Distances between subspaces

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Motivation

- Start with k objects (images, text, etc.) with N features.
- I.e. a collection of k vectors of dimension N.

Example

If we start with k images, we can split it into p squares and take the grayscale values to get k vectors in $\mathbb{R}^p$.

- Then we turn these vectors into some kind of subspace. The three types we will consider are:
  - linear subspaces (vector subspaces),
  - affine subspaces (shifted vector subspaces),
  - ellipsoids (higher-dimensional ellipses).
- Before doing anything else with these subspaces, we want to develop some notion of distance between them.

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Review: linear subspaces

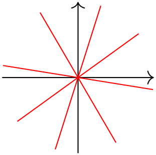
- Consider the real vector space $\mathbb{R}^N$.
- A *linear subspace of* $\mathbb{R}^N$ is a subset which is also a vector space.
- In particular, it **contains** 0**.**

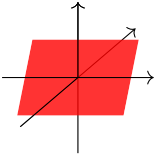
Example

Linear subspaces of $\mathbb{R}^2$ are lines **through the origin**.

Example

The 2-dimensional linear subspaces of $\mathbb{R}^3$ are planes **through the origin**.





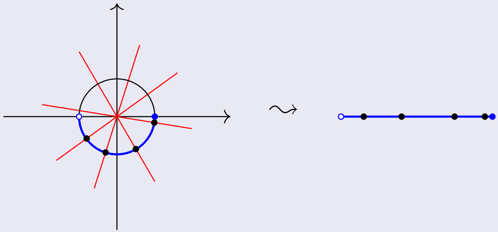
Distance

Question

What is the distance between two linear subspaces?

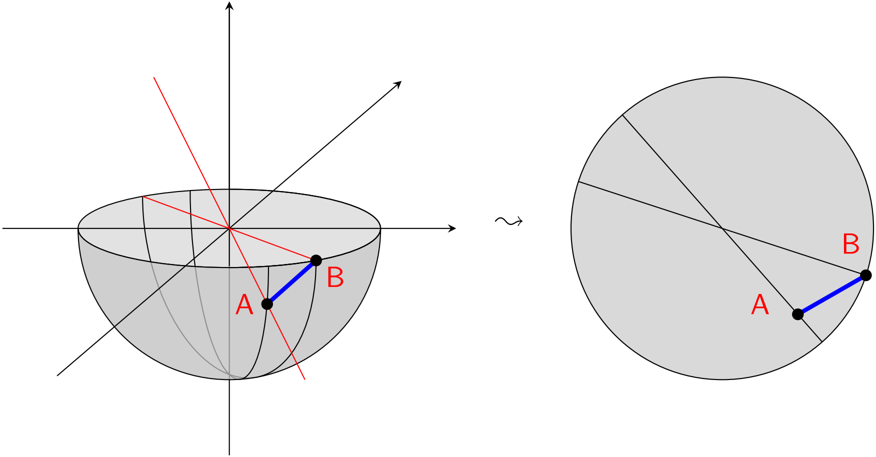
Example

For lines in $\mathbb{R}^2$, we just need to take the angle.



So now we want to formalize this in high dimensions.

Higher-dimensional picture



distance (A,B) = blue.

Higher-dimensional setup

Let $a_1, \ldots, a_k \in \mathbb{R}^N$ and $b_1, \ldots, b_k \in \mathbb{R}^N$ be (separately) linearly independent sets of vectors. Write their spans as:

$$A \coloneqq \operatorname{Span}\{a_1, \ldots, a_k\} \subset \mathbb{R}^N \qquad B \coloneqq \operatorname{Span}\{b_1, \ldots, b_k\} \subset \mathbb{R}^N \ .$$

Since the vectors were linearly independent, A and B are both k-dimensional linear subspaces of $\mathbb{R}^N$.

Therefore A and B are points of the *Grassmannian*.

$$A, B \in \operatorname{Gr}(k, N) \coloneqq \left\{ k - \text{dim'l linear subspaces of } \mathbb{R}^N \right\} \ .$$

Principal vectors and angles

- Write $\widehat{a}_1 \in A$ and $\widehat{b}_1 \in B$ for the vectors which

$$\begin{aligned} \text{maximize} \quad & a^T b \\ \text{such that} \quad & \|a\| = \|b\| = 1 \end{aligned}$$

  for $a \in A$, $b \in B$.
- Write $\widehat{a}_2 \in A$ and $\widehat{b}_2 \in B$ for the vectors which

$$\begin{aligned} \text{maximize} \quad & a^T b \\ \text{such that} \quad & \|a\| = \|b\| = 1 \\ & a^T \widehat{a}_1 = 0, \quad b^T \widehat{b}_1 = 0 \end{aligned}$$

  for $a \in A$ and $b \in B$.
- In general we ask for $\widehat{a}_j$ (resp. $\widehat{b}_j$) to be orthogonal to $\widehat{a}_i$ (resp. $\widehat{b}_i$) for all $i < j$.

Grassmann distance

- Tl;dr: $\widehat{a}_1$ and $\widehat{b}_1$ are unit vectors which have minimal angle between them. The vectors $\widehat{a}_i$ and $\widehat{b}_i$ are defined the same way, except you insist that they are orthogonal to the previously chosen vectors.
- We can think of the principal vectors as forming a basis which is convenient for measuring angles.
- Define the *principal angles* θ_j by

$$\cos\theta_j = \widehat{a}_j^T \widehat{b}_j \ .$$

  Note that $\theta_1 \leq \ldots \leq \theta_k$.
- The *Grassmann distance* between the linear subspaces A and B is given by:

$$d_k(A, B) = \left(\sum_{i=1}^{k} \theta_i^2 \right)^{1/2} \ .$$

Computing principal angles

- For any basis of A (resp. B) we can store the vectors as columns, to represent A as a matrix M_A (resp. M_B).
- Then we can compute the singular value decomposition (SVD):

$$M_A^T M_B = U \Sigma V^T$$

where

$$\Sigma = \begin{pmatrix} \sigma_1 & & 0 \\ & \ddots & \\ 0 & & \sigma_k \end{pmatrix} .$$

- The principal angles then satisfy

$$\cos \theta_i = \sigma_i \ .$$

- The principal vectors are the columns of:

$$M_A U \qquad\qquad\qquad M_B V \ .$$

An example

- By separating images into three regions and taking the grayscale values we get:

$$2 \text{ images of someone's face } \rightsquigarrow v_1, v_2 \in \mathbb{R}^3$$

- If v_1 and v_2 are linearly independent, we get a plane:

$$F := \operatorname{Span}(v_1, v_2) = \{m_1 v_1 + m_2 v_2 \mid m_1, m_2 \in \mathbb{R}\} \subset \mathbb{R}^3 .$$

- For two new photos of someone, again we get a plane

$$2 \text{ images} \rightsquigarrow \text{plane}$$

  and we can take the distance to F as a way to compare to the original photos.
- But what if I only have one picture of someone, and I want to compare it to the two I started with?

Question

How do we compare subspaces of different dimensions?

Schubert varieties

- For $k \leq \ell$, we would like a notion of distance between

$$A \in \mathrm{Gr}(k, N) \qquad\qquad B \in \mathrm{Gr}(\ell, N) \ .$$

- Consider the set of ℓ-planes containing A:

$$\Omega_+(A) := \{P \in \mathrm{Gr}(\ell, N) \mid A \subseteq P\}$$

  and the set of all k-planes containing B:

$$\Omega_-(B) := \{P \in \mathrm{Gr}(k, N) \mid P \subseteq B\} \ .$$

  E.g.

$$\Omega_+(\text{the line}) = \{\text{planes containing the line}\}$$
$$\Omega_-(\text{plane}) = \{\text{lines contained in the plane}\} \ .$$

- **Strategy:** measure distance from A to $\Omega_-(B)$, and B to $\Omega_+(A)$ and compare.

Distance between linear subspaces of different dimensions

The distance from A to $\Omega_+(A)$ is given by:

$$\delta_+ = \min\left\{ d_\ell(P,B) \,\middle|\, P \in \Omega_+(A) \right\} \ .$$

and the distance from B to $\Omega_-(B)$ is given by

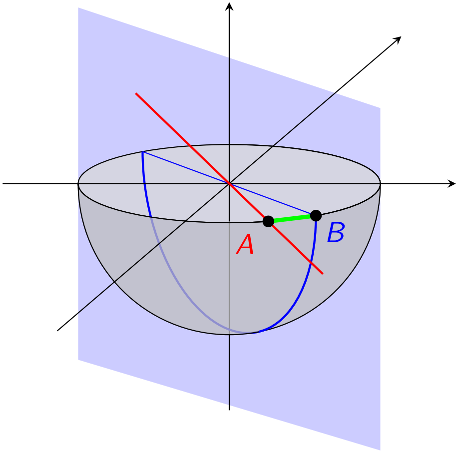
$$\delta_- = \min\left\{ d_k(P,A) \,\middle|\, P \in \Omega_-(B) \right\} \ .$$

Theorem 1 (Ye-Lim 2016 [YL16])

$\delta_+ = \delta_-$, and the common value is:

$$\delta(A,B) = \left(\sum_{i=1}^{\min(k,\ell)} \theta_i^2 \right)^{1/2} \ .$$

Now A is still a line, but B is a plane, both still in $\mathbb{R}^3$.

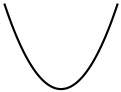


The distance is the only principal angle that can be defined: the first one. So

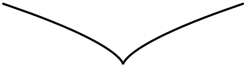
$$\delta\left(\mathrm{A}, \mathrm{B}\right) = \text{green} \;.$$

Digression: Schubert varieties

- In algebraic geometry, Schubert varieties primarily act as one of the most important (and well-studied) *singular varieties*.
- Classically, a *variety* is a subspace (of e.g. $\mathbb{R}^N$) defined as the points where some polynomials vanish.



- These can be nice and smooth: e.g. $y - x^2 = 0$ in $\mathbb{R}^2$.



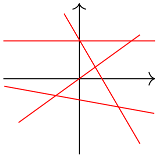
- Or not nice and *singular*: e.g. $y^3 - x^2 = 0$ in $\mathbb{R}^2$.
- So these Schubert varieties are actually the subset where some polynomials vanish inside of some huge $\mathbb{R}^D$.

Affine subspaces

- Let $A \in \mathrm{Gr}(k, N)$ be a k-dimensional linear subspace and $b \in \mathbb{R}^N$ to be thought of as the "shift away" from the origin.
- Write $\{a_1, \ldots, a_k\}$ for some basis of A.
- The associated *affine subspace* is:

$$A + b := \left\{ m_1 a_1 + \ldots + m_k a_k + b \in \mathbb{R}^N \,\middle|\, \lambda_i \in \mathbb{R} \right\} \subset \mathbb{R}^N \ .$$

In particular, they don't have to contain the origin.



Together, the affine subspaces form the *affine Grassmannian*:

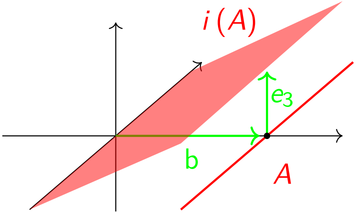
$$\mathrm{Graff}(k, N) = \left\{ k\text{-dim'l affine subspaces of } \mathbb{R}^N \right\} \ .$$

Distance via embedding Graff in (bigger) Gr

$$\operatorname{Graff}(k, N) \xhookrightarrow{i} \operatorname{Gr}(k+1, N+1)$$

$$A + b \longmapsto \operatorname{Span}(A \cup \{b + e_{n+1}\})$$

Under i, this red line in $\operatorname{Graff}(1, 2)$ goes to the red plane in $\operatorname{Gr}(2, 3)$.



We use this embedding to define the distance between two affine subspaces:

$$d_{\operatorname{Graff}(k,N)}(A + b, B + c) := d_{\operatorname{Gr}(k+1,N+1)}(i(A + b), i(B + c)) \ .$$

Remarks about Graff distance

- If $b = c = 0$, this is just the usual Grassmannian distance.
- Just as the distance between linear subspaces was calculated using the principal angles, there are *affine principal angles* such that this distance is written as before.
- These angles are also computationally manageable.

An example

- By separating images into three regions and taking the grayscale values we get $v_1, v_2 \in \mathbb{R}^3$.
- If linearly independent, we get an affine subspace (line) L which contains those points:

$$L := \{m_1 v_1 + m_2 v_2 \mid m_1 + m_2 = 1, m_1, m_2 \in \mathbb{R}\} \subset \mathbb{R}^3 .$$

  This is called the *affine span/hull of v_1 and v_2*, following e.g. [SR20].
- The affine hull is the smallest affine subspace containing the data. In particular, it is contained in the linear subspace F from before.
- For two new photos of someone, again we get a line

$$2 \text{ images} \rightsquigarrow \text{line}$$

  and we can take the distance to L to compare to the originals.

Question

How do we compare subspaces of different dimensions?

Distance for inequidimensional affine subspaces

For $k \leq \ell$, we would like a notion of distance between

$$A + b \in \mathrm{Graff}\,(k, N) \qquad\qquad B + c \in \mathrm{Graff}\,(\ell, N)\ .$$

As in the linear case, define

$$\begin{aligned}\Omega_+ (A + b) &\coloneqq \{P + q \in \mathrm{Graff}\,(\ell, N) \mid A + b \subseteq P + q\}\\ \Omega_- (B + c) &\coloneqq \{P + q \in \mathrm{Graff}\,(k, N) \mid P + q \subseteq B + c\}\ .\end{aligned}$$

Theorem 2 (Lim-Wong-Ye 2018 [LWY18])

$d_{\mathrm{Graff}(k,N)} (A + b, \Omega_- (B + c)) = d_{\mathrm{Graff}(\ell,N)} (B + c, \Omega_+ (A + b))$, *and it is explicitly given via the affine principle angles.*

Ellipsoids

- $M \in \mathbb{R}^{k \times k}$ is a real symmetric positive definite matrix
  $\iff$ all eigenvalues of M are positive,
  $\iff$ $\forall$ non-zero column vectors z we have $z^T M z > 0$.
- Such a matrix M determines an *ellipsoid*:

$$E_M := \left\{ x \in \mathbb{R}^k \,\middle|\, x^T M x \leq 1 \right\} .$$

Example

If M is the identity matrix, then this is just the closed ball of dimension N.

- We will define a distance between E_A and E_B by finding one between the matrices A and B.

PDS cone and distance between ellipsoids

$\mathbb{S}^k_{++}$ = the cone of real symmetric positive definite matrices.

Good distance on $\mathbb{S}^k_{++}$:

$$\mathbb{S}^k_{++} \times \mathbb{S}^k_{++} \xrightarrow{\quad\delta_2\quad} \mathbb{R}_+$$

$$(A, B) \xmapsto{\delta_2} \left(\sum_{j=1}^{n} \log^2\left(\lambda_j\left(A^{-1}B\right)\right)\right)^{1/2} .$$

This is good because it is very *invariant*. I.e. it satisfies:

$$\begin{aligned} \delta_2\left(XAX^T, XBX^T\right) &= \delta_2(A, B) \\ \delta_2\left(XAX^{-1}, XBX^{-1}\right) &= \delta_2(A, B) \\ \delta_2\left(A^{-1}, B^{-1}\right) &= \delta_2(A, B) . \end{aligned}$$

δ_2 has applications to computer vision, medical imaging, radar signal processing, statistical inference, and other areas.

An example

- Assume we are given k articles written about Halloween, and we count the occurrences of the terms
  - pumpkins,
  - skeletons, and
  - trick-or-treating

  to yield k vectors in $\mathbb{R}^3$.
- Write E for the smallest ellipsoid in $\mathbb{R}^3$ containing these vectors. If they are linearly independent, it is k-dimensional.
- For some other collection of k articles, we can count the same three words and form a second ellipsoid. Then we can measure the distance to E.
- The inverse of the distance gives the likelihood that the new articles are about Halloween.
- If we wanted to compare fewer than k articles to the originals, we would have needed to compare E to an ellipsoid of dim $\lneq k$.

Sub-ellipsoids

- There is a partial order on $\mathbb{S}^k_{++}$ given by:

$$A \preccurlyeq B \qquad \Longleftrightarrow \qquad B - A \in \mathbb{S}^k_+ \ ,$$

where $\mathbb{S}^k_+$ consists of real symmetric positive semi-definite matrices.
- $A \preccurlyeq B$ iff $E_B \subseteq E_A$.
- If I want to compare $A \in \mathbb{S}^k_{++}$ to $M \in \mathbb{S}^\ell_{++}$ (for $k \leq \ell$) then I can write

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{12}^T & M_{22} \end{pmatrix} \ , \tag{1}$$

where M_{11} is the upper left $k \times k$ block of M, and compare A to M_{11}.
- We will use this notion of containment to define the analogues of Schubert varieties.

Analogue of Schubert varieties

For $k \leq \ell$, we would like a notion of distance between

$$A \in \mathbb{S}_{++}^{k} \qquad\qquad B \in \mathbb{S}_{++}^{\ell} \ .$$

Define the convex set of ellipsoids containing/contained in E_A/E_B:

$$\Omega_+(A) \coloneqq \left\{ M = \begin{pmatrix} M_{11} & M_{12} \\ M_{12}^T & M_{22} \end{pmatrix} \in \mathbb{S}_{++}^{\ell} \,\middle|\, M_{11} \preccurlyeq A \right\}$$
$$\Omega_-(B) \coloneqq \left\{ M \in \mathbb{S}_{++}^{k} \,\middle|\, B_{11} \preccurlyeq M \right\}$$

where B_{11} is the upper left $k \times k$ block of B, M_{11} is the upper left $k \times k$ block of M.

Distance between inequidimensional ellipsoids

Theorem 3 (Lim-Sepulchre-Ye 2019 [LSY19])

$\delta_2\left(A, \Omega_-\left(B\right)\right) = \delta_2\left(B, \Omega_+\left(A\right)\right)$. *The common value is*

$$\delta_2^+\left(A, B\right) = \left(\sum_{j=1}^{k} \log^2 \lambda_j\left(A^{-1} B_{11}\right)\right)^{1/2}$$

where k *is such that*

$$\lambda_j\left(A^{-1} B_{11}\right) \leq 1$$

for $j = k+1, \ldots, m$.

Future directions

- A *category* is (roughly) a collection of objects and arrows between the objects which satisfy some conditions.
- In [DHKK13], the authors define a notion of distance between any two objects of a category.

Example

The collection of half-dimensional subspaces of a given even-dimensional manifold[a] fit naturally into a category called the *Fukaya category*. Roughly, we have an object for every subspace, and an arrow whenever they intersect.

[a] Technically they're Lagrangians in a symplectic manifold.

Question

Is this a useful distance for our purposes? Is it computable?

Summary:

Assume we have a way to pass from raw data to a subspace:

$$\text{raw data} \quad \rightsquigarrow \quad \{v_i\} \in \mathbb{R}^N \quad \rightsquigarrow \quad \text{subspace} \subseteq \mathbb{R}^N$$

When the subspace is linear, affine, or an ellipsoid, there is a notion of distance which is realistic to calculate.

So we can distinguish data by measuring the distance between the associated subspaces.

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