorem (Hausmann and Knutson, 1997)

*The space of length-2 closed polygons in the plane **up to rotation and translation** is double-covered by  $G_2(\mathbb{R}^n)$ .*

Conclusion

*The right way to compare shapes is to compute distances in the Grassmann manifold! This is a description of polygon space that's simple and easy to work with, and also won't be confused by simply rotating or translating the polygon.*

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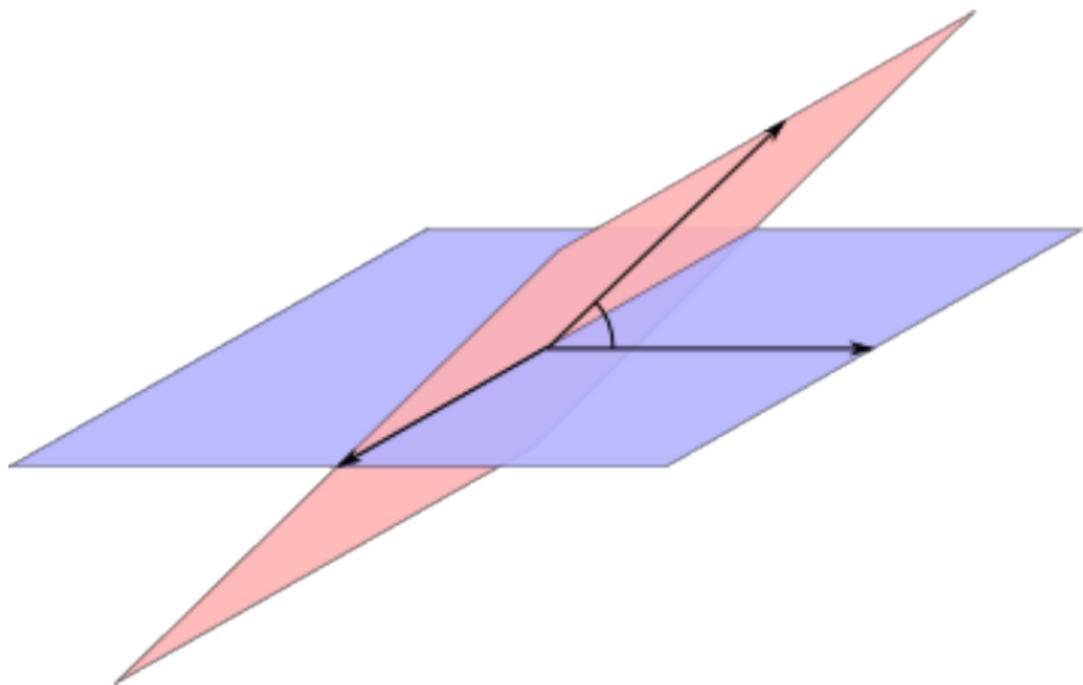
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# Jordan Angles and the Distance Between Planes

## Question

*How far apart are two planes in  $\mathbb{R}^n$ ?*



# Jordan Angles and the Distance Between Planes

## Theorem (Jordan)

Any two planes in  $\mathbb{R}^n$  have a pair of orthonormal bases  $\vec{v}_1, \vec{w}_1$  and  $\vec{v}_2, \vec{w}_2$  so that

- 1  $\vec{v}_2$  minimizes the angle between  $\vec{v}_1$  and any vector on plane  $P_2$ .  $\vec{w}_2$  minimizes the angle between the vector  $\vec{w}_1$  perpendicular to  $\vec{v}_1$  in  $P_1$  and any vector in  $P_2$ .
- 2 (vice versa)

The angles between  $\vec{v}_1$  and  $\vec{v}_2$  and  $\vec{w}_1$  and  $\vec{w}_2$  are called the **Jordan angles** between the two planes. The rotation carrying  $\vec{v}_1 \rightarrow \vec{v}_2$  and  $\vec{w}_1 \rightarrow \vec{w}_2$  is called the **direct rotation** from  $P_1$  to  $P_2$  and it is the shortest path from  $P_1$  to  $P_2$  in the Grassmann manifold  $G_2(\mathbb{R}^n)$ .

## Theorem (Jordan)

- Let  $\Pi_1$  be the map  $P_1 \rightarrow P_1$  given by orthogonal projection  $P_1 \rightarrow P_2$  followed by orthogonal projection  $P_2 \rightarrow P_1$ . The basis  $\vec{v}_1, \vec{w}_1$  is given by the eigenvectors of  $\Pi_1$ .
- Let  $\Pi_2$  be the map  $P_2 \rightarrow P_2$  given by orthogonal projection  $P_2 \rightarrow P_1$  followed by orthogonal projection  $P_1 \rightarrow P_2$ . The basis  $\vec{v}_2, \vec{w}_2$  is given by the eigenvectors of  $\Pi_2$ .

## Conclusion

*The bases  $\vec{v}_1, \vec{w}_1$  and  $\vec{v}_2, \vec{w}_2$  give the rotations of polygons  $P_1$  and  $P_2$  that are closest to one another in the Stiefel manifold  $V_2(\mathbb{R}^n)$ . This is how we should align polygons in the plane!*

Theorem (with Cantarella, Chapman, and Needham)

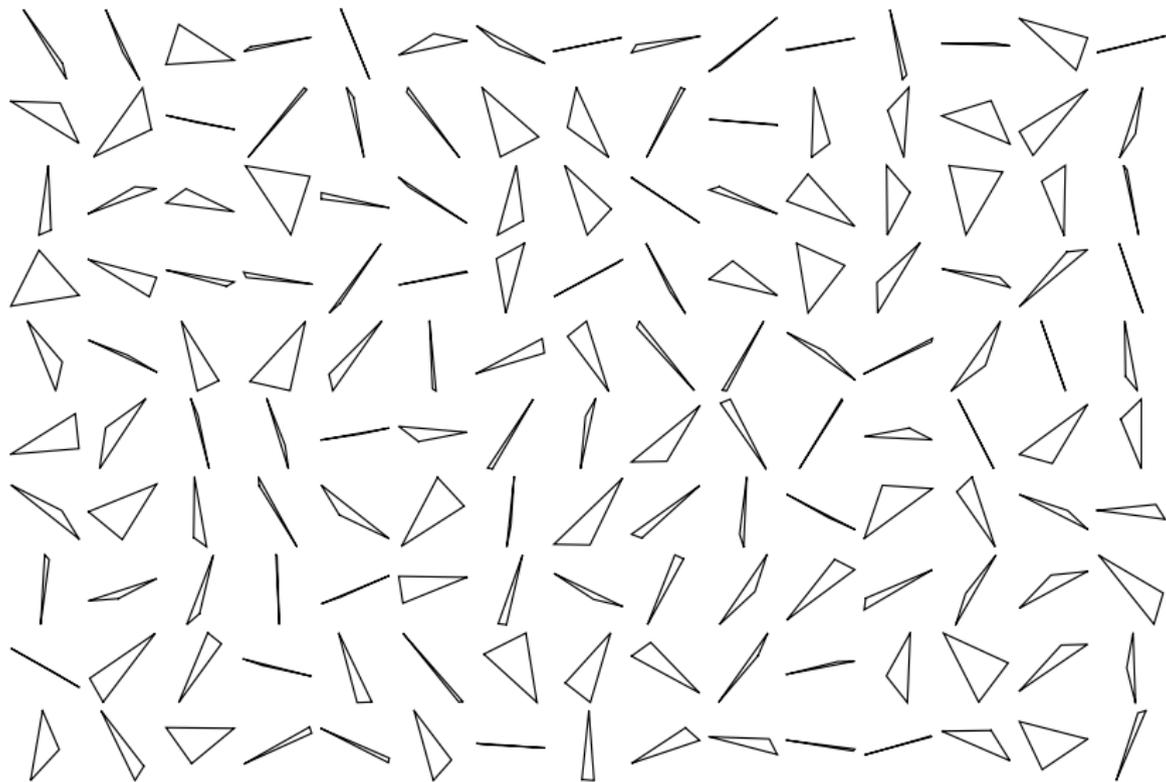
*With respect to the symmetric measure on planar triangles, the fraction of acute triangles is exactly*

$$\frac{\ln 8}{\pi} - \frac{1}{2} \simeq 0.161907$$



The acute triangles inside  $G_2(\mathbb{R}^3) \cong \mathbb{RP}^2$ .

# 150 Random Triangles



# What about the square root of a space polygon? Quaternions

## Definition

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

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

In other words, elements of  $\mathbb{H}$  are of the form

$$q = a + b\mathbf{i} + c\mathbf{j} + d\mathbf{k}.$$

We can think of the “square root” of a vector  $\vec{v} \in \mathbb{R}^3$  as the quaternion  $q$  so that

$$\vec{v} = \bar{q}\mathbf{i}q.$$

Then we get a square root description of space polygons by taking the “square root” of each edge in the polygon.

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More precisely, if  $\text{Hopf} : \mathbb{H}^n \rightarrow \{\text{polygonal arms in } \mathbb{R}^3\}$  is given by

$$\text{Hopf}(q_1, \dots, q_n) = (\bar{q}_1 \mathbf{i} q_1, \dots, \bar{q}_n \mathbf{i} q_n),$$

then we see that the total perimeter of an arm  $\text{Hopf}(q_1, \dots, q_n)$

is

$$\sum_{\ell} |\bar{q}_{\ell} \mathbf{i} q_{\ell}| = \sum_{\ell} |q_{\ell}|^2.$$

Therefore, the sphere  $S^{4n-1}(\sqrt{2}) \subset \mathbb{H}^n$  of radius  $\sqrt{2}$  is mapped onto the space of polygonal arms of total perimeter 2.

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# From Arm Space to Closed Polygon Space

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

$$(\vec{u}, \vec{v}, \theta) \mapsto \sqrt{2}(\cos \theta \vec{u} + \sin \theta \vec{v} \mathbf{j})$$

where  $\vec{u}, \vec{v} \in \mathbb{C}^n$  lie in the unit sphere and  $\theta \in [0, \pi/2]$ .

We focus on

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

Proposition (Hausmann–Knutson '97)

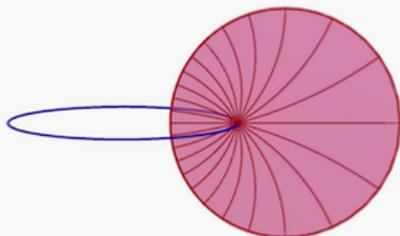
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$$(\vec{u}, \vec{v}, \theta) \mapsto \sqrt{2}(\cos \theta \vec{u} + \sin \theta \vec{v} \mathbf{j})$$

where  $\vec{u}, \vec{v} \in \mathbb{C}^n$  lie in the unit sphere and  $\theta \in [0, \pi/2]$ .



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We focus on

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

Proposition (Hausmann–Knutson '97)

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

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**Proposition (Hausmann–Knutson '97)**

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# The proof is (a computation) worth doing!

In complex form, the map  $\text{Hopf}(q)$  can be written as

$$\text{Hopf}(a + bj) = (\overline{a + bj})i(a + bj) = i(|a|^2 - |b|^2 + 2\bar{a}bj)$$

Thus the polygon closes  $\iff$

$$\begin{aligned} \left| \sum \text{Hopf}(q_i) \right|^2 &= \left| \sum 2|\cos \theta u_i|^2 - \sum 2|\sin \theta v_i|^2 \right. \\ &\quad \left. + 4 \cos \theta \sin \theta \sum \bar{u}_i v_i \right|^2 \\ &= \left| 2 \cos^2 \theta - 2 \sin^2 \theta \right|^2 + |4 \cos \theta \sin \theta \langle u, v \rangle|^2 \\ &= 4 \cos^2 2\theta + 4 \sin^2 2\theta |\langle u, v \rangle|^2 = 0 \end{aligned}$$

or  $\iff \theta = \pi/4$  and  $\vec{u}, \vec{v}$  are orthogonal.

# Sampling random polygons (directly!)

## Proposition (with Cantarella and Deguchi)

*The natural (Haar) measure on  $V_2(\mathbb{C}^n)$  (and hence the symmetric measure on  $\widetilde{\text{FPol}}(n)$  or  $\widetilde{\text{Pol}}(n)$ ) 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]];

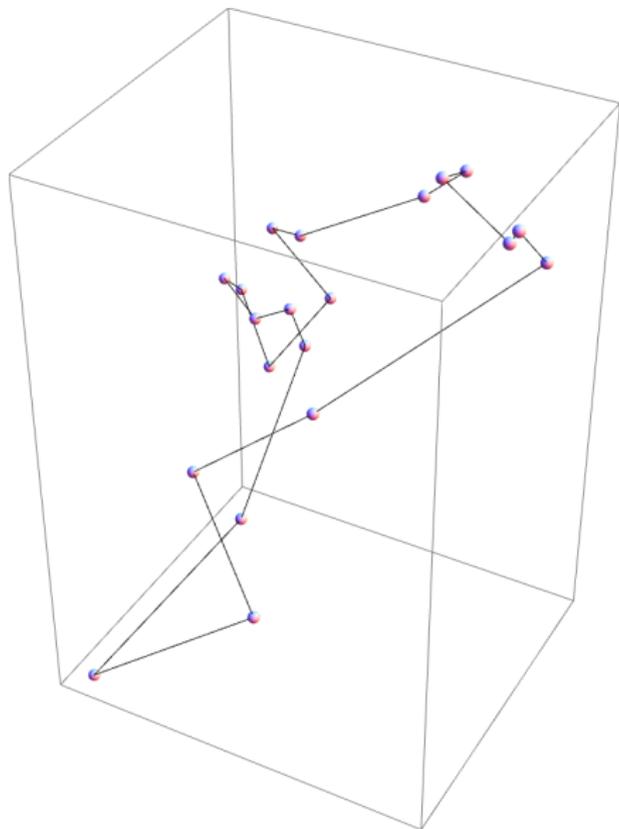
ComplexDot[A_, B_] := Dot[A, Conjugate[B]];
ComplexNormalize[A_] := (1 / Sqrt[Re[ComplexDot[A, A]]]) A;

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}
];
```

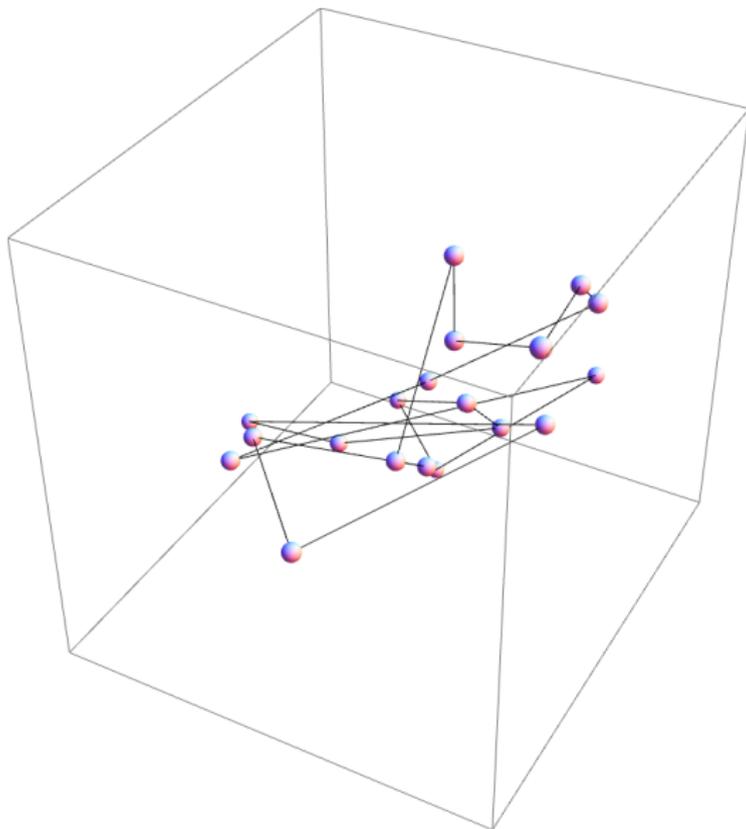
Now we need only apply the Hopf map to generate an edge set:

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

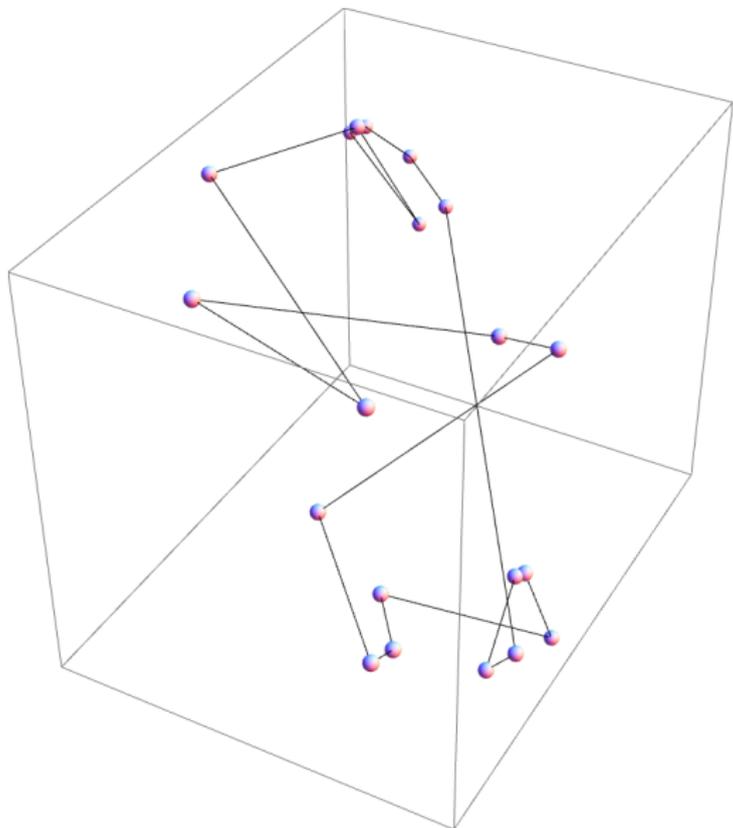
# Examples of 20-gons



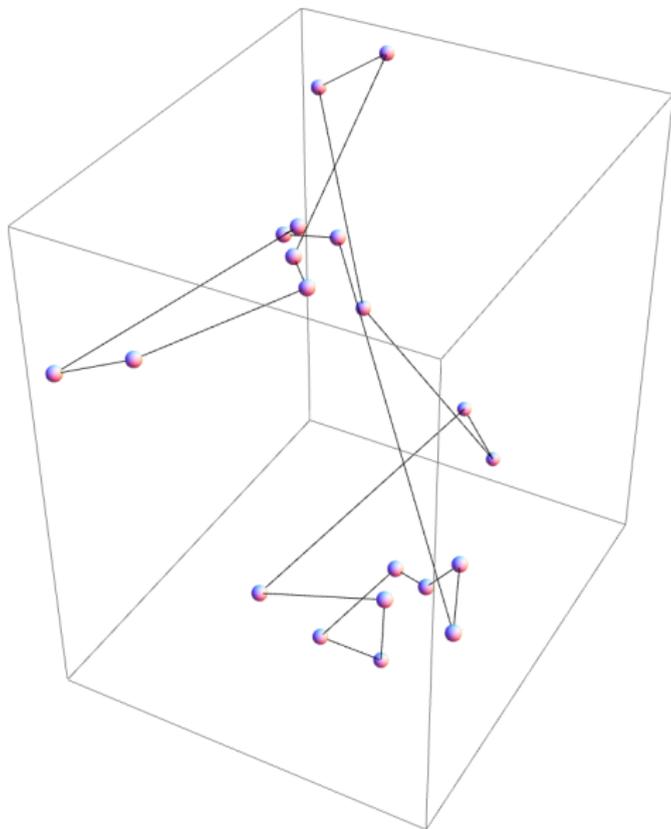
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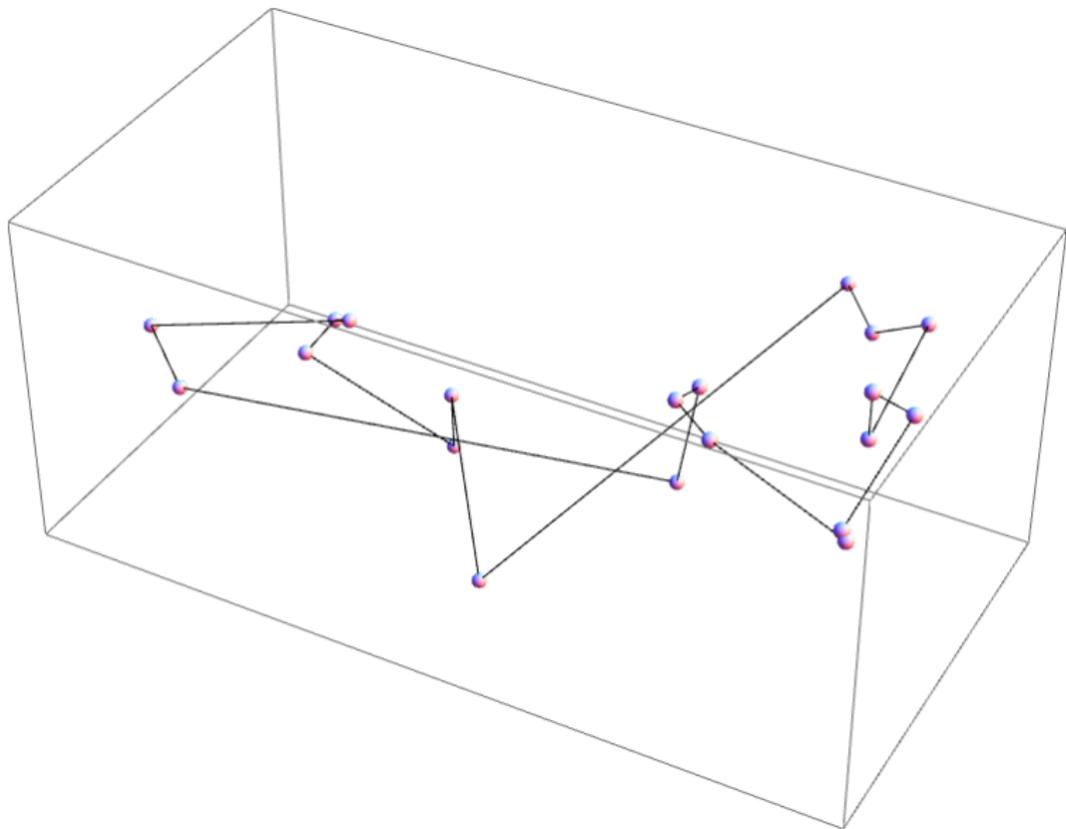
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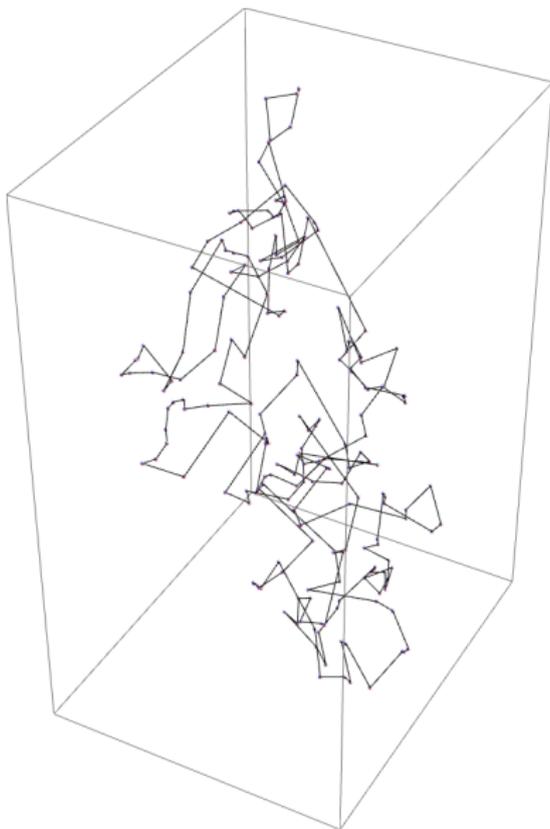
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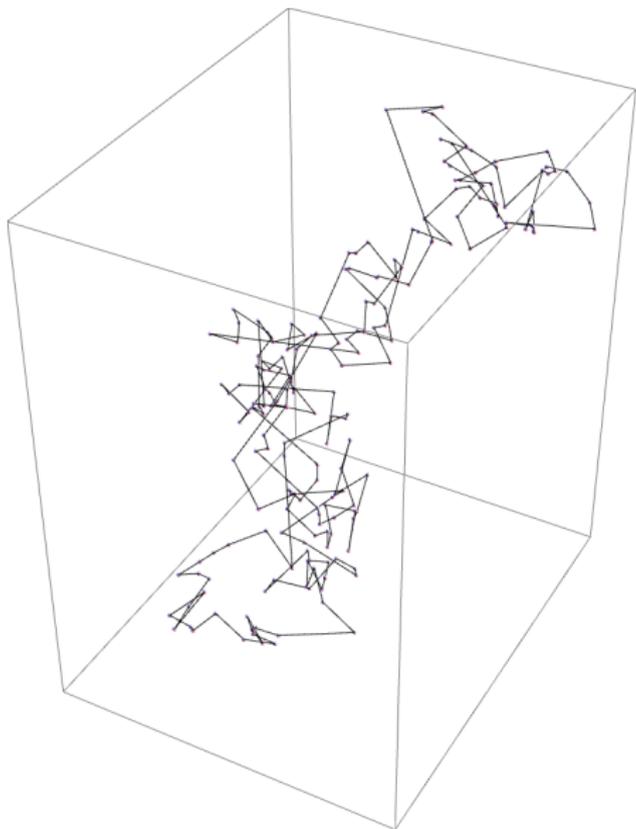
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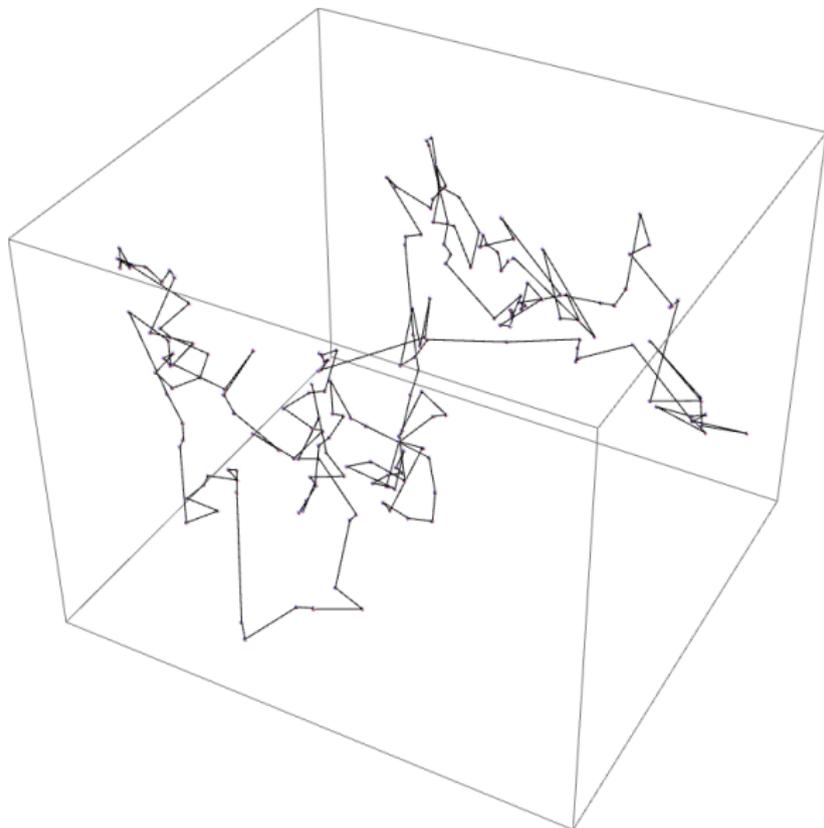
# Examples of 200-gons



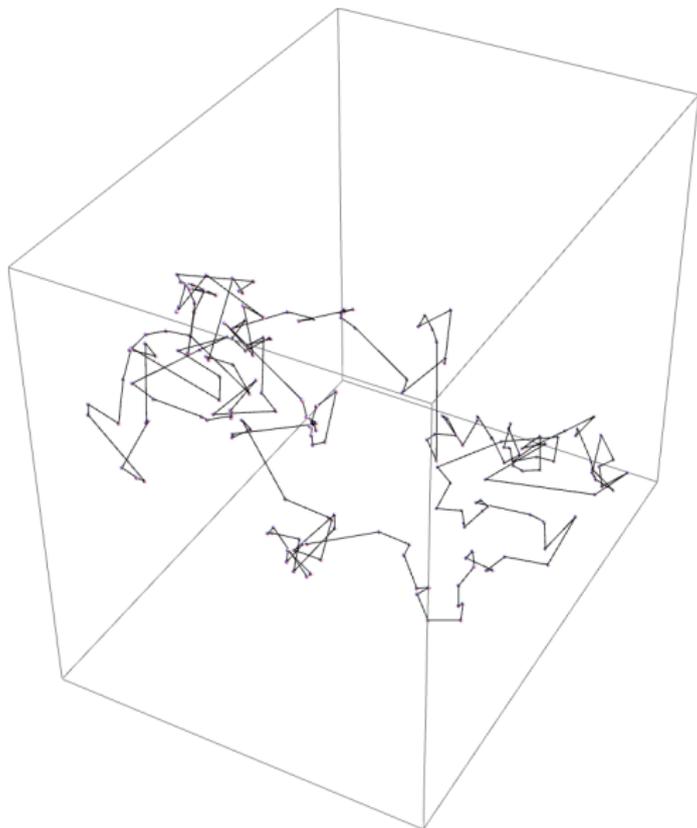
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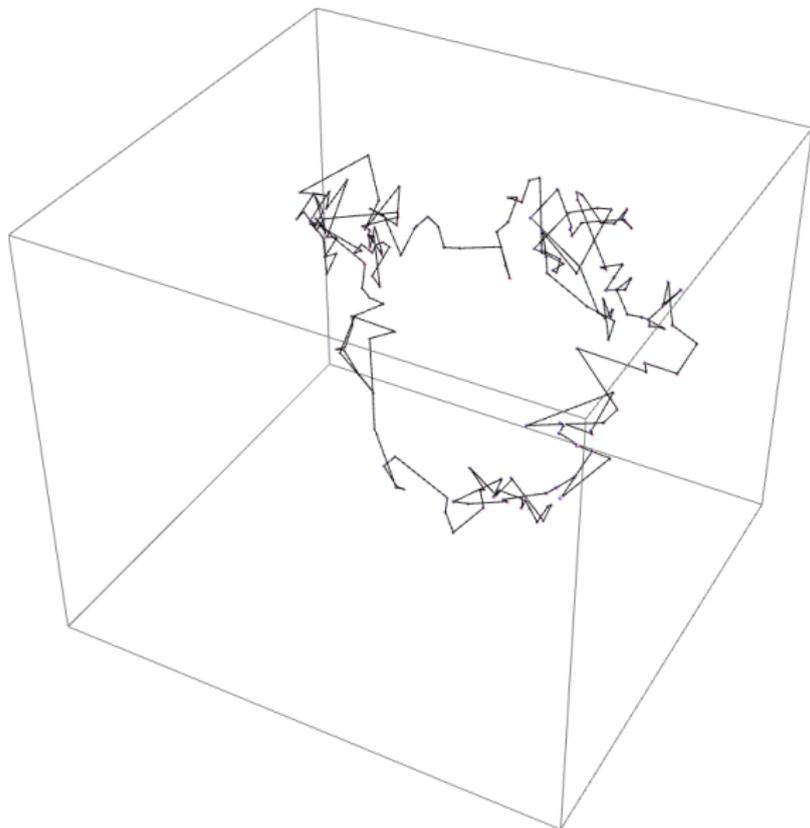
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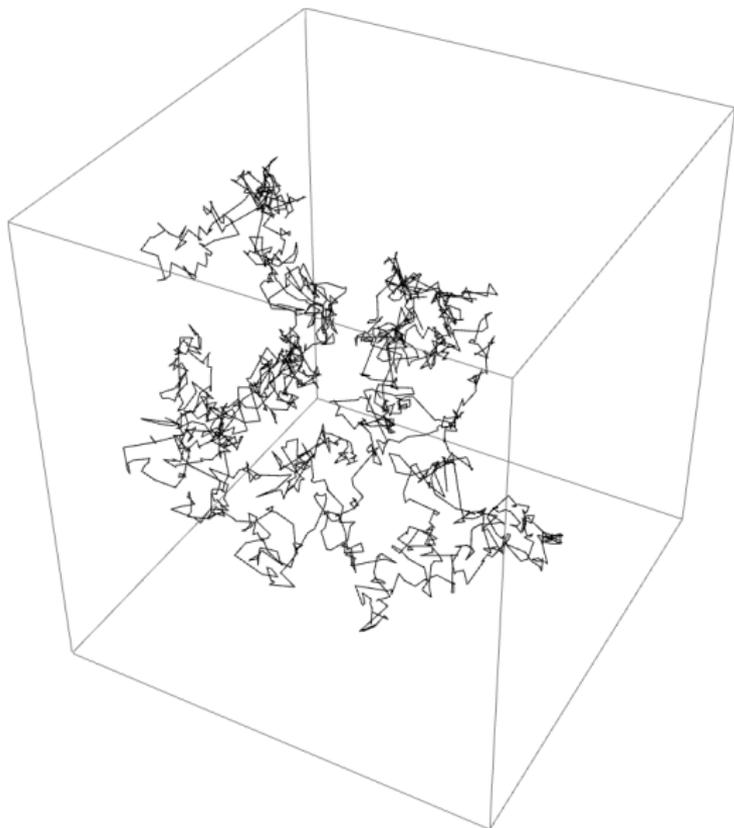
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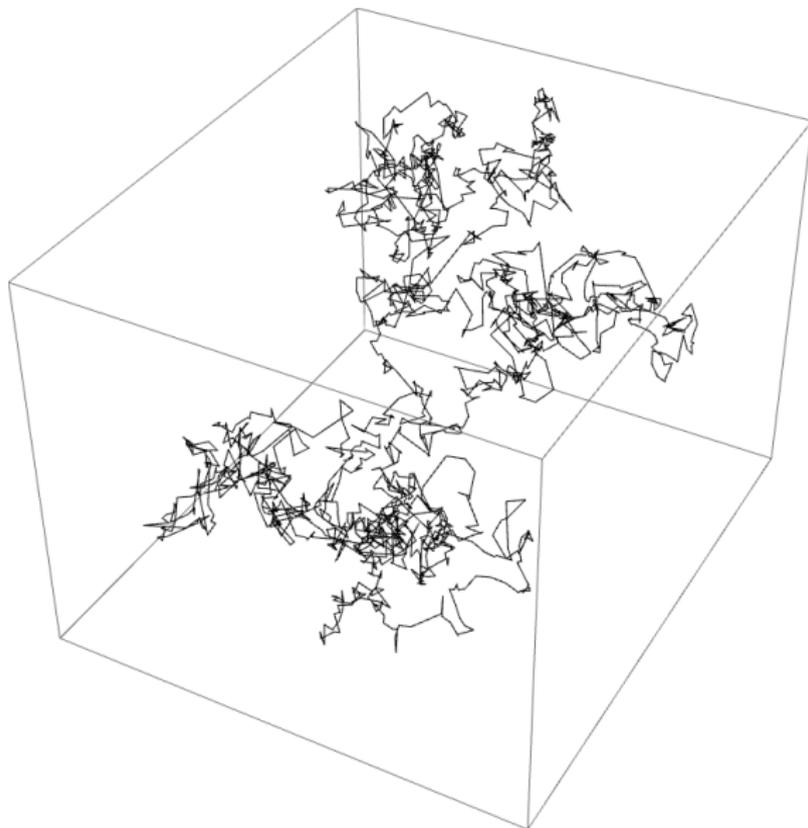
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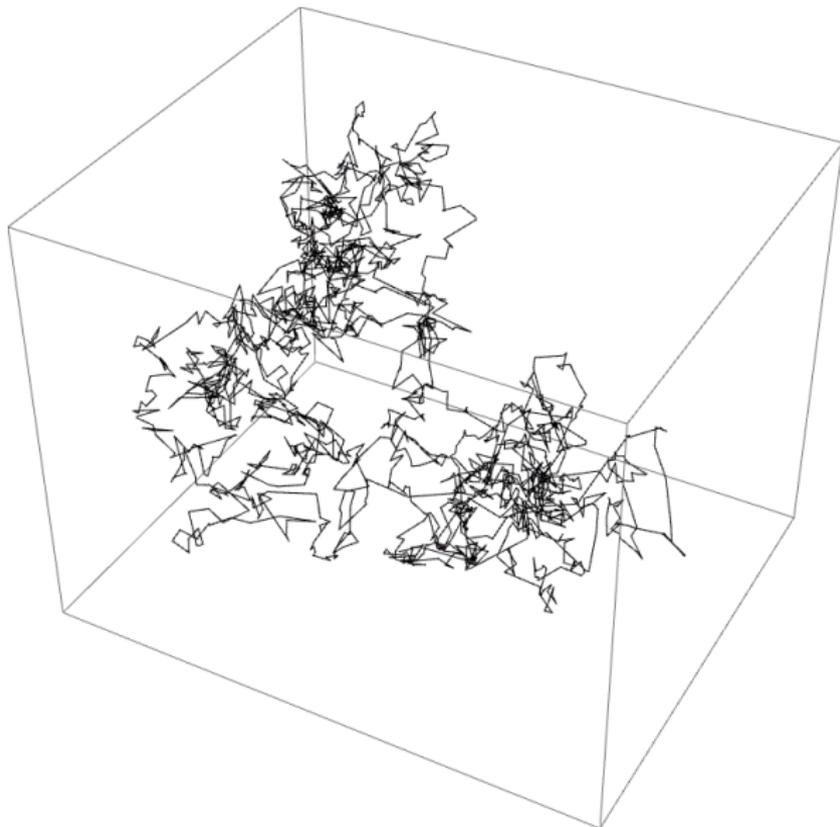
# Examples of 2,000-gons



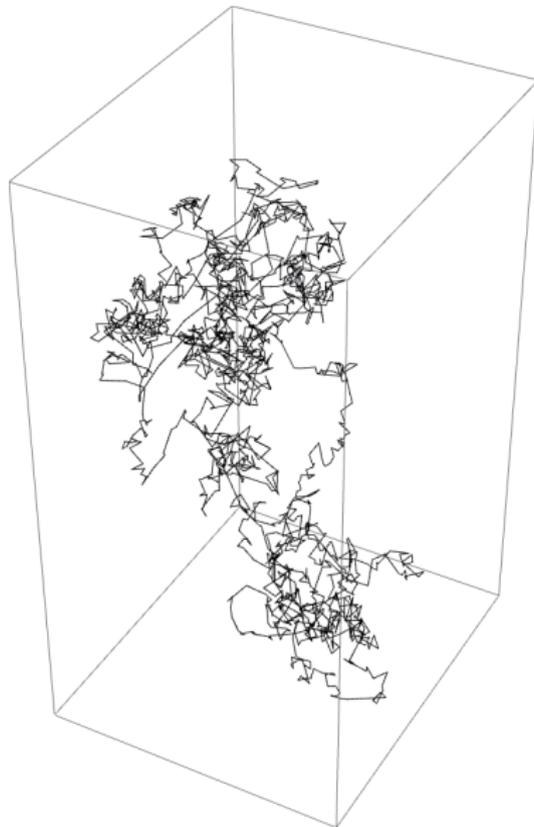
# Examples of 2,000-gons



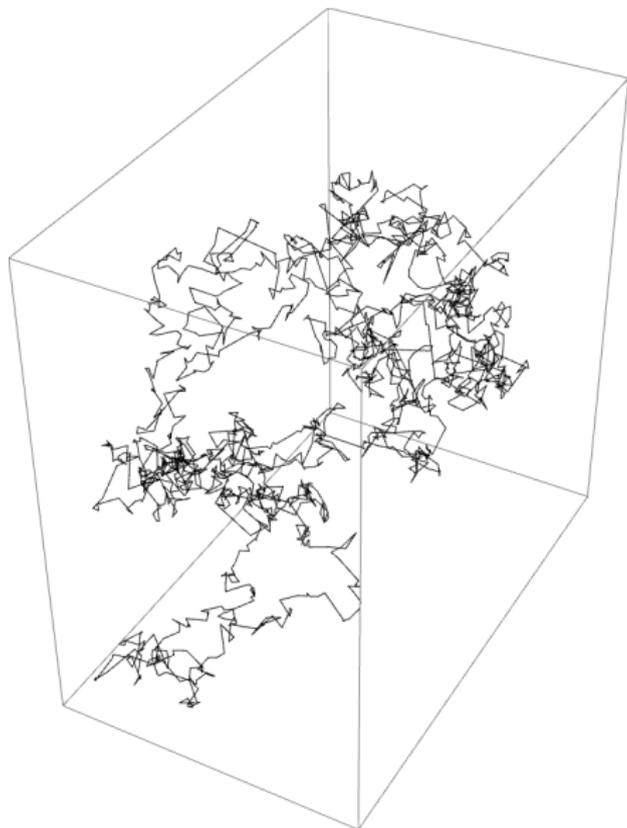
# Examples of 2,000-gons



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Thank you for inviting me and for spending so much time listening to what I had to say.