# A non parametric PLSDA

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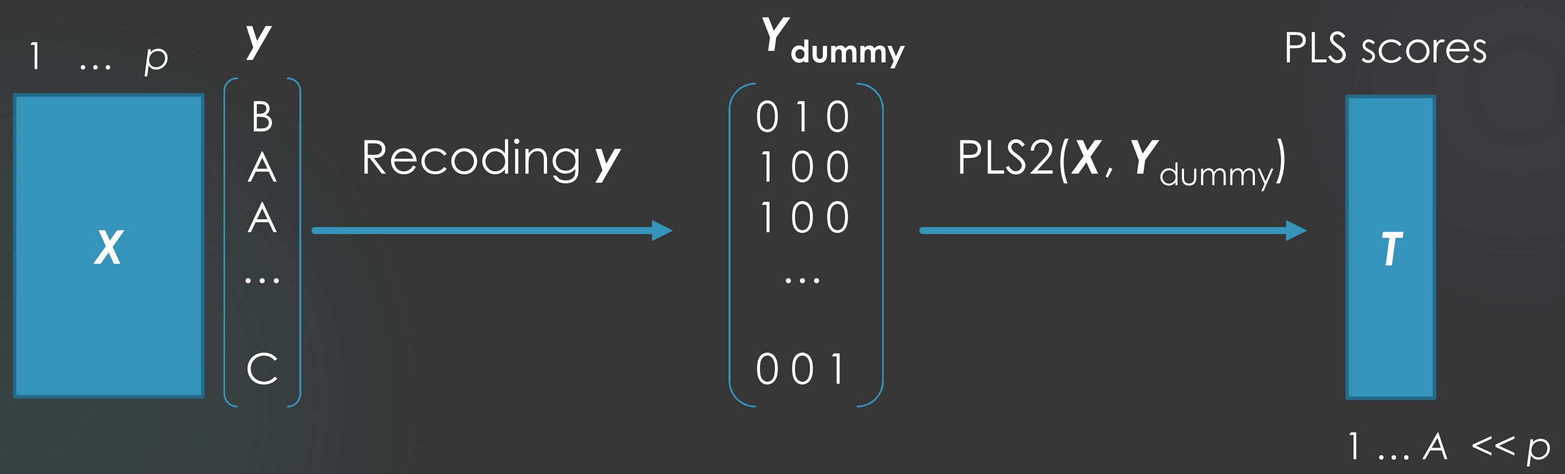
# "PLSDA" PLS discriminant analysis

**Step 1) Dimension reduction**



## Step 2) Several alternatives

A) Regression $\boldsymbol{Y}_{\textbf{dummy}}$ on $\boldsymbol{T}$ $\Rightarrow$ PLSR-DA = usual "PLSDA"

$$\hat{Y}_{dummy}$$

$$\begin{pmatrix} -.2 & 3.7 & -1.5 \\ .3 & .4 & -1.7 \\ \boxed{.9 \quad -.1 \quad .2} \\ & \cdots & \\ -.7 & -.1 & 1.8 \end{pmatrix} \longrightarrow \text{class A} \quad \text{(highest prediction)}$$

~ **unbounded** estimates of class-membership probabilities

(**Rk:** The same prediction table is usually returned by deep learning pipelines. In general, they transform the predictions by applying a final softmax function to come back to the scale of a probability [0, 1] but, in principle, it is not mandatory)

## B) or Probabilistic DA on $\boldsymbol{T}$

Objective: $\hat{P}(\boldsymbol{y}_i = Class\ \ j \mid \boldsymbol{x}_i)$

$$\begin{pmatrix} .1 & .8 & .1 \\ .4 & .5 & .1 \\ .8 & .0 & .2 \\ & \cdots & \\ \\ .2 & .1 & .7 \end{pmatrix} \quad \longrightarrow \quad \text{class A}$$

a) Parametric hypothesis on the distribution of $\boldsymbol{T}$

- e.g. **Gaussian** distribution(s)
  - LDA $\Rightarrow$ PLS-LDA
  - QDA $\Rightarrow$ PLS-QDA

b) Non parametric: No hypothesis on the distribution of $\boldsymbol{T}$

- e.g. **Kernel density estimation** (KDE) $\Rightarrow$ PLS-KDE-DA

## a) Parametric Gaussian probability density

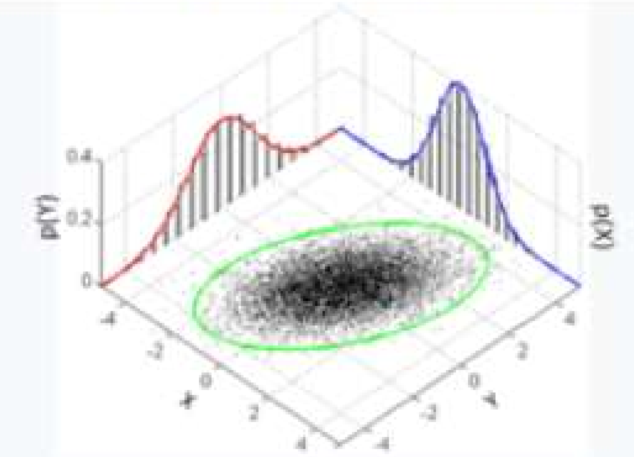


| PDF | $(2\pi)^{-k/2}\det(\boldsymbol{\Sigma})^{-1/2}\exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathsf{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right),$ exists only when $\boldsymbol{\Sigma}$ is positive-definite |
|---|---|

$\Sigma$ = ***X*** covariance matrix

**Multivariate normal**

**Probability density function**




https://en.wikipedia.org/wiki/Multivariate_normal_distribution

- **LDA** Same $\Sigma$ for all classes
- **QDA** One $\Sigma$ per class

# b) Non parametric

## Univariate KDE

$$\hat{f}_K(x) = \frac{1}{nh}\sum_{i=1}^{n} K\left(\frac{x - x_i}{h}\right) = \frac{1}{n}\sum_{i-1}^{n} K_h(x - x_i)\ ,$$

Density estimate at obs. **x**

Bandwidth (= smoothing)
Parameter to tune

Kernel function (integral sums to 1)
e.g. Gaussian pdf

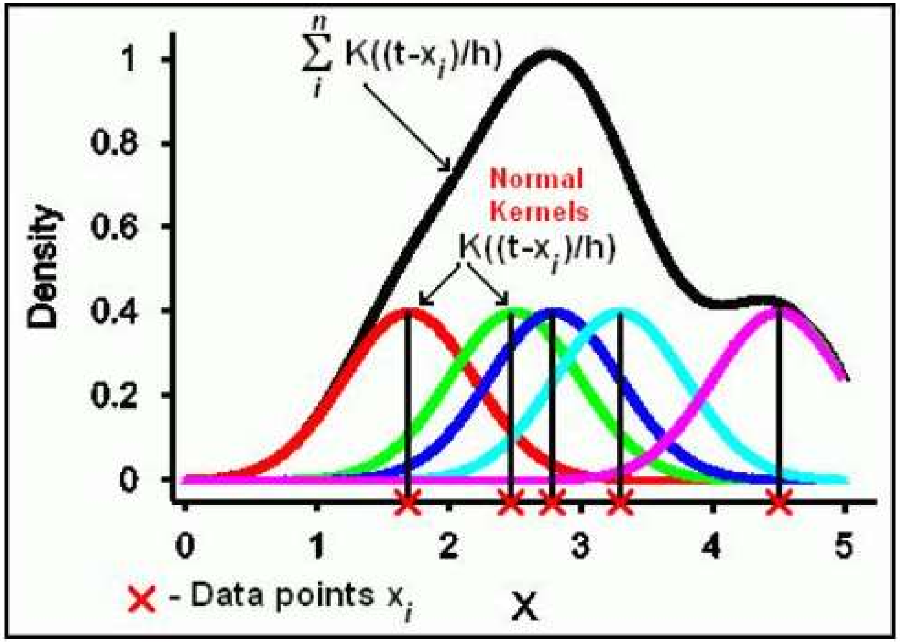
~ similarity index to **x**

Scott DW, Sain SR. - Multidimensional Density Estimation. In: Rao CR, Wegman EJ, Solka JL, eds. Handbook of Statistics. Vol 24. Data Mining and Data Visualization. Elsevier; 2005:229-261. doi:10.1016/S0169-7161(04)24009-3.

```
fh(t) = the sum of (K(t-xi)/h)/(nh) from i = 1...n
```

where n denotes the sample size. The choice of kernel function K is not very critical for the resulting estimate fh(t) and so a Gaussian kernel is used.

The following graph showing the sum of the normal kernels at 5 data points illustrates the ideas behind the kernel density estimation.




Univariate KDE

**Source: https://genstat.kb.vsni.co.uk/knowledge-base/kernel-density-estimation**

## Gaussian univariate KDE

$$\hat{f}(x) = \frac{1}{n}\sum_{i=1}^{n} \frac{1}{h\sqrt{2\pi}} exp\left\{-\frac{1}{2}\left(\frac{x - x_i}{h}\right)^2\right\}$$

$$= \frac{1}{nh}\sum_{i=1}^{n} K(u_i)$$

with $\quad u_i = \frac{x - x_i}{h}$

and $\quad K(u_i) = \frac{1}{\sqrt{2\pi}} exp\left\{-\frac{1}{2}\, u_i^2\right\}$ **pdf Normal(0, 1)**

## Gaussian multivariate KDE

The extension of the kernel estimator to vector-valued data, $\mathbf{x} \in \Re^d$, is straightforward for a normal kernel, $K \sim N(0, \Sigma)$:

$$\hat{f}(\mathbf{x}) = \frac{1}{n(2\pi)^{d/2}|\Sigma|^{1/2}} \sum_{i=1}^{n} \exp[-\frac{1}{2}(\mathbf{x}-\mathbf{x}_i)'\Sigma^{-1}(\mathbf{x}-\mathbf{x}_i)]\,. \tag{16}$$

Bandwidth matrix

$p \times p$ Positive-definite, symmetric

**To tune**

**Scott & Sain 2005**

$$\hat{f}(\mathbf{x}) = \frac{1}{n(2\pi)^{d/2}|\Sigma|^{1/2}} \sum_{i=1}^{n} \exp[-\frac{1}{2}(\mathbf{x}-\mathbf{x}_i)'\Sigma^{-1}(\mathbf{x}-\mathbf{x}_i)] \,. \tag{16}$$

**Assuming $\Sigma$ to be diagonal in (16)**
simplifies a lot the computations and tuning

$\Rightarrow$ Multiplicative Gaussian KDE

= product of univariate KDEs

# Illustration on iris data



***X***

| Row | sepal_length Float64 | sepal_width Float64 | petal_length Float64 | petal_width Float64 |
|---|---|---|---|---|
| 1 | 5.1 | 3.5 | 1.4 | 0.2 |
| 2 | 4.9 | 3.0 | 1.4 | 0.2 |
| 3 | 4.7 | 3.2 | 1.3 | 0.2 |

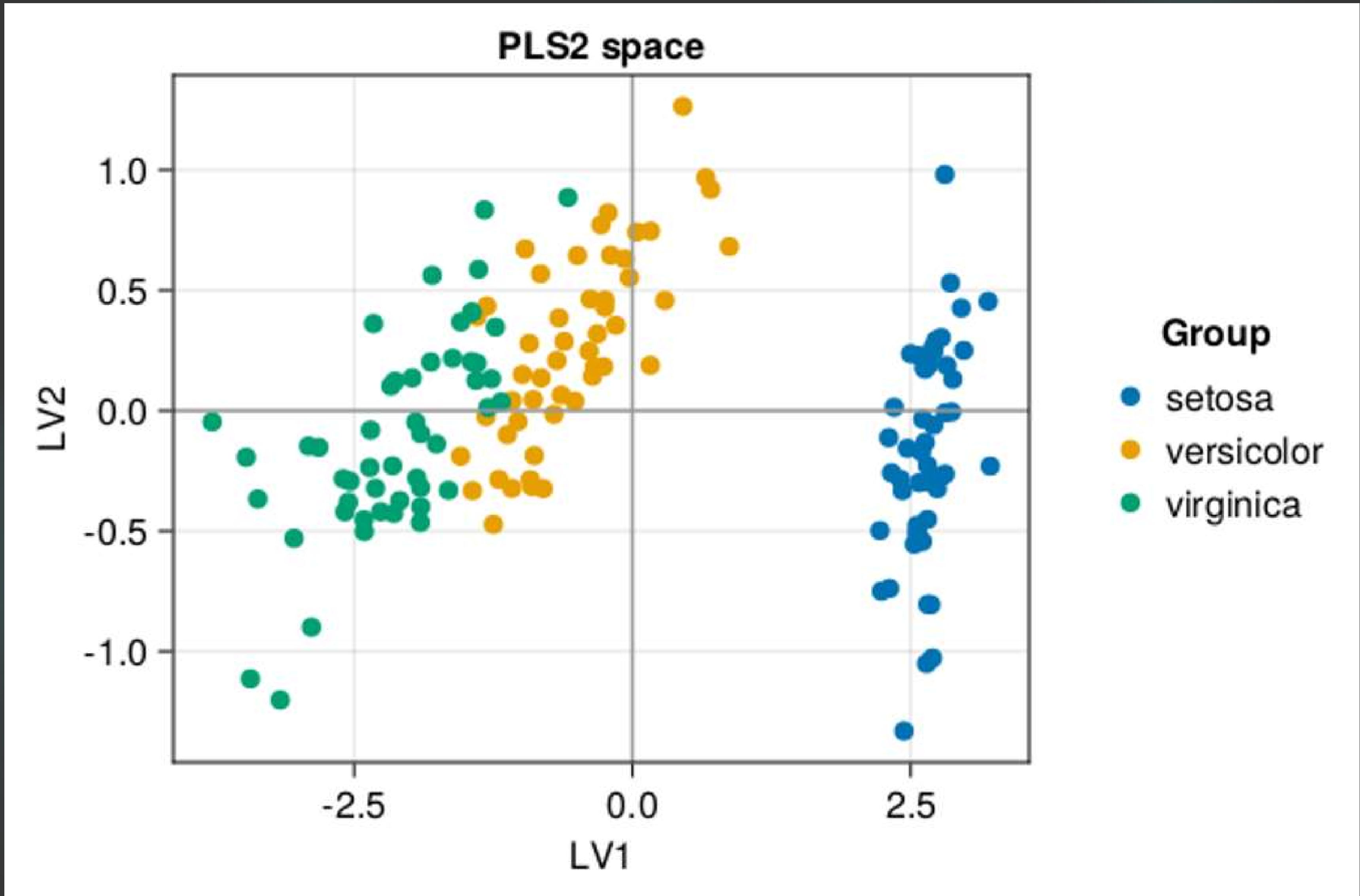
... (150, 4)

***y***: 3 classes

```
"setosa"     => 50
"versicolor" => 50
"virginica"  => 50
```

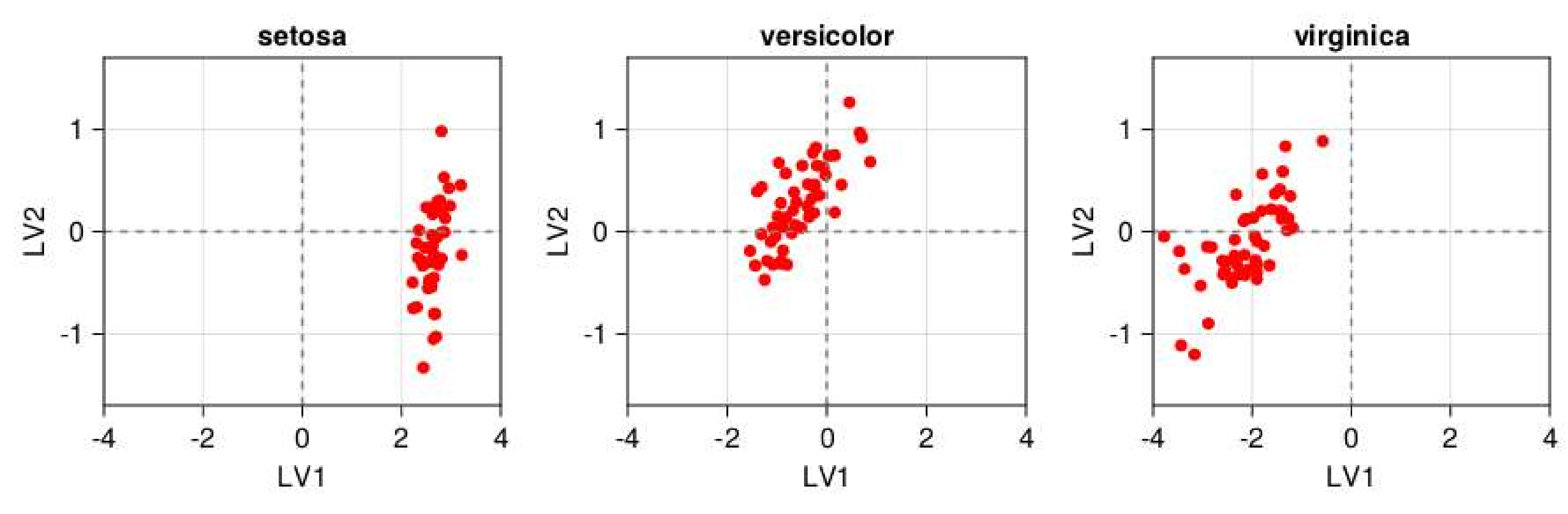
PLS2($\mathbf{X}$, $\mathbf{Y}_{\text{dummy}}$)   nb. LVs = 2

$\Rightarrow$ $\mathbf{T}$ ($n \times 2$)

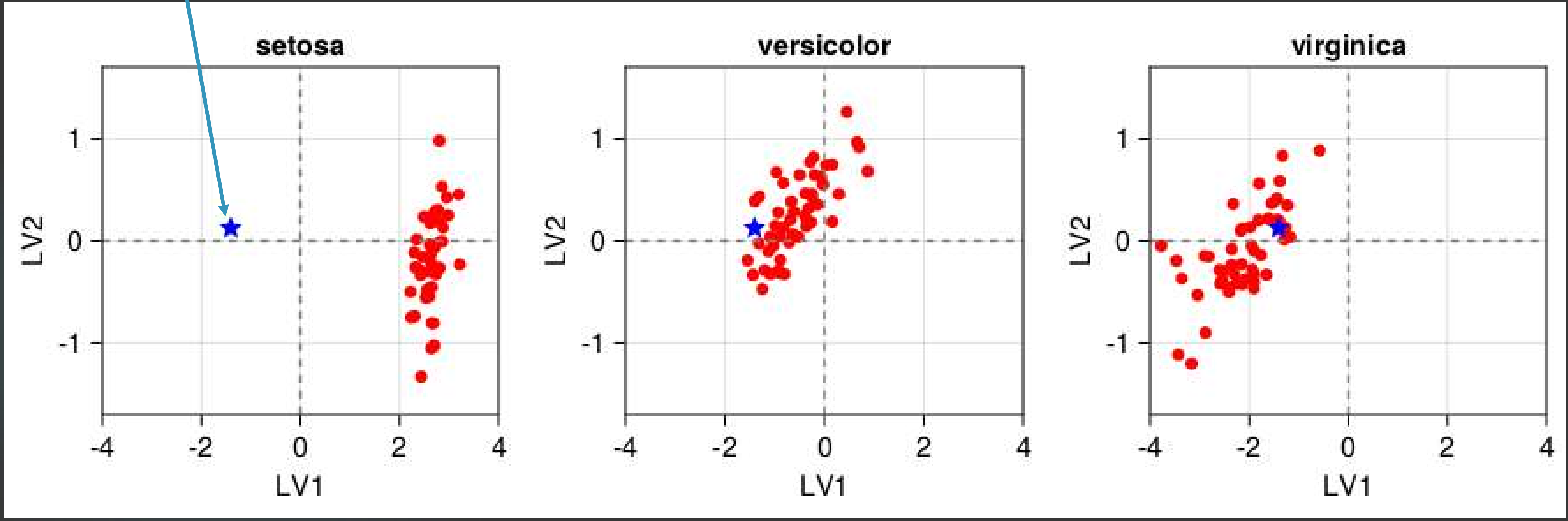

PLS2 space
LV2
1.0
0.5
0.0
-0.5
-1.0
-2.5
0.0
2.5
LV1
Group
setosa
versicolor
virginica

**Probabilistic DA**

⇒ Estimate the multivariate **probability density function (pdf)** of ***T*** in each class

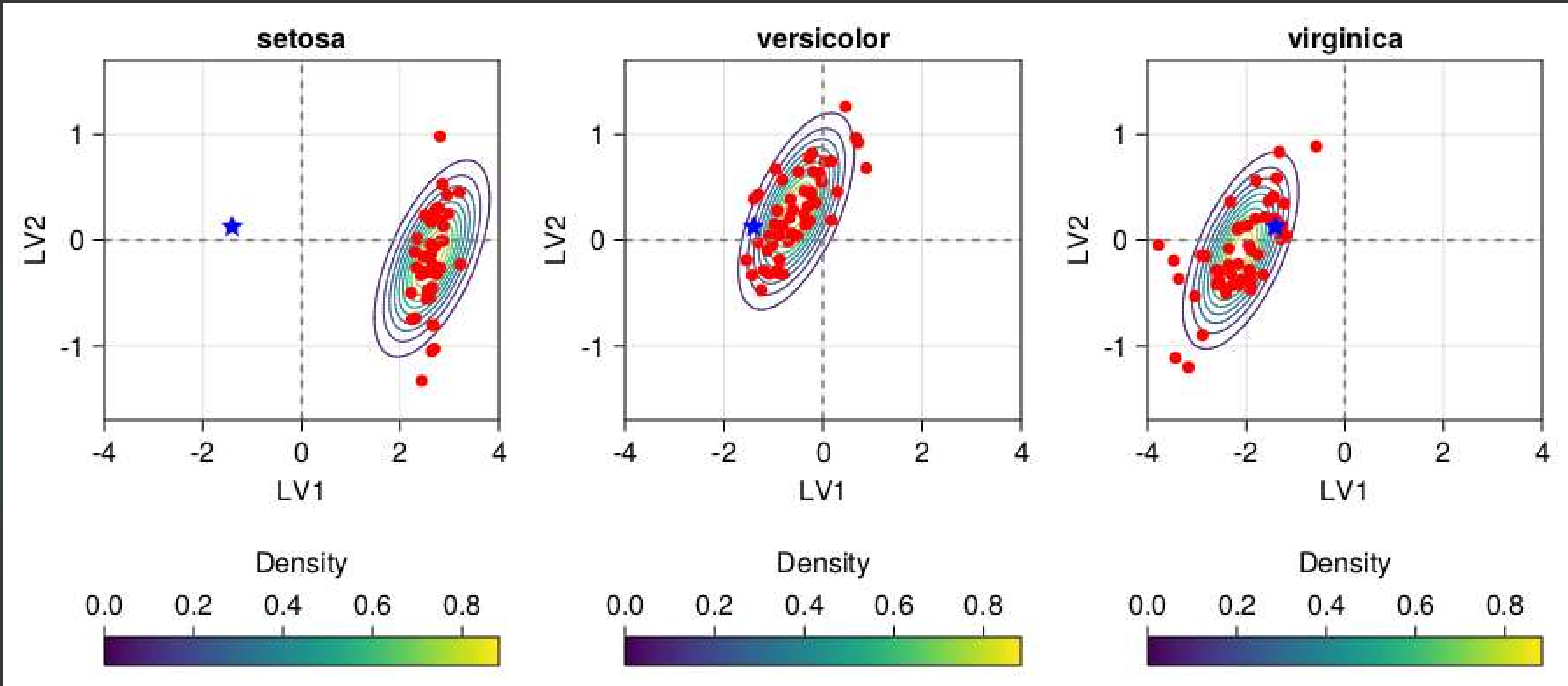


New observation to predict
= which class? ⇔ where is located the new obs. compared to the class pdf



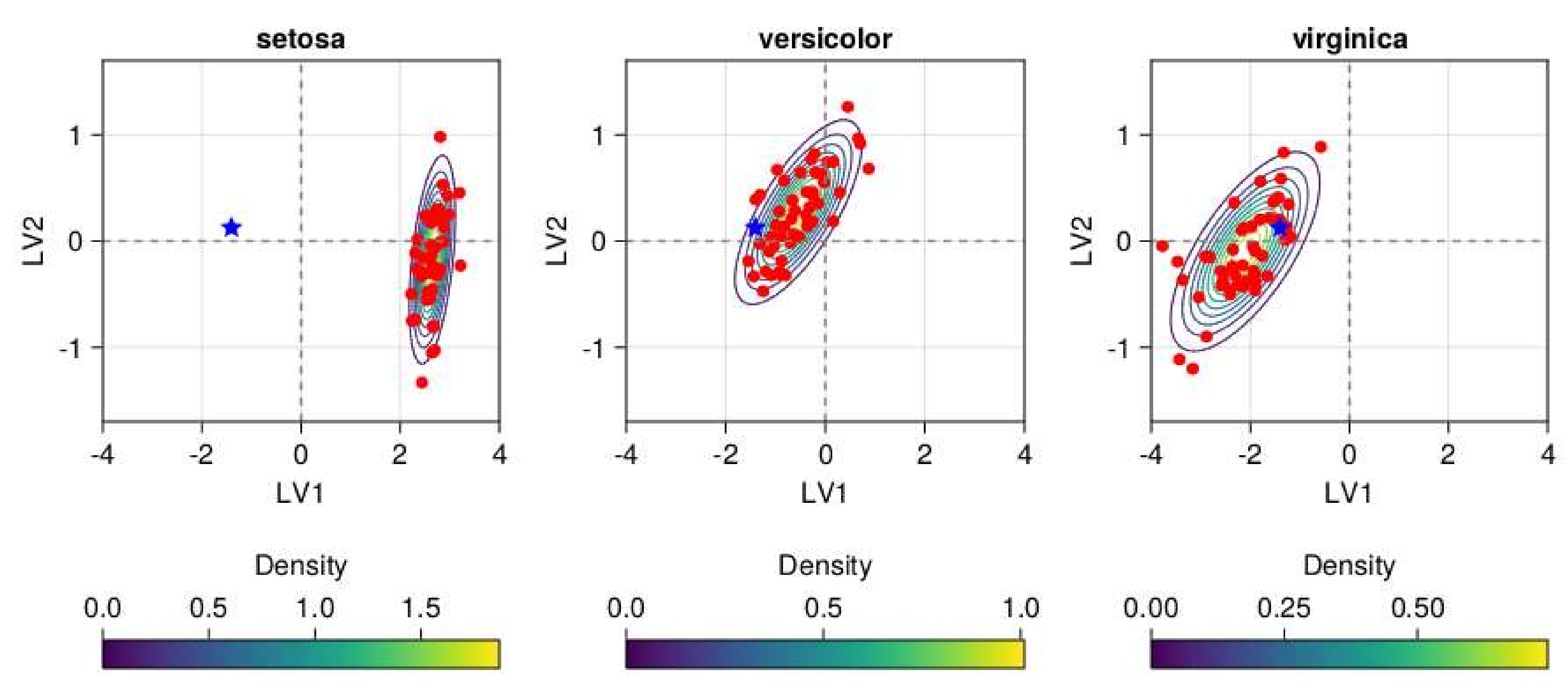
**LDA** **Same covariance matrix** $\Sigma$ estimated for all classes





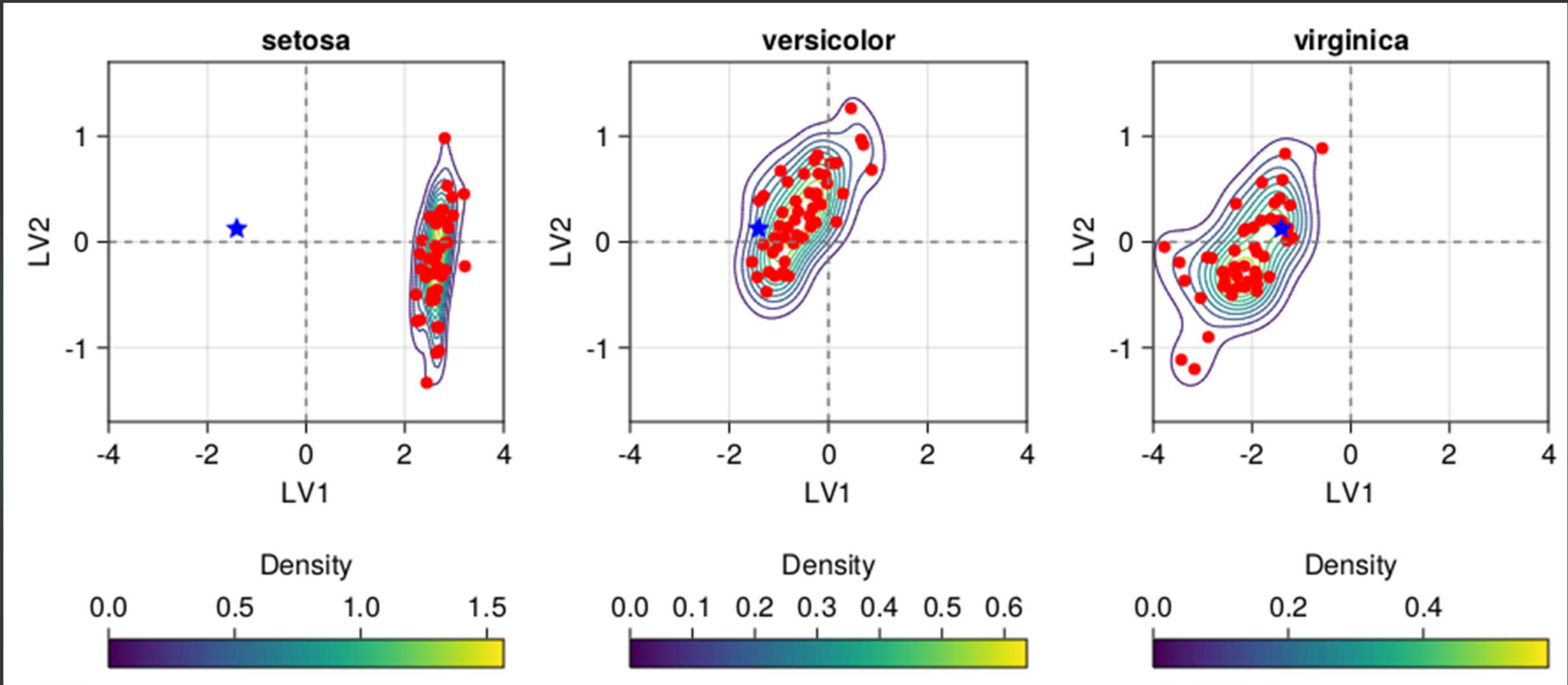
## QDA One covariance matrix $\Sigma_j$ estimated per class





## Multiplicative Gaussian KDE

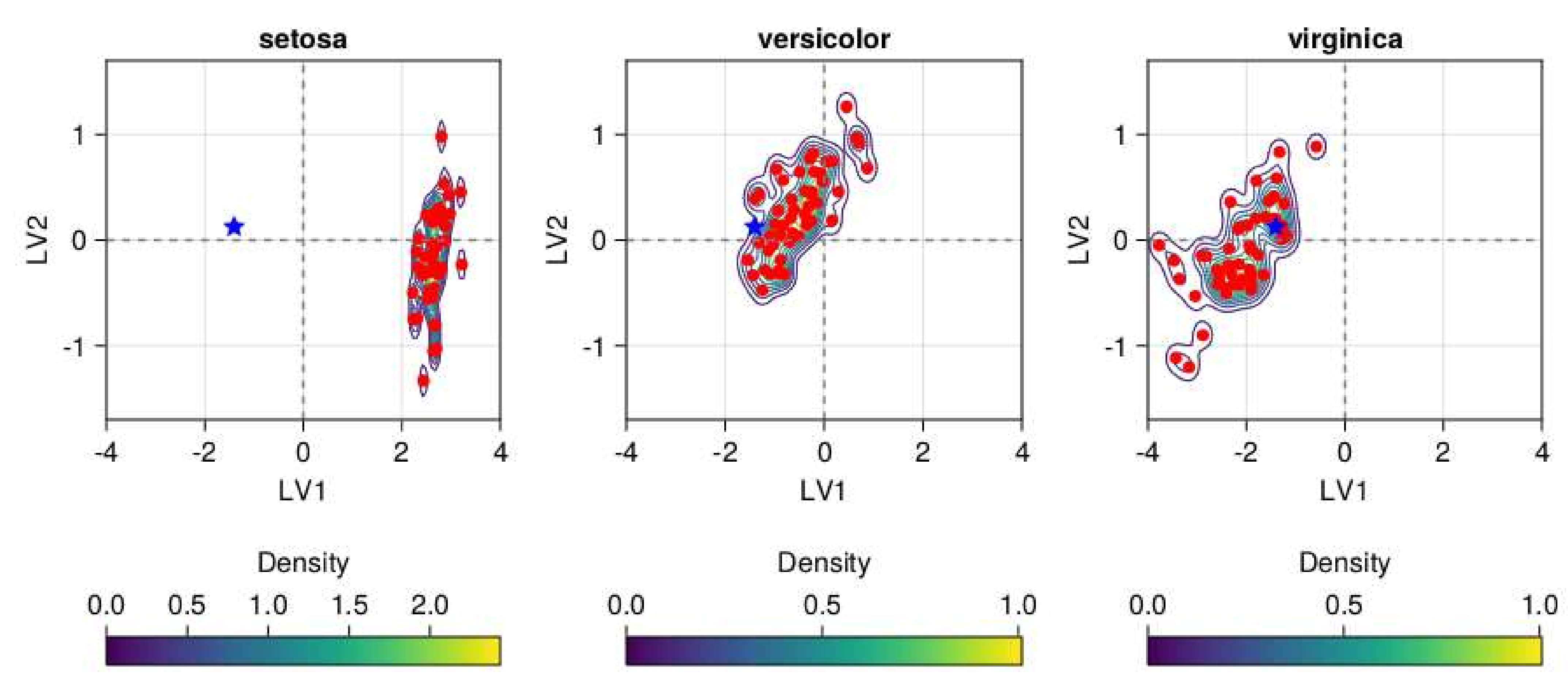
Smoothing level *a* = 1



## Multiplicative Gaussian KDE

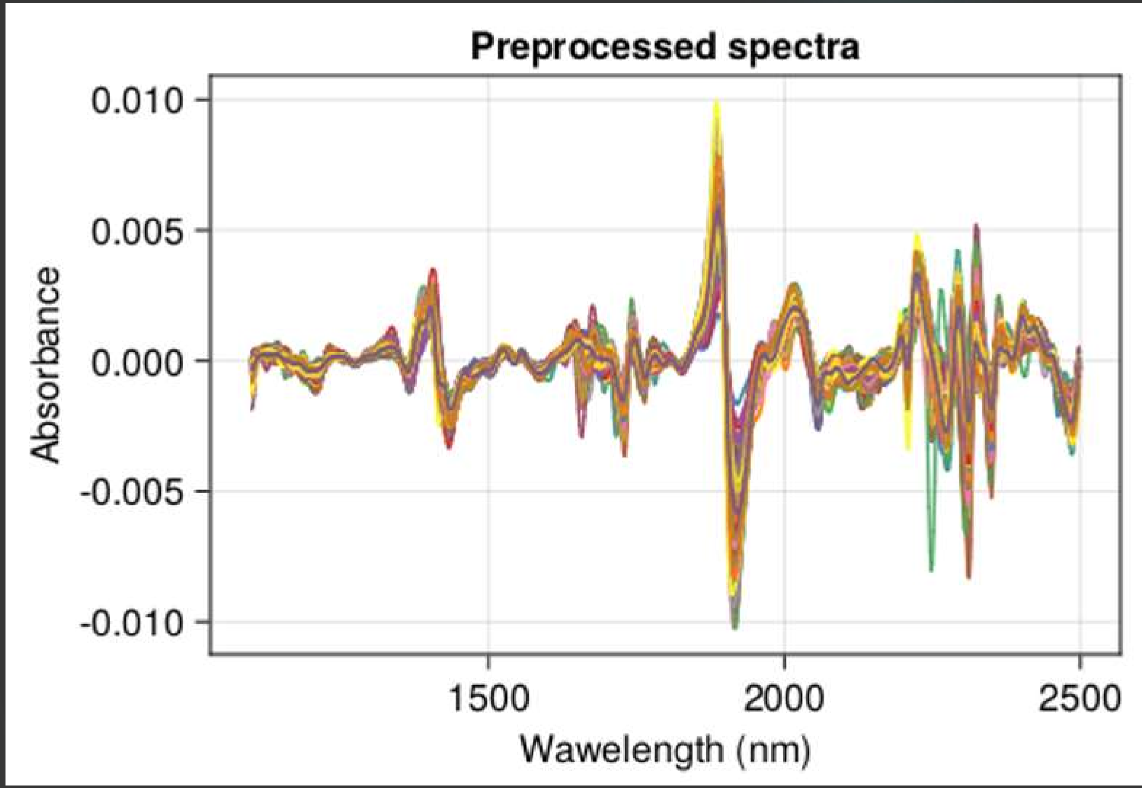
Smoothing level *a* = .5





# **Another illustration**
## NIR Forages

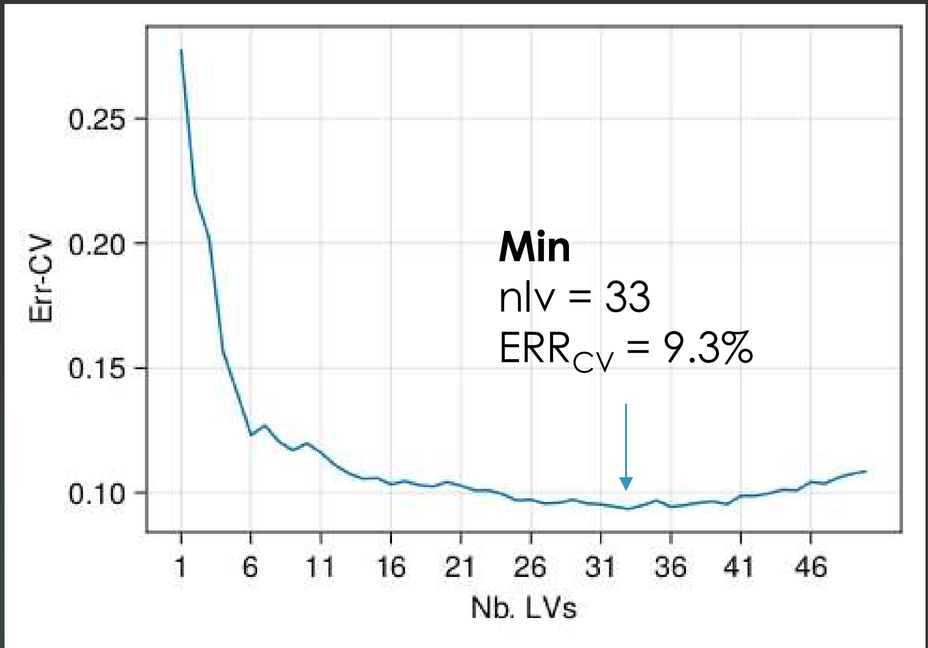
ntot = 485
ntrain = 323 (CV)
ntest = 162




***y***: 3 classes

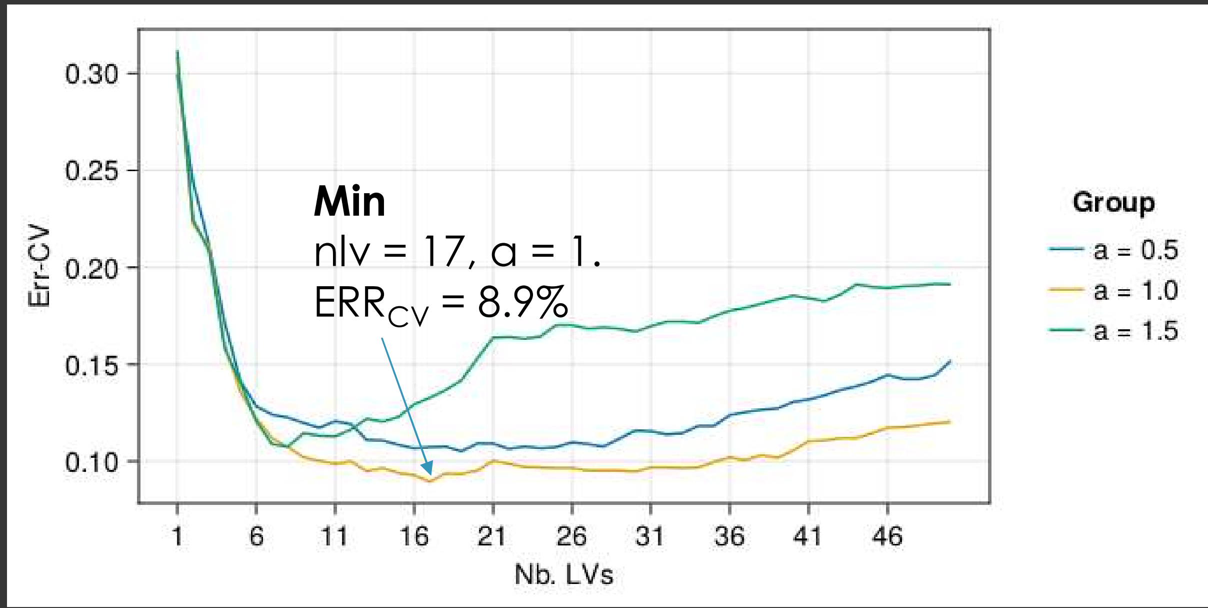
```
"Legume forages"
"Forage trees"
"Cereal and grass forages"
```

## PLS-LDA




ERR$_{Test}$ = 8%

## PLS-KDE-DA




ERR$_{Test}$ = 7%

Often, PLS-KDE-DA has a performance close to those of parametric methods, but it can overperform if some classes have clear internal multimodal distributions (eg. when a class contains several sub-groups that do not span the same sub-spaces of the PLS space)

Function **plskdeda** available in package Jchemo
https://github.com/mlesnoff/Jchemo.jl
https://github.com/mlesnoff/JchemoDemo

```
model = plskdeda(nlv = 15, a = .5)
fit!(model, Xtrain, ytrain)
pred = predict(model, Xtest).test
```