COMP229: Introduction to Data Science
Lecture 20: Isometries

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Lecture plan

- Why linear algebra?
- Kernel trick overview.
- What is an isometry?
- Isometries via reflections.

Reminder: Algebra and geometry from linear maps

- A linear map preserves the operations of *vector addition* and *scalar multiplication*.
- Any linear map is determined by images of basis vectors and can be represented by the matrix whose columns are these images.
- The matrix multiplication is motivated by the composition of linear maps: $(BA)_{ij} = \sum_{s=1}^{k} b_{is} a_{sj}$.
- Any *affine* map $\mathbb{R}^m \to \mathbb{R}^k$ is $\vec{v} \mapsto A\vec{v} + \vec{u}$ for a fixed $k \times m$ matrix A, a fixed vector $\vec{u} \in \mathbb{R}^k$.

Why linear algebra?

The *expected value* of a random variable is linear:

for any random variables X and Y:

$E[X+Y] = E[X] + E[Y]$ and $E[aX] = aE[X]$.

The variance of a random variable is not linear.

Differentiation is a linear map from the space of all differentiable functions to the space of all functions:

$\frac{d}{dx}(af(x) + bg(x)) = a\frac{df(x)}{dx} + b\frac{dg(x)}{dx}$.

The derivative at a point is a linear approximation of the function at that point.

Definite integral is a linear map from the space of all real-valued integrable functions to $\mathbb{R}$:

$\int_u^v (af(x) + bg(x))\, dx = a\int_u^v f(x)dx + b\int_u^v g(x)dx$.

From linear to kernel methods

Generalisation of the scalar product:

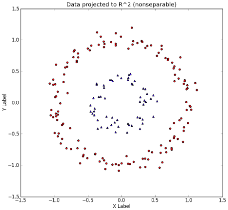
an inner product is a map $\langle \cdot, \cdot \rangle : V \times V \to \mathbb{R}$ such that for all vectors $x, y, z \in V$ and all scalars $a, b \in \mathbb{R}$

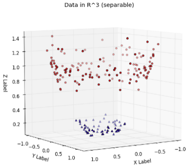
1) symmetry $\langle x, y \rangle = \langle y, x \rangle$.

2) linearity $\langle ax + by, z \rangle = a\langle x, z \rangle + b\langle y, z \rangle$.

3) positive-definiteness: if x is not zero, then $\langle x, x \rangle > 0$.

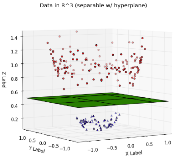
The kernel method allows to use linear methods after adding dimentionality via a *feature map* φ. In this example $\varphi : [x, y] \to [x, y, x^2 + y^2]$.

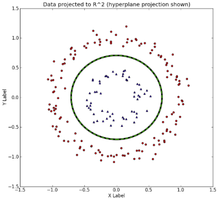




Images courtesy to this blog.

Kernel trick and inner product





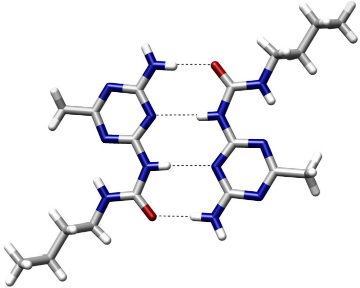
We can even use the resultant separating hyperplane to make predictions back in the initial space.

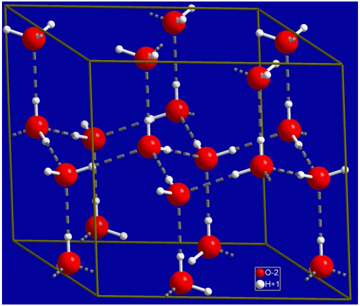
Calculations in higher dimentions are computationally expensive. Luckily, linear methods rely on *scalar products*. Those can be replaced by a **kernel** function in the initial space $k(\mathbf{x}, \mathbf{y}) = \langle \varphi(\mathbf{x}), \varphi(\mathbf{y}) \rangle$ as long as there exists such inner product representation. In this case there is even no need to write the feature map φ. A function can serve as a kernel iff matrix of k it is symmetric and positive definite.

Hence we can try several popular kernel functions (Polynomial, RBF), and choose the best result via K-fold validation.

How to compare rigid bodies

A body is *rigid* if the distance between any points is preserved. Many parts of cars, aircrafts and other machines are classified up to rigid motions.





Crystals are rigid since atoms have chemical bonds.

Isometries in Euclidean space $\mathbb{R}^m$

Definition 20.1. An **isometry**(or **congruence**) of $\mathbb{R}^m$ is any map $f : \mathbb{R}^m \to \mathbb{R}^m$ that is defined on the whole space $\mathbb{R}^m$ and preserves the Euclidean L_2-metric, i.e.
$L_2(p, q) = L_2(f(p), f(q))$ for any $p, q \in \mathbb{R}^m$.

An isometry is often confusingly called a **rigid** motion. A reflection over a line is an isometry not realisable as a continuous motion in the plane.

A translation by a vector $\vec{u}$ can be considered as a continuous motion of translations by $t\vec{u}$, $t \in [0, 1]$.

A non-example of an isometry

Problem 20.2. Which maps are isometries of $\mathbb{R}^2$?

$$\begin{pmatrix} x \\ y \end{pmatrix} \mapsto \begin{pmatrix} -2x \\ 3y \end{pmatrix}, \begin{pmatrix} x \\ y \end{pmatrix} \mapsto \begin{pmatrix} 2-x \\ y+3 \end{pmatrix}.$$

If yes, prove. If not, give a counter-example.

Solution 20.2. $\begin{pmatrix} x \\ y \end{pmatrix} \mapsto \begin{pmatrix} -2x \\ 3y \end{pmatrix}$ isn't an isometry.

$\begin{pmatrix} 0 \\ 0 \end{pmatrix} \mapsto \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \end{pmatrix} \mapsto \begin{pmatrix} -2 \\ 0 \end{pmatrix}$, the distance 1 between original points becomes distance 2 between their images under the map.

An example of an isometry

$\begin{pmatrix} x \\ y \end{pmatrix} \mapsto \begin{pmatrix} 2-x \\ y+3 \end{pmatrix}$ is an isometry, because the squared Euclidean distance between the images of any given points $\begin{pmatrix} x_1 \\ y_1 \end{pmatrix}, \begin{pmatrix} x_2 \\ y_2 \end{pmatrix} \in \mathbb{R}^2$ equals

$((2-x_1)-(2-x_2))^2+((y_1+3)-(y_2+3))^2 = (x_1-x_2)^2+(y_1-y_2)^2$, which is equal to the squared distance between the original points.

Isometries are bijective

Theorem 20.3. Any isometry $f : \mathbb{R}^m \to \mathbb{R}^m$ is *bijective*, hence any different points $p \neq q$ have different images under f, i.e. $f(p) \neq f(q)$.

Half proof. The injectivity is easy : the first metric axiom says that $d(p, q) = 0 \Leftrightarrow p = q$. Assume $f(p) = f(q)$. Conclude that $0 = d(f(p), f(q)) = d(p, q)$, hence $p = q$, again by the first axiom.
The surjectivity is harder, this year a proof isn't need for the exam.

Translations of $\mathbb{R}^m$ are isometries

Claim 20.4. For any fixed vector $\vec{u} \in \mathbb{R}^m$, the translation $t_{\vec{u}}(\vec{p}) = \vec{p} + \vec{u}$, $p \in \mathbb{R}^m$, is an isometry.

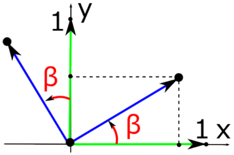
The algebraic form of the *translation* by a fixed vector $\vec{u} = \begin{pmatrix} s \\ t \end{pmatrix}$ is $\begin{pmatrix} x \\ y \end{pmatrix} \mapsto \begin{pmatrix} x+s \\ y+t \end{pmatrix}$.

Claim 20.5. For any isometries $f, g : \mathbb{R}^m \to \mathbb{R}^m$, the composition $f \circ g : \mathbb{R}^m \to \mathbb{R}^m$ is an isometry.

Rotations in the plane

Definition 20.6. The anticlockwise **rotation** about a point $O \in \mathbb{R}^2$ through an angle $\beta \in [0, 2\pi)$ maps p to the point q so that $\angle pOq = \beta$, $|Op| = |Oq|$.

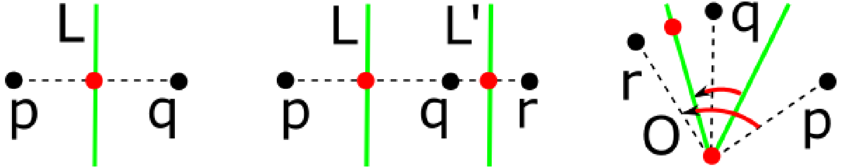
Claim 20.7. The rotation about $0 \in \mathbb{R}^2$ through an angle β is $\vec{v} \mapsto A\vec{v}$ with matrix $A = \begin{pmatrix} \cos\beta & -\sin\beta \\ \sin\beta & \cos\beta \end{pmatrix}$.



Proof. The basis vectors map to the columns $\begin{pmatrix} \cos\beta \\ \sin\beta \end{pmatrix}$, $\begin{pmatrix} -\sin\beta \\ \cos\beta \end{pmatrix}$ of A.

The reflection over a line in $\mathbb{R}^2$

Definition 20.8. The **reflection** over a line L maps any point $p \in \mathbb{R}^2$ to the point q such that L is the perpendicular bisector of the line segment $[p, q]$.

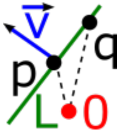


Theorem 20.9. Any isometry $f : \mathbb{R}^m \to \mathbb{R}^m$ decomposes into at most $m+1$ reflections, hence

f is bijective and has the inverse $f^{-1} : \mathbb{R}^m \to \mathbb{R}^m$.

A vector equation of a line

Theorem 20.9 allows us to represent any isometry (defined geometrically) in an algebraic matrix form.



For any line $L \subset \mathbb{R}^2$, let $p \in L$ and $\vec{v}$ be a unit length vector *perpendicular* to L.

Then L consists of all points q such that

$(\vec{q} - \vec{p}) \perp \vec{v}$,

or the scalar product $(\vec{q} - \vec{p}) \cdot \vec{v} = 0$ or $\vec{q} \cdot \vec{v} = const$.

A reflection in a vector form

Problem 20.10. For a line L passing via $0 \in \mathbb{R}^2$, how does the reflection R_L map any point $q \in \mathbb{R}^2$?

Solution 20.10. Any vector $\vec{q} \in \mathbb{R}^2$ is a sum of two: one $\vec{q}_v$ parallel to the given unit length $\vec{v}$ and another $\vec{q}_L$ perpendicular to $\vec{v}$ or parallel to $L \perp \vec{v}$.

The projection of $\vec{q}$ to the straight line through $\vec{v}$ is $\vec{q}_v = \vec{v}|\vec{q}|\cos\alpha = (\vec{q} \cdot \vec{v})\vec{v}$. The reflection R_L over the line $L \perp \vec{v}$ keeps the projection $\vec{q}_L$ parallel to L and reverses the sign of the projection $\vec{q}_v = (\vec{q} \cdot \vec{v})\vec{v}$ perpendicular to the line L. Then $\vec{q} = \vec{q}_L + \vec{q}_v$ maps to $R_L(\vec{q}) = \vec{q}_L - \vec{q}_v = (\vec{q} - \vec{q}_v) - \vec{q}_v = \vec{q} - 2(\vec{q} \cdot \vec{v})\vec{v}$.

From coordinates to a matrix

Similarly to the argument above for $m = 2$, in $\mathbb{R}^m$ for a unit vector $\vec{v}$ normal to a hyperspace L passing through $\vec{0}$, the reflection is $R_L(\vec{q}) = \vec{q} - 2(\vec{q} \cdot \vec{v})\vec{v}$.

In $\mathbb{R}^2$, let $\vec{q} = \begin{pmatrix} x \\ y \end{pmatrix}$ and the unit vector $\vec{v} = \begin{pmatrix} v_x \\ v_y \end{pmatrix}$.

Then $R_L(\vec{q}) = \vec{q} - 2(\vec{q} \cdot \vec{v})\vec{v}$ has the coordinates
$x - 2(xv_x + yv_y)v_x = (1 - 2v_x^2)x - (2v_xv_y)y$ and
$y - 2(xv_x + yv_y)v_y = -(2v_xv_y)x + (1 - 2v_y^2)y$.

A reflection in a matrix form

$$R_L(\vec{q}) = \begin{pmatrix} 1 - 2v_x^2 & -2v_x v_y \\ -2v_x v_y & 1 - 2v_y^2 \end{pmatrix} \vec{q} = (I - 2\vec{v}\vec{v}^T)\vec{q}.$$

Hence, the reflection R_L over a line $L \perp \vec{v}$ via $\vec{0} \in \mathbb{R}^2$ is the linear map $\vec{q} \mapsto (I - 2\vec{v}\vec{v}^T)\vec{q}$, where $I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $\vec{v}\vec{v}^T = \begin{pmatrix} v_x^2 & v_x v_y \\ v_x v_y & v_y^2 \end{pmatrix}$ is the product of the vector-column $\vec{v} = \begin{pmatrix} v_x \\ v_y \end{pmatrix}$ and $\vec{v}^T = (v_x, v_y)$.

Any isometry is affine

Theorem 20.11. Any isometry of $\mathbb{R}^m$ is affine.

Indeed, any reflection is an affine map, hence any composition of reflections is affine.

Affine maps are not linear, but it's possible to deal with them similarly:
If a line L doesn't pass via the origin $\vec{0}$, shift L to the parallel line $M||L$ that goes via $\vec{0}$, reflect over M, shift back.

Reflection over the line $x + y = 1$

Problem 20.12. Write down the reflection over the line L given by $x + y = 1$ in a matrix form.

Solution 20.12. Translate L by $\vec{u} = -\frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$. The line L has the normal unit vector $\vec{v}^T = \frac{1}{\sqrt{2}}(1, 1)$ with $\vec{v}\vec{v}^T = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$. The reflection R_M is

$\vec{q} \mapsto (I - 2\vec{v}\vec{v}^T)\vec{q} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}\vec{q}$, then

$t_{-\vec{u}} \circ R_M \circ t_{\vec{u}}(\vec{q}) = (I - 2\vec{v}\vec{v}^T)(\vec{q} + \vec{u}) - \vec{u}$.

Reflection in the affine form

$$\vec{q} = \begin{pmatrix} x \\ y \end{pmatrix} \mapsto (I - 2\vec{v}\vec{v}^T)(\vec{q} + \vec{u}) - \vec{u} =$$

$$\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} x - 0.5 \\ y - 0.5 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix} =$$

$$\begin{pmatrix} 0.5 - y \\ 0.5 - x \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 - y \\ 1 - x \end{pmatrix} =$$

$$\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

Draw and check how points are reflected, e.g. $(0, 0) \leftrightarrow (1, 1)$.

Time to revise and ask questions

Theoretical abstraction is the key to any good practical tool!

An isometry

- preserves distances,
- decomposes into reflections and
- is an affine map.

Problem 20.13. Write an affine map from the triangle on $(0,0), (4,0), (0,3)$ to $(4,3), (0,3), (4,0)$.

References

- Dot product and duality: video explaining the idea behind kernel trick on dot product example.
- Everything You Wanted to Know about the Kernel Trick (But Were Too Afraid to Ask) by Eric Kim.
- Inner product.