

Model-based Statistical Learning



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The curse of dimensionality

The **curse of dimensionality**:

- this term was first used by R. Bellman in the introduction of his book “Dynamic programming” in 1957:

*All [problems due to high dimension] may be subsumed under the heading “**the curse of dimensionality**”. Since this is a curse, [...], **there is no need to feel discouraged about the possibility of obtaining significant results despite it.***

- ✓ he used this term to talk about the difficulties to find an optimum in a high-dimensional space using an exhaustive search,
- ✓ in order to promote dynamic approaches in programming.

The curse of dimensionality

In the mixture model context:

- the building of the data partition mainly depends on:

$$H_k(x) = -2 \log(\pi_k f(x, \theta_k)),$$

- model Full-GMM:

$$H_k(x) = (x - \mu_k)^T \Sigma_k^{-1} (x - \mu_k) + \log(\det \Sigma_k) - 2 \log(\pi_k) + \gamma.$$

Consequently:

- it is necessary to invert Σ_k which have a number of parameters proportional to p^2 ,
- if n is small compared to p^2 , the estimates of Σ_k are ill-conditionned or singular and it will be difficult or impossible to invert Σ_k .

\Rightarrow if n is too small compared to p , it won't be possible to run an EM algorithm with a full-GMM!

The curse of dimensionality

From the estimation point of view:

- let us consider the normalized trace $\tau(\Sigma) = \text{tr}(\Sigma^{-1})/p$ of the inverse covariance matrix Σ^{-1} of a multivariate Gaussian distribution $\mathcal{N}(0, \Sigma)$,
- the estimation of τ from a sample of n observations $\{x_1, \dots, x_n\}$ conduced to:

$$\tau(\hat{\Sigma}) = \tau(\hat{\Sigma}) = \frac{1}{p} \text{tr}(\hat{\Sigma}^{-1}), \quad \checkmark$$

$$E[\tau(\hat{\Sigma})] = \left(1 - \frac{p}{n-1}\right)^{-1} \tau(\Sigma).$$

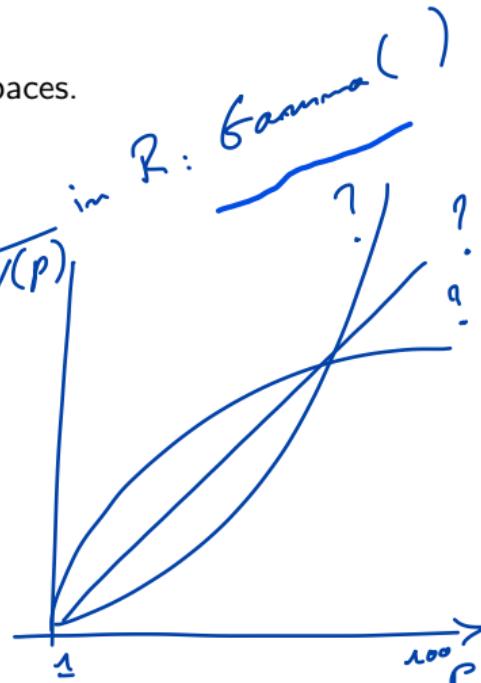
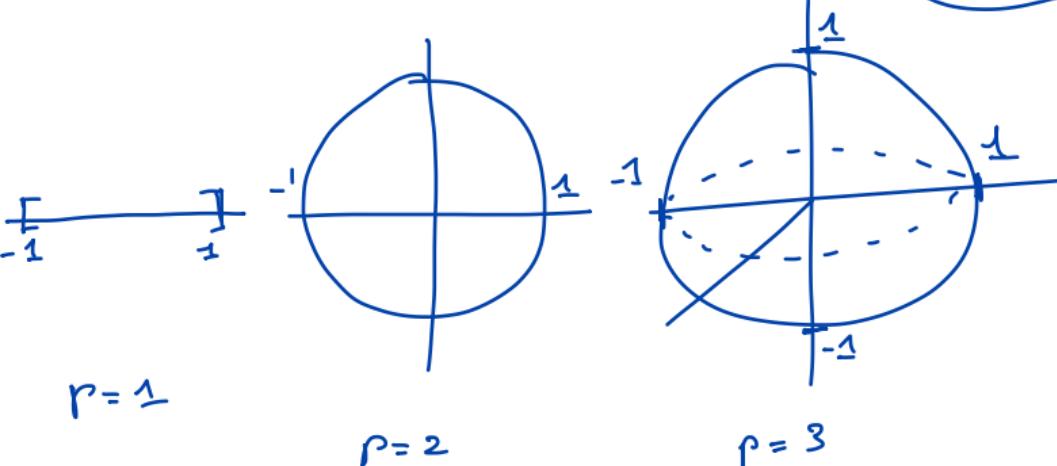
- consequently, if the ratio $p/n \rightarrow 0$ when $n \rightarrow +\infty$, then $E[\tau(\hat{\Sigma})] \rightarrow \tau(\Sigma)$,
- however, if the dimension p is comparable with n , then $E[\tau(\hat{\Sigma})] \rightarrow \underline{c} \tau(\Sigma)$ when $n \rightarrow +\infty$, where $c = \lim_{n \rightarrow +\infty} p/n$.

The blessings of dimensionality

As Bellman thought:

- all is not bad in high-dimensional spaces (hopefully!)
- there are interesting things which happen in high-dimensional spaces.

First example: volume of the unit sphere is $V(p) = \frac{\pi^{p/2}}{\Gamma(p/2+1)}$,



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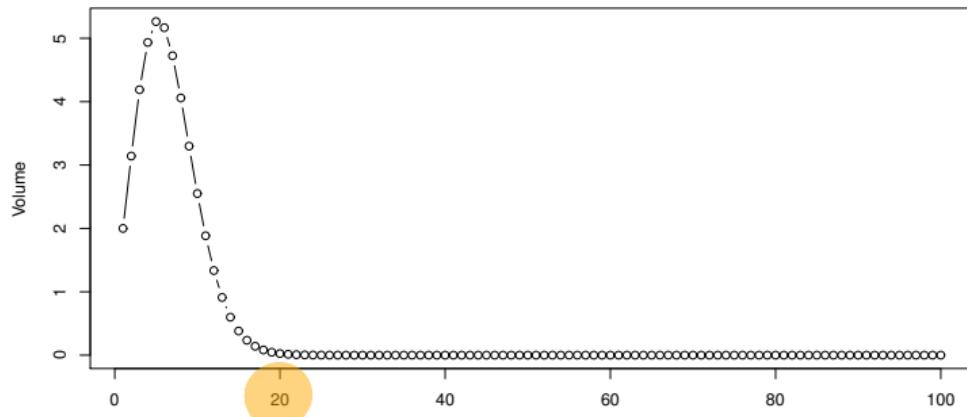
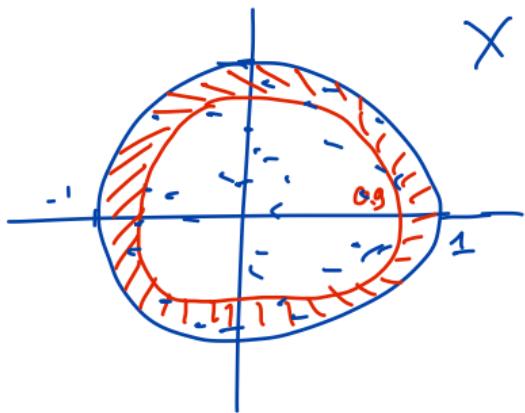


Fig. Volume of a sphere of radius 1 regarding to the dimension p .

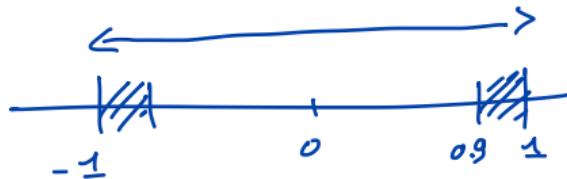
The blessings of dimensionality

Second example: probability that a uniform variable on the unit sphere belongs to the shell between the spheres of radius 0.9 and 1 is

$$P(X \in S_{0.9}(p)) = 1 - 0.9^p \xrightarrow{p \rightarrow \infty} 1$$



$$X \sim U(\text{HS1})$$

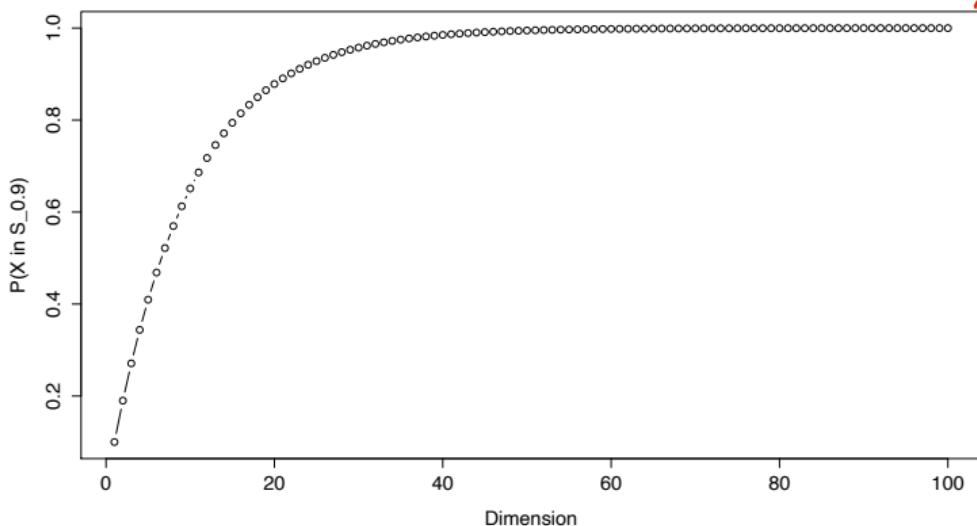


$$P(X \in S_{0.9}) = 0.1$$

The blessings of dimensionality

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$$P(X \in S_{0.9}(p)) = 1 - 0.9^p \xrightarrow{p \rightarrow \infty} 1$$



A) The message here is that HD spaces are mostly empty. The data are located in subspaces of lower dimensionalities.
⇒ the "empty space phenomenon"

Fig. Probability that X belongs to the shell $S_{0.9}$ regarding to the dimension p .

The blessings of dimensionality

Third example:

- since high-dimensional spaces are almost empty,
- it should be easier to separate groups in high-dimensional space with an adapted classifier,
- a way to observe this is to look at the Bayes classifier behaviour.

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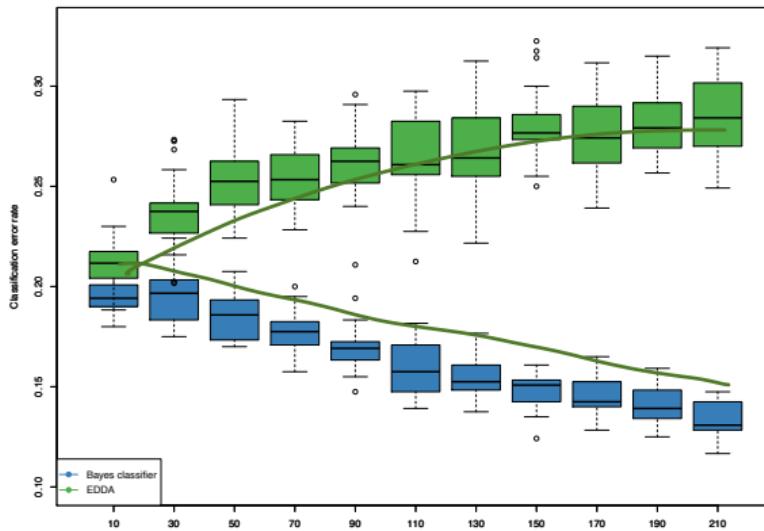


Fig. Classification error rate of the optimal classifier (blue) and EDDA (green) versus the data dimension on simulated data.

Classical ways to avoid the curse of dimensionality

Dimension reduction:

- the problem comes from that p is too large,
- therefore, reduce the data dimension to $d \ll p$,
- such that the curse of dimensionality vanishes!

Regularization:

- the problem comes from that parameter estimates are unstable,
- therefore, regularize these estimates, 
- such that the parameters are correctly estimated!

$$\hat{\Sigma}^{-1} = (\hat{\Sigma} + \epsilon I)^{-1}$$

$\epsilon \approx 0.01$

Parsimonious models:

- the problem comes from that the number of parameters to estimate is too large,
- therefore, make restrictive assumptions on the model,
- such that the number of parameters to estimate becomes more "decent"!

$$\hat{\Sigma} = \frac{1}{n} I$$

Outline

1. Introduction
2. Reminder on the learning process
3. Learning in high-dimensions
4. Dimension reduction
5. Clustering and classification

Dimension reduction

A common phantasm about dimension reduction:

- believe that dimension reduction helps for classification,
- this is not true because, most of the time, dimension reduction implies an information loss which would be discriminative.

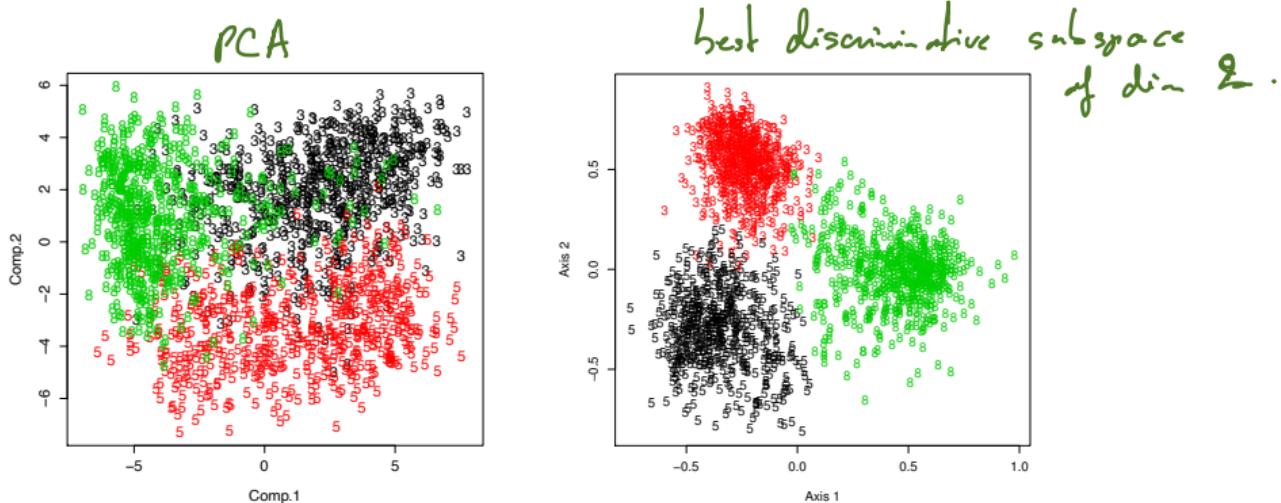
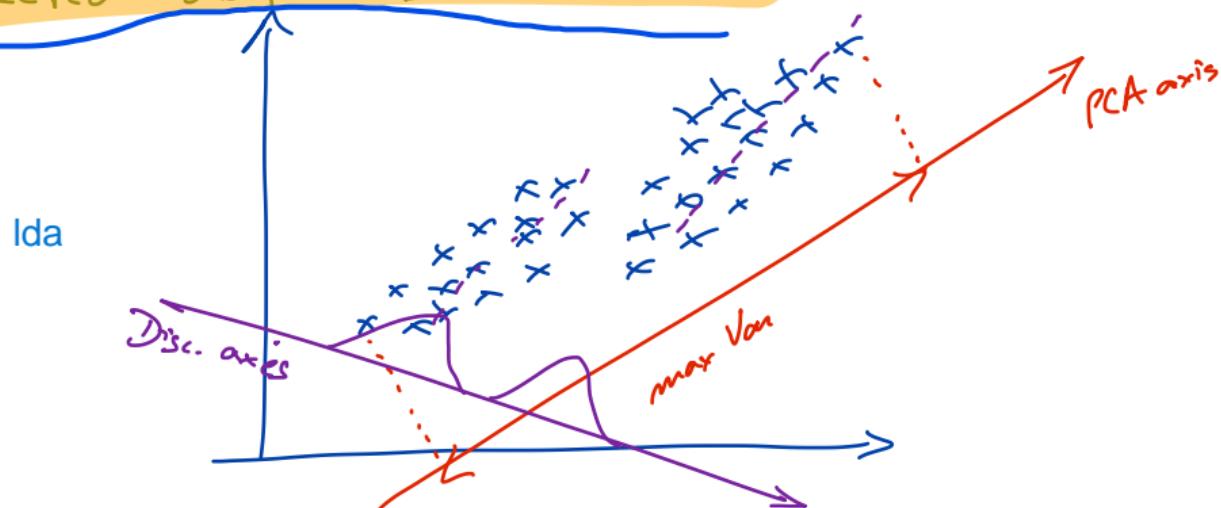


Figure: Projection of the 256-dimensional USPS data with PCA (left, unsupervised) and FDA (right, supervised).

PCA: principal component analysis

The goal of PCA is to find d new axes build on the p original axes by linear combinations such that the variance of the projected data is maximum.



PCA: the principle

The goal of PCA : $\underset{\substack{U \\ p \times d}}{\operatorname{argmax}} \operatorname{Var}(\underline{\underline{X}}^t U)$

$\underline{\underline{X}}$

projection of
 X in the d -
dimensional space

Solution : the d PCA axes u_1, \dots, u_d are the
eigen vectors of $\underline{\underline{X}}^t \underline{\underline{X}} = S$ associated with the largest
eigenvalues $\lambda_1, \dots, \lambda_d$ of S .

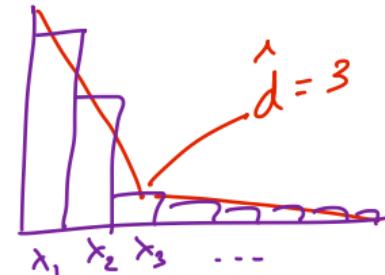
In practice :

- 1) compute $S = \underline{\underline{X}}^t \underline{\underline{X}}$ where $\underline{\underline{X}}$ are the centered data
- 2) do the eigen decomposition of S .
- 3) keep the eigenvectors of S associated with the largest λ_j .

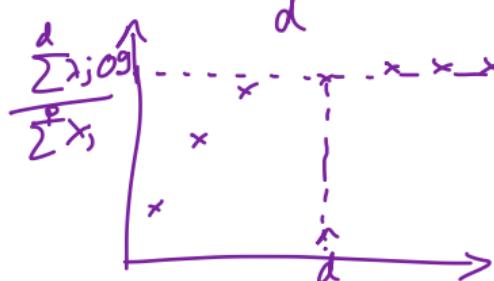
PCA: the principle

How to choose d ?:

1) the "elbow" method: plot the eigenvalue scree and select d in the place of the elbow in the scree

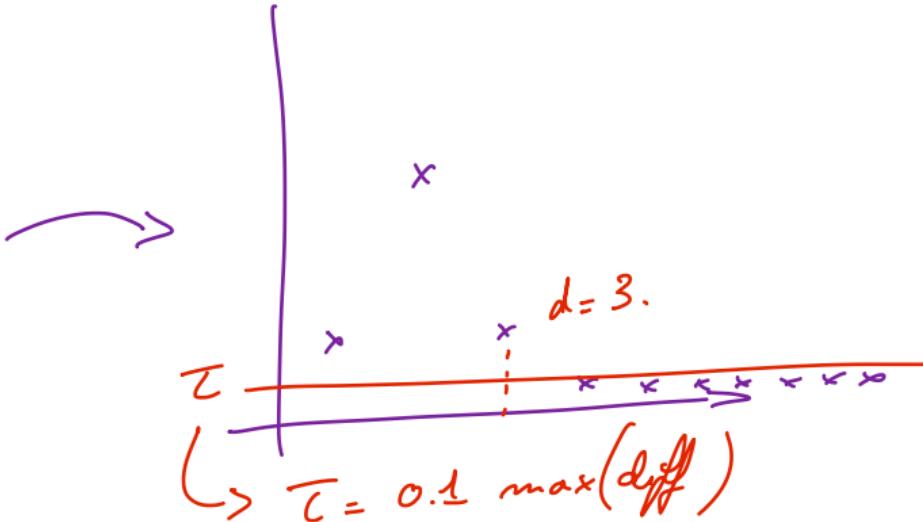
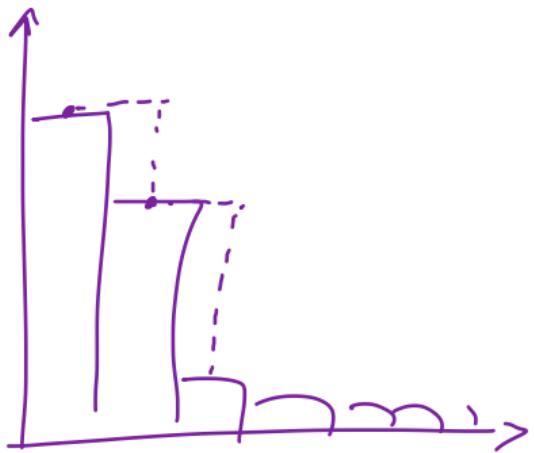


2) the "90%" rule:

$$\hat{d} = \underset{d}{\operatorname{argmin}} \frac{\sum_{j=1}^d \lambda_j}{\sum_{j=1}^p \lambda_j} \geq 90\%.$$


3) the scree-test of Cattell

Compute the differences between consecutive eigenvalues and select d when all differences after d are smaller than a threshold



A general remark: in case of hesitation, it is better to keep too much dimensions than too few!

PCA: projection

$$Y = X \cdot \hat{U}$$

will contain the projected data points on the d-dimensional PCA subspace.

↑
principal scores

the loading matrix.

Dimensions:
 $n \times d$ $n \times p$ $p \times d$

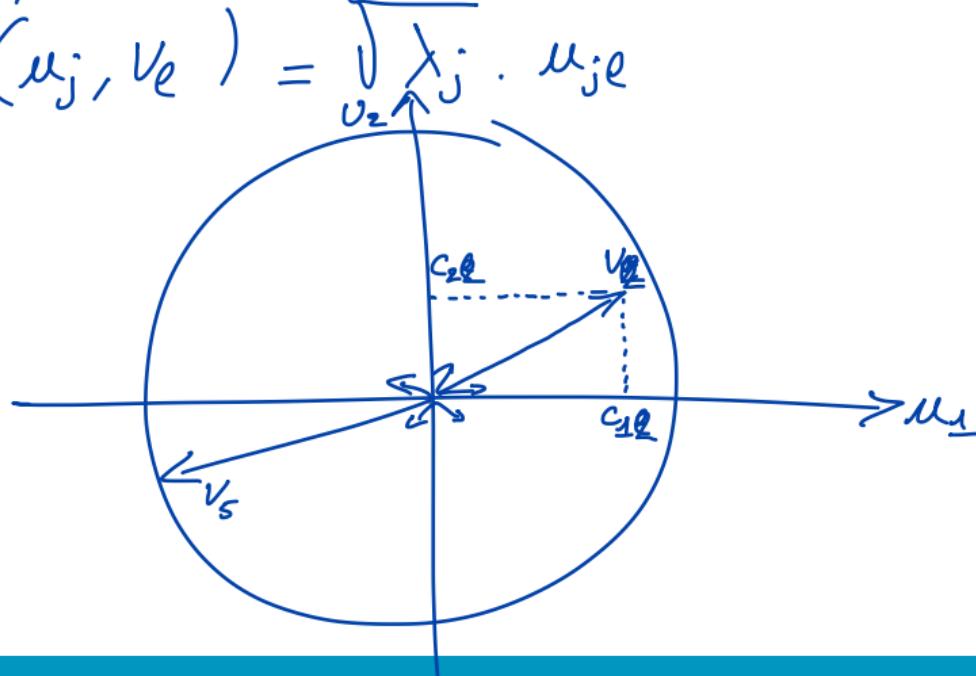
PCA: how many axes?

PCA: how many axes?

PCA: correlation circle

It is easy to relate the PCA axes with the original variables by calculating the correlation between them:

$$c_{je} = \text{Cor}(u_j, v_e) = \sum u_{je}$$



PCA: analysis of the marathon data

PPCA: a probabilistic version of PCA

Probabilistic PCA (Tipping & Bishop, 1999) extends PCA in a statistical framework. PPCA justifies PCA under the Gaussian assumption.

PPCA assumes a linear link between X the observed variable and Y a **latent** low-dimensional variable:

$$X = U^t Y + \varepsilon$$

where $X \in \mathbb{R}^P$
 $Y \in \mathbb{R}^d$ with $d \ll P$
 $\varepsilon \in \mathbb{R}^P$ is a noise term.
 U is a $p \times d$ matrix

PPCA: a probabilistic version of PCA

PPCA adds some statistical assumptions:

$$\epsilon \sim N(0, \sigma^2 I_p)$$

$$y \sim N(\mu, I_d) \quad \text{with } \mu \in \mathbb{R}^d$$

Interestingly, the marginal distribution of x is:

$$x \sim N(U\mu, UU^T + \sigma^2 I_p)$$

Let's introduce $\Theta = \{\mu, \sigma^2, U\}$, the set of model parameters

Thanks to this statistical model, we have now a new way to perform PCA: estimate the model parameters of PPCA from the data.

performing PCA (\Rightarrow estimate the models of PPCA).

Maximum Likelihood can be used for that, through the EM algorithm.

Lemma: the estimation of U through the EM algo is the eigenvectors of $S = \bar{X}^t \bar{X}$ associated with the largest eigenvalues of S .

PPCA: why is it interesting?

- i) PPCA offers a theoretical justification of PCA under the Gaussian assumption.
- ii) it also helps to understand the limitation of PCA
- iii) we can rely on model selection (AIC, BIC, ...) to select d
- iv) new statistical models can be elaborated from PPCA.

PPCA in practice...

$$\hat{U} = \text{eigen}(\text{cov}(X))$$

i) Let's do PCA as before / $\hat{\mu} = \text{mean}(X\hat{U})$
 $\hat{\Sigma} = \text{mean}(\text{diag}(\text{cov}(X - X\hat{U}\hat{U}^T)))$

ii) Use Bic to select d:

$$\text{BIC}(d) = \log L(X; \hat{\theta}_{\text{PPCA}}) - \frac{\gamma(d)}{2} \log(n)$$

where $\gamma(d) = d + \frac{1}{\hat{\sigma}^2} + p \frac{(d+1)}{2}$

$\begin{matrix} \uparrow & \uparrow & \uparrow \\ \mu & \hat{\sigma}^2 & U \\ & & p \times d \end{matrix}$

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5. Clustering ~~and classification~~ in HD spaces

The limits of GMM in high dimensional spaces

- ⊕ Empty HD spaces \Rightarrow good for clustering
 - ⊖ Model-based approaches are usually over-parametrized which is problem when learning!
- \Rightarrow The solution: adapt the statistical techniques to HD spaces by taking into account the properties of those spaces.

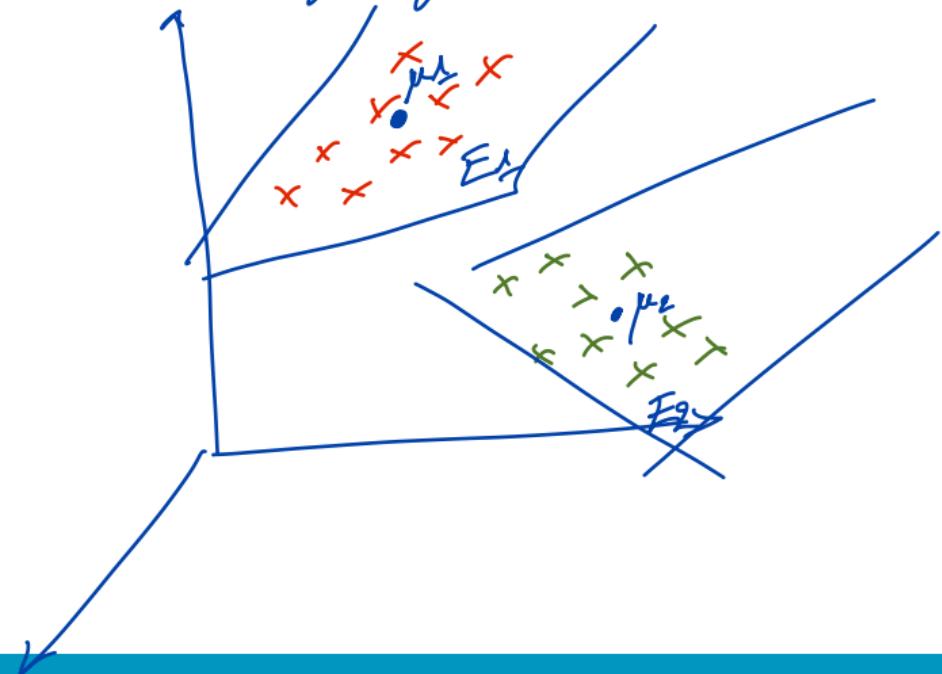
Parsimonious models for GMM



Figure: The parsimonious models of Mclust.

The solutions : Subspace clustering

The idea of subspace clustering is to assume that each group leaves in a specific low-dimensional subspace.



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The mixture of PPCA

Tipping & Bishop proposed in 1996 the mixture of PPCA

$$Z \sim \mathcal{H}(1; \pi) \quad \pi = (\pi_1, \dots, \pi_K)$$

$$X_{|Z=h} = \gamma U_h + \epsilon_h \quad \text{where } U_h \text{ is a } p \times d \text{ matrix}$$

$$\epsilon_h \sim N(0, \Sigma_h \mathbb{I}_p)$$

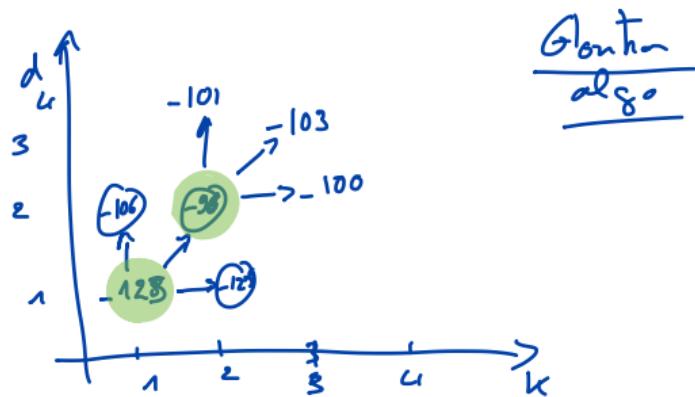
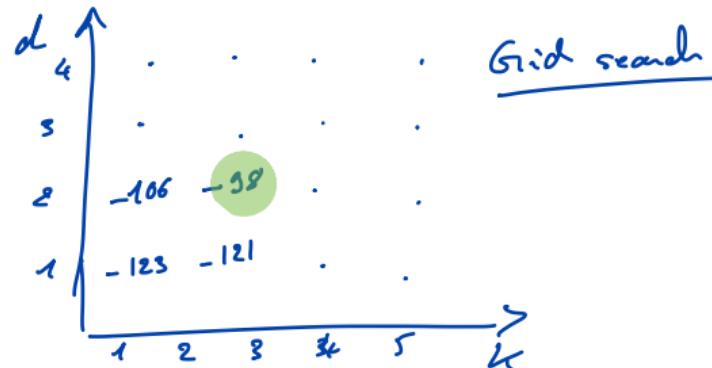
$$Y|Z=h \sim N(\mu_h, I_d)$$

$$\Rightarrow X \sim \sum_{h=1}^K \pi_h \phi(\mu_h U_h, U_h^t U_h + \Sigma_h^{-1})$$

The mixture of PPCA

The inference of MPPCA can be done using the EM algorithm.

The choice of both K and d can be done using model selection, with BIC for instance.



HDDC (High Dimensional Data Clustering, Bouveyron 06)

The idea of HDDC is to extend NPPCA on 2 directions:

- 1) allows the intrinsic dimensions of the subspaces to be different : $d \rightarrow d_k$.
- 2) allows sub-models of NPPCA to fit in different situations with fewer data.

HDDC

the model of HDDC, $Z \sim \text{cl}(1, \pi)$

$$X_{|Z=k} = YU_k + \varepsilon_k \quad \text{where } U_k \text{ is a } p \times d_k \text{ orthonormal matrix}$$

$$\varepsilon_k \sim N(0, \sigma_k^2 I_p)$$

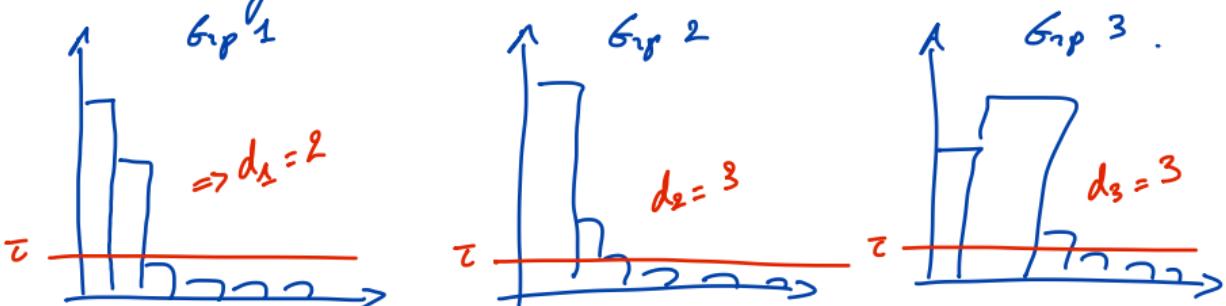
$$Y \sim N(\mu_k, \alpha_k I_{d_k}) \quad \text{where } \alpha_k \in \mathbb{R}^{d_k}$$

$$\Rightarrow X \sim \sum_{k=1}^n \pi_k N\left(\mu_k U_k, (\alpha_k U_k)(\alpha_k U_k)^T \sigma_k^2 I_p\right)$$

HDDC

Inferring this HDDC model is still possible with ER, but model selection is now very difficult because we have $(K+1)$ discrete hyper-parameters to choose.

A solution to avoid this combinatorial problem: the scree-test of Cattell



\Rightarrow Model selection here resumes to choosing K and τ .

In HDDC, it is also possible to get more parsimonious models by constraining some model parameters to be common between or within groups.

$$\forall h, d_h = d \Rightarrow \text{PPCA}$$

$$\forall h, \sigma_h^2 = \sigma^2 \Rightarrow [a_{hj} \ b_{hj} \ Q_h \ d_h]$$

$$a_{hj} = a_h \Rightarrow [a_h \ b_h \ Q_h \ d_h]$$

$$\sigma_h^2 = \sigma^2 \ \& \ a_{hj} = a_h \Rightarrow [a_h \ b \ Q_h \ d_h]$$

(...)

$$\Rightarrow [a \ b \ Q \ d]$$

\Rightarrow the R Library `HDDC` classif implements it.

\Rightarrow the Python package `HDDA` for Python github.com/mfauvel/HDDA

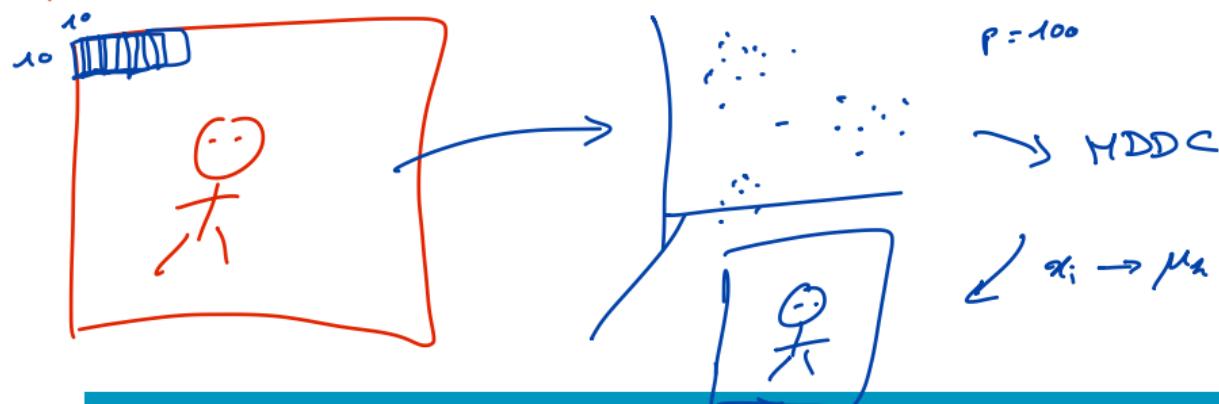
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28 submodels.
which can be selected thanks to model selection.

In the supervised case: HDDA

In the supervised case, HDDA implements all the 28 models (including MPPCA) for supervised classification.

A remark: HDDC for image denoising turns out to be extremely performant: HDTI method implements it.



Conclusion on subspace clustering / classif.:

- ⊕ extremely performant models for HD data.
- ⊖ no easy way to visualize the data in the latent subspaces.
↳ the Fisher-EP algorithm aims to solve this visualization problem while keeping the idea of subspace clustering.