Unlocking the geometry of polygon space by taking square roots

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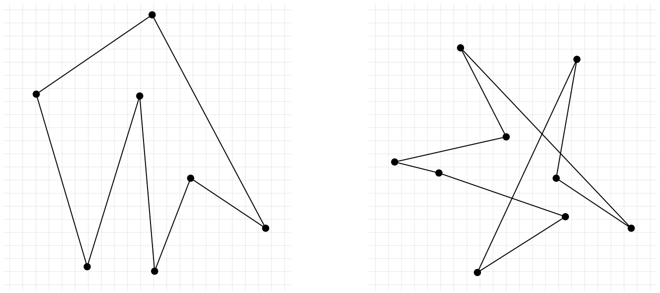
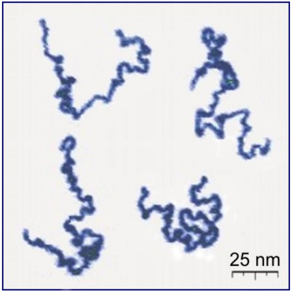
Definition

A polygon given by vertices $v_1, \ldots, v_n$ is a collection of line segments in the plane 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:

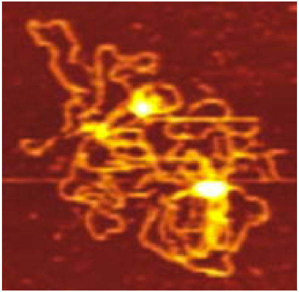
$$\vec{e}_i = v_i - v_{i-1} \quad \text{(and } \vec{e}_0 = v_1 - v_n\text{)}.$$



Applications of Polygon Model

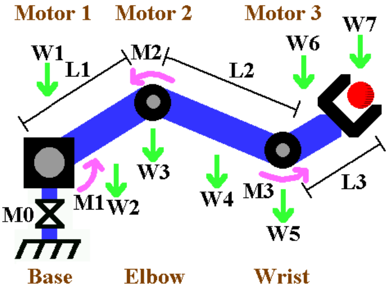


Protonated P2VP
Roiter/Minko
Clarkson University

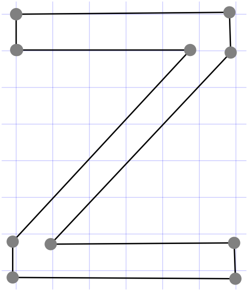


Plasmid DNA
Alonso-Sarduy, Dietler Lab
EPF Lausanne

Applications of Polygon Model



Robot Arm
Society Of Robots



Polygonal Letter Z

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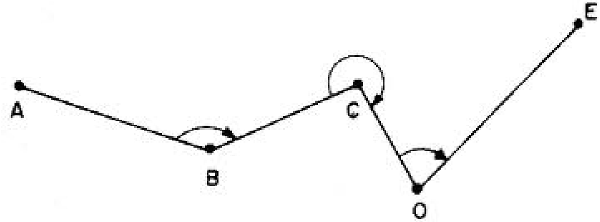
The space of possible shapes of a polygon (with a fixed number of edges) is called a *configuration space*.



Theorem

The configuration space of n-edge open polygons is the set of $n-1$ turning angles $\theta_1, \ldots, \theta_{n-1}$. This space is called an $(n-1)$-torus.

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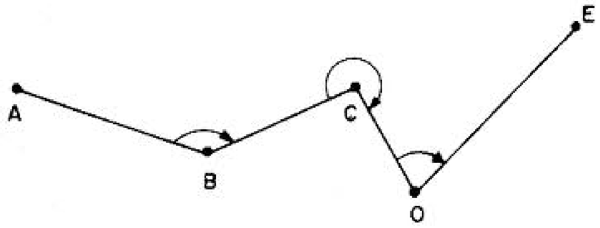

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How can we describe closed plane polygons?

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?)
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Complex Numbers and the Square Root of a Polygon

Definition

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

Definition

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

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

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

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

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

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

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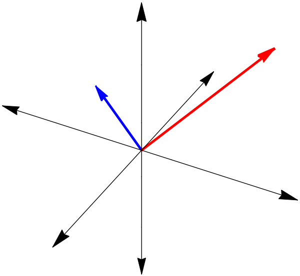
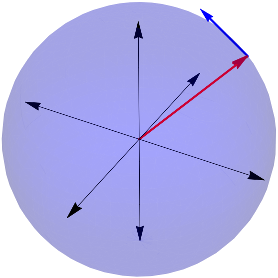
The *Stiefel manifold* $V_2(\mathbb{R}^n)$ is the space of orthonormal pairs of vectors in $\mathbb{R}^n$.

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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Proposition (Hausmann and Knutson, 1997)

The rotation by angle ϕ 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* $-\sin(\phi/2)\vec{a} + \cos(\phi/2)\vec{b}$.

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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 ϕ, we rotate each $\vec{e}_k$ by ϕ and the new polygon is given by

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

So

$$\begin{aligned} u_k &= r_k e^{i(\theta_k + \frac{\phi}{2})} \\ &= r_k \cos(\theta_k + \frac{\phi}{2}) + r_k \sin(\theta_k + \frac{\phi}{2}) i \\ &= (a_k \cos\frac{\phi}{2} + b_k \sin\frac{\phi}{2}) + (-a_k \sin\frac{\phi}{2} + b_k \cos\frac{\phi}{2}) i. \end{aligned}$$

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Putting it all together II

Definition

The *Grassmann manifold* $G_2(\mathbb{R}^n)$ is the space of 2-dimensional linear subspaces of $\mathbb{R}^n$.

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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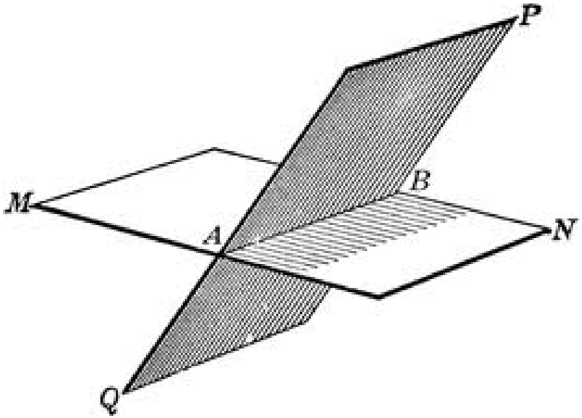
Question

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



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 $\vec{v}_1 \to \vec{v}_2$ and $\vec{w}_1 \to \vec{w}_2$ 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 Π_1 be the map $P_1 \to P_1$ given by orthogonal projection $P_1 \to P_2$ followed by orthogonal projection $P_2 \to P_1$. The basis $\vec{v}_1, \vec{w}_1$ is given by the eigenvectors of Π_1.*
- *Let Π_2 be the map $P_2 \to P_2$ given by orthogonal projection $P_2 \to P_1$ followed by orthogonal projection $P_1 \to P_2$. The basis $\vec{v}_2, \vec{w}_2$ is given by the eigenvectors of Π_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!

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 **i**, **j**, and **k** so that

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

We can identify quaternions with frames in SO(3) via the Hopf map

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

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

Proposition

The unit quaternions (S^3) double-cover SO(3) *via the Hopf map.*

Thank you!

- *Probability Theory of Random Polygons from the Quaternionic Viewpoint*
  Cantarella, Deguchi, and Shonkwiler
  arXiv:1206.3161
  Communications on Pure and Applied Mathematics
  (2013), doi:10.1002/cpa.21480.

- *The Expected Total Curvature of Random Polygons*
  Cantarella, Grosberg, Kusner, and Shonkwiler
  arXiv:1210.6537.

- *The symplectic geometry of closed equilateral random walks in 3-space*
  Cantarella and Shonkwiler
  arXiv:1310.5924.

Thank you for inviting me!