Unlocking the geometry of polygon space by taking square roots

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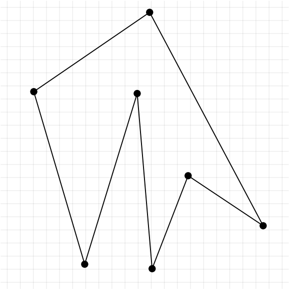
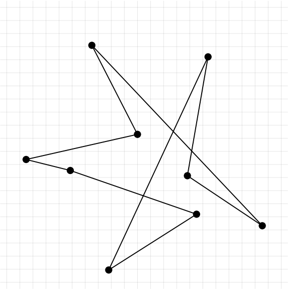
Definition

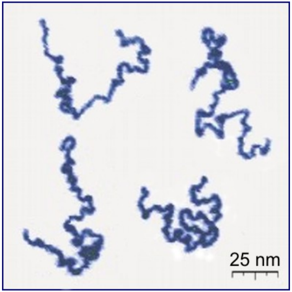
A polygon given by vertices $v_1, \ldots, v_n$ is a collection of line segments in the plane joining each v_i to v_{i+1} (and v_n to v_1). The *edge vectors* $\vec{e}_i$ of the polygons are the differences between vertices:

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

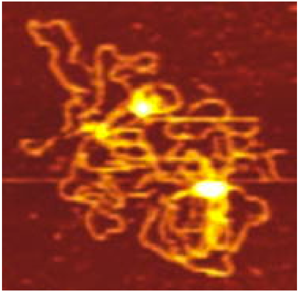




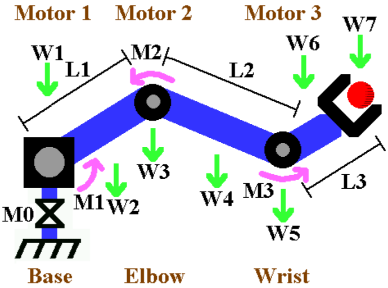
Applications of Polygon Model



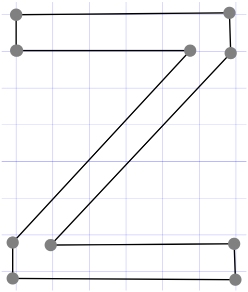
Protonated P2VP
Roiter/Minko
Clarkson University



Plasmid DNA
Alonso-Sarduy, Dietler Lab
EPF Lausanne



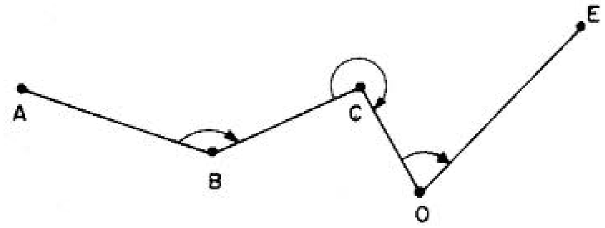
Robot Arm
Society Of Robots



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 $\theta_1, \ldots, \theta_{n-1}$. This space is called an $(n-1)$-torus.

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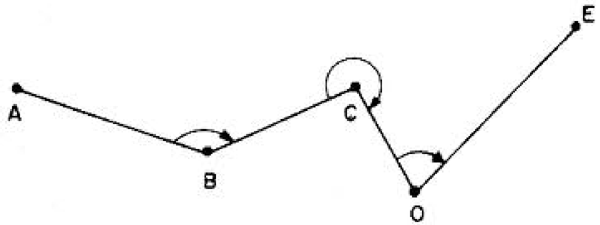

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Question

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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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 $\iff$ $\vec{e}_1 + \cdots + \vec{e}_n = \vec{0}$.

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 $w_1, \ldots w_n$ 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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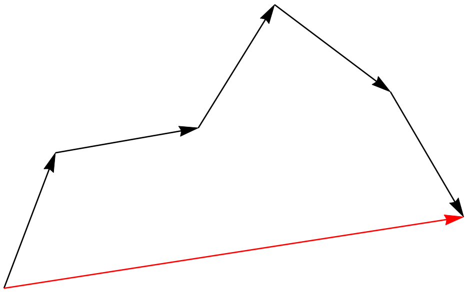

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Closure and The Square Root Description

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 $w_k = a_k + b_k i$.

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

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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

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

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Length and The Square Root Description

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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 $w_k = a_k + b_k i$.

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

Proof.

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

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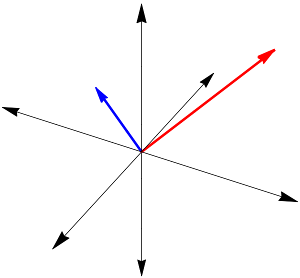
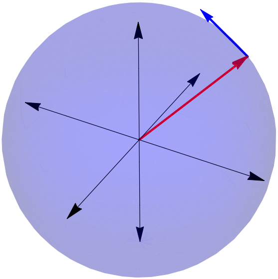
Definition

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 $V_2(\mathbb{R}^n)$.*

Conclusion

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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* $\sin(\phi/2)\vec{a} + \cos(\phi/2)\vec{b}$.

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

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Definition

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

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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.

Putting it all together II

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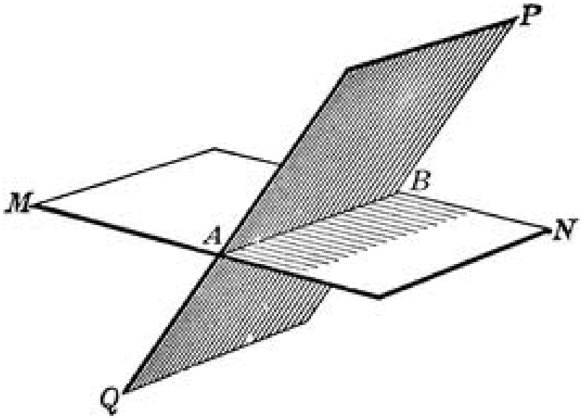
Question

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 $\vec{v}_1 \to \vec{v}_2$ 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!

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.

What about the square root of a space polygon? Quaternions

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Thank you!

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