Tutorial on Dimensionality Reduction

Some recents approches in statistics and Machine Learning

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General Introduction

Exploratory analysis of (modern) data sets

Assume a table with n individuals described by p features/variables

Questions

Look for **patterns** or **structures** to summarize the data by

- Finding groups of "similar" individuals
- Finding variables important for these data
- Performing visualization

Challenges

- Size data may be large ("big data": large n large p)
- Dimension data may be high dimensional (more variables than individual or $n \ll p$)
- Redundancy many variables may carry the same information
- Unsupervised we don't necessary know what we are looking after

An example in genetics: ‘snp’

Genetics variant in European population

Description: *medium/large data, high-dimensional*}

500, 000 Genetics variants (SNP – Single Nucleotide Polymorphism) for 3000 individuals (1 meter × 166 meter (height × width)

- SNP : 90 % of human genetic variations
- coded as 0, 1 or 2 (10, 1 or 2 allel different against the population reference)

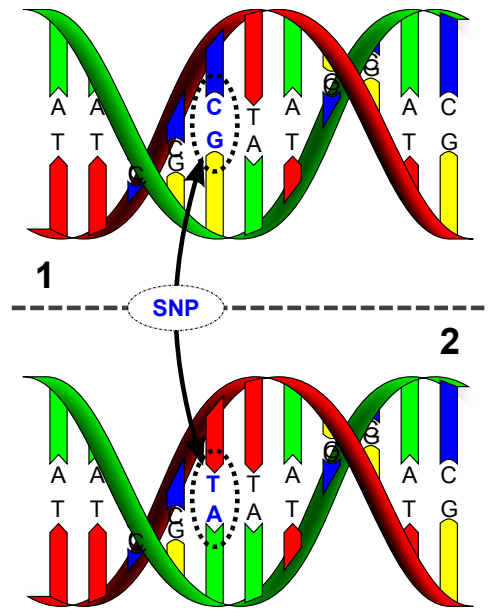


Figure 1: SNP (wikipedia)

Summarize 500,000 variables with 2 features

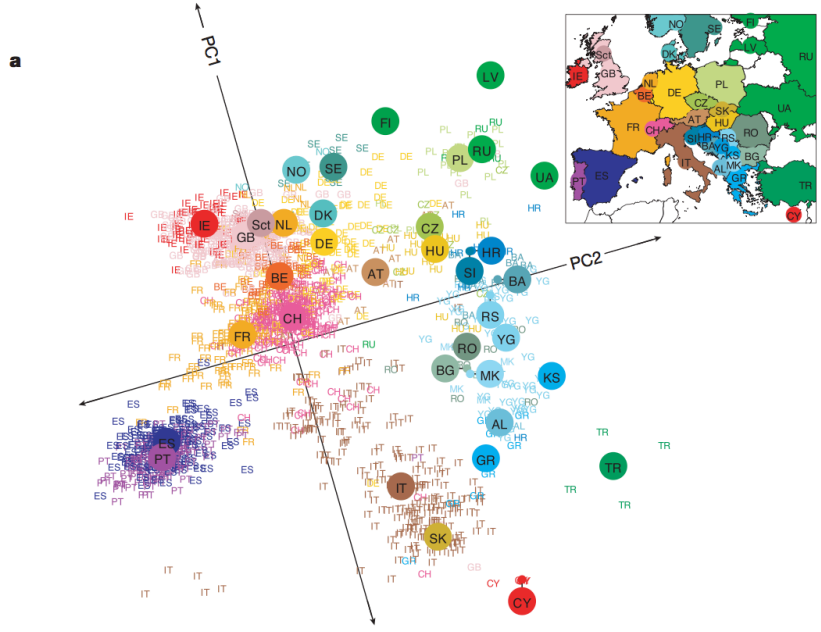


Figure 2: Dimension reduction + labels {source: Nature "Gene Mirror Geography Within Europe", 2008}

In the original messy $3,000 \times 500,000$ table, we may find - an extremely strong structure between individuals (**"clustering"**) - a very simple subspace where it is obvious (**"dimension reduction"**)

Theoretical argument: dimensionality Curse

Theorem (Folks theorem)

If $\mathbf{x}_1, \dots, \mathbf{x}_n$ in the hypercube of dimension p such that their coordinates are i.i.d then

$$p^{-1/2}\left(\max \|\mathbf{x}_i - \mathbf{x}_{i'}\|_2 - \min \|\mathbf{x}_i - \mathbf{x}_{i'}\|_2\right) = 0 + O\left(\sqrt{\frac{\log n}{p}}\right)$$

$$\frac{\max \|\mathbf{x}_i - \mathbf{x}_{i'}\|_2}{\min \|\mathbf{x}_i - \mathbf{x}_{i'}\|_2} = 1 + O\left(\sqrt{\frac{\log n}{p}}\right).$$

$\rightsquigarrow$ When p is large, all the points are almost equidistant\

Hopefully, the data **are not really leaving in p** dimension (think of the SNP example)

Dimension reduction: general goals

Main objective:

find a **low-dimensional representation** that captures the "essence" of (high-dimensional) data

Application in Machine Learning

Preprocessing, Regularization

- Compression, denoising, anomaly detection
- Reduce overfitting in supervised learning

Application in Statistics/Data analysis}

Better understanding of the data

- descriptive/exploratory methods
- visualization (difficult to plot and interpret $> 3d$!)

Dimension reduction: problem setup

Settings

- Training data : $\mathscr{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\} \in \mathbb{R}^p$, (i.i.d.)
- Space $\mathbb{R}^p$ of possibly high dimension ($n \ll p$)

Dimension Reduction Map

Construct a map Φ from the space $\mathbb{R}^p$ into a space $\mathbb{R}^q$ of smaller dimension:

$$\begin{aligned} \Phi : \quad & \mathbb{R}^p \to \mathbb{R}^q, q \ll p \\ & \mathbf{x} \mapsto \Phi(\mathbf{x}) \end{aligned}$$

How should we design/construct Φ?

Criterion

- Geometrical approach
- Reconstruction error
- Relationship preservation

Form of the map Φ

- **Linear** or non-linear ?
- tradeoff between **interpretability** and versatility ?
- tradeoff between high or **low** computational resource

Background: Principal Component Analysis

Outline

1 Geometric approach to PCA

2 Principal axes and variance maximization

3 Representation and interpretation

4 Additional tools and Complements

Cloud of observation in $\mathbb{R}^p$

Individuals can be represented in the variable space $\mathbb{R}^p$ as a point cloud

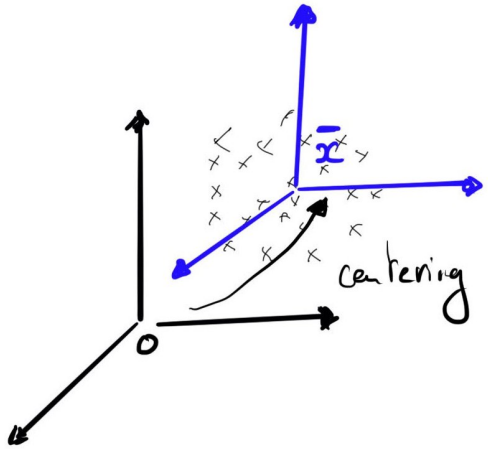


Figure 3: Example in $\mathbb{R}^3$

Center of Inertia

(or barycentrum, or empirical mean)

$$\bar{\mathbf{x}} = \frac{1}{n}\sum_{i=1}^{n}\mathbf{x}_i = \begin{pmatrix} \sum_{i=1}^{n} x_{i1}/n \\ \sum_{i=1}^{n} x_{i2}/n \\ \vdots \\ \sum_{i=1}^{n} x_{ip}/n \end{pmatrix}$$

We center the cloud $\mathbf{X}$ around $\mathbf{x}$ denote this by $\mathbf{X}^c$

$$\mathbf{X}^c = \begin{pmatrix} x_{11} - \bar{x}_1 & \dots & x_{1j} - \bar{x}_j & \dots & x_{1p} - \bar{x}_p \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{i1} - \bar{x}_1 & \dots & x_{ij} - \bar{x}_j & \dots & x_{ip} - \bar{x}_p \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{n1} - \bar{x}_1 & \dots & x_{nj} - \bar{x}_j & \dots & x_{np} - \bar{x}_p \end{pmatrix}$$

Inertia and Variance

Total Inertia:

distance of the individuals to the center of the cloud

$$I_T = \frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{p}(x_{ij} - \bar{x}_j)^2 = \frac{1}{n}\sum_{i=1}^{n}\|\mathbf{x}_i - \bar{\mathbf{x}}\|^2 = \frac{1}{n}\sum_{i=1}^{n}\text{dist}^2(\mathbf{x}_i, \bar{\mathbf{x}})$$

Proportional to the total variance

Let $\hat{\mathbf{\Sigma}}$ be the empirical variance-covariance matrix

$$I_T = \frac{1}{n}\sum_{j=1}^{p}\sum_{i=1}^{n}(x_{ij} - \bar{x}_j)^2 = \sum_{j=1}^{p}\frac{1}{n}\|\mathbf{x}^j - \bar{x}_j\|^2 = \sum_{j=1}^{p}\mathbb{V}(\mathbf{x}^j) = \text{trace}\left(\hat{\mathbf{\Sigma}}\right)$$

⇝ Good representation has large inertia (much variability)

⇝ Large dispertion ∼ Large distances between points

Inertia with respect to an axis

The Inertia of the cloud wrt axe Δ is the sum of the distances between all points and their orthogonal projection on Δ.

$$I_\Delta = \frac{1}{n} \sum_{i=1}^{n} \text{dist}^2(\mathbf{x}_i, \Delta)$$

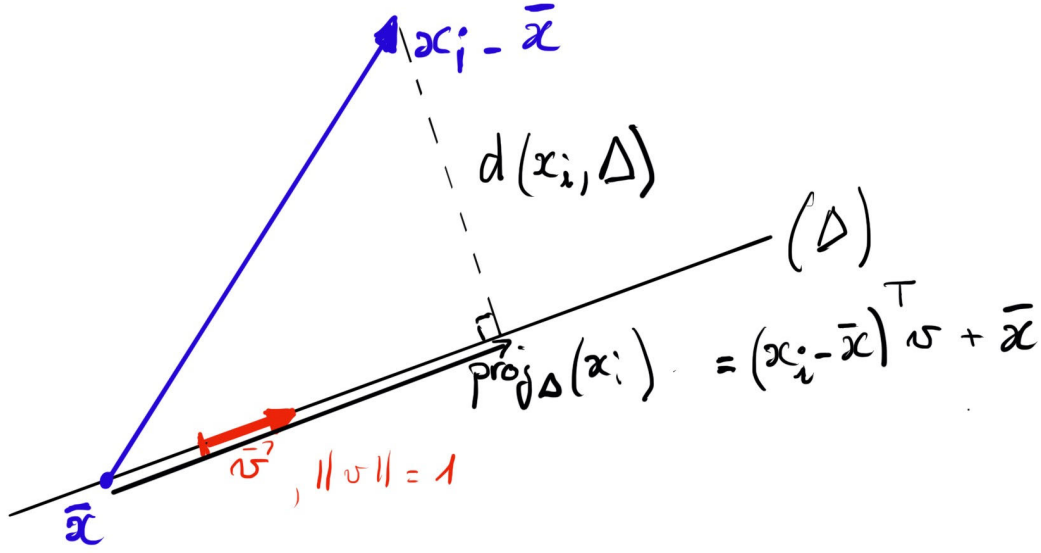
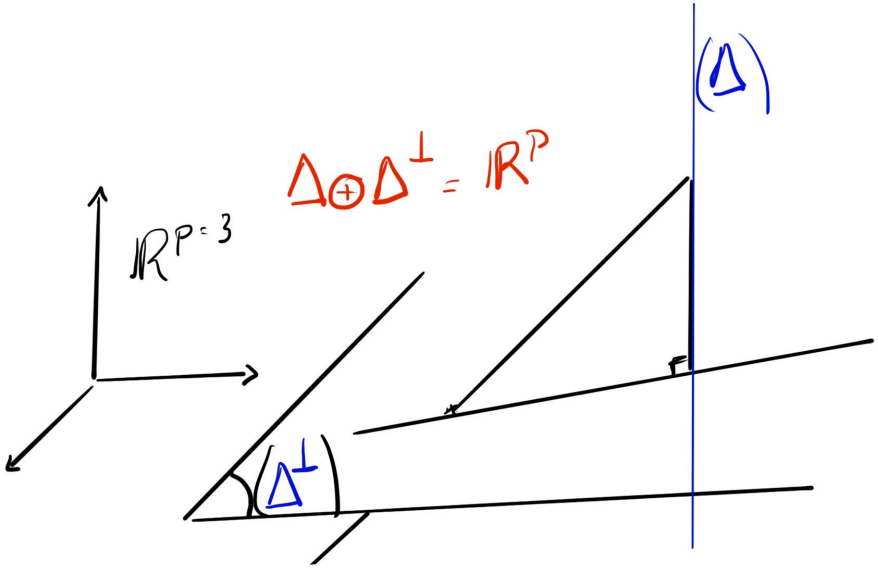


Figure 4: Projection of $\mathbf{x}_i$ onto a line Δ passing through $\bar{\mathbf{x}}$

Decomposition of total Inertia (1)

Let $\Delta^\perp$ be the orthogonal subspace of Δ in $\mathbb{R}^p$



Theorem (Huygens)

A consequence of the above (Pythagoras Theorem) is the decomposition of the following total inertia:

$$I_T = I_\Delta + I_{\Delta^\perp}$$

By projecting the cloud $\mathbf{X}$ *onto* Δ*, with loss the inertia measured by* $\Delta^\perp$

Decomposition of total Inertia (2)

Consider only subspaces with dimension 1 (that is, lines or axes). We can decompose $\mathbb{R}^p$ as the sum of p othogonal axis.

$$\mathbb{R}^p = \Delta_1 \oplus \Delta_2 \oplus \cdots \oplus \Delta_p$$

⇝ These axes form a new basis for representing the point cloud.

Theorem (Huygens)

$$I_T = I_{\Delta_1} + I_{\Delta_2} + \cdots + I_{\Delta_p}$$

Outline

1 Geometric approach to PCA

2 Principal axes and variance maximization

3 Representation and interpretation

4 Additional tools and Complements

Finding the best axis (1)

Definition of the problem

- The best axis Δ_1 is the "closest" to the point cloud
- Inertia of Δ_1 measures the distance between the data and Δ_1
- Δ_1 is defined by the director vector $\mathbf{u}_1$, such as $\|\mathbf{u}_1\| = 1$
- $\Delta_1^\perp$ is defined by the normal vector $\mathbf{u}_1$, such as $\|\mathbf{u}_1\| = 1$

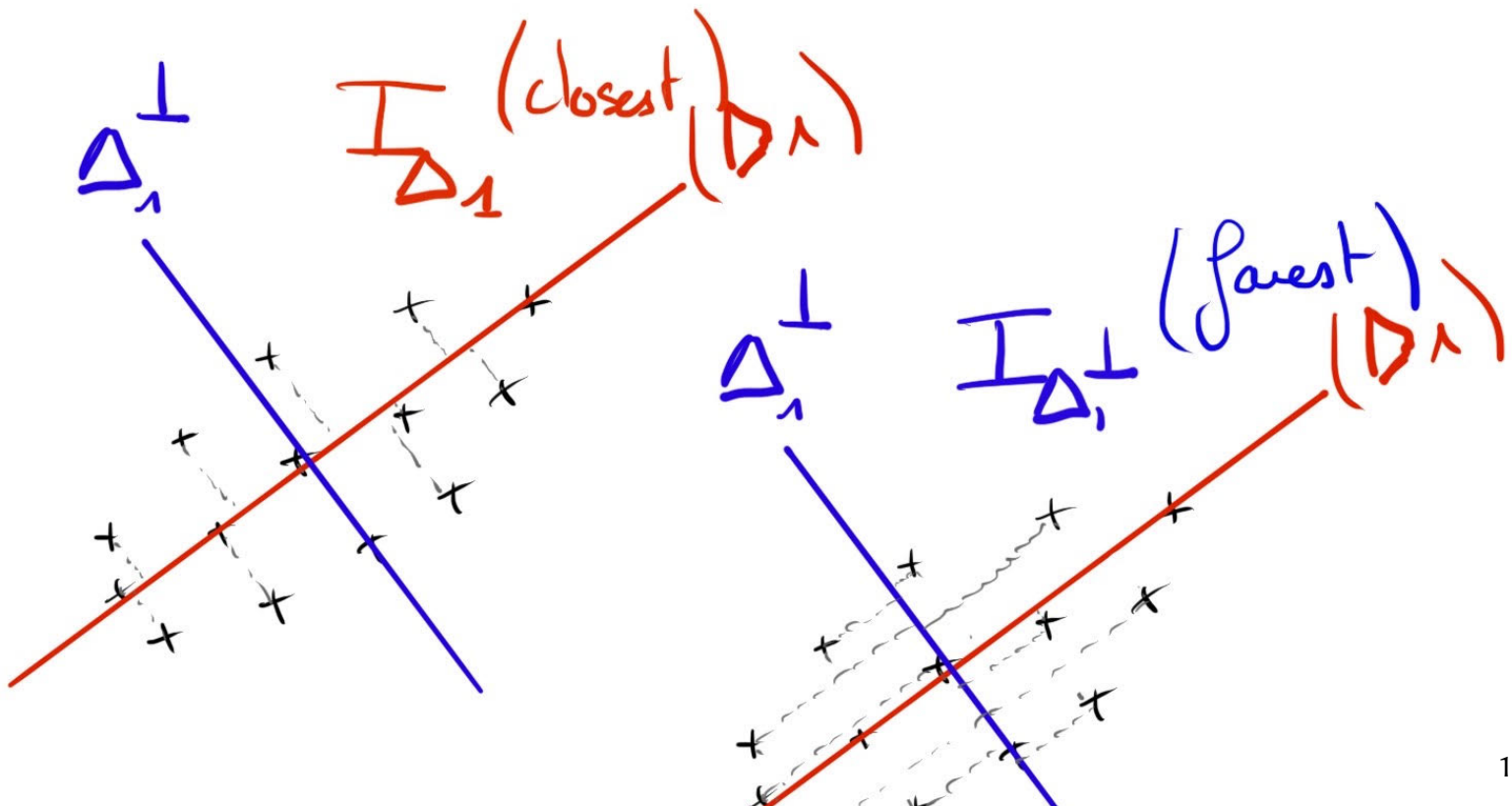
$\rightsquigarrow$ The best axis Δ_1 is the one with the minimal Inertia.

Finding the best axis (2)

Stating the optimization problem

Since $\Delta_1 \oplus \Delta_1^\perp = \mathbb{R}^p$ and $I_T = I_{\Delta_1} + I_{\Delta_1^\perp}$, then

$$\underset{\mathbf{u}\in\mathbb{R}^p : \|\mathbf{u}\|=1}{\text{minimize}} \; I_{\Delta_1} \;\Leftrightarrow\; \underset{\mathbf{u}\in\mathbb{R}^p : \|\mathbf{u}\|=1}{\text{maximize}} \; I_{\Delta_1^\perp}$$



Finding the best axis (3)

Stating the problem (algebraically)

Find $\mathbf{u}_1; \|\mathbf{u}_1\| = 1$ that maximizes

$$
\begin{aligned}
I_{\Delta_1^\perp} &= \frac{1}{n} \sum_{i=1}^{n} \text{dist}(\mathbf{x}_i, \Delta_1^\perp)^2 \\
&= \frac{1}{n} \sum_{i=1}^{n} \mathbf{u}_1^\top (\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^\top \mathbf{u}_1 \\
&= \mathbf{u}_1^\top \left(\sum_{i=1}^{n} \frac{1}{n} (\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^\top \right) \mathbf{u}_1 \\
&= \mathbf{u}_1^\top \hat{\mathbf{\Sigma}} \mathbf{u}_1
\end{aligned}
$$

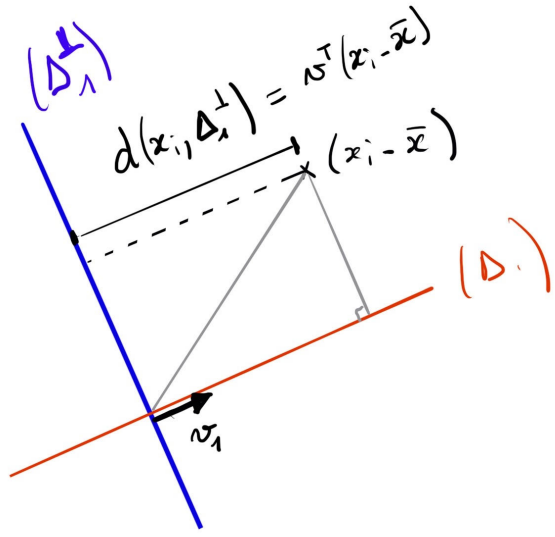


Figure 5: Geometrical insight

Finding the best axis (4)

We solve a simple constraint maximization problem with the method of Lagrange multipliers:

$$\underset{\mathbf{u}_1 : \|\mathbf{u}_1\|=1}{\text{maximize}}\, \mathbf{u}_1^\top \hat{\mathbf{\Sigma}} \mathbf{u}_1 \Leftrightarrow \underset{\mathbf{u}_1 \in \mathbb{R}^p, \lambda_1 > 0}{\text{maximize}}\, \mathbf{u}_1^\top \hat{\mathbf{\Sigma}} \mathbf{u}_1 - \lambda_1 (\|\mathbf{u}_1\|^2 - 1)$$

By straightforward (vector) differentiation, an using that $\mathbf{u}_1^\top \mathbf{u}_1 = 1$

$$\begin{cases} 2\hat{\mathbf{\Sigma}}\mathbf{u}_1 - 2\lambda_1 \mathbf{u}_1 = 0 \\ \mathbf{u}_1^\top \mathbf{u}_1 - 1 = 0 \end{cases} \Leftrightarrow \begin{cases} \hat{\mathbf{\Sigma}}\mathbf{u}_1 = \lambda_1 \mathbf{u}_1 \\ \mathbf{u}_1^\top \hat{\mathbf{\Sigma}} \mathbf{u}_1 = \lambda_1 \mathbf{u}_1^\top \mathbf{u}_1 = \lambda_1 = I_{\Delta_1}^\perp \end{cases}$$

- $\mathbf{u}_1$ is the first (normalized) eigen vector of $\hat{\mathbf{\Sigma}}$
- λ_1 is the first eigen value of $\hat{\mathbf{\Sigma}}$

$\boxtimes$ **Δ_1 is defined by the first eigen vector of $\hat{\Sigma}$**

$\boxtimes$ **Variance "carried" by Δ_1 is equal to the largest eigen value of $\hat{\Sigma}$**

Finding the following axes

Second best axis

Find Δ_2 with dimension 1, director vector $\mathbf{u}_2$ orthogonal to Δ_1 solving

$$\underset{\mathbf{u}_2 \in \mathbb{R}^p}{\text{maximize}}\, I_{\Delta_2^\perp} = \mathbf{u}_2^\top \hat{\mathbf{\Sigma}} \mathbf{u}_2, \quad \text{with } \|\mathbf{u}_2\| = 1, \mathbf{u}_1^\top \mathbf{u}_2 = 0.$$

$\rightsquigarrow$ $\mathbf{u}_2$ is the second eigen vector of $\hat{\mathbf{\Sigma}}$ with eigen value λ_2

And so on!

PCA is roughly a matrix factorisation problem

$$\hat{\mathbf{\Sigma}} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\top, \quad \mathbf{U} = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2, & \dots & \mathbf{u}_p \end{pmatrix}, \quad \mathbf{\Lambda} = \text{diag}(\lambda_1, \dots, \lambda_p)$$

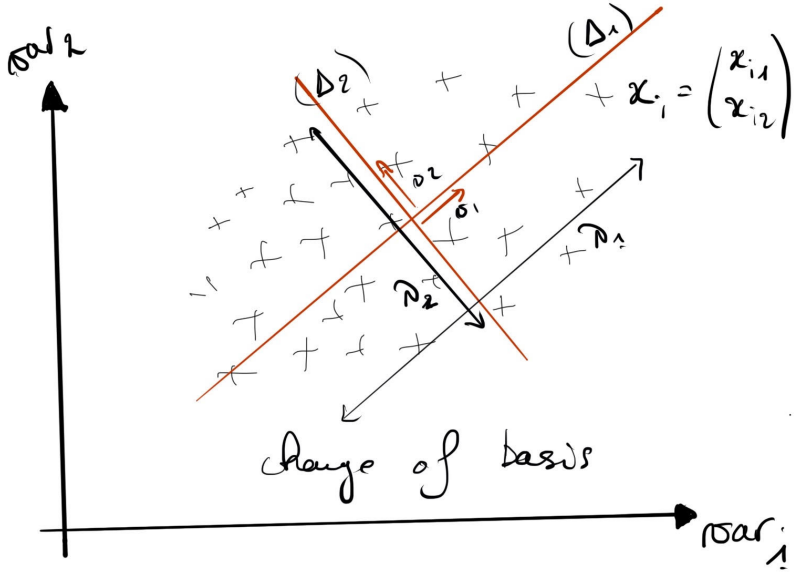
- $\mathbf{U}$ is an orthogonal matrix of normalized eigen vectors.
- $\mathbf{\Lambda}$ is diagonal matrix of ordered eigen values.

Interpretation in $\mathbb{R}^p$

$\mathbf{U}$ describes a new orthogonal basis and a rotation of data in this basis

$\rightsquigarrow$ PCA is an appropriate rotation on axes that maximizes the variance

$$\begin{cases} \Delta_1 & \oplus & \dots & \oplus & \Delta_p \\ \mathbf{u}_1 & \perp & \dots & \perp & \mathbf{u}_p \\ \lambda_1 & > & \dots & > & \lambda_p \\ I_{\Delta_1^\perp} & > & \dots & > & I_{\Delta_p^\perp} \end{cases}$$



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Contribution of each axis and quality of the representation}

Δ_k is carrying inertia/variance defined by its orthogonal, thus

$$I_T = I_{\Delta_1^\perp} + \cdots + I_{\Delta_p^\perp} = \lambda_1 + \cdots + \lambda_p$$

Relative contribution of axis k

$$\text{contrib}(\Delta_k) = \frac{\lambda_k}{\sum_{k=1}^{p} \lambda_j} = \frac{\lambda_k}{\text{trace}\left(\hat{\Sigma}\right)} \times 100$$

$\rightsquigarrow$ Percentage of explained inertia/variance explained

Global quality of the representation on the first k axes

$$\text{contrib}(\Delta_1, \ldots, \Delta_k) = \frac{\lambda_1 + \cdots + \lambda_k}{\text{trace}\left(\hat{\Sigma}\right)} \times 100$$

A few axes may explain a large proportion of the total variance.

$\rightsquigarrow$ This paves the way for dimension reduction

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Individuals: representation in the new basis

Projection

The projection of $\mathbf{x}_i$ onto axis Δ_k is $c_{ik}\mathbf{u}_k$, with

$$c_{ik} = \mathbf{u}_k^\top(\mathbf{x}_i - \bar{\mathbf{x}}),$$

the coordinate of i in the basis $\mathbf{u}_k$ (along axis Δ_k).

Coordinates

Coordinates of i in the new basis $\{\mathbf{u}_1, \dots, \mathbf{u}_p\}$ is thus

$$\mathbf{c}_i = (\mathbf{U}^\top(\mathbf{x}_i - \bar{\mathbf{x}}))^\top = (\mathbf{x}_i - \bar{\mathbf{x}})^\top\mathbf{U} = \mathbf{X}_i^c\mathbf{U}, \quad \mathbf{c}_i \in \mathbb{R}^p.$$

- $\mathbf{U}$ are often the called the **loadings**, or **weights**
- $\mathbf{c}_i$ are the **scores** or **coordinates** in the new space for the individuals

Warning: about distances after projection

Close projection doesn't mean close individuals!

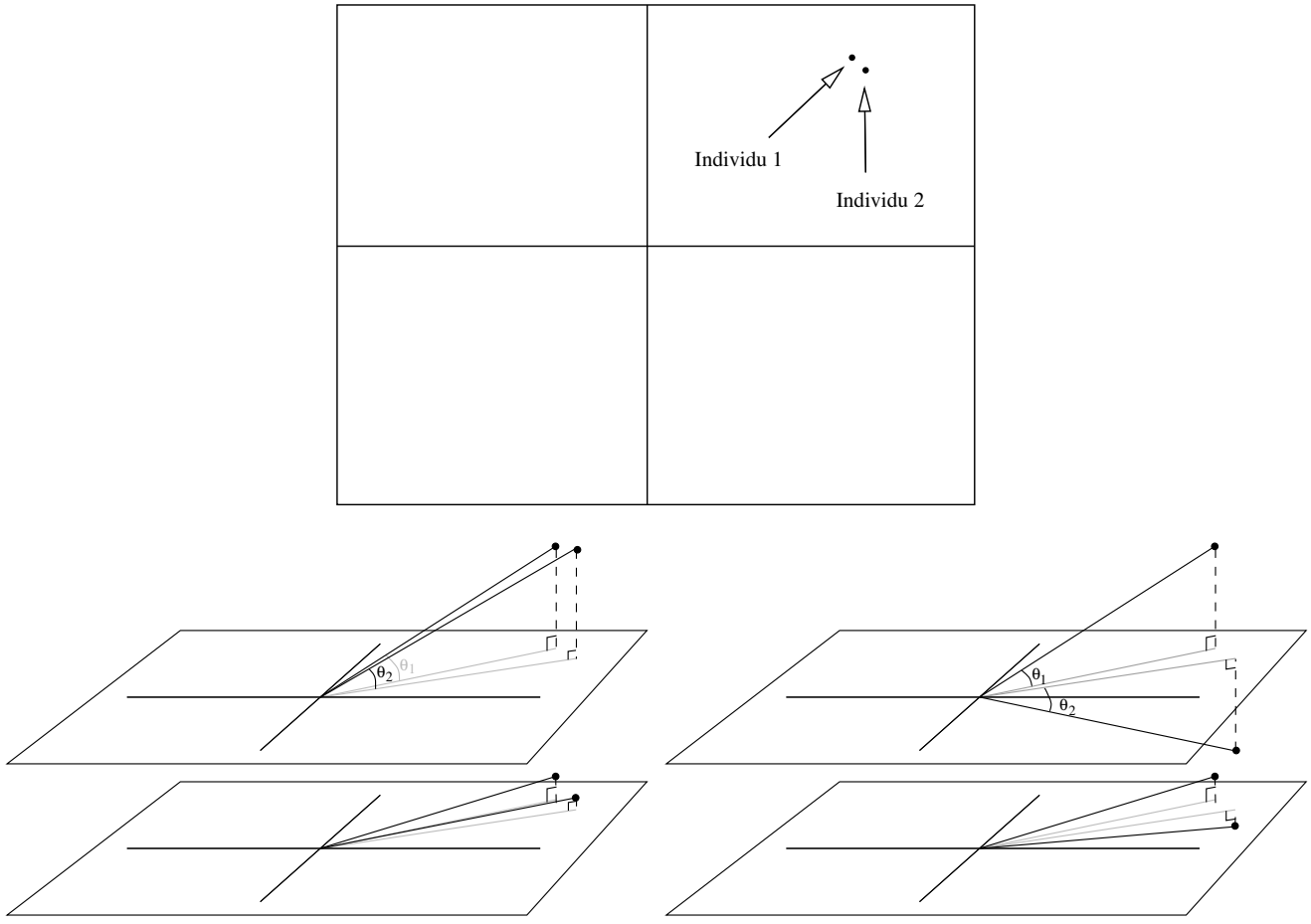


Figure 6: Same projections but different situations (source: E. Matzner)

⇝ Only work when individuals are well represented in the lower space

Individual: representation

Quality

- An individual i is well represented by Δ_k if it is close to this axis.
- In other word, vector $\mathbf{x}_i - \bar{\mathbf{x}}$ and $\mathbf{u}_k$ are close to collinear

Use the cosine of the angle between $\mathbf{x}_i - \bar{\mathbf{x}}$ and $\mathbf{u}_k$ to measure collinearity:

$$\cos^2(\theta_{ik}) = \frac{\left(\mathbf{u}_k^\top(\mathbf{x}_i - \bar{\mathbf{x}})\right)^2}{\|\mathbf{x}_i - \bar{\mathbf{x}}\|^2 \|\mathbf{u}_k\|^2}$$

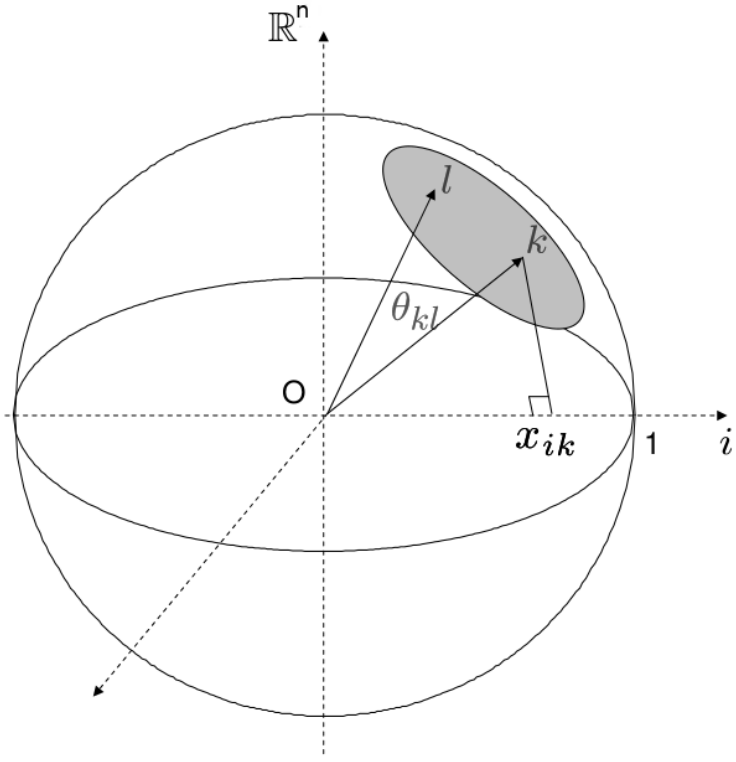
Contribution

- Inertia "explained" by Δ_k is inertia of $\Delta_k^\perp$
- $I_{\Delta_k^\perp} = n^{-1} \sum_{i=1}^n \text{dist}^2(\Delta_k^\perp, \mathbf{x}_i)$

Contribution is the proportion of variance/inertia carried by individual i:

$$n^{-1}\text{dist}^2(\Delta_k^\perp, \mathbf{x}_i) \qquad \left(\mathbf{u}_k^\top(\mathbf{x}_i - \bar{\mathbf{x}})\right)^2$$

Cloud of variables



Direct equivalence between geometry and statistics (collinearity ≡ correlation)

$$\cos(\theta_{kl}) = \frac{\langle \mathbf{x}^k, \mathbf{x}^\ell \rangle}{\|\mathbf{x}^k\| \|\mathbf{x}^\ell\|} = \rho(\mathbf{x}^k, \mathbf{x}^\ell)$$

Principal Components

Dual representation

A symmetric reasoning can be made in $\mathbb{R}^n$ for the variables, like with the individuals in $\mathbb{R}^p$.
$\rightsquigarrow$ New axes are linear combinaison of the original variables, which can be seen as **new variables** in the new latent space

Principal component

It is the linear combinasion formed by the orginal variables with weights given by the loadings $\mathbf{u}_k = (u_{k1}, \dots, u_{kj}, \dots, u_{kp})$

$$\mathbf{f}_k = \sum_{j=1}^{p} u_{kj}(\mathbf{x}^j - \bar{x}_j) = \mathbf{X}^c \mathbf{u}_k, \quad \mathbf{f}_k \in \mathbb{R}^n$$

Sometimes called "factors" in factor analysis, as latent (hidden) variables.

Variable representation in the new space

Connection with original variables

- essential for interpretation
- answer to the question: how to read the axes of the individual map
- use correlation to measure connection to original variable

$$\mathbb{V}(\mathbf{f}_k) = \frac{1}{n}\mathbb{V}(\mathbf{X}^c\mathbf{u}_k) = \mathbf{u}_k^\top \frac{1}{n}(\mathbf{X}^c)^\top \mathbf{X}^c\mathbf{u}_k = \mathbf{u}_k^\top \hat{\mathbf{\Sigma}}\mathbf{u}_k = \lambda_k$$

$$\text{cov}(\mathbf{f}_k, (\mathbf{x}^j - \bar{x}_j)) = \mathbf{u}_k \top \mathbf{X}^{c\top}\mathbf{X}^c e_j = \mathbf{u}_k \lambda_k e_j = \lambda_k \mathbf{u}_{kj}$$

$$\text{cor}(\mathbf{f}_k, (\mathbf{x}^j - \bar{x}_j)) = \sqrt{\frac{\lambda_k}{\mathbb{V}(\mathbf{x}^j)}}\mathbf{u}_{kj}$$

Warning: about angle after projection

Close projection doesn't mean close variable!

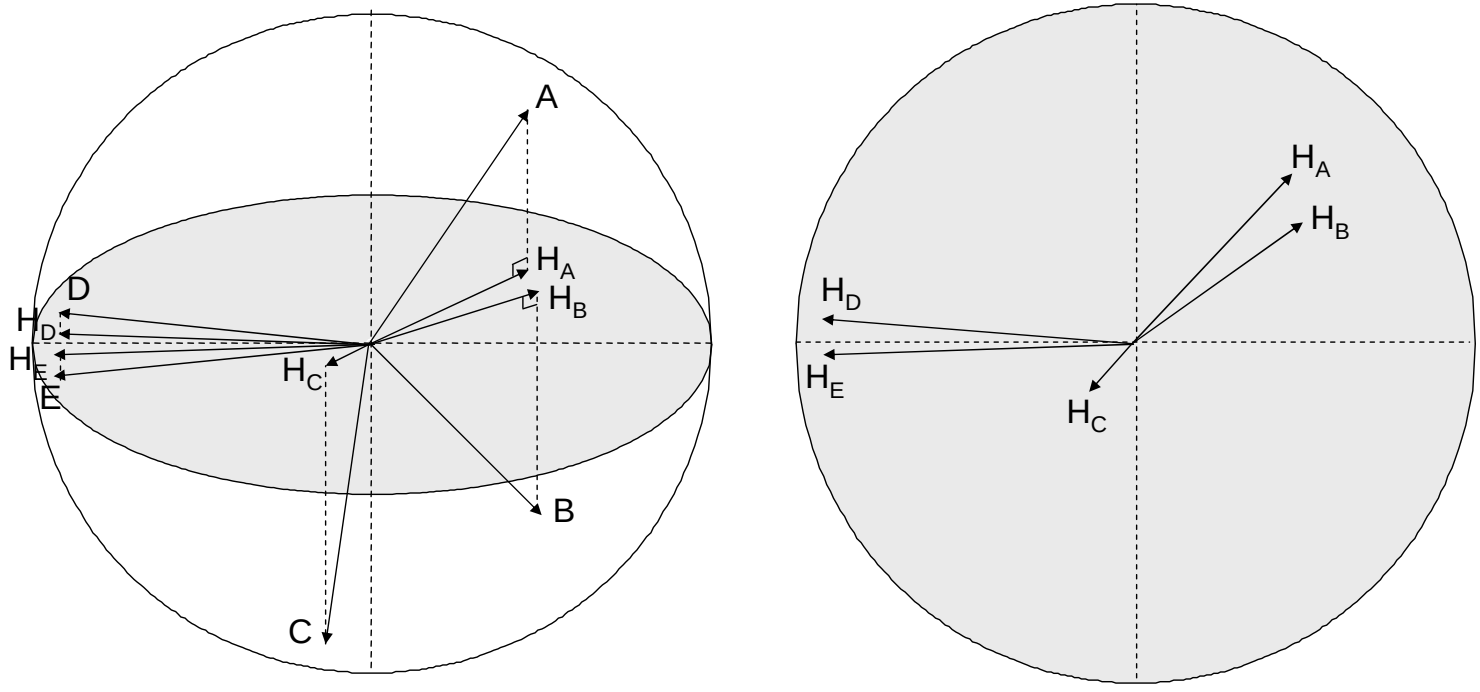


Figure 7: Same angle but different situations {(source: J. Josse)}

⇝ Only work when variables are well represented in the latent space

Variable representation

Quality

- An variable j is well represented by Δ_k if its projection is close to $\mathbf{f}_k$.
- High collinearity means high absolute correlation and high cosine.
- use cosine to the square of the angle between the original and new variables.

$\rightsquigarrow$ The projection of j must be close to the boundary of the correlation circle

Contribution

Similarly to individuals, we can measure the contribution of the original variables to the construction of the new ones.

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Unifying view of variables and individuals

Principal components

The full matrix of principal component connects individual coordinates to latent factors:

$$\text{PC} = \mathbf{X}^c\mathbf{U} = \begin{pmatrix} \mathbf{f}_1 & \mathbf{f}_2 & \dots & \mathbf{f}_p \end{pmatrix} = \begin{pmatrix} \mathbf{c}_1^\top \\ \mathbf{c}_2^\top \\ \dots \\ \mathbf{c}_n^\top \end{pmatrix}$$

- new variables (latent factor) are seen column-wise
- new coordinates are seen row-wise

⇝ Everything can be interpreted on a single plot, called the biplot

Reconstruction formula

Recall that $\mathbf{F} = (\mathbf{f}_1, \ldots, \mathbf{f}_p)$ is the matrix of Principal components. Then,

- $\mathbf{f}_k = \mathbf{X}^c \mathbf{u}_k$ for projection on axis k
- $\mathbf{F} = \mathbf{X}^c \mathbf{U}$ for all axis.

Using orthogonality of $\mathbf{U}$, we get back the original data as follows, without loss ($\mathbf{U}^T$ performs the inverse rotation of $\mathbf{U}$):

$$\mathbf{X}^c = \mathbf{F}\mathbf{U}^\top$$

We obtain an approximation $\tilde{\mathbf{X}}^c$ (compression) of the data $\mathbf{X}^c$ by considering a subset $\mathcal{S}$ of PC, typically $\mathcal{S} = 1, \ldots, q$ with $q \ll p$.

$$\tilde{\mathbf{X}}^c = \mathbf{F}_{\mathcal{S}} \mathbf{U}_{\mathcal{S}}^\top = \mathbf{X}^c \mathbf{U}_{\mathcal{S}} \mathbf{U}_{\mathcal{S}}^\top$$

$\rightsquigarrow$ This is a rank-q approximation of $\mathbf{X}$ (information captured by the first q axes).

PCA (and linear methods) limitations

Do not account for ‘complex’ data distribution

- PCA is tied to a hidden **Gaussian assumption**
- Fails with **Count data**
- Fails with **Skew data**
- Linear methods like PCA are robust but badly shaped for complex geometries
- High-dim. datas are characterized by multiscale properties (local / global structures)

Possible solutions

- Probabilistic (non Gaussian) models
- Need transformed (non-linear) input space (preserving local characteristics of distances)

Dimension reduction: revisiting the problem setup

Settings

- Training data : $\mathscr{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\} \in \mathbb{R}^p$, (i.i.d.)
- Space $\mathbb{R}^p$ of possibly high dimension ($n \ll p$)

Dimension Reduction Map

Construct a map Φ from the space $\mathbb{R}^p$ into a space $\mathbb{R}^q$ of smaller dimension:

$$\begin{aligned} \Phi : \quad & \mathbb{R}^p \to \mathbb{R}^q, q \ll p \\ & \mathbf{x} \mapsto \Phi(\mathbf{x}) \end{aligned}$$

How should we design/construct Φ?

Geometrical approach

(**see slides on PCA**)

Idea to go beyond linear approaches

- Modify the model by amending the **reconstruction error**
- Focus on **Relationship preservation**

Form of the map Φ

- Linear or **non-linear ?**
- tradeoff between interpretability and **versatility ?**
- tradeoff between **high** or low computational resource

Reconstruction error approach

1. Construct a map Φ from the space $\mathbb{R}^p$ into a space $\mathbb{R}^q$ of smaller dimension:

$$\begin{aligned} \Phi : \quad & \mathbb{R}^p \to \mathbb{R}^q, q \ll p \\ & \mathbf{x} \mapsto \Phi(\mathbf{x}) = \tilde{\mathbf{x}} \end{aligned}$$

2. Construct $\tilde{\Phi}$ from $\mathbb{R}^q$ to $\mathbb{R}^p$ (reconstruction formula)
3. Control an error ϵ between $\mathbf{x}$ and its reconstruction $\hat{\mathbf{x}} = \tilde{\Phi}(\Phi(\mathbf{x}))$

For instance, the error measured with the Frobenius between the original data matrix $\mathbf{X}$ and its approximation:

$$\epsilon(\mathbf{X}, \hat{\mathbf{X}}) = \left\|\mathbf{X} - \hat{\mathbf{X}}\right\|_F^2 = \sum_{i=1}^{n} \left\|\mathbf{x}_i - \tilde{\Phi}(\Phi(\mathbf{x}_i))\right\|^2$$

Reinterpretation of PCA

PCA model

Let $\mathbf{V}$ be a $p \times q$ matrix whose columns are of q orthonormal vectors.

$$\Phi(\mathbf{x}) = \mathbf{V}^\top(\mathbf{x} - \boldsymbol{\mu}) = \tilde{\mathbf{x}}$$

$$\mathbf{x} \simeq \tilde{\Phi}(\tilde{\mathbf{x}}) = \boldsymbol{\mu} + \mathbf{V}\tilde{\mathbf{x}}$$

↝ Model with **Linear assumption + ortho-normality constraints**

PCA reconstruction error

$$\underset{\boldsymbol{\mu} \in \mathbb{R}^p, \mathbf{V} \in \mathcal{O}_{p,q}}{\text{minimize}} \sum_{i=1}^{n} \left\| (\mathbf{x}_i - \boldsymbol{\mu}) - \mathbf{V}\mathbf{V}^\top(\mathbf{x}_i - \boldsymbol{\mu}) \right\|^2$$

Solution (explicit)

- $\boldsymbol{\mu} = \bar{\mathbf{x}}$ the empirical mean
- $\mathbf{V}$ an orthonormal basis of the space spanned by the q first eigenvectors of the empirical covariance matrix

Important digression: SVD

Singular Value Decomposition (SVD)

The SVD of $\mathbf{M}$ a $n \times p$ matrix is the factorization given by

$$\mathbf{M} = \mathbf{U}\mathbf{D}\mathbf{V}^\top,$$

where $r = \min(n, p)$ and

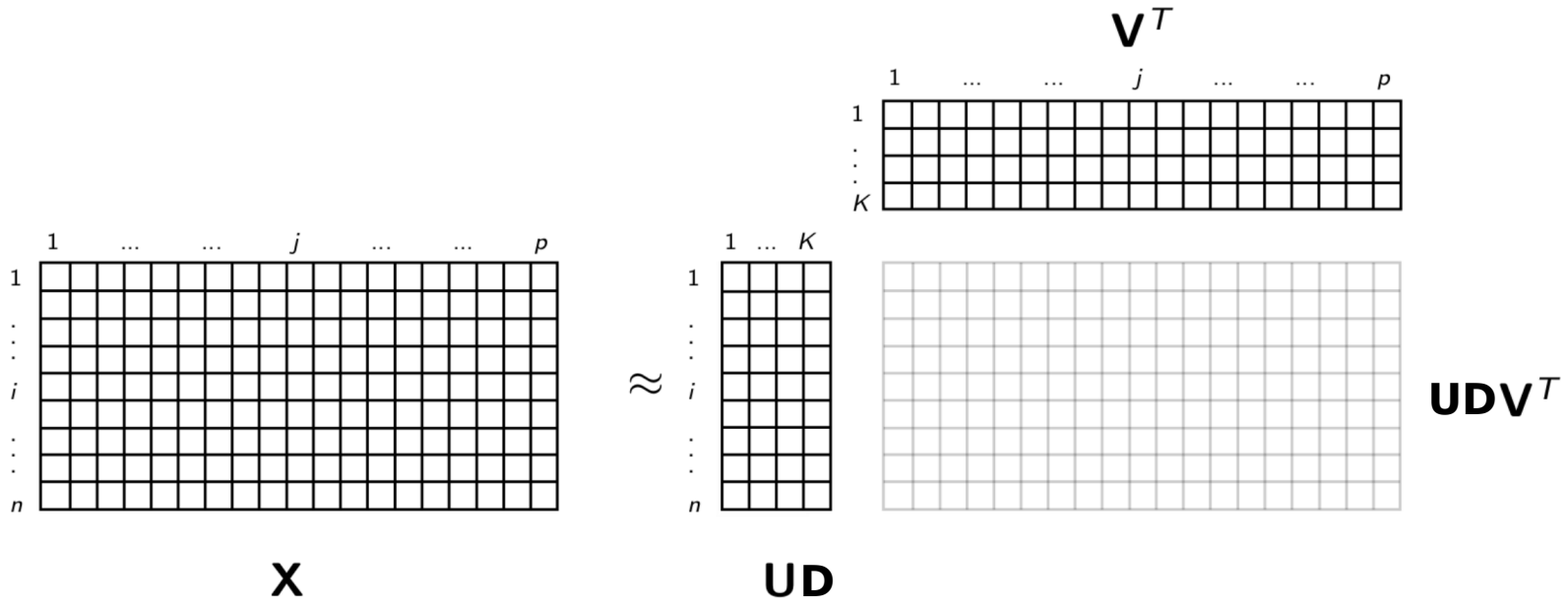
- $\mathbf{D}_{r \times r} = \text{diag}(\delta_1, ...\delta_r)$ is the diagonal matrix of singular values.
- $\mathbf{U}$ is orthonormal, whose columns are eigen vectors of $(\mathbf{M}\mathbf{M}^T)$
- $\mathbf{V}$ is orthonormal whose columns are eigen vectors of $(\mathbf{M}^T\mathbf{M})$

  ⇝ Time complexity in $\mathcal{O}(npqr)$ (less when $k \ll r$ components are required)

Connection with eigen decomposition of the covariance matrix

$$\begin{aligned}\mathbf{M}^\top\mathbf{M} &= \mathbf{V}\mathbf{D}\mathbf{U}^\top\mathbf{U}\mathbf{D}\mathbf{V}^\top \\ &= \mathbf{V}\mathbf{D}^2\mathbf{V}^\top = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^\top\end{aligned}$$

PCA solution is given by SVD of the centered data matrix



Since $\tilde{\mathbf{X}} = \mathbf{X}^c\mathbf{V} = \mathbf{U}\mathbf{D}\mathbf{V}^\top\mathbf{V} = \mathbf{U}\mathbf{D}$, PCA can be rephrased as

$$\hat{\mathbf{X}}^c = \mathbf{F}\mathbf{V}^\top = \underset{\mathbf{F}\in\mathscr{M}_{n,q},\mathbf{V}\in\mathcal{O}_{p,q}}{\arg\min} \left\|\mathbf{X}^c - \mathbf{F}\mathbf{V}^\top\right\|_F^2 \text{ with } \|\mathbf{A}\|_F^2 = \sum_{ij} a_{ij}^2,$$

$\left.\tilde{\mathbf{X}} \in \mathbb{R}^{n\times q}, \mathbf{V} \in \mathbb{R}^{p\times q}\right\}$ Best linear low-rank representation of $\mathbf{X}$

Non-negative Matrix Factorization – NMF

Setup

Assume that $\mathbf{X}$ contains only non-negative entries (i.e. ≥ 0).

Model

Linear assumption + non-negativity constraints on both $\mathbf{V}$ and $\tilde{\mathbf{x}}$

$$\Phi(\mathbf{x}) = \mathbf{V}^\top \mathbf{x} = \tilde{\mathbf{x}}$$

$$\mathbf{x} \simeq \tilde{\Phi}(\tilde{\mathbf{x}}) = \mathbf{V}\tilde{\mathbf{x}}$$

For the whole data matrix $\mathbf{X}$,

$$\hat{\mathbf{X}} = \underbrace{\tilde{\mathbf{X}}}_{\mathbf{F}\text{, the factors}} \mathbf{V}^\top$$

NMF reconstruction errors

Build $\hat{\mathbf{X}} = \mathbf{F}\mathbf{V}^\top$ to minimize a distance $D(\hat{\mathbf{X}}, \mathbf{X})$. Several choice, e.g:

- Least-square loss (distance measured by Frobenius norm)

$$\hat{\mathbf{X}}^{\text{ls}} = \underset{\substack{\mathbf{F}\in\mathscr{M}(\mathbb{R}_+)_{n,q} \\ \mathbf{V}\in\mathscr{M}(\mathbb{R}_+)_{p,q}}}{\arg\min} \left\|\mathbf{X} - \mathbf{F}\mathbf{V}^\top\right\|_F^2,$$

- Generalized Kullback-Leibler divergence ("distance" for distributions)

$$\begin{aligned}\hat{\mathbf{X}}^{\text{kl}} &= \underset{\substack{\mathbf{F}\in\mathscr{M}(\mathbb{R}_+)_{n,q} \\ \mathbf{V}\in\mathscr{M}(\mathbb{R}_+)_{p,q}}}{\arg\min} \sum_{i,j} x_{ij}\log\left(\frac{x_{ij}}{(\mathbf{F}\mathbf{V}^\top)_{ij}}\right) + (\mathbf{F}\mathbf{V}^\top)_{ij} \\ &= \underset{\substack{\mathbf{F}\in\mathscr{M}(\mathbb{R}_+)_{n,q} \\ \mathbf{V}\in\mathscr{M}(\mathbb{R}_+)_{p,q}}}{\arg\max} \sum_{i,j} x_{ij}\log((\mathbf{F}\mathbf{V}^\top)_{ij}) - (\mathbf{F}\mathbf{V}^\top)_{ij},\end{aligned}$$

NMF: limitations

Caveats

- Basis $\mathbf{V}$ formed by standard NMF is not orthogonal!
- Visualization is questionable ...
- Used to performed matrix factorization rather than exploratory analysis

Other model-based approaches

Use a probabilistic-based model to better described non-negative data

- Look for models handling**surdispersion** \{multivariate Poisson-lognormal model, Poisson-Gamma, etc.}
- Look for **zero-inflated** distributions

$$\mathbb{P}(\mathbf{x}_i) = \pi_0 \, \delta_0 + (1 - \pi_0) f(\mathbf{x}_i)$$

Kernel-PCA

Principle: non linear transformation of $\mathbf{x}$ prior to linear PCA

1. Project the data into a higher space where it is linearly separable
2. Apply PCA to the transformed data

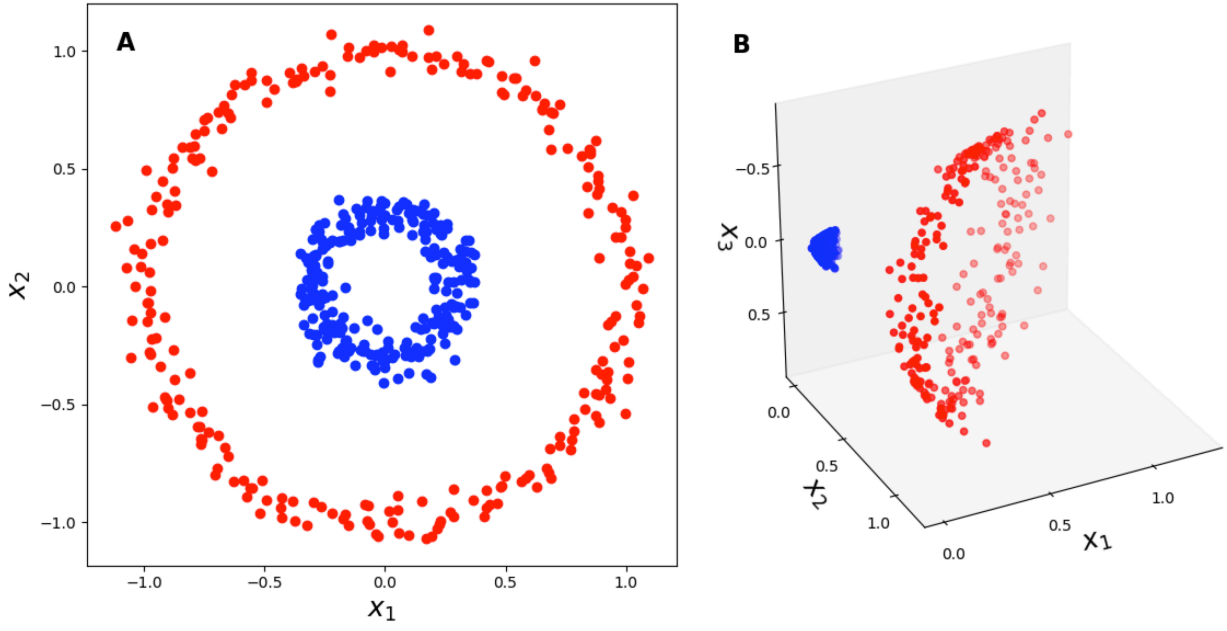


Figure 8: Transformation $\Psi : \mathbf{x} \rightarrow \Psi(\mathbf{x})$ (illustration in presence of existing labels)

Kernel-PCA

Kernel PCA Model

Assume a non linear transformation $\Psi(\mathbf{x}_i)$ where $\Psi : \mathbb{R}^p \to \mathbb{R}^n$, then perform linear PCA, with $\mathbf{U}$ a $n \times q$ orthonormal matrix

$$\Phi(\mathbf{x}) = \mathbf{U}^\top \Psi(\mathbf{x} - \boldsymbol{\mu}) = \tilde{\mathbf{x}}$$

Kernel trick

Never calculate $\Psi(\mathbf{x}_i)$ thanks to the kernel trick:

$$K = k(\mathbf{x}, \mathbf{y}) = (\Psi(\mathbf{x}), \Psi(\mathbf{y})) = \Psi(\mathbf{x})^T \Psi(\mathbf{y})$$

Solution

Eigen-decomposition of the doubly centered kernel matrix $\mathbf{K} = k(\mathbf{x}_i, \mathbf{x}_{i'})$

$$\tilde{\mathbf{K}} = (\mathbf{I} - \mathbf{1}\mathbf{1}^\top/n)\mathbf{K}(\mathbf{I} - \mathbf{1}\mathbf{1}^\top/n) = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^\top$$

Choice of a kernel

A symmetric positive definite function $k(\mathbf{x}, \mathbf{y}) \in \mathbb{R}$, which depends on the kind of **similarity** assumed

Some common kernels

- **Polynormial Kernel**

$$k(\mathbf{x}_i, \mathbf{x}_{i'}) = (\mathbf{x}_i^\top \mathbf{x}_{i'} + c)^d$$

- **Gaussian (radial) kernel**

$$k(\mathbf{x}_i, \mathbf{x}_{i'}) = \exp \frac{-\|\mathbf{x}_i - \mathbf{x}_{i'}\|^2}{2\sigma^2}$$

- **Laplacian kernel**

$$k(\mathbf{x}_i, \mathbf{x}_{i'}) = \exp \frac{-\|\mathbf{x}_i - \mathbf{x}_{i'}\|}{\sigma}$$

↝ Kernel PCA suffers from the choice of the Kernel

(Variational) Auto-encoders

Highly non-linear model

Find Φ and $\tilde{\Phi}$ with **two** neural-networks, controlling the error.

$$\epsilon(\mathbf{X}, \hat{\mathbf{X}}) = \sum_{i=1}^{n} \left\| \mathbf{x}_i - \tilde{\Phi}(\Phi(\mathbf{x}_i)) \right\|^2 + \text{regularization}(\Phi, \tilde{\Phi})$$

- # layers and neurons determine the **model complexity**
- Need regularization to avoid **overfitting**
- Fitted with optimization tools like stochastic gradient descent
- Require more data and more computational resources
- **Interpretation questionable**

Manifold learning (preserving pairwise relations)

Pairwise Relation

Focus on pairwise relation $\mathscr{R}(\mathbf{x}_i, \mathbf{x}_{i'})$.

Distance Preservation

Construct a map Φ from the space $\mathbb{R}^p$ into a space $\mathbb{R}^q$ of smaller dimension:

$$\begin{aligned} \Phi : \quad & \mathbb{R}^p \to \mathbb{R}^q, q \ll p \\ & \mathbf{x} \mapsto \Phi(\mathbf{x}) \end{aligned}$$

$$\text{such that} \quad \mathscr{R}(\mathbf{x}_i, \mathbf{x}_{i'}) \sim \mathscr{R}'(\tilde{\mathbf{x}}_i, \tilde{\mathbf{x}}_{i'})$$

Multidimensional scaling

A.k.a PCoA (Principal Coordinates Analysis)
Try to preserve inner product related to the distance (e.g. Euclidean)

t-SNE – Stochastic Neighborhood Embedding

Try to preserve relations with close neighbors with Gaussian kernel

Multidimensional scaling

a.k.a Principale Coordinates Analysis

Problem setup

Consider a collection of points $\mathbf{x}_i \in \mathbb{R}^p$ and assume either

- $D = d_{ii'}$ a $n \times n$ dissimilarity matrix, or
- $S = s_{ii'}$ a $n \times n$ similarity matrix, or

Goal: find $\tilde{\mathbf{x}}_i \in \mathbb{R}^q$ while preserving S/D in the latent space

↝ Don't need access to the position in $\mathbb{R}^p$ (only D or S ↝ 'kernel').

Classical MDS model

Measure similarities with the (centered) **inner product** and minimize

$$\sum_{i \neq i'} \left((\mathbf{x}_i - \boldsymbol{\mu})^\top (\mathbf{x}_i - \boldsymbol{\mu}) - \tilde{\mathbf{x}}_i^\top \tilde{\mathbf{x}}_{i'} \right)^2,$$

assuming a linear model $\tilde{\mathbf{x}} = \mathbf{V}^\top (\mathbf{x}_i - \boldsymbol{\mu})$, with $\mathbf{V} \in \mathcal{O}_{p \times q}$.

Classical MDS: solution

With the linear model $\tilde{\mathbf{x}} = \Phi(\mathbf{x}) = \mathbf{V}^\top(\mathbf{x}_i - \boldsymbol{\mu})$, we aim at minimizing

$$\begin{aligned}\text{Stress}^{cMDS} &= \sum_{i \neq i'} \left((\mathbf{x}_i - \boldsymbol{\mu})^\top (\mathbf{x}_{i'} - \boldsymbol{\mu}) - \tilde{\mathbf{x}}_i^\top \tilde{\mathbf{x}}_{i'} \right)^2, \\ &= \sum_{i \neq i'} \left((\mathbf{x}_i - \boldsymbol{\mu})^\top (\mathbf{x}_{i'} - \boldsymbol{\mu}) - (\mathbf{x}_i - \boldsymbol{\mu})^\top \mathbf{V}\mathbf{V}^\top (\mathbf{x}_{i'} - \boldsymbol{\mu}) \right)^2,\end{aligned}$$

It can be showed that $\underset{\boldsymbol{\mu} \in \mathbb{R}^p, \mathbf{V} \in \mathcal{O}_{pq}}{\text{minimize}}\ \text{Stress}^{cMDS}(\tilde{\mathbf{x}}_i)$ is dual to principal component analysis and leads to

$$\tilde{\mathbf{x}} = \mathbf{X}^c\mathbf{V} = \mathbf{U}\mathbf{D}\mathbf{V}^\top\mathbf{V} = \mathbf{U}\mathbf{D}.$$

↝ The principal coordinates in $\mathbb{R}^q$ correspond to the scores of the n individuals projected on the first q principal components.

Metric Multidimensional Scalings

Idea to generalize classical MDS:

preserving similarities in term of **inner product** amounts to preserve dissimilarity in terms of Euclidean distance

Least-squares/Kruskal-Shephard scaling

Use a distance base formulation with the following loss (Stress) function:

$$\text{Stress}^{SK} = \sum_{i \neq i'} \left(d_{ii'} - \|\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_{i'}\|\right)^2,$$

- Almost equivalent to classical MDS when d is the Euclidean distance
- Generalize to any **quantitative** dissimilarity/distance d

Sammong mapping - Variant of the loss (Stress) function

$$\text{Stress}^{SM} = \sum_{i \neq i'} \frac{\left(d_{ii'} - \|\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_{i'}\|\right)^2}{d_{ii'}}.$$

Stochastic Neighbor Embedding (SNE)

Let $(\mathbf{x}_1, \dots, \mathbf{x}_n)$ be the original points in $\mathbb{R}^p$, and measure similarities by

$$p_{ij} = (p_{j|i} + p_{i|j})/2n$$

where

$$\begin{aligned} p_{j|i} &= \frac{\exp(-\|\mathbf{x}_j - \mathbf{x}_i\|^2/2\sigma_i^2)}{\sum_{k\neq i}\exp(-\|\mathbf{x}_k - \mathbf{x}_i\|^2/2\sigma_i^2)}, \\ &= \frac{\exp(-d_{ij}^2/2\sigma_i^2)}{\sum_{k\neq i}\exp(-d_{ki}^2/2\sigma_i^2)} \end{aligned}$$

- SNE preserves relations with **close neighbors** with Gaussian kernels
- σ smooths the data (linked to the regularity of the target manifold)

The perplexity parameter

The variance σ_i^2 should adjust to local densities (neighborhood of point i)

Perplexity: a smoothed effective number of neighbors

The perplexity is defined by

$$Perp(p_i) = 2^{H(p_i)}, \qquad H(p_i) = -\sum_{j=1}^{n} p_{j|i} \log_2 p_{j|i}$$

where H is the Shannon entropy of $p_i = (p_{1|i}, \dots, p_{n|i})$.\
↝ SNE performs a binary search for the value of σ_i that produces a p_i with a fixed perplexity that is specified by the user.

tSNE and Student / Cauchy kernels

Consider $(\tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_n)$ are points in the low dimensional space $\mathbb{R}^{q=2}$

- Consider a similarity between points in the new representation:

$$q_{i|j} = \frac{\exp(-\|\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_j\|^2)}{\sum_{k \neq i} \exp(-\|\tilde{\mathbf{x}}_k - \tilde{\mathbf{x}}_j\|^2)}$$

- Robustify this kernel by using Student(1) kernels (ie Cauchy)

$$q_{i|j} = \frac{(1 + \|\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_j\|^2)^{-1}}{\sum_{k \neq i} (1 + \|\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_k\|^2)^{-1}}$$

Optimizing tSNE

- Minimize the KL between p and q so that the data representation minimizes:

$$C(y) = \sum_{ij} KL(p_{ij}, q_{ij})$$

- The cost function is not convex

$$\left[\frac{\partial C(y)}{\partial y}\right]_i = \sum_j (p_{ij} - q_{ij})(y_i - y_j)$$

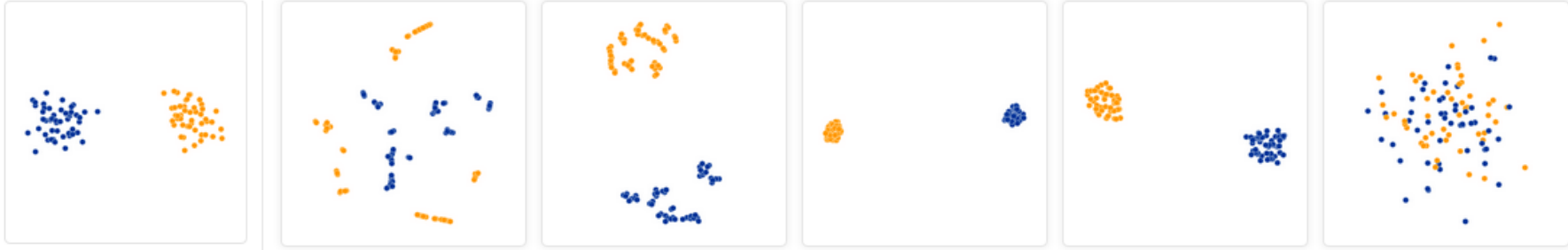
- Gradient update (adaptive learning rate η) with momentum $\alpha(t)$

$$Z^{(t)} = Z^{(t-1)} + \eta \frac{\partial C(Z)}{\partial Z} + \alpha(t)(Z^{(t-1)} - Z^{(t-2)})$$

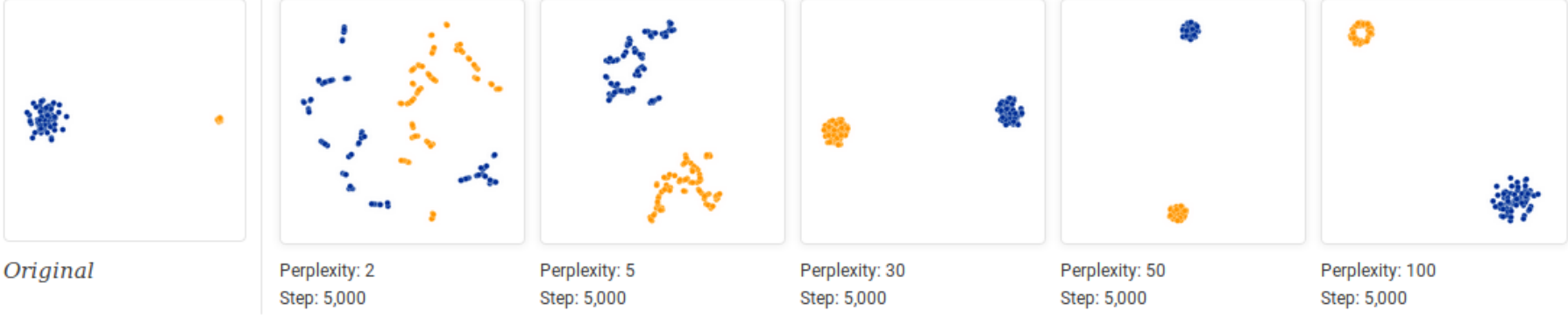
- Initialization $Z_i^{(0)} \sim \mathcal{N}(0, \delta I)$, δ small.

Empirical properties of tSNE (1)

Effect of Hyperparameters : Perplexity



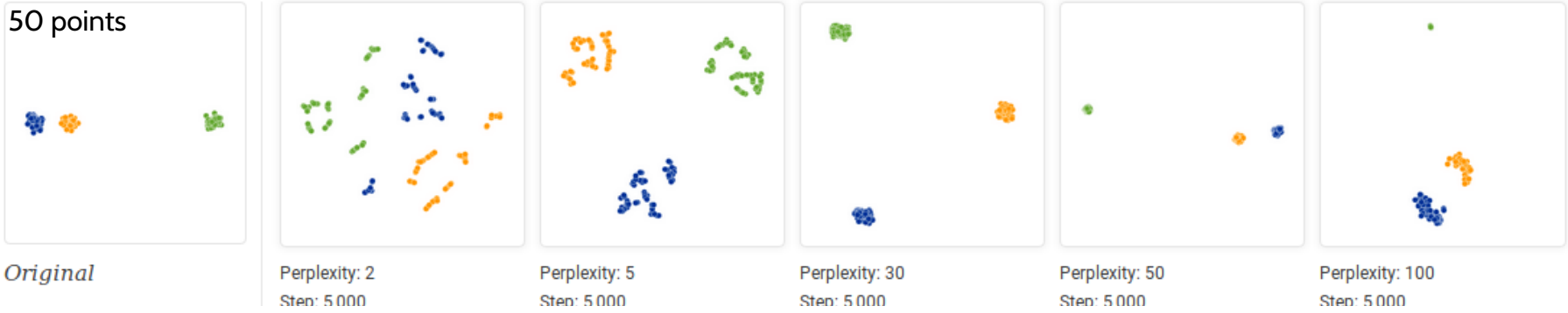
tSNE does not account for heteroscedasticity

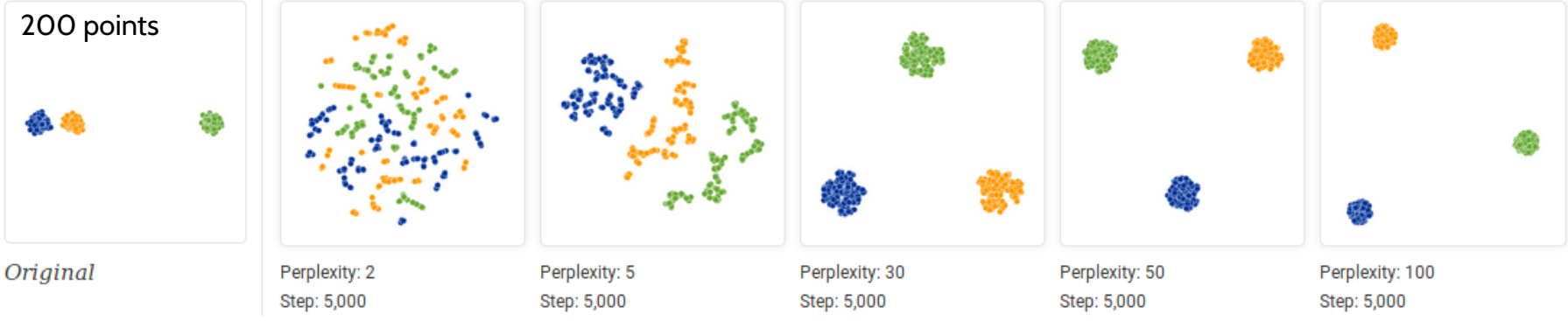


https://distill.pub/2016/misread-tsne/

Empirical properties of tSNE (2)

tSNE does not account for between-cluster distance



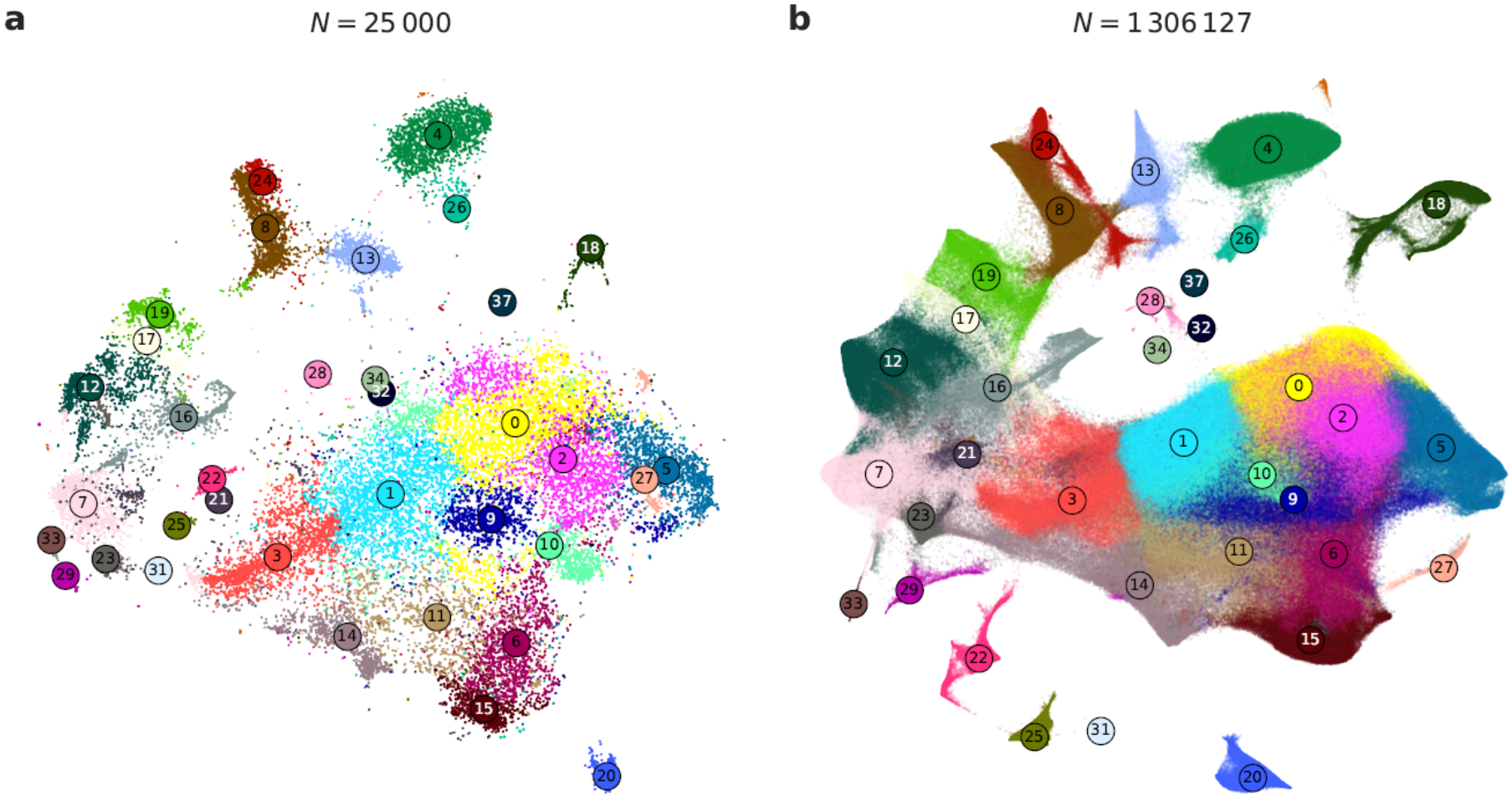


What about random noise ?

Empirical properties of tSNE (3)

Catching Complex Geometries

tSNE on single cell Gene Expression data [1]



t-SNE: pros/cons

Properties

- good at preserving local distances (intra-cluster variance)
- not so good for global representation (inter-cluster variance)
- good at creating clusters of close points, bad at positioning clusters wrt each other

Limitations

- importance of preprocessing: initialize with PCA and feature selection plus log transform (non linear transform)
- percent of explained variance ? interpretation of the q distribution ?
- Lack of reproducibility due to stochastic optimization

Uniform Manifold Approximation and Projection [2]

For j in the k-neighborhood of i, define the conditional distribution

$$p_{j|i} = \exp\left(-\frac{\|X_i - X_j\|_2^2 - \rho_i}{\sigma_i}\right) \quad \text{with } \rho_i = \min_{j \neq i} \|X_i - X_j\|^2$$

and its symmetrized version

$$p_{ij} = p_{j|i} + p_{i|j} - p_{j|i} p_{i|j}.$$

Rely on a generalized Student-distribution with a, b fitted on the data:

$$q_{ij} = \left(1 + a\|Z_i - Z_j\|_2^{2b}\right)^{-1}$$

UMAP solves the following problem:

$$\min_{Z \in \mathbb{R}^{n \times d}} \quad -\sum_{i<j} p_{ij} \log q_{ij} + (1 - p_{ij}) \log(1 - q_{ij})$$

References

[1] Kobak, D. and Berens, P. (2018). The art of using t-SNE for single-cell transcriptomics. *bioRxiv*.

[2] McInnes, L., Healy, J. and Melville, J. (2018). UMAP: Uniform manifold approximation and projection for dimension reduction. *Arxiv* 1–63.