

Unlocking the geometry of polygon space by taking square roots

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University of Georgia

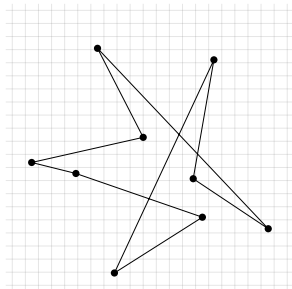
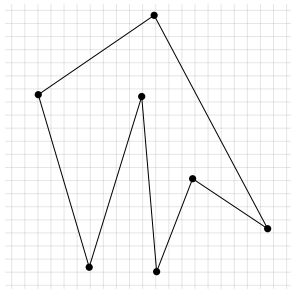
Gettysburg College

February 11, 2014

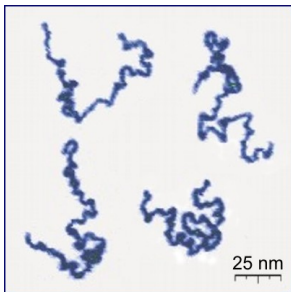
Definition

A polygon given by vertices v_1, \dots, 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:

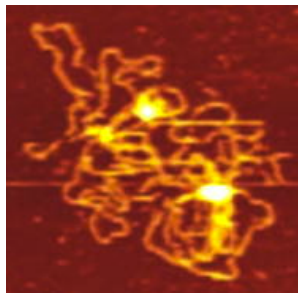
$$\vec{e}_i = v_{i+1} - v_i \quad (\text{and } \vec{e}_n = v_1 - v_n).$$



Applications of Polygon Model

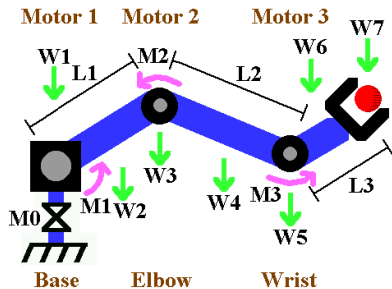


Protonated P2VP
Roiter/Minko
Clarkson University

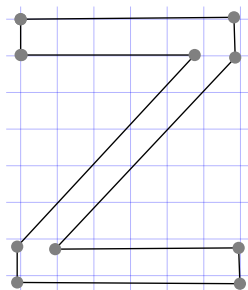


Plasmid DNA
Alonso-Sarduy, Dietler Lab
EPF Lausanne

Applications of Polygon Model



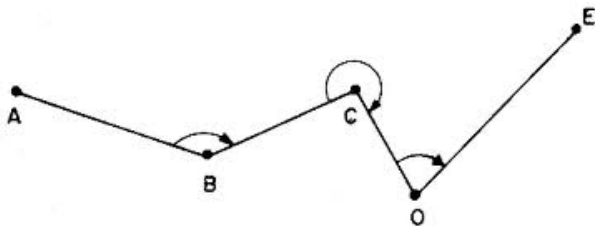
Robot Arm
Society Of Robots



Polygonal Letter Z

Definition

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

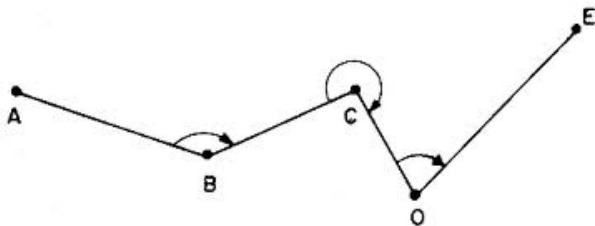


Theorem

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?)
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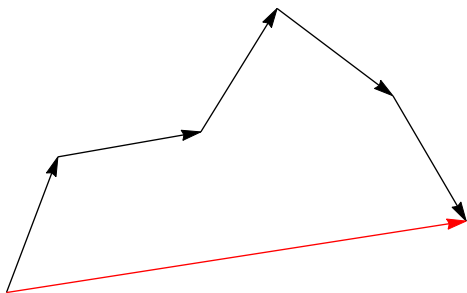
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Edge Vectors and the Closure Condition

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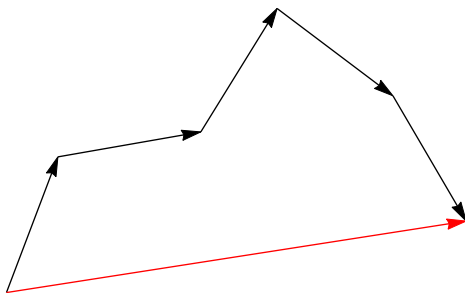
An n -edge polygon could be given by a collection of edge vectors $\vec{e}_1, \dots, \vec{e}_n$ of the polygon. The polygon closes $\iff \vec{e}_1 + \dots + \vec{e}_n = \vec{0}$.



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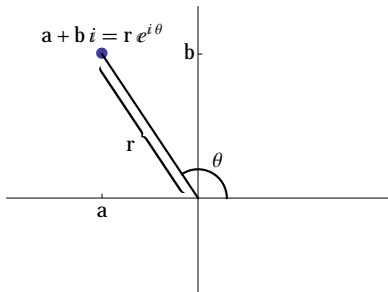
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Complex Numbers and the Square Root of a Polygon

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

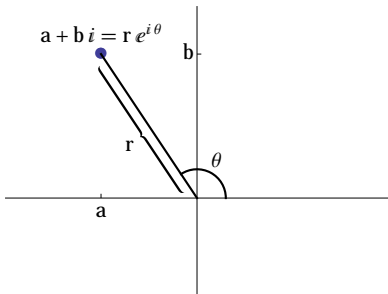
$$\vec{e}_k = w_k^2$$

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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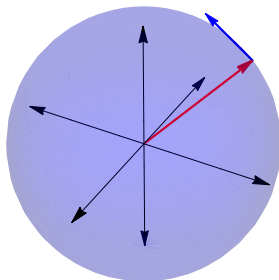
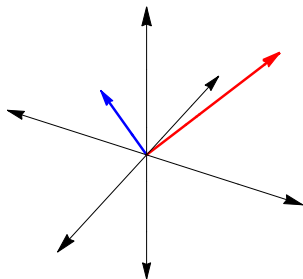


Definition

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 (a.k.a., *orthonormal*).

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

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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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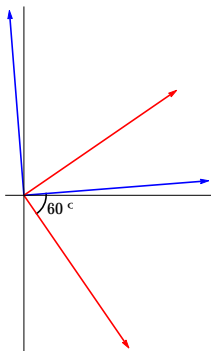
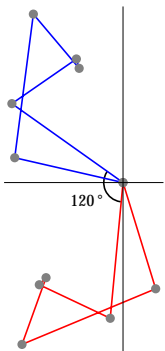
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Rotation and the Square Root Description

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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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 ϕ , we rotate each \vec{e}_k by ϕ 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 $u_k = r_k e^{i(\theta_k + \frac{\phi}{2})}$

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

$$= (a_k \cos \frac{\phi}{2} - b_k \sin \frac{\phi}{2}) + (a_k \sin \frac{\phi}{2} + b_k \cos \frac{\phi}{2})i.$$

Definition

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

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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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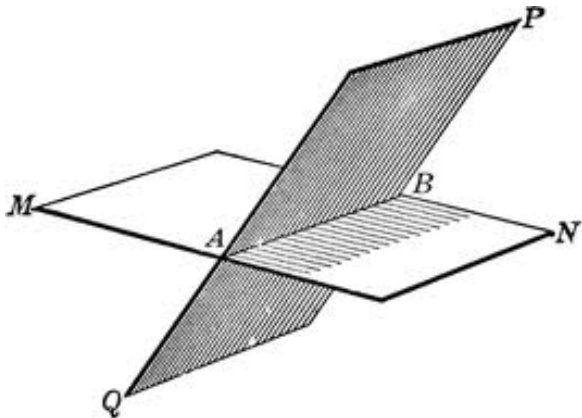
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Jordan Angles and the Distance Between Planes

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 Π_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 Π_1 .
- Let Π_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 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 \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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Thank you for inviting me!