Analyse de Données

Slides 1ère année Sciences du Numérique

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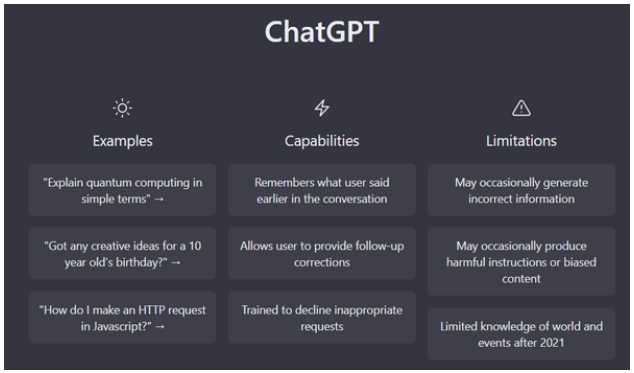
Octobre 2023

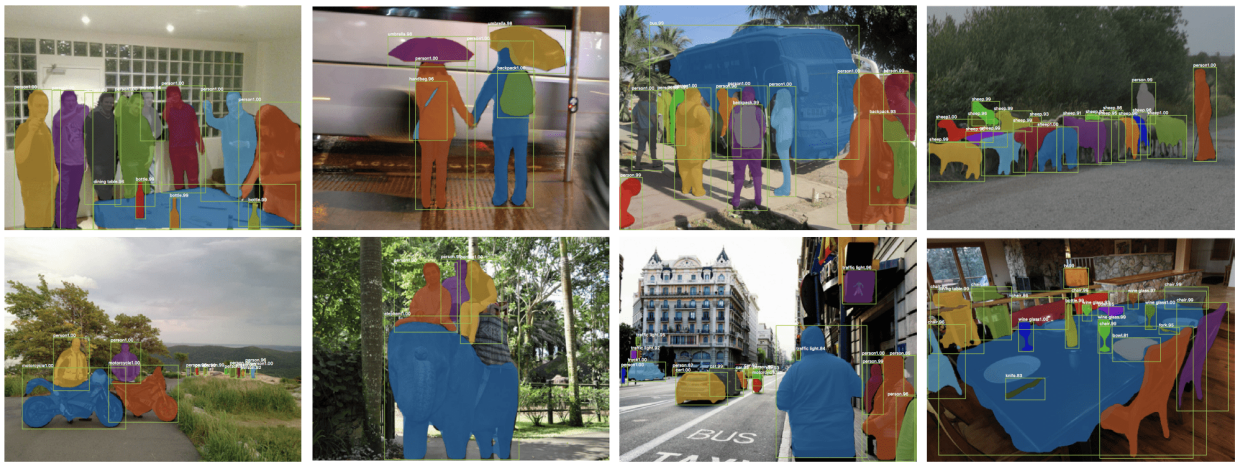
References

- R. O. Duda, P. E. Hart and D. G. Stork, Pattern Classification, 2nd edition, Wiley, 2000.
- S. Theodoridis and K. Koutroumbas, Pattern Recognition, 4th edition, Academic Press, 2008.
- A. Jain, R. Duin and J. Mao, Statistical Pattern Recognition: A Review, IEEE Transactions Pattern Analysis and Machine Intelligence, vol. 22, no. 1, pp. 4-37, Jan. 2000.

Summary

Classification Applications





Machine Learning

Machine Learning is a field of study that gives computers the ability to learn without being explicitly programmed.

Arthur Samuel (1959)

A computer program is said to learn from experience E, with respect to a task T and a performance measure P, if its performance P on task T improves with experience E.

Tom Mitchell (1998)

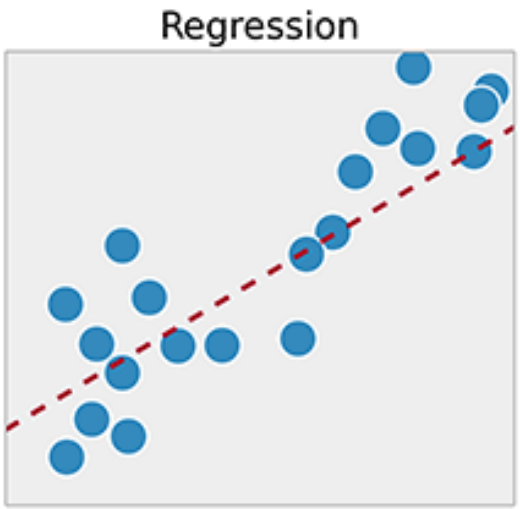
2 main types of learning

Supervised learning

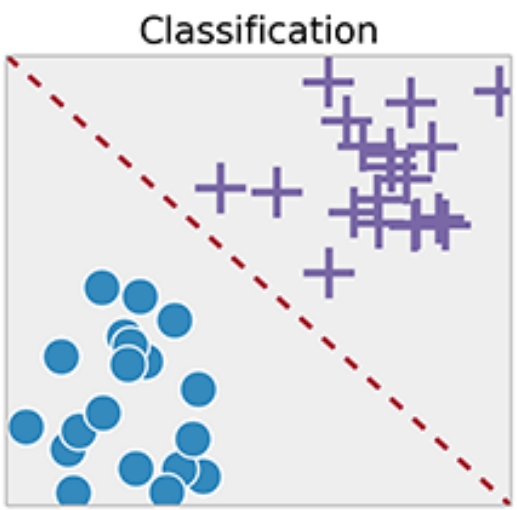
- An oracle (expert) provides a training set (data, labels) :

$$\mathcal{D} = \{(\boldsymbol{x}^{(1)}, y^{(1)}), ..., (\boldsymbol{x}^{(m)}, y^{(m)})\}$$

- A model (predictor) is trained to minimize the difference between ground truth and predicted labels.
- Often costly because it requires large databases to be annotated by humans.



$\boldsymbol{y}$ continuous

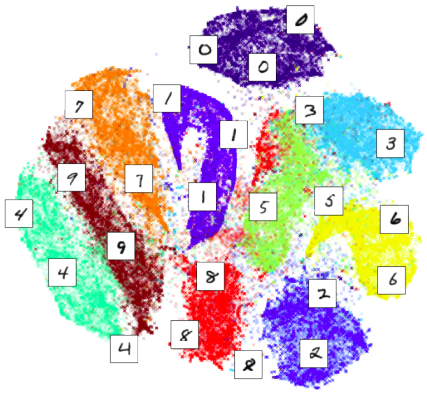


$\boldsymbol{y}$ discrete

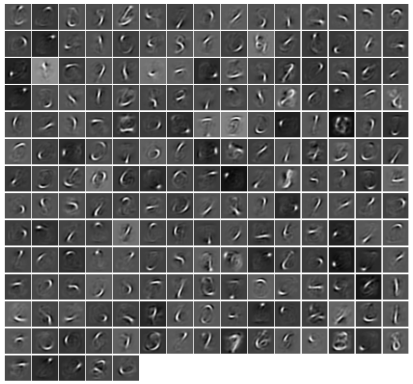
2 types of learning

In **unsupervised learning**, information should be inferred from data only (no labels) :

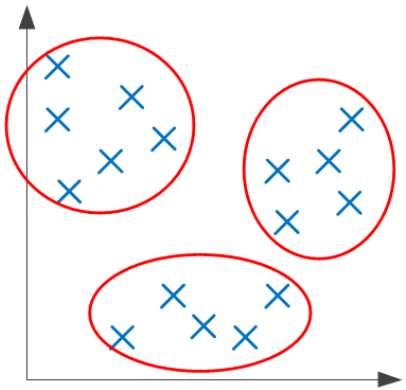
$$\mathcal{D} = \{\boldsymbol{x}^{(1)}, ..., \boldsymbol{x}^{(m)}\}.$$



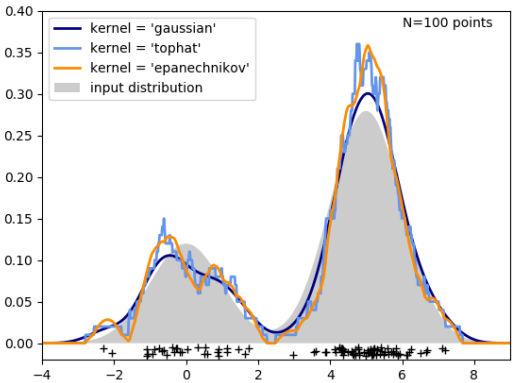
Dimension reduction



Feature extraction



Clustering



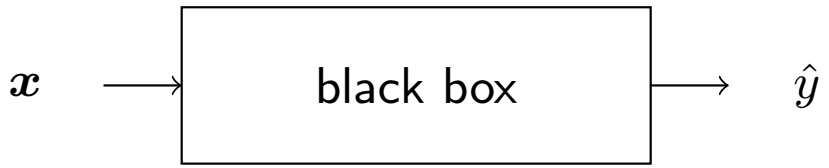
Density estimation

Supervised learning

The **supervised learning** framework assumes we have observations (or data) and labels (or targets) which constitute a training set, that we denote :

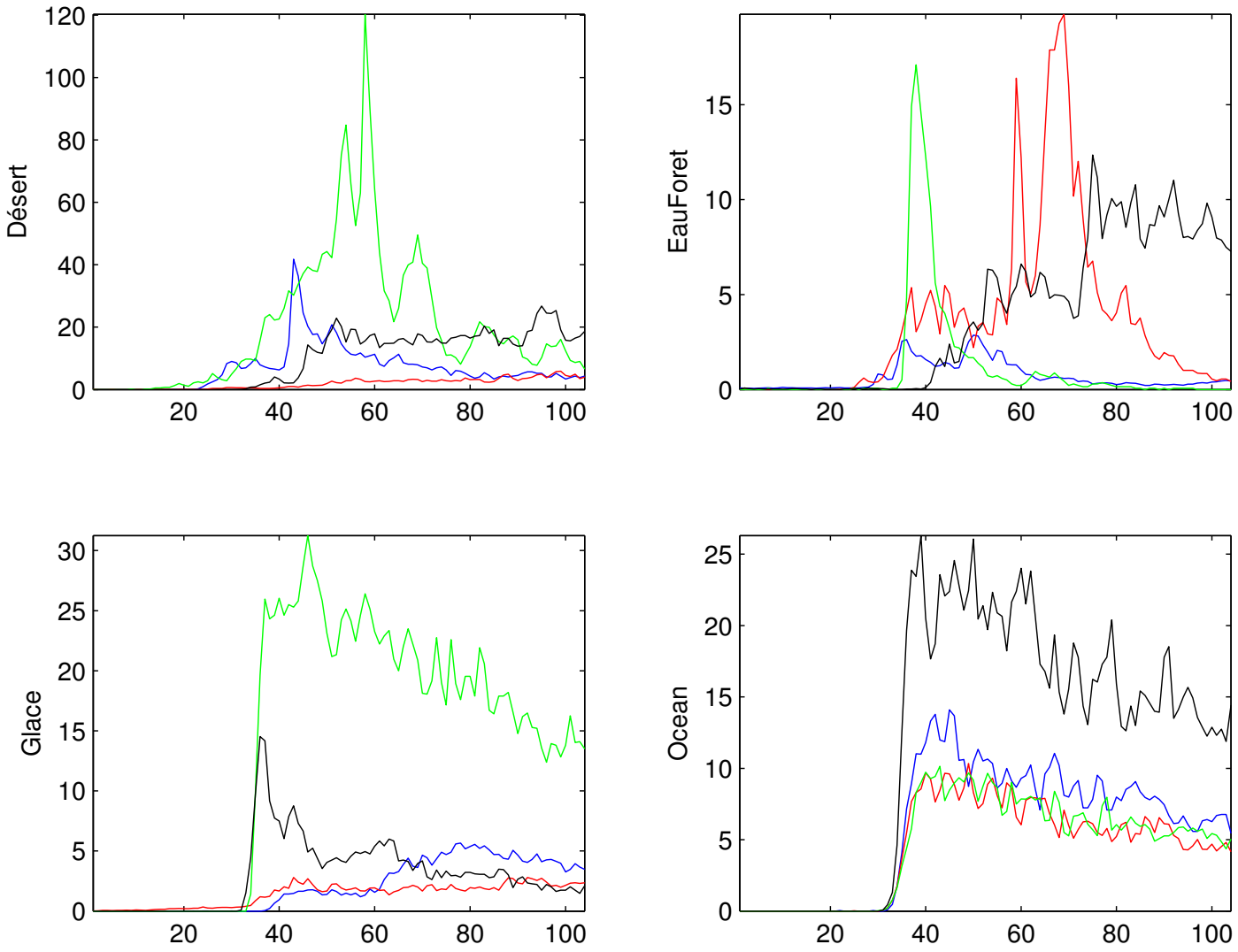
$$\mathcal{D} = \{(\boldsymbol{x}^{(1)}, y^{(1)}), .., (\boldsymbol{x}^{(m)}, y^{(m)})\}.$$

The model is trained to reproduce the correspondences between observations and labels.

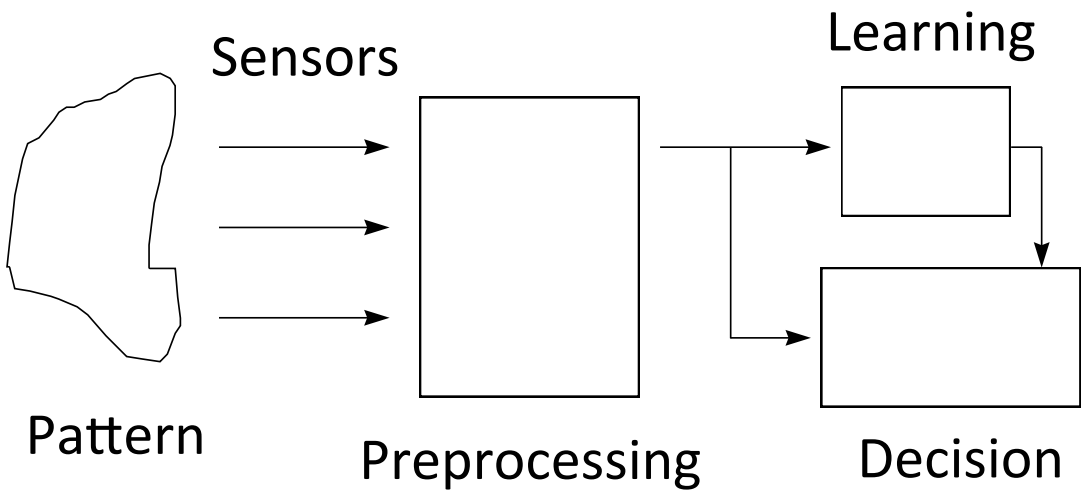


The "black-box" model

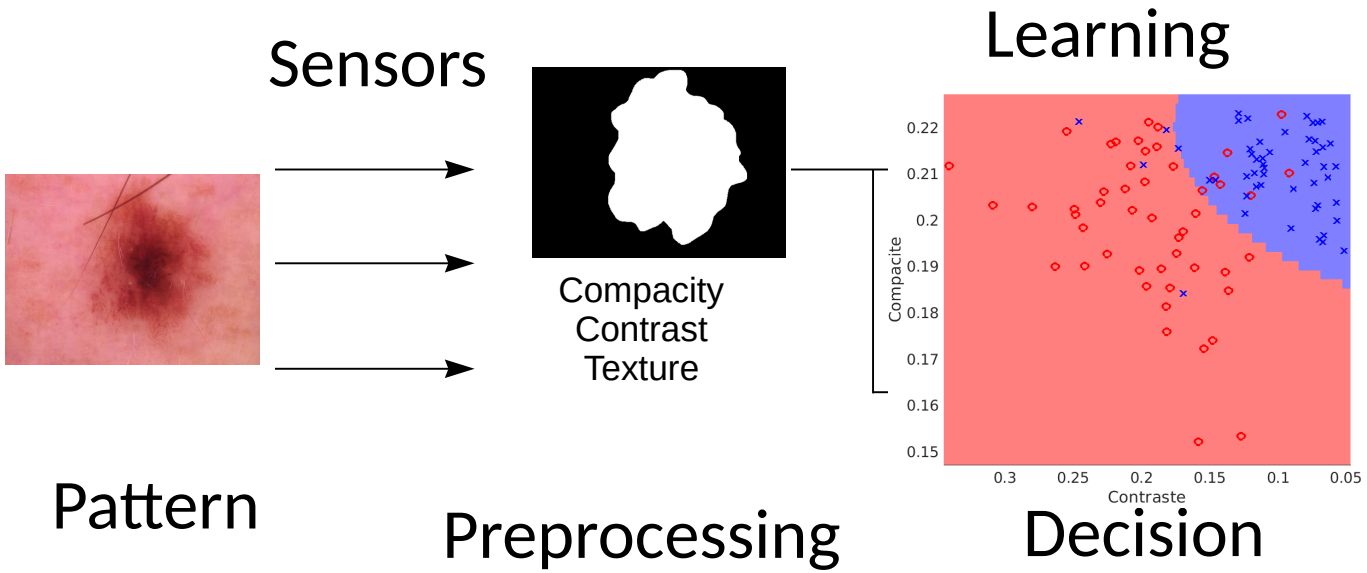
Example : Classification of Altimetric Signals



Classification pipeline

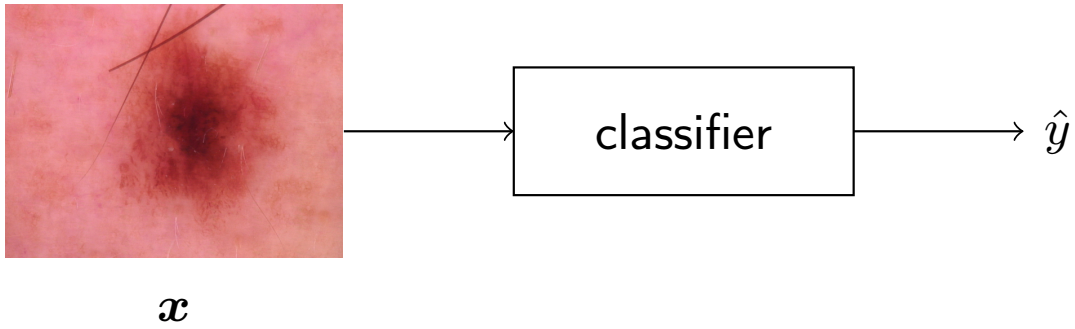


Classification pipeline: lab example



Summary

Evaluating classifiers



In this example, y and $\hat{y} \in \{\text{benign}, \text{malignant}\}$
y is called the ground truth associated with $\boldsymbol{x}$, while $\hat{y}$ is the classifier prediction.

How to assess the quality of a classifier?
What makes a good classifier?

Accuracy

Accuracy: The accuracy measures the overall correctness of the classifier.

$$Accuracy = \frac{\text{Number of Correctly Classified Instances}}{\text{Total Number of Instances}}$$

Example:
Let's consider a binary classification task with 100 instances. The classifier correctly classifies 85 instances. The accuracy is:

$$Accuracy = \frac{85}{100} = 0.85 \quad \text{(or 85\%)}$$

Confusion Matrix

The confusion matrix provides a detailed view of a classifier's performance.

Example:
Consider a binary classification task with 100 instances. The confusion matrix for a classifier is as follows:

	Predicted Negative	Predicted Positive
Actual Negative	60	10
Actual Positive	5	25

The confusion matrix reveals:

- 60 True Negatives and 25 True Positives
- False Positives (in statistics, false alarms): 10
- False Negatives (in statistics, non detections): 5

In our lab example, this means the classifier tends to raise false alarms (i.e. to predict cancer) more often than to miss actual cancers.

Precision, Recall, and F1-score

Precision, recall, and F1-score evaluate the performance of a classifier in terms of positive predictions.
Precision quantifies the proportion of correctly predicted positive instances out of all instances predicted as positive.

$$Precision = \frac{\text{True Positives}}{\text{True Positives} + \text{False Positives}}$$

Recall calculates the ratio of correctly predicted positive instances to the actual number of positive instances.

$$Recall = \frac{\text{True Positives}}{\text{True Positives} + \text{False Negatives}}$$

F1-score combines precision and recall into a single metric by calculating their harmonic mean.

$$F1\text{-}score = 2 \times \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

Precision, Recall, and F1-score

Example:
Consider a binary classification task with 100 instances. The confusion matrix for a classifier is as follows:

	Predicted Negative	Predicted Positive
Actual Negative	60	10
Actual Positive	5	25

$$Precision = \frac{25}{25+10} \approx 0.71$$

$$Recall = \frac{25}{25+5} \approx 0.83$$

$$F1\text{-}score = 2 \times \frac{0.71 \times 0.83}{0.71+0.83} = 0.76$$

Summary

Empirical risk and Expected risk

Empirical risk: average prediction error on the training set.

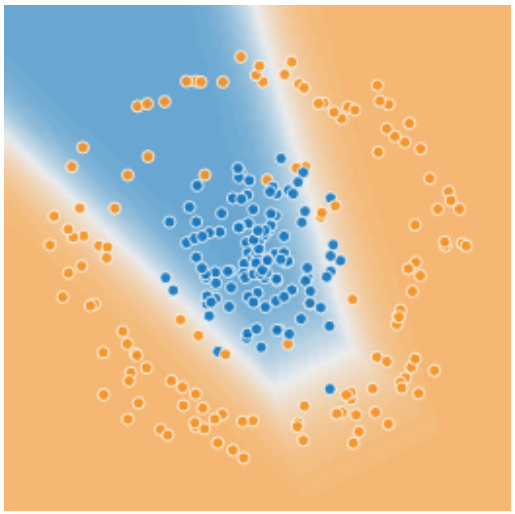
Expected risk (or generalization risk) : average prediction error on the target population... **Unknown** !

The training objective of any machine learning algorithm is to minimize the **Empirical Risk**, but in fact what we are really interested in is to minimize the **Expected Risk**.

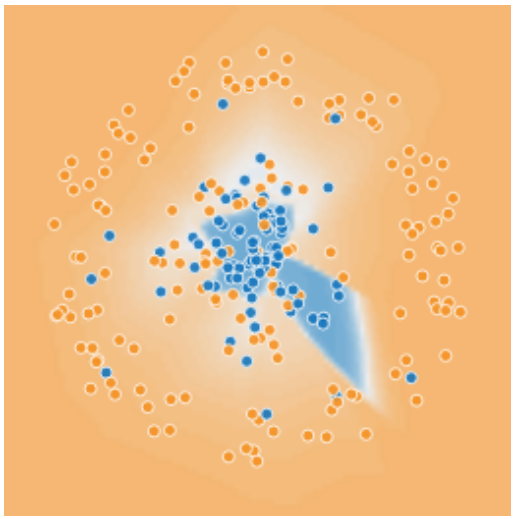
Under/Overfitting

We speak of **underfitting** when the learned model explains the training set too poorly. *Empirical risk is high.*

We speak of **overfitting** when the learned model explains the training set too well; this model then badly generalizes to the target population. *Empirical risk is low, but expected risk is high!*

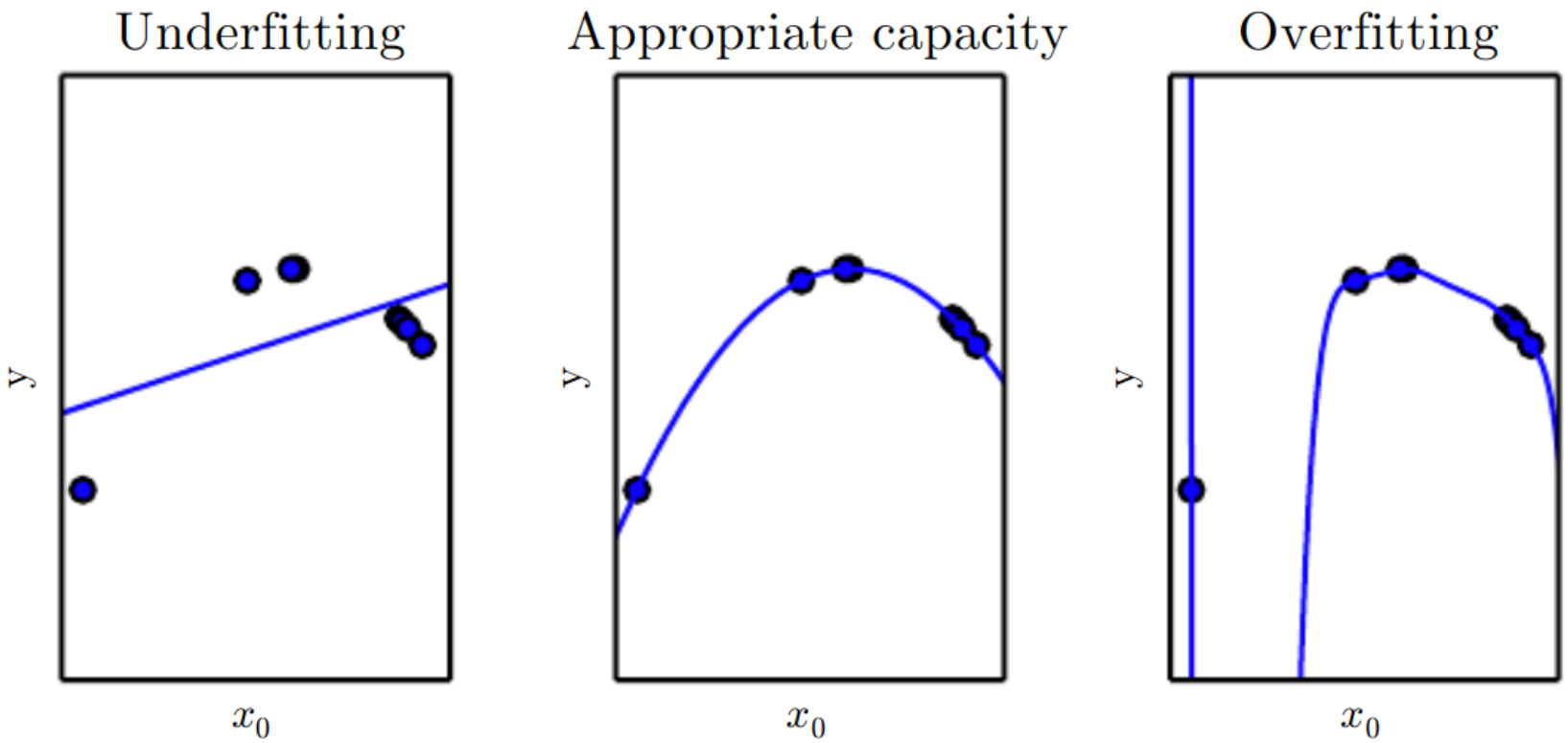


Underfitting



Overfitting

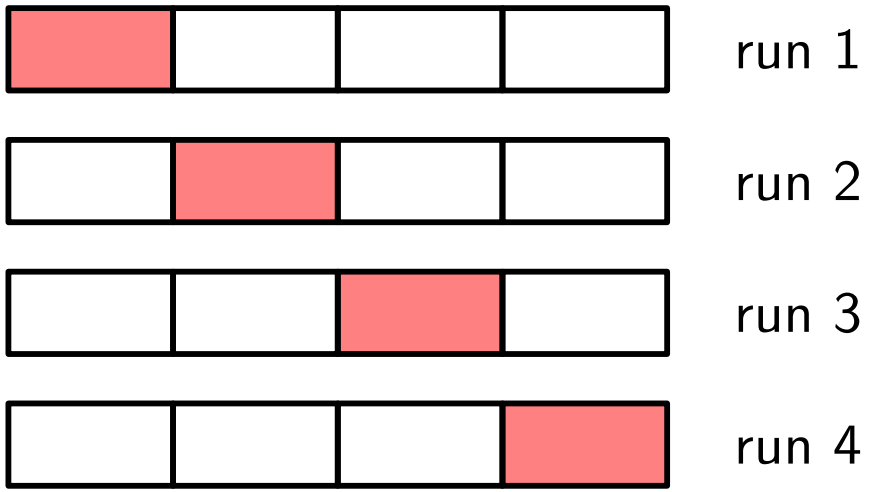
Under/Overfitting : model **capacity**



Models with low capacity compared to the task complexity will tend to underfit, while models with large capacity will tend to overfit.

Image from [Goodfellow et al. 2015] Deep Learning

Detecting Under/Overfitting



Cross Validation is a way to jointly evaluate empirical risk and expected risk when the size of the dataset is limited.

In the case we have a sufficient number of data samples, we can split the dataset into two parts for learning and testing.

Summary

Classification

Notations

- K classes $\omega_1, ..., \omega_K$
- $\boldsymbol{x} = [x(1), ..., x(p)]^T$ measurements $\in X = \mathbb{R}^p$
- A: set of possible actions $a_1, ..., a_q$ where $a_k =$ "assign the vector $\boldsymbol{x}$ to the class ω_k", $\forall k = 1, ..., K$

Definition

$$d : \begin{array}{l} X \to A \\ \boldsymbol{x} \mapsto d(\boldsymbol{x}) \end{array}$$

Remark

Classification with reject option: $A = \{a_0, a_1, ..., a_K\}$ where $a_0 =$ "do not classify the vector $\boldsymbol{x}$"

Bayesian Rule

Hypothesis: Probabilistic Model

- *A priori* probability of class ω_k

$$P(\omega_k)$$

- Probability density function of the observation vector $\boldsymbol{x}$ conditionally to class ω_k

$$f(\boldsymbol{x}|\omega_k)$$

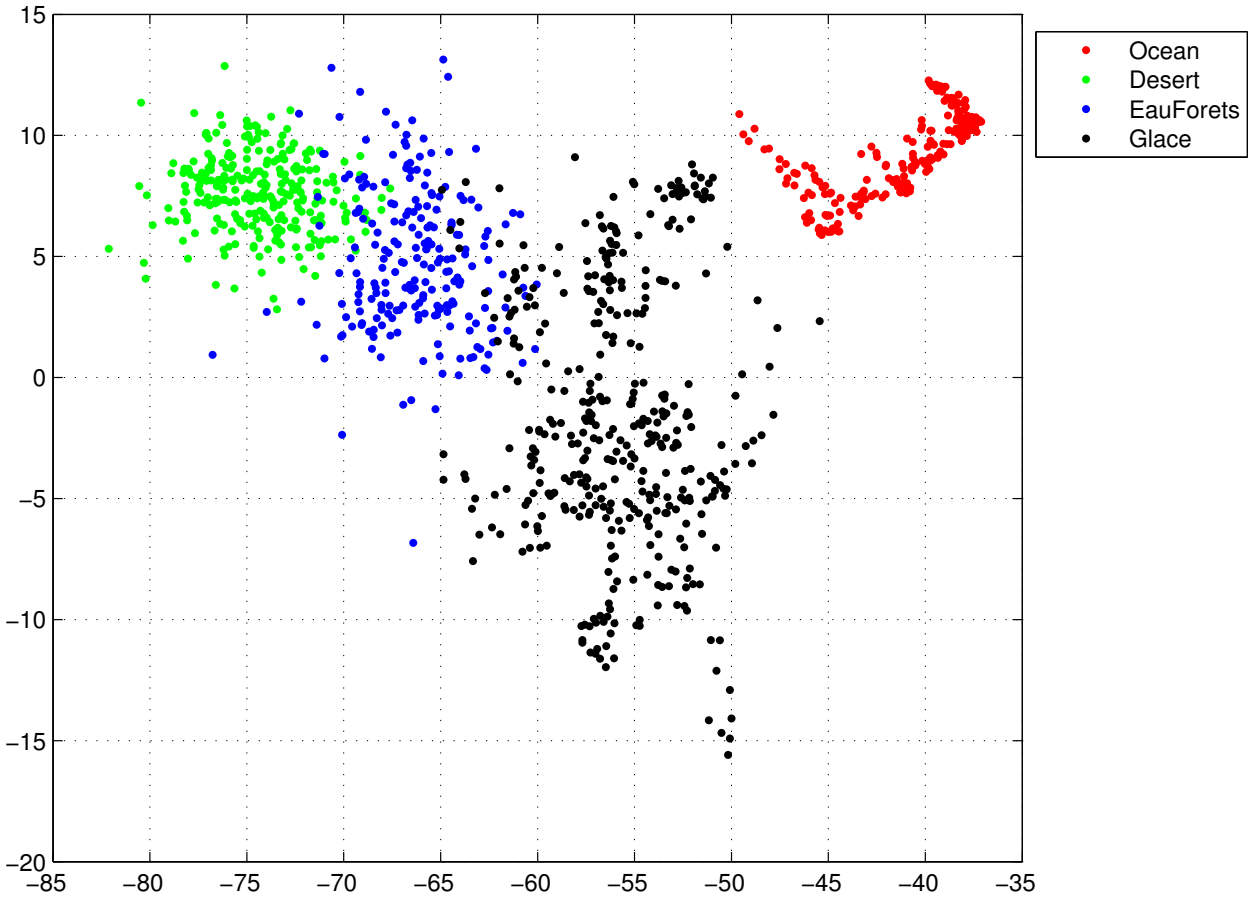
Conclusion

- *A posteriori* probability that $\boldsymbol{x}$ belongs to class ω_k

$$P(\omega_k|\boldsymbol{x}) = \frac{f(\boldsymbol{x}|\omega_k)\,P(\omega_k)}{f(\boldsymbol{x})}$$

with $f(\boldsymbol{x}) = \sum_{k=1}^{K} f(\boldsymbol{x}|\omega_k)\,P(\omega_k)$.

Example


15
10
5
0
−5
−10
−15
−20
−85
−80
−75
−70
−65
−60
−55
−50
−45
−40
−35
Ocean
Desert
EauForets
Glace

MAP Classifier

Definition

$$d^*(\boldsymbol{x}) = a_j \Leftrightarrow P(\omega_j | \boldsymbol{x}) \geq P(\omega_k | \boldsymbol{x}), \forall k \in \{1, ..., K\}$$

Equiprobable Classes: Maximum Likelihood Classifier

$$d^*(\boldsymbol{x}) = a_j \Leftrightarrow f(\boldsymbol{x} | \omega_j) \geq f(\boldsymbol{x} | \omega_k), \forall k \in \{1, ..., K\}$$

Property

The MAP classifier minimizes the probability of error

Proof (2 classes)

$$\begin{aligned} P_e &= P\left[d\left(\boldsymbol{x}\right) = a_1 \cap \boldsymbol{x} \in \omega_2\right] + P\left[d\left(\boldsymbol{x}\right) = a_2 \cap \boldsymbol{x} \in \omega_1\right] \\ &= P\left[d\left(\boldsymbol{x}\right) = a_1 \mid \boldsymbol{x} \in \omega_2\right] P\left(\omega_2\right) + P\left[d\left(\boldsymbol{x}\right) = a_2 \mid \boldsymbol{x} \in \omega_1\right] P\left(\omega_1\right) \end{aligned}$$

Let $R_i = \{\boldsymbol{x} \in \mathbb{R}^p / d(\boldsymbol{x}) = a_i\}$ be the acceptance region for class ω_i

$$\begin{aligned} P_e &= \int_{R_1} P\left(\omega_2\right) f\left(\boldsymbol{x} \,|\omega_2\,\right) d\boldsymbol{x} + \int_{R_2} P\left(\omega_1\right) f\left(\boldsymbol{x} \,|\omega_1\,\right) d\boldsymbol{x} \\ &= P\left(\omega_2\right)\left[1 - \int_{R_2} f\left(\boldsymbol{x} \,|\omega_2\,\right) d\boldsymbol{x}\right] + \int_{R_2} P\left(\omega_1\right) f\left(\boldsymbol{x} \,|\omega_1\,\right) d\boldsymbol{x} \\ &= P\left(\omega_2\right) + \int_{R_2} \left[P\left(\omega_1\right) f\left(\boldsymbol{x} \,|\omega_1\,\right) - P\left(\omega_2\right) f\left(\boldsymbol{x} \,|\omega_2\,\right)\right] d\boldsymbol{x} \\ &= P\left(\omega_2\right) - \int_{R_2} \left[P\left(\omega_2 \,|\boldsymbol{x}\,\right) - P\left(\omega_1 \,|\boldsymbol{x}\,\right)\right] f\left(\boldsymbol{x}\right) d\boldsymbol{x} \end{aligned}$$

P_e is minimum when $R_2 = \{\boldsymbol{x} / P\left(\omega_2 \,|\boldsymbol{x}\,\right) > P\left(\omega_1 \,|\boldsymbol{x}\,\right)\}$

Probability of Error (K classes)

Definition

$$P_e = \sum_{k=1}^{K} P\left[d\left(\boldsymbol{x}\right) = a_k \cap \boldsymbol{x} \notin \omega_k\right]$$

Property (admitted)

The MAP classifier minimizes the probability of error

Gaussian Case

Densities

$$f\left(\boldsymbol{x}\left|\omega_k\right.\right) = \frac{1}{(2\pi)^{p/2}\sqrt{\det \Sigma_k}} \exp\left[-\frac{1}{2}\left(\boldsymbol{x}-\boldsymbol{m}_k\right)^T \boldsymbol{\Sigma}_k^{-1}\left(\boldsymbol{x}-\boldsymbol{m}_k\right)\right]$$

General Case

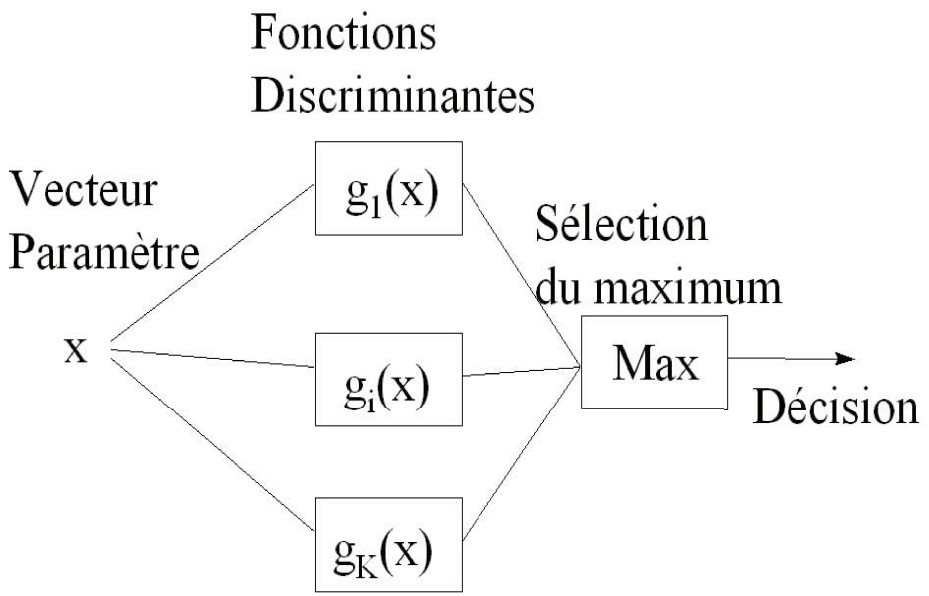
$$d^*\left(\boldsymbol{x}\right) = a_i \Leftrightarrow g_i\left(\boldsymbol{x}\right) \geq g_k\left(\boldsymbol{x}\right) \qquad \forall k = 1, ..., K$$

with

$$g_i\left(\boldsymbol{x}\right) = -\left(\boldsymbol{x}-\boldsymbol{m}_i\right)^T \boldsymbol{\Sigma}_i^{-1}\left(\boldsymbol{x}-\boldsymbol{m}_i\right) - \ln\det \boldsymbol{\Sigma}_i + 2\ln P\left(\omega_i\right)$$

Gaussian Case

Classifier



Discriminant functions

Quadratic term + linear term + constant

Identical covariance matrices ($\Sigma_i = \Sigma$)

Equiprobable classes - Centroid Distance Rule

$$d^*(\boldsymbol{x}) = a_i \Leftrightarrow d_M(\boldsymbol{x}, \boldsymbol{m}_i) \leq d_M(\boldsymbol{x}, \boldsymbol{m}_k) \qquad \forall k = 1, ..., K$$

where d_M is the Mahalanobis distance

$$d_M(\boldsymbol{x}, \boldsymbol{m}_k) = \sqrt{(\boldsymbol{x} - \boldsymbol{m}_k)^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{m}_k)}$$

Non equiprobable classes: affine discriminant functions

$$d^*(\boldsymbol{x}) = a_i \Leftrightarrow \left[\boldsymbol{x} - \frac{1}{2}(\boldsymbol{m}_i + \boldsymbol{m}_k)\right]^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{m}_i - \boldsymbol{m}_k) \geq \ln \frac{P(\omega_k)}{P(\omega_i)}, \ \forall k$$

Exemple

- Exemple 1

  En communications numériques, on veut transmettre un symbole x binaire défini par :

  $$\text{Classe } 1 : x = 0$$
  $$\text{Classe } 2 : x = 1$$

  Le symbole émis x passe par un canal de transmission, où il est perturbé par un bruit n supposé Gaussien centré de variance σ^2. Le signal reçu est alors $z = x + n$. Le problème est de retrouver le symbole émis à partir du signal reçu.
  1) Énoncez la règle de décision Bayésienne lorsque les deux valeurs 0 et 1 ont la même probabilité d'apparition.
  2) Calculer la probabilité d'erreur correspondante que l'on exprimera à l'aide de la fonction de répartition de la loi normale $\mathcal{N}(0, 1)$ définie par

  $$F(x) = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{u^2}{2}\right) du.$$

  Montrer que cette probabilité d'erreur tend vers 0 lorsque σ tend vers 0 et commenter.
  3) Comment la règle de décision Bayésienne est modifiée si les deux valeurs $x = 0$ et $x = 1$ ont des probabilités d'apparition notées P_0 et P_1 ? Interpréter ce résultat lorsque $P_0 > P_1$.
  4) On envoie N fois le même symbole x et on reçoit $z_i = x + n_i$. En supposant que les variables aléatoires $n_1, ..., n_N$ sont indépendantes, quelle est la règle de décision Bayésienne dans le cas de deux symboles équiprobables ?

- Exemple 2

  Généralisation à 4 symboles $\boldsymbol{x} \in \{(0, 0), (0, 1), (1, 0), (1, 1)\}$

Summary

Parametric methods

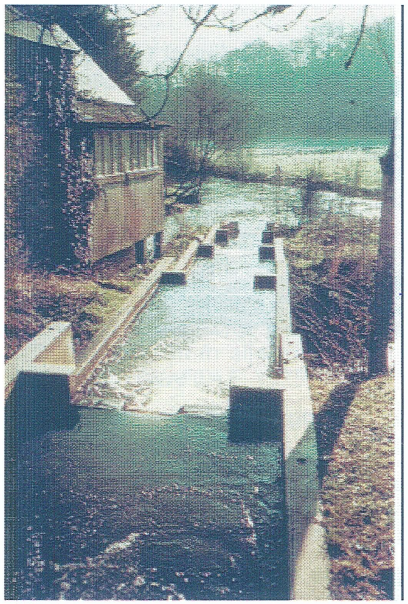
Principle

Assume that the distribution of $\boldsymbol{x} = (x_1, ..., x_n)^T$ is characterized by a parametric probability density function, which depends on an unknown parameter vector $\theta \in \mathbb{R}^p$ and estimate this parameter vector using a method considered in statistics

- Maximum likelihood method
- Method of moments
- MMSE or MAP estimators

Contexte de l'étude

Les passes à poissons

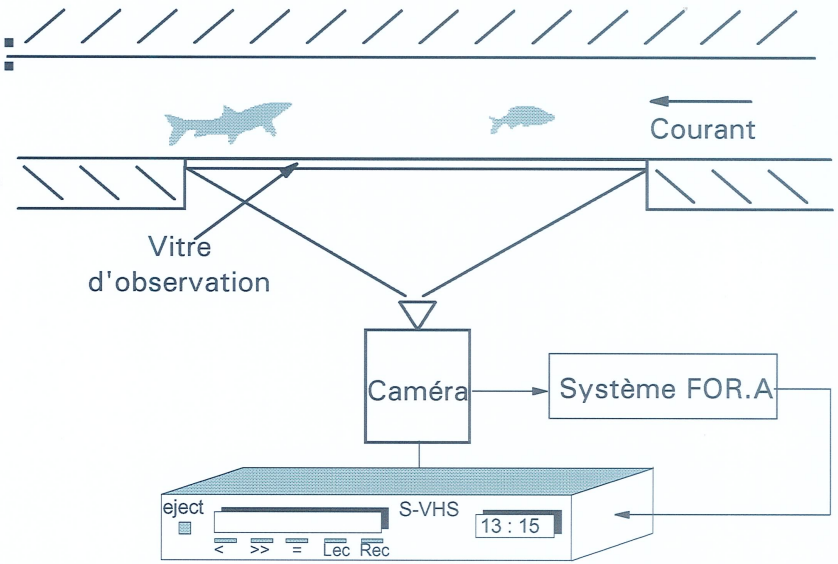

à bassins successifs


à ralentisseurs


ascenseur

Suivi des passes à poissons

- Dispositif vidéo actuel de comptage par espèces :

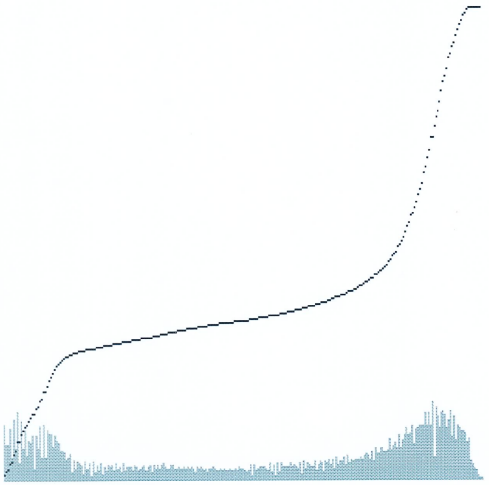


- Dépouillement des bandes vidéo enregistrées par un opérateur humain

Acquisition des images

Nouvelles conditions d'acquisition

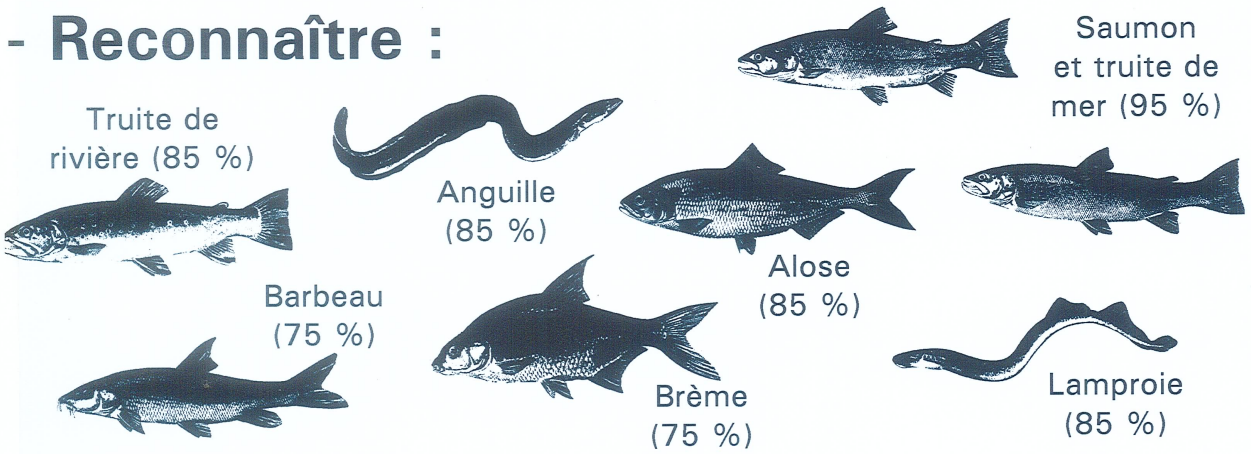
Image



Histogramme : bimodal

Cahier des charges du système de vision automatique

- Compter les poissons, toutes espèces confondues, au delà d'une certaine taille
- Reconnaître :



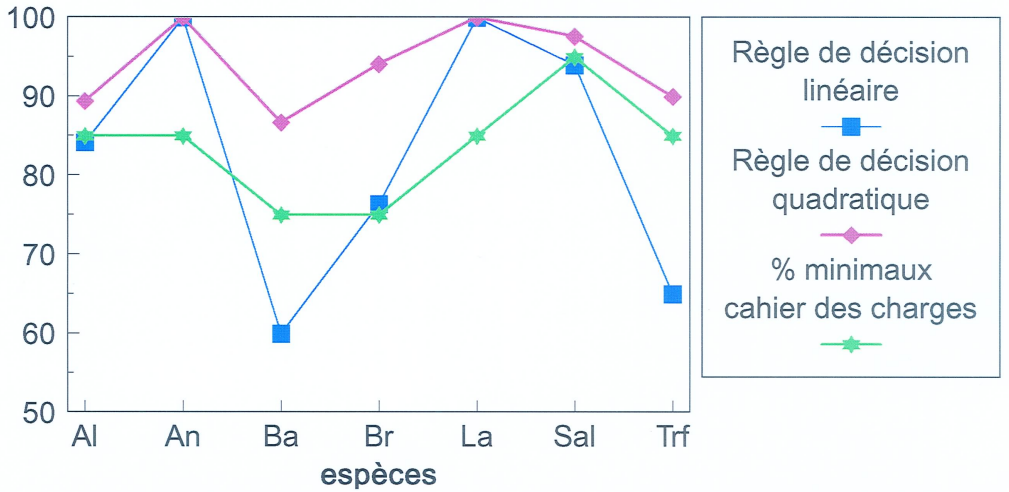
- Fournir : La comptabilisation des différentes espèces
  Les dates et heures de passage

Mesure d'efficacité de la règle de classement

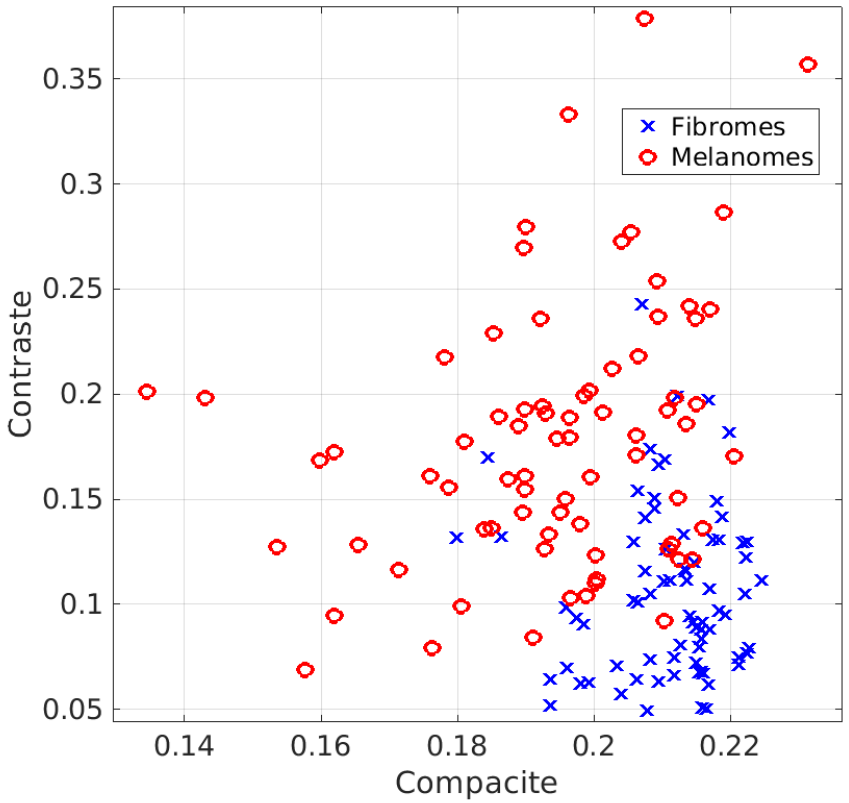
Résultats obtenus sur la BDT

% de reconnaissance dynamiques sur la base de données test

(comparaison des règles de décision quadratique et linéaire)

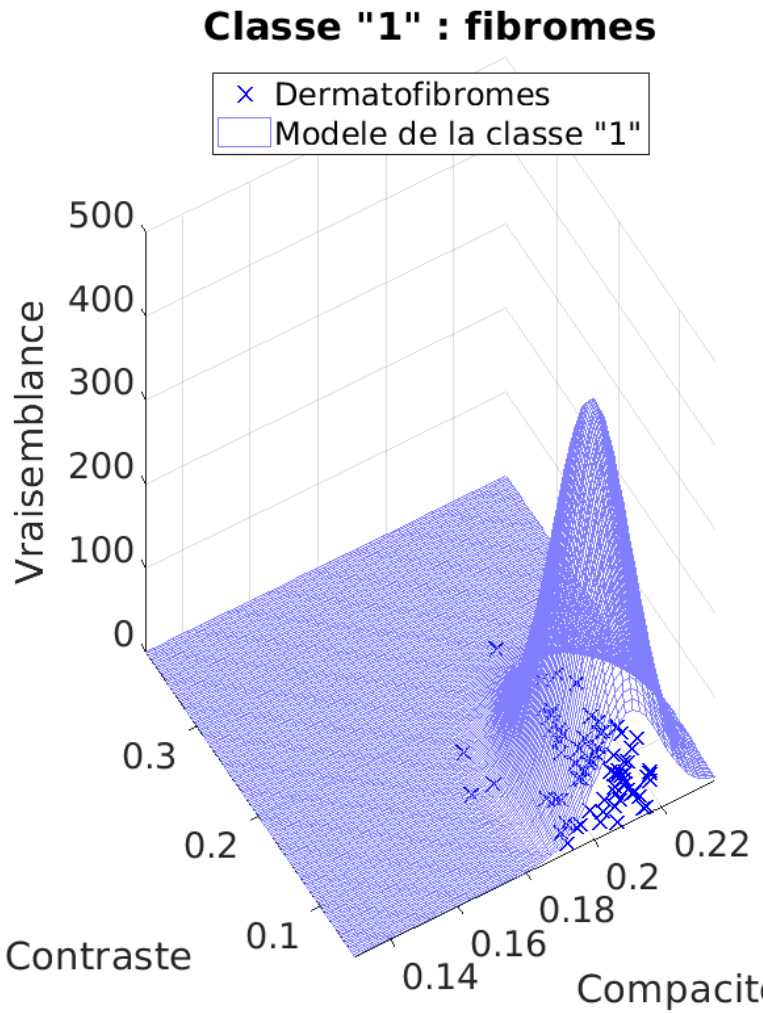


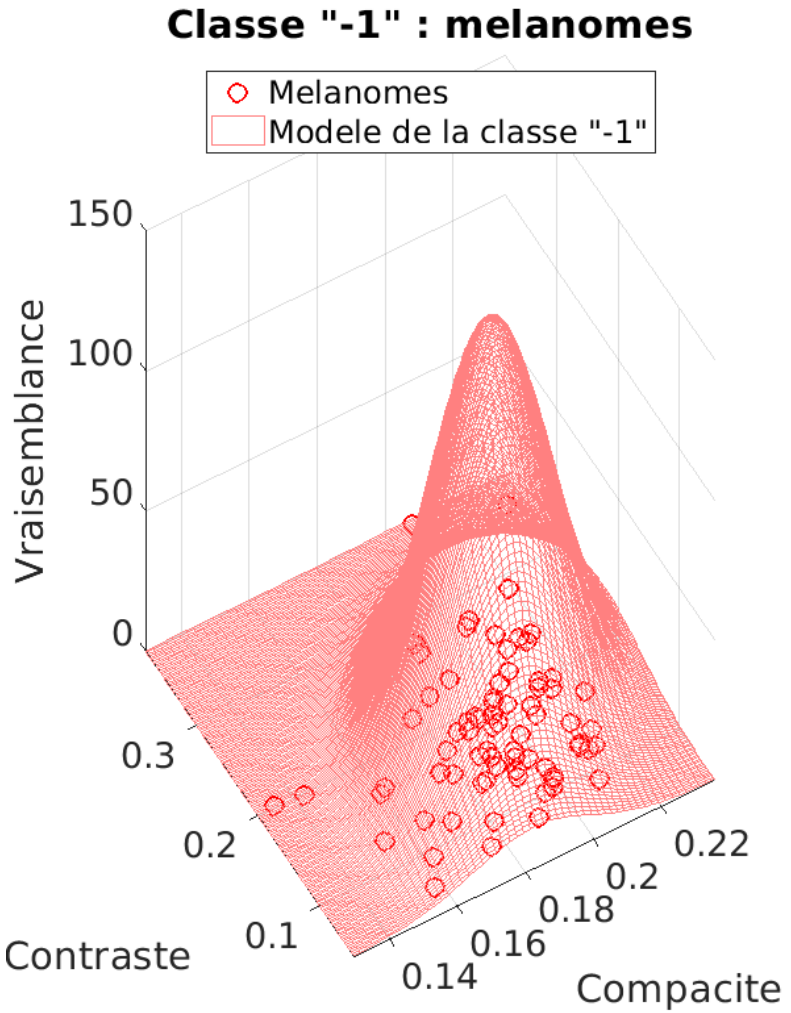
Lab example



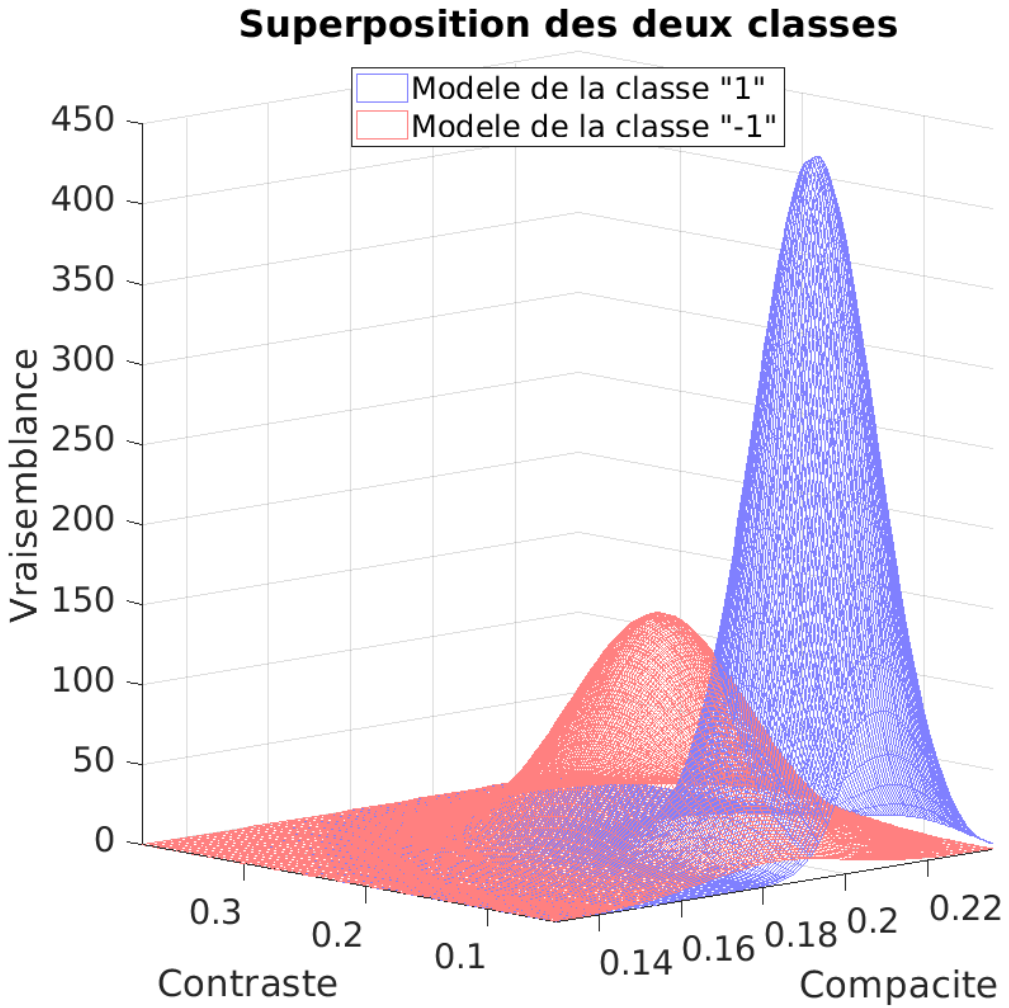
We choose to model the distributions of each class with a Gaussian model.

Lab example

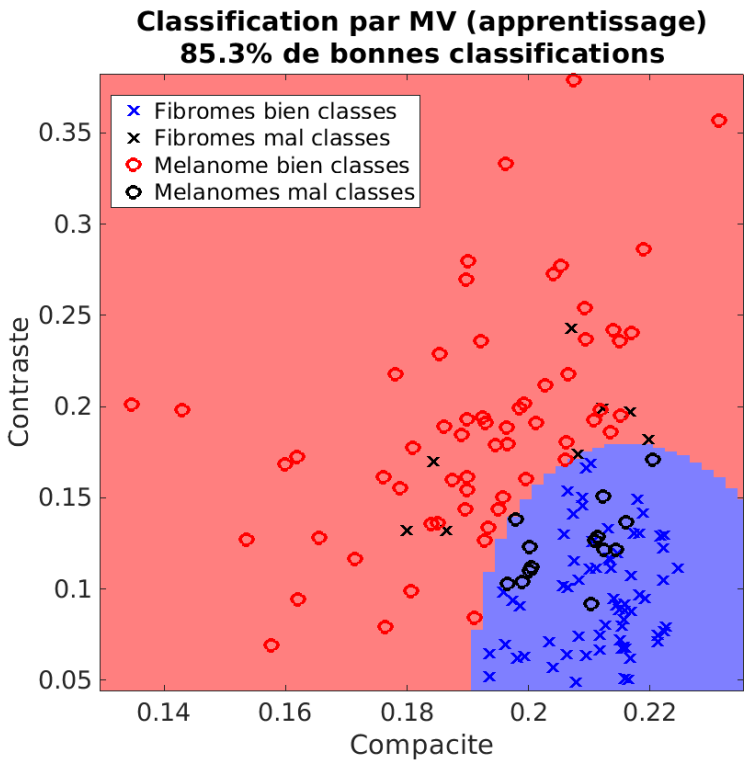

Classe "1" : fibromes
Dermatofibromes
Modele de la classe "1"
Vraisemblance
500
400
300
200
100
0
0.3
0.2
0.1
Contraste
0.14
0.16
0.18
0.2
0.22
Compacite

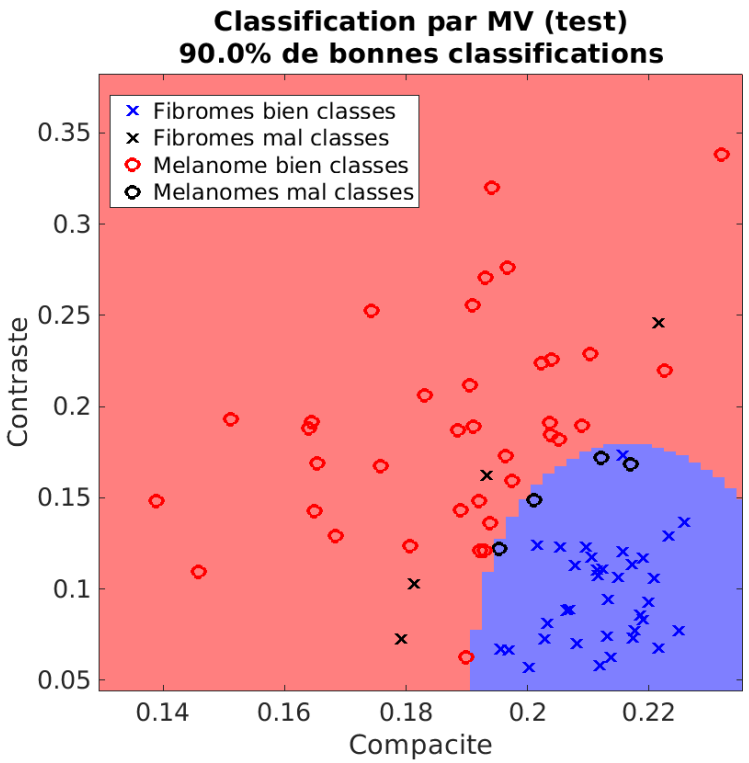

Classe "-1" : melanomes
Melanomes
Modele de la classe "-1"
Vraisemblance
150
100
50
0
0.3
0.2
0.1
Contraste
0.14
0.16
0.18
0.2
0.22
Compacite

Lab example


Superposition des deux classes
Modele de la classe "1"
Modele de la classe "-1"
Vraisemblance
450
400
350
300
250
200
150
100
50
0
0.3
0.2
0.1
Contraste
0.14
0.16
0.18
0.2
0.22
Compacite

Lab example





In this example, the model is too simple and seems to underfit. However the results on the test set are satisfying.

A non-parametric method: the k-nearest neighbor rule

the nearest neighbor rule

$$\boxed{d(x) = a_j \text{ if the nearest neighbor of } x \text{ belongs to } \omega_j}$$

The observed vector $\boldsymbol{x}$ is affected to the class of its nearest neighbor.

Inequality of Cover and Hart

$$P^* \leq P_1 \leq P^* \left(2 - \frac{K}{K-1} P^*\right)$$

The k-nearest neighbor rule

$\boldsymbol{x}$ is assigned to the class most common amongst its k-nearest neighbors (with a given distance measure)

Probability of error

Inequalities

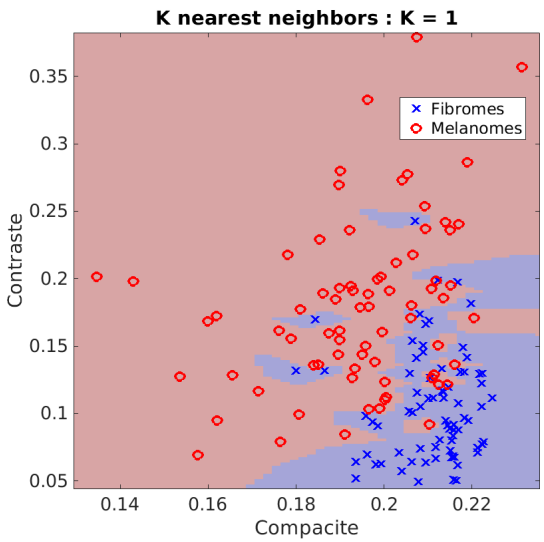
$$P^* \leq P_k \leq P^* + \frac{1}{\sqrt{ke}} \text{ or } P^* \leq P_k \leq P^* + \sqrt{\frac{2P_1}{k}}$$

Approximations

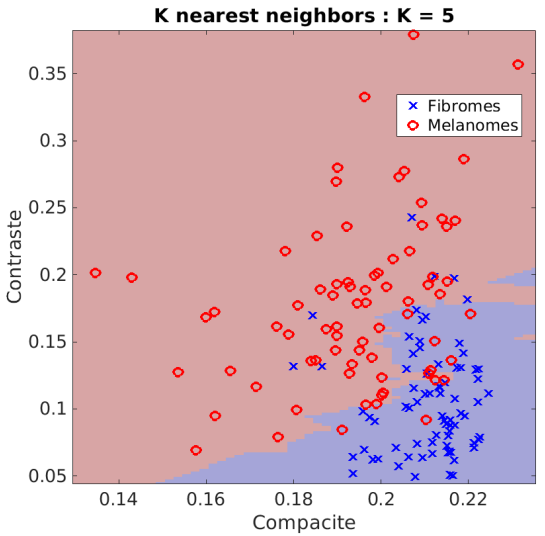
When P^* is small, the following results can be obtained

$$P_1 \approx 2P^* \text{ and } P_3 \approx P^* + 3\left(P^*\right)^2$$

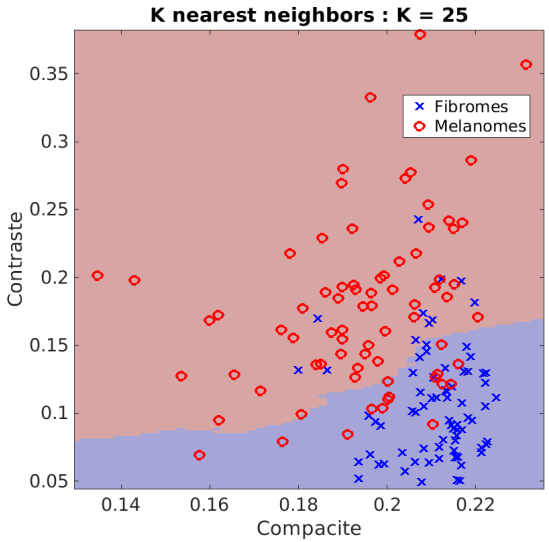
Lab example



Test accuracy: 87.5%



Test accuracy: 91.2%



Test accuracy: 93.8%

- A smaller K tends to perfectly reproduce the training data but generalizes poorly (*overfitting*)
- A larger K tends to regularize the decision boundary, which helps generalization.

Summary

Comparing and selecting classifiers.

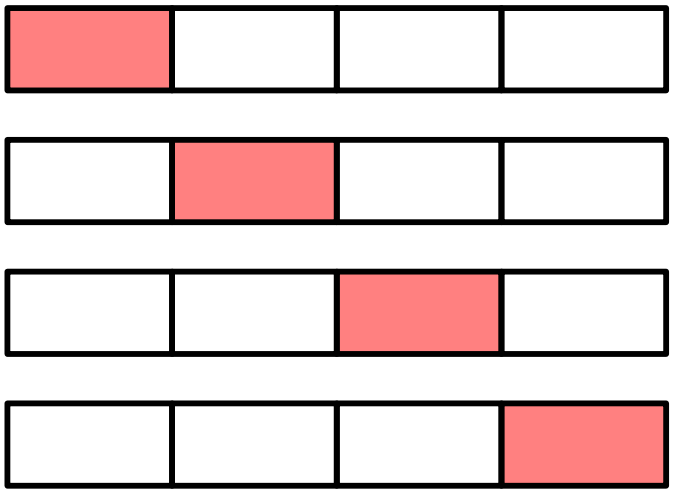
- We just saw how a "k-nearest-neighbors" (knn) classifier works and the rationale behind such a non-parametric method.
- How should we select k? is a remaining question.

S-fold cross-validation

- S-fold cross-validation involves taking the available data and partitioning it into S groups. Then $S-1$ of the groups are used to train a set of models that are then evaluated/tested on the remaining group (termed ζ in the sequel).
- This procedure is then repeated for all S possible choices for the held-out group, indicated here by the red blocks, and the performance scores from the S runs are then averaged.

S-fold Cross-Validation

4-fold cross-validation



CV score for each k and $\zeta(j)$ is the jth group used as testing data

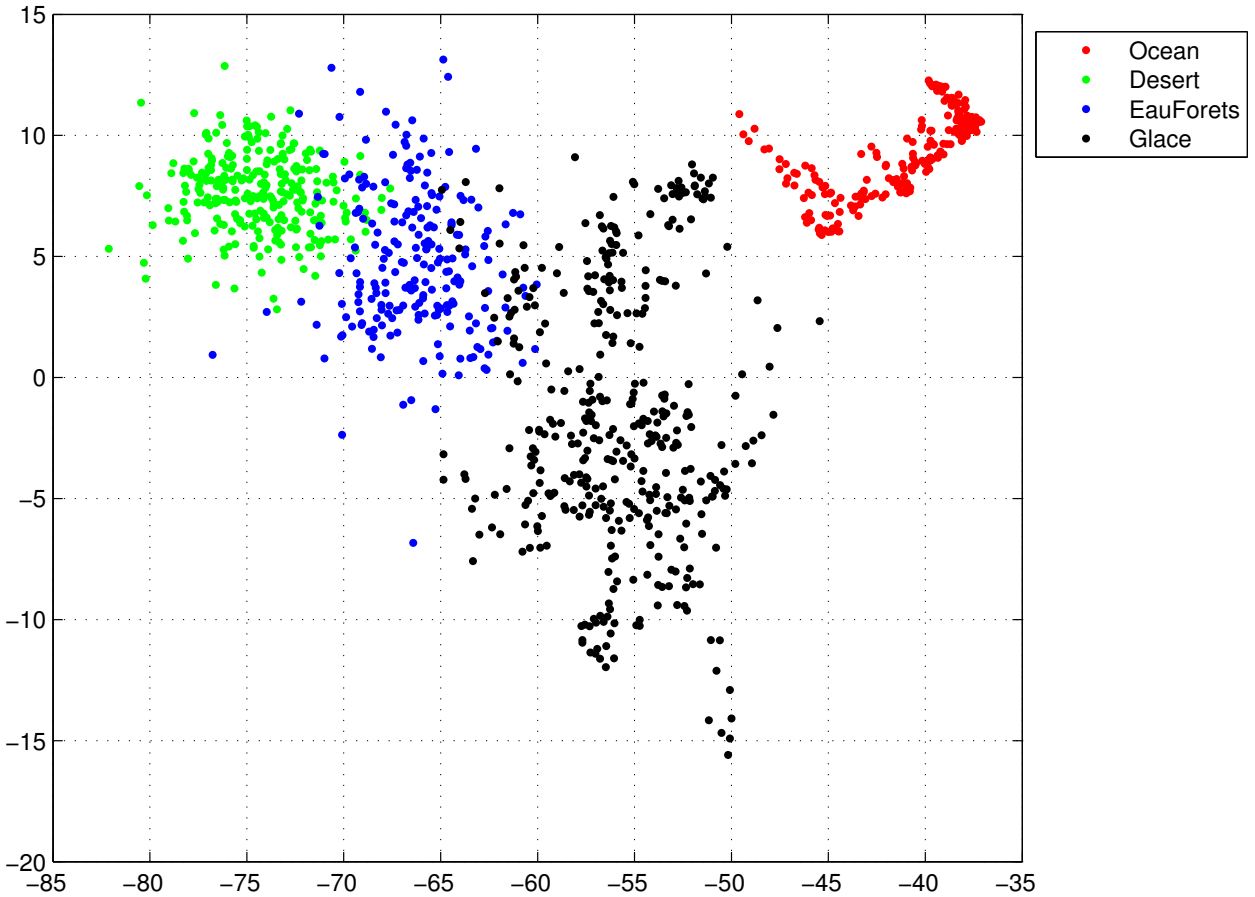
$$CV(k) = \frac{1}{S} \sum_{\textbf{run } j=1}^{S} \frac{1}{|\zeta(j)|} \sum_{(\mathbf{x}', y') \in \zeta(j)} c(f_{k\text{nn}}^{D-\zeta(j)}(\mathbf{x}'), y')$$

Leave-One-Out (LOO) score for each k

$$\text{CV}(k) = \frac{1}{n} \sum_{i=1}^{n} c(f_{k\text{nn}}^{D-\{(\boldsymbol{x_i}, y_i)\}}(\boldsymbol{x_i}), y_i)$$

Summary

Example


15
10
5
0
−5
−10
−15
−20
−85
−80
−75
−70
−65
−60
−55
−50
−45
−40
−35
Ocean
Desert
EauForets
Glace

Some classification results

Bayesian Classification (Gaussian densities)

Classes	*Ocean*	*Desert*	*Forest*	*Ice*
Ocean	**99.6**	0.0	0.0	0.0
Desert	0.0	**95.3**	1.8	0.0
Forest	0.0	4.4	**97.7**	0.8
Ice	0.4	0.4	0.5	**99.2**

1-PPV Method

Classes	*Ocean*	*Desert*	*Forest*	*Ice*
Ocean	**100**	0.0	0.0	0.0
Desert	0.0	**96.0**	5.4	0.0
Forest	0.0	4.0	**93.2**	0.0
Ice	0.0	0.0	1.4	**100**

Some classification results

5-PPV Method

Classes	*Ocean*	*Desert*	*Forest*	*Ice*
Ocean	**100**	0.0	0.0	0.0
Desert	0.0	**93.8**	5.9	0.3
Forest	0.0	6.2	**93.2**	0.0
Ice	0.0	0.0	0.9	**99.7**

Neural Networks

Classes	*Ocean*	*Desert*	*Forest*	*Ice*
Ocean	**100**	0.0	0.0	0.0
Desert	0.0	**96.0**	5.4	0.0
Forest	0.0	4.0	**92.8**	0.8
Ice	0.0	0.0	1.8	**99.2**

Summary

Support vector machines (SVMs)

Learning set

$$\mathcal{B} = \{(\boldsymbol{x}_1, y_1), ..., (\boldsymbol{x}_n, y_n)\}$$

where $\boldsymbol{x}_1, ..., \boldsymbol{x}_n$ are n vectors of $\mathbb{R}^p$ and $y_1, ..., y_n$ are binary variables

$$y_i = 1 \text{ if } \boldsymbol{x}_i \in \omega_1, \quad y_i = -1 \text{ if } \boldsymbol{x}_i \in \omega_2$$

Hyperplane definition

$$g_{\boldsymbol{w},b}(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x} - b = 0$$

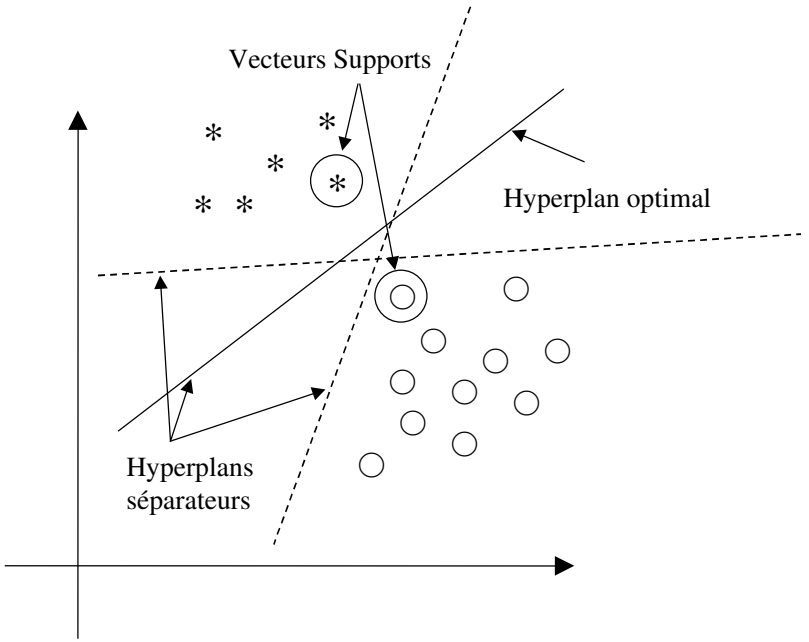
with

$$g_{\boldsymbol{w},b}(\boldsymbol{x}_i) > 0 \text{ if } \boldsymbol{x}_i \in \omega_1, \quad g_{\boldsymbol{w},b}(\boldsymbol{x}_i) < 0 \text{ if } \boldsymbol{x}_i \in \omega_2$$

Classification rule

$$f(\boldsymbol{x}) = \text{sign}\left[g_{\boldsymbol{w},b}(\boldsymbol{x})\right] \tag{1}$$

Illustration



Summary

Problem formulation

Margin of $\boldsymbol{x}_i$ with label y_i (algebraic distance to the hyperplane)

$$\gamma_i\left(\widetilde{\boldsymbol{w}}\right) = \frac{y_i\left(\boldsymbol{w}^T\boldsymbol{x}_i - b\right)}{\|\boldsymbol{w}\|}$$

with $\widetilde{\boldsymbol{w}} = (\boldsymbol{w}, b)$ ($\boldsymbol{x}_i$ is correctly classified by (1) if $\gamma_i\left(\widetilde{\boldsymbol{w}}\right) > 0$)

Margin of the learning set

$$\gamma_{\mathcal{B}}\left(\widetilde{\boldsymbol{w}}\right) = \min_{i\in\{1,\ldots,n\}} \frac{y_i\left(\boldsymbol{w}^T\boldsymbol{x}_i - b\right)}{\|\boldsymbol{w}\|}$$

Since $\gamma_{\mathcal{B}}\left(a\widetilde{\boldsymbol{w}}\right) = \gamma_{\mathcal{B}}\left(\widetilde{\boldsymbol{w}}\right)$, $\forall a > 0$, $\widetilde{\boldsymbol{w}}$ is not unique!

Constraints for the hyperplane: one forces the training samples that are the closest to the hyperplane to satisfy

$$y_i\left(\boldsymbol{w}^T\boldsymbol{x}_i - b\right) = 1 \Rightarrow \min_{i\in\{1,\ldots,n\}} y_i\left(\boldsymbol{w}^T\boldsymbol{x}_i - b\right) = 1$$

The vectors $\boldsymbol{x}_i$ satisfying $y_i\left(\boldsymbol{w}^T\boldsymbol{x}_i - b\right) = 1$ are called support vectors.

Problem formulation

Canonical hyperplane

$$y_i \left(\boldsymbol{w}^T \boldsymbol{x}_i - b \right) \geq 1, \quad \forall i = 1, ..., n$$

Classifier margin for a canonical hyperplane

$$\gamma_{\mathcal{B}} \left(\widetilde{\boldsymbol{w}} \right) = \frac{1}{\|\boldsymbol{w}\|}$$

We want to **maximize the margin**, i.e. minimize $\|\boldsymbol{w}\|$, which leads to the

Primal formulation

$$\begin{cases} \min\limits_{\boldsymbol{w} \in \mathbb{R}^n, b \in \mathbb{R}} \left\{ \frac{1}{2} \|\boldsymbol{w}\|^2 \right\} \\ \textbf{s.c.} \quad y_i \left(\boldsymbol{w}^T \boldsymbol{x}_i - b \right) \geq 1, \forall i \in \{1, \ldots, n\} \end{cases}$$

Simple problem since the cost function to optimize is quadratic and the constraints are linear!

Summary

Optimization

Lagrangian

$$L(\widetilde{\boldsymbol{w}}, \alpha) = \frac{1}{2}\boldsymbol{w}^T\boldsymbol{w} - \sum_{i=1}^{n} \alpha_i \left[y_i \left(\boldsymbol{w}^T \boldsymbol{x}_i - b \right) - 1 \right]$$

Set to zero the partial derivatives of L with respect to b and w

$$\sum_{i=1}^{n} \alpha_i y_i = 0 \text{ and } \boldsymbol{w} = \sum_{i=1}^{n} \alpha_i y_i \boldsymbol{x}_i$$

Kuhn and Tucker multipliers

For a convex optimization problem (convex function $f(x)$ to optimize and convex constraints $G_i(\boldsymbol{x}) \leq 0$), an optimality condition is the existence of parameters $\alpha_i \geq 0$ such that the Lagrangian derivative is zero, i.e.,

$$L'(\boldsymbol{x}) = f'(\boldsymbol{x}) + \sum_{i=1}^{n} \alpha_i G_i'(\boldsymbol{x}) = 0$$

with $\alpha_i = 0$ if $G_i(\boldsymbol{x}) < 0$ (i.e., $\alpha_i G_i(\boldsymbol{x}) = 0$).

Dual problem

Solve $L'(\boldsymbol{x}) = 0$

$$\boldsymbol{w} = \sum_{\text{Support vectors}} \alpha_i y_i \boldsymbol{x}_i = \boldsymbol{x}^T \boldsymbol{Y} \boldsymbol{\alpha} \tag{2}$$

with $\boldsymbol{\alpha} = (\alpha_1, ..., \alpha_n)^T$, $\boldsymbol{x} = (x_1, ..., x_n)^T$, $\boldsymbol{Y} = \text{diag}\,(y_1, ..., y_n)$ and

$$\begin{cases} \alpha_i = 0 \text{ if the constraint is a strict inequality} \\ \alpha_i > 0 \text{ if the constraint is an equality} \end{cases}$$

After replacing the expression of w in the Lagrangian, we obtain

$$U(\alpha) = -\frac{1}{2} \boldsymbol{\alpha}^T \boldsymbol{Y} \left(\boldsymbol{x} \boldsymbol{x}^T \right) \boldsymbol{Y} \boldsymbol{\alpha} + \sum_{i=1}^{n} \alpha_i$$

that has to be maximized in the domain defined by $\alpha_i \geq 0, \forall i$ and $\sum_{i=1}^{n} \alpha_i y_i = 0$.

Dual problem

Dual formulation

$$\left\{ \begin{array}{l} \max\limits_{\boldsymbol{\alpha} \in \mathbb{R}^n} \left\{ -\frac{1}{2} \boldsymbol{\alpha}^T \boldsymbol{Y} \left(\boldsymbol{x}\boldsymbol{x}^T \right) \boldsymbol{Y} \boldsymbol{\alpha} + \sum_{i=1}^n \alpha_i \right\} \\ \quad \textbf{s.c.} \left\{ \begin{array}{l} \sum\limits_{i=1}^n \alpha_i \, y_i = 0 \\ \alpha_i \geq 0, \qquad \forall \, i \in \{1, \ldots, n\} \end{array} \right. \end{array} \right.$$

The solutions of this dual problem are also solutions of the primal problem.

Simple optimization problem

Quadratic (hence convex) function to optimize and linear constraints

Remarks

Decision rule

Norm of the solution $\boldsymbol{w}_0$

$$\|\boldsymbol{w}_0\|^2 = \sum_{\text{support vectors}} \alpha_i^0 \left(1 + y_i b\right) = \sum_{\text{support vectors}} \alpha_i^0$$

because of the constraint $\sum_{i=1}^n \alpha_i y_i = 0$.

Classifier margin

$$\boxed{\gamma = \frac{1}{\|\boldsymbol{w}_0\|} = \left(\sum \alpha_i^0\right)^{-1/2}}$$

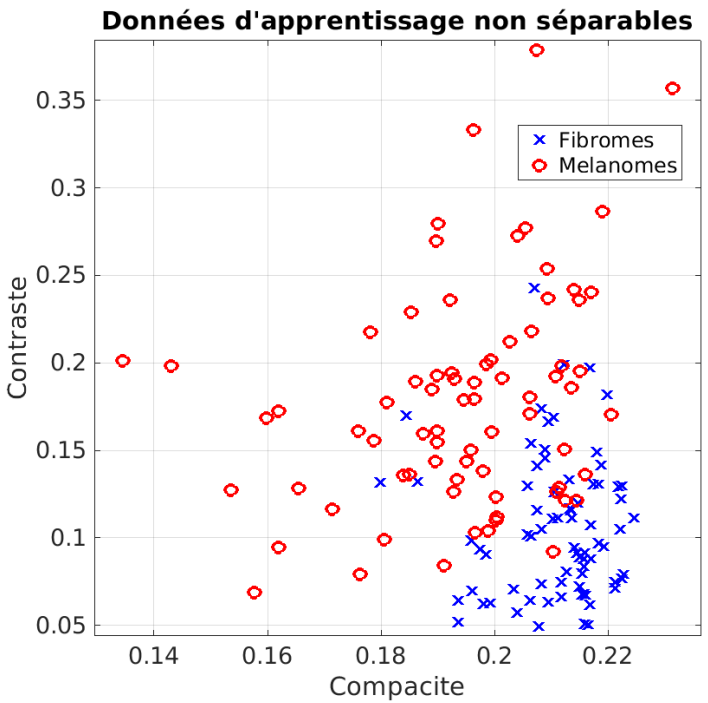
Classification rule for a vector $\boldsymbol{x}$

$$f(\boldsymbol{x}) = \text{sign}\left(\sum_{x_i \text{ support vectors}} \alpha_i^0 y_i \boldsymbol{x}_i^T \boldsymbol{x} - b_0\right), \quad b_0 = \frac{1}{2}\left(\boldsymbol{w}_0^T \boldsymbol{x}^+ + \boldsymbol{w}_0^T \boldsymbol{x}^-\right),$$

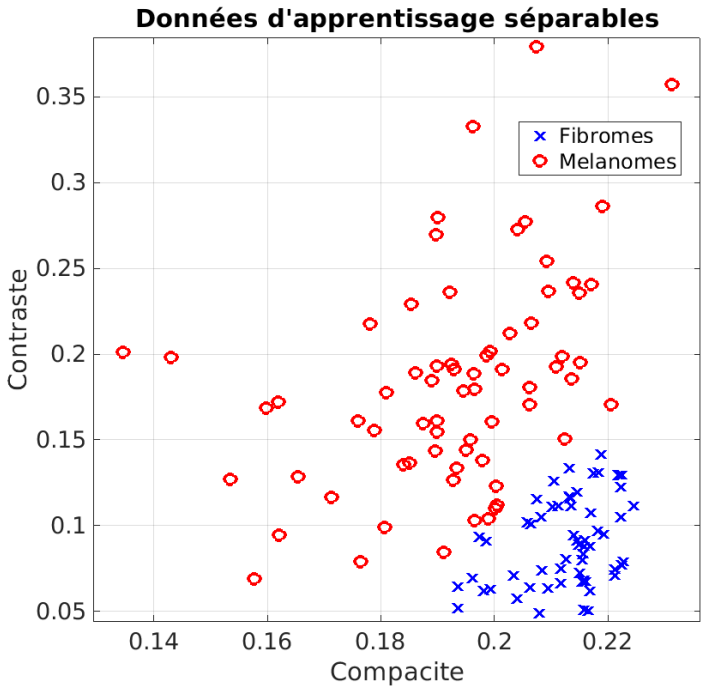
where $\boldsymbol{x}^+$ (resp. $\boldsymbol{x}^-$) is a support vector belonging to the 1st (resp. 2nd) class.

Remarks

The quadratic optimization can only converge when the data is linearly separable:



No convergence

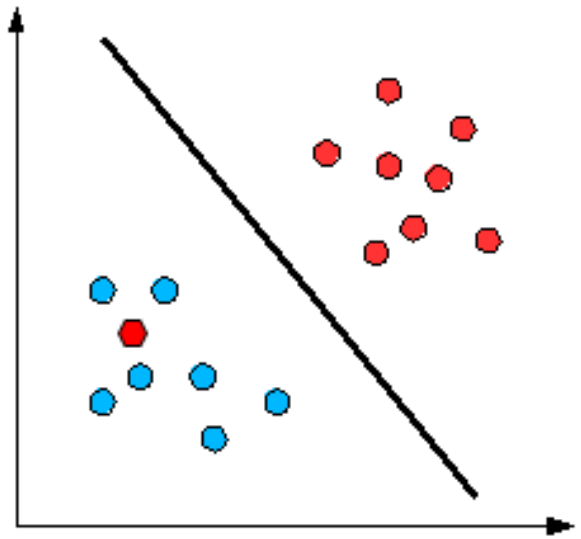


Convergence

Summary

Non-linear separability

Real-world data are often noisy and may not be linearly separable.

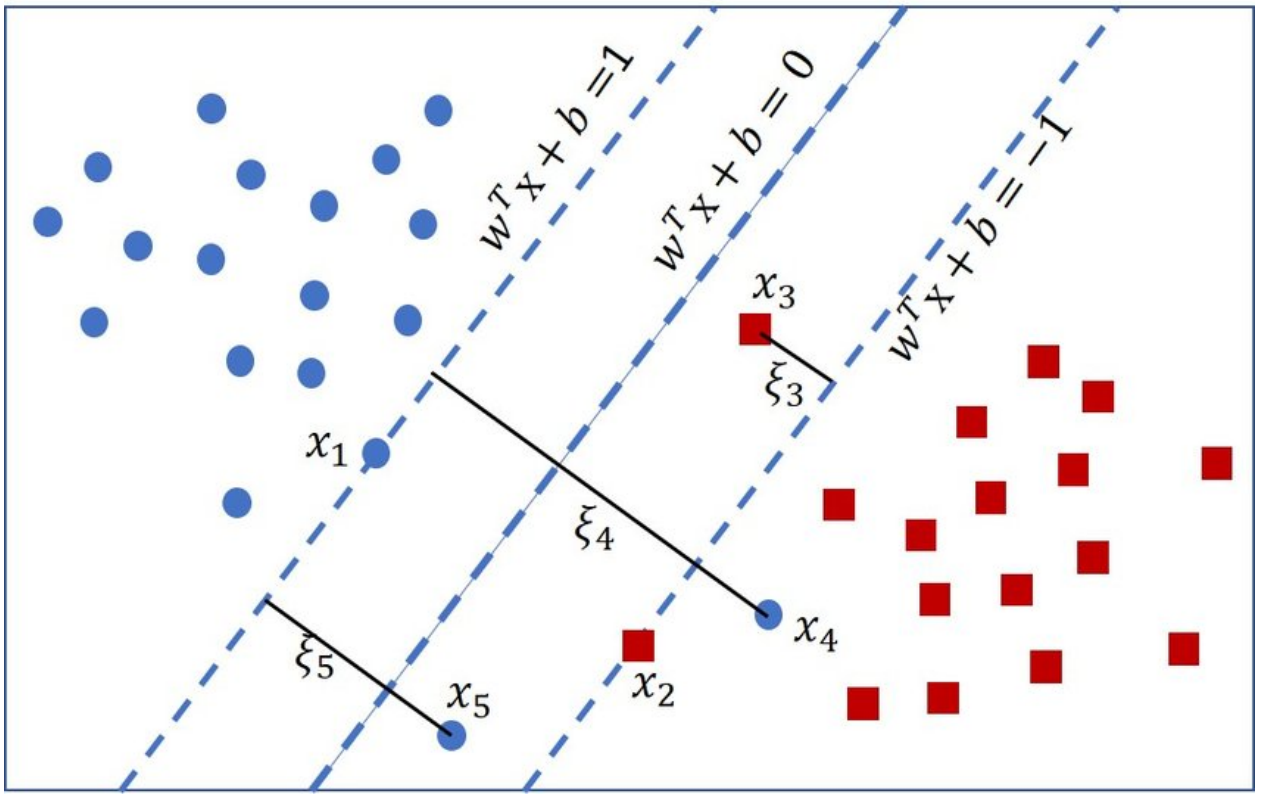


In that case, the SVM does not admit any solution to the primal (nor dual) optimization problem.

Soft-margin SVM: Slack variables

We introduce slack variables $\xi_i \geq 0$ to relax the canonical hyperplane constraints:

$$y_i \left(\boldsymbol{w}^T \boldsymbol{x}_i - b \right) \geq 1 - \xi_i \qquad \forall\, i \in \{1, \ldots, n\}$$



Soft-margin SVM: problem formulation

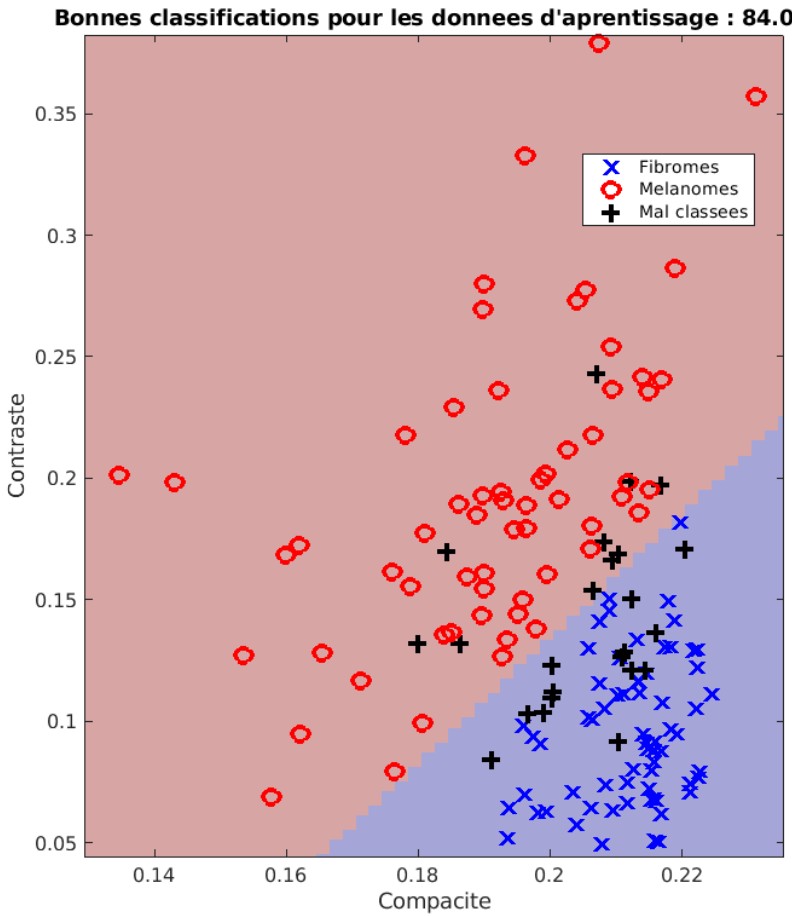
The problem becomes:

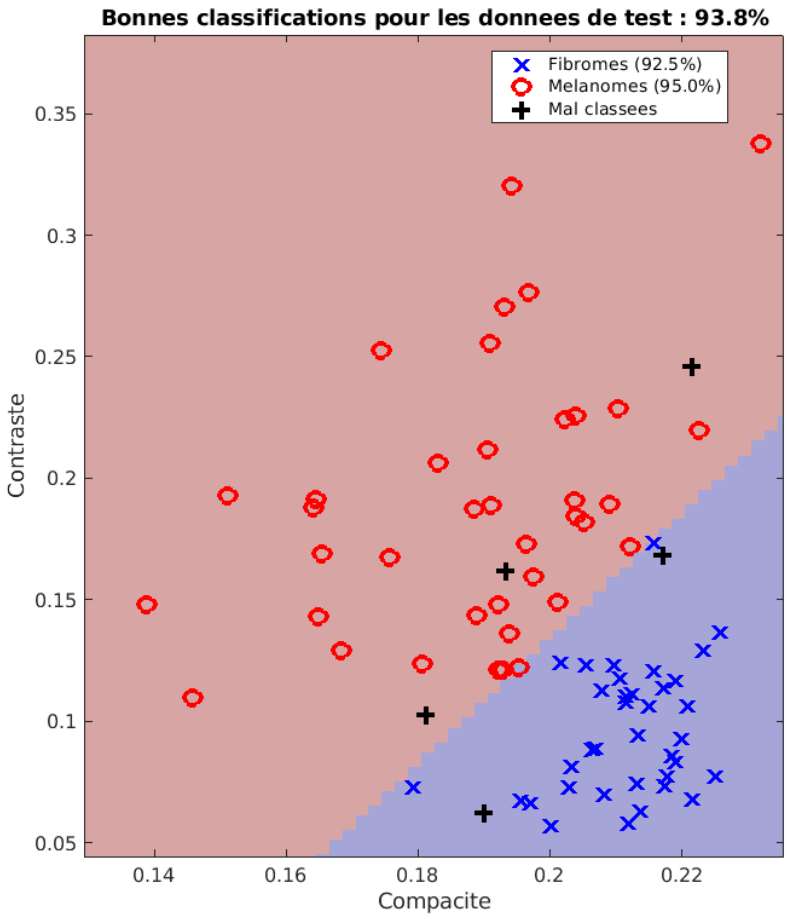
$$\begin{cases} \min\limits_{\substack{\boldsymbol{w}\in\mathbb{R}^n, b\in\mathbb{R} \\ (\xi_1,\dots,\xi_n)\in\mathbb{R}^n}} \left\{ \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum\limits_{i=1}^{n}\xi_i \right\} \\ \quad \textbf{u.c.} \begin{cases} y_i\left(\boldsymbol{w}^T\boldsymbol{x}_i - b\right) \geq 1-\xi_i & \forall i\in\{1,\dots,n\} \\ \xi_i \geq 0 & \forall i\in\{1,\dots,n\} \end{cases} \end{cases}$$

C is a hyperparameter that can be tuned using cross-validation:

- When C is 0, the problem is the same as in the "hard-margin" SVM.
- When C is low (but not 0), we allow many points to violate the margin.
- As C becomes larger, less and less points can violate the margin (when $C=\infty$, one tends to the hard-margin SVM)

Lab example





This simple linear model underfits but generalizes well!

Extensions

The ν-SVM classifier

Minimize $\frac{1}{2}\|\boldsymbol{w}\|^2 + \frac{1}{n}\sum_{i=1}^{n}\xi_i - \nu\gamma$

with the constraints

$y_i\left(\boldsymbol{w}^T\boldsymbol{x}_i - b\right) \geq \gamma - \xi_i, \forall i,$

$\xi_i \geq 0, \forall i,$

$\gamma \geq 0$

This formulation introduces a new hyperparameter ν that is an upper bound of the fraction of points that violate the margin.

Summary

Non-linear preprocessing

Search a non-linear transformation $\phi : \mathbb{R}^p \to \mathbb{R}^q$ ensuring linear separability.

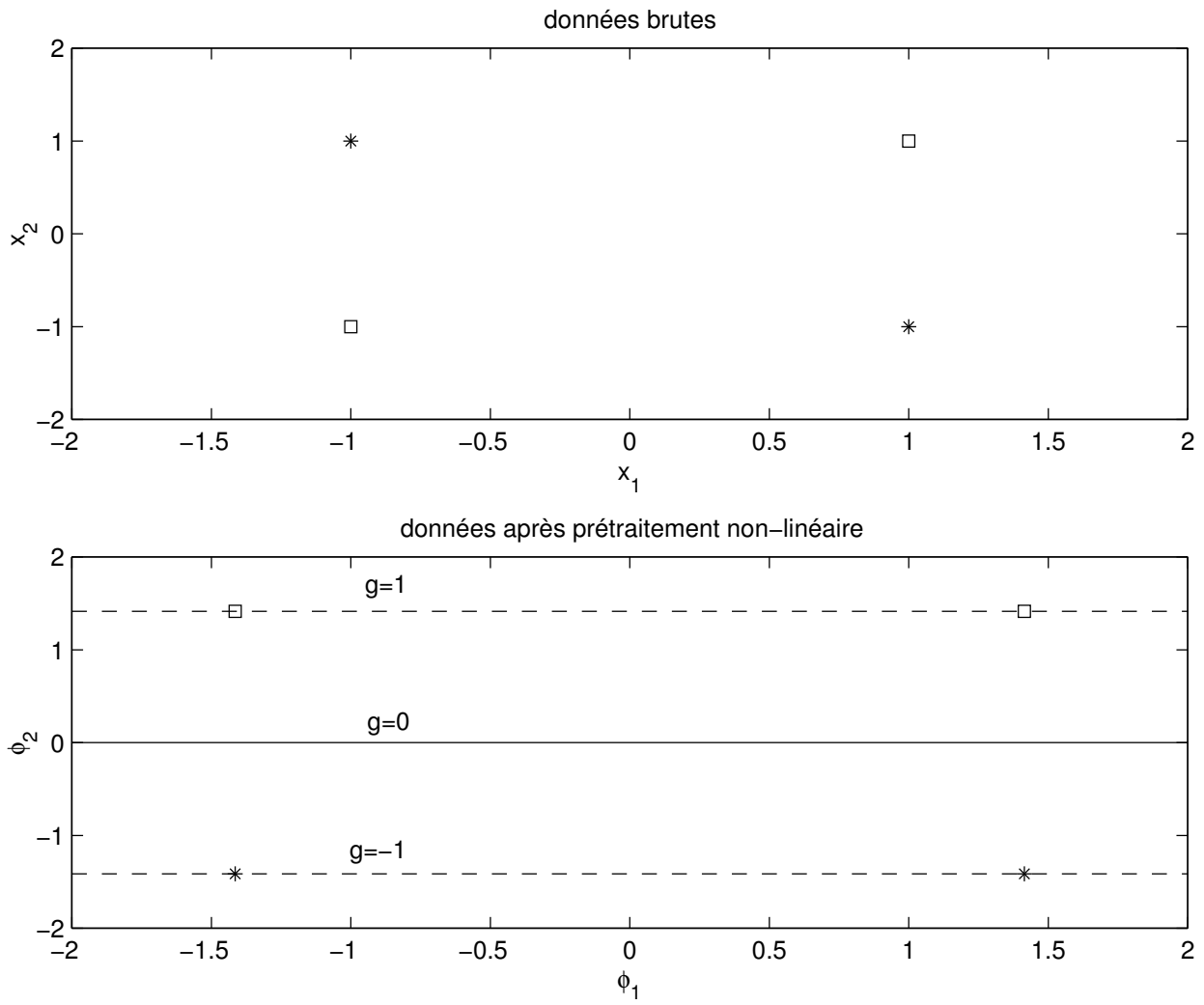
Classical example

The classes $\chi_1 = \{(1,1), (-1,-1)\}$ and $\chi_2 = \{(1,-1), (-1,1)\}$ are not linearly separable. Consider the application ϕ defined by

$$\phi : \begin{array}{l} \mathbb{R}^2 \to \mathbb{R}^6 \\ (x_1, x_2)^T \mapsto \left(\sqrt{2}x_1, \sqrt{2}x_1x_2, 1, \sqrt{2}x_2, x_1^2, x_2^2\right)^T \end{array}$$

The data are separable in the plane (ϕ_1, ϕ_2)

Example of separability



Non-linear SVM classifier

Decision rule after preprocessing

$$\begin{aligned} f(\tilde{\boldsymbol{x}}) &= \text{sign}\left(g_{\boldsymbol{w},b}(\tilde{\boldsymbol{x}})\right) = \text{sign}\left(\boldsymbol{w}^T\phi\left(\boldsymbol{x}\right) - b\right) \\ &= \text{sign}\left(\sum_{\text{support vectors}} \alpha_i^0 y_i \phi\left(\boldsymbol{x}_i\right)^T \phi\left(\boldsymbol{x}\right) - b_0\right) \end{aligned}$$

Cost function to optimize

$$\boxed{U\left(\boldsymbol{\alpha}\right) = -\tfrac{1}{2}\boldsymbol{\alpha}^T\boldsymbol{Y}\boldsymbol{G}\boldsymbol{Y}^T\alpha + \sum_{i=1}^n \alpha_i}$$

where $\boldsymbol{G}$ is the Gram matrix defined by $G_{ij} = \phi\left(\boldsymbol{x}_i\right)^T \phi\left(\boldsymbol{x}_j\right)$. The cost function $U\left(\alpha\right)$ has to be maximized under the constraints

$$\boxed{0 \leq \alpha_i \leq \tfrac{1}{n},\ \forall i} \quad \text{and} \quad \boxed{\sum_{i=1}^n \alpha_i \geq \nu}$$

Conclusions: the cost function and the decision rule only depend on the inner products $\phi\left(\boldsymbol{x}_i\right)^T \phi\left(\boldsymbol{x}_j\right)$ and $\phi\left(\boldsymbol{x}_i\right)^T \phi\left(\boldsymbol{x}\right)$.

Kernels

A kernel $k(\boldsymbol{x}, \boldsymbol{y}) = \phi(\boldsymbol{x})^T \phi(\boldsymbol{y})$ allows inner products $\phi(\boldsymbol{x}_i)^T \phi(\boldsymbol{x}_j)$ and $\phi(\boldsymbol{x}_i)^T \phi(\boldsymbol{x})$ to be computed with a reduced computational cost.

Example: $\boldsymbol{x} = (x_1, x_2)^T$ and $\phi(\boldsymbol{x}) = \left(x_1^2, x_2^2, \sqrt{2}x_1 x_2\right)$

$$\begin{aligned} \phi(\boldsymbol{x})^T \phi(\boldsymbol{y}) &= \begin{pmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1 x_2 \end{pmatrix} . \begin{pmatrix} y_1^2 \\ y_2^2 \\ \sqrt{2}y_1 y_2 \end{pmatrix} \\ &= x_1^2 y_1^2 + x_2^2 y_2^2 + 2x_1 x_2 y_1 y_2 \\ &= \left(\boldsymbol{x}^T \boldsymbol{y}\right)^2 \end{aligned}$$

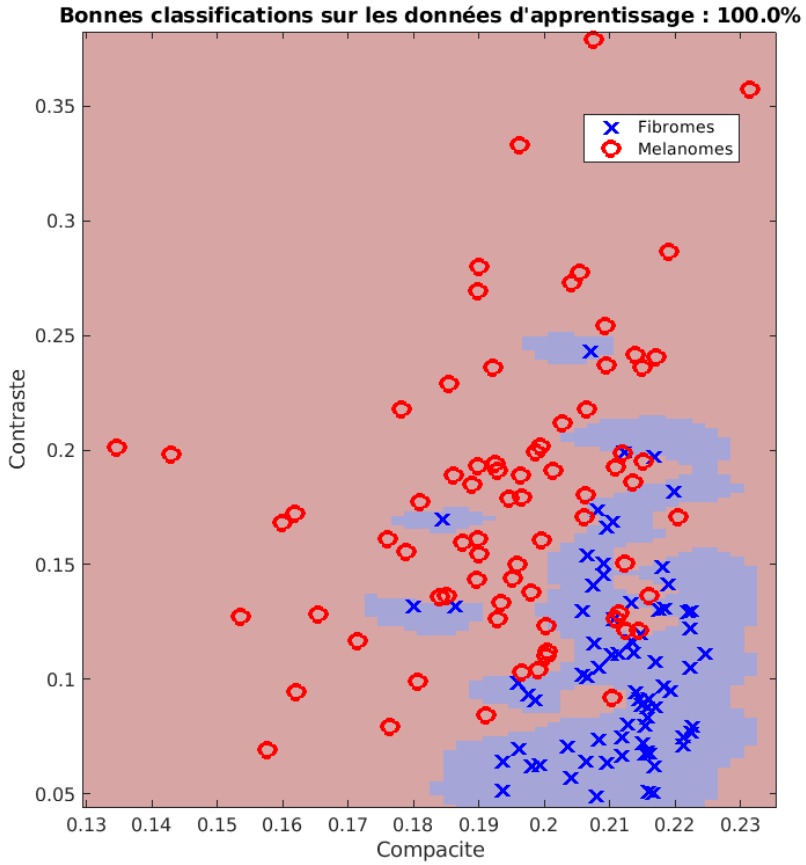
Mercer kernels can be expressed as inner products

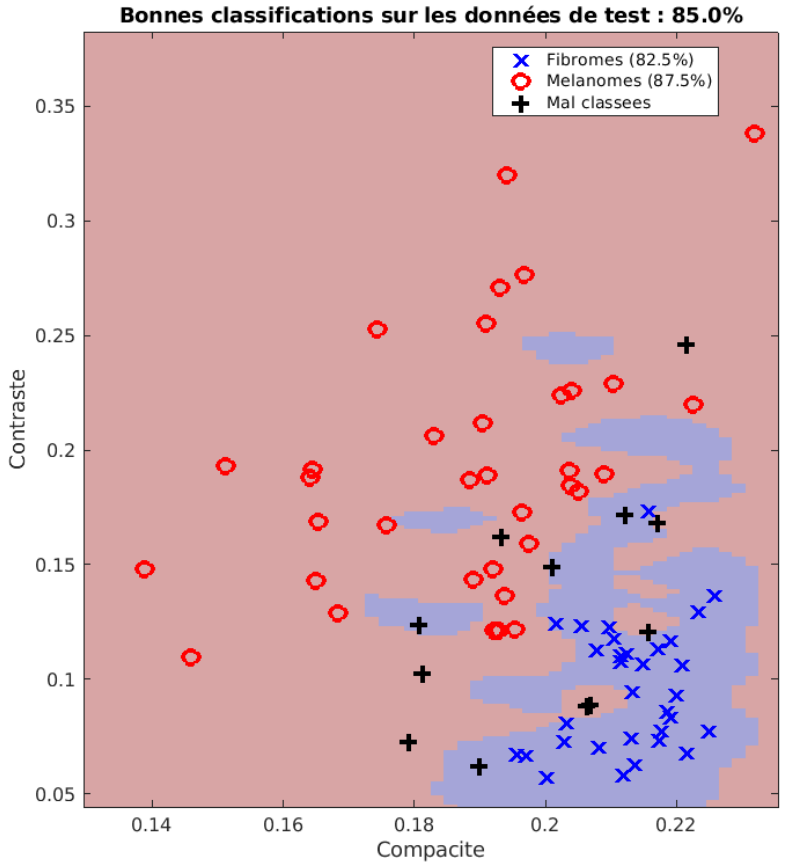
$$k(\boldsymbol{x}, \boldsymbol{y}) = \phi(\boldsymbol{x})^T \phi(\boldsymbol{y})$$

Classical kernels

Kernel	Expression
Polynomial (of degree q)	$k(\boldsymbol{x}, \boldsymbol{y}) = (\langle \boldsymbol{x}, \boldsymbol{y} \rangle)^q$ $q \in \mathbb{N}^+$
Full polynomial	$k(\boldsymbol{x}, \boldsymbol{y}) = (\langle \boldsymbol{x}, \boldsymbol{y} \rangle + c)^q$ $c \in \mathbb{R}^+$, $q \in \mathbb{N}^+$
RBF (Gaussian)	$k(\boldsymbol{x}, \boldsymbol{y}) = \exp\left(-\frac{\|\boldsymbol{x}-\boldsymbol{y}\|^2}{2\sigma^2}\right)$ $\sigma \in \mathbb{R}^+$
Mahalanobis	$k(\boldsymbol{x}, \boldsymbol{y}) = \exp\left[-(\boldsymbol{x}-\boldsymbol{y})^T \boldsymbol{\Sigma} (\boldsymbol{x}-\boldsymbol{y})\right]$ $\boldsymbol{\Sigma} = \text{diag}\left(\frac{1}{\sigma_1^2}, ..., \frac{1}{\sigma_p^2}\right)$, $\sigma_i \in \mathbb{R}^+$

Lab example





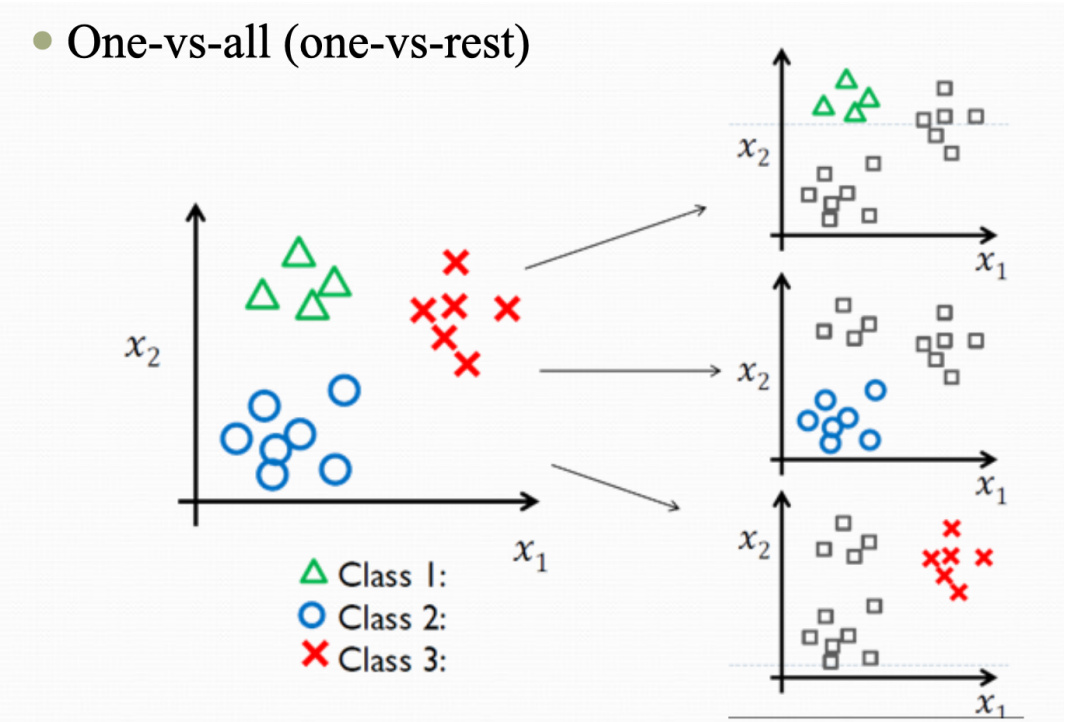
The model (Gaussian kernel) overfits the training data in this example.

Summary

Multi-class classification: one-versus-all

Assign $\boldsymbol{x}$ to ω_i if $i = \arg \max_{k=1,\ldots,K} g_k(\boldsymbol{x})$

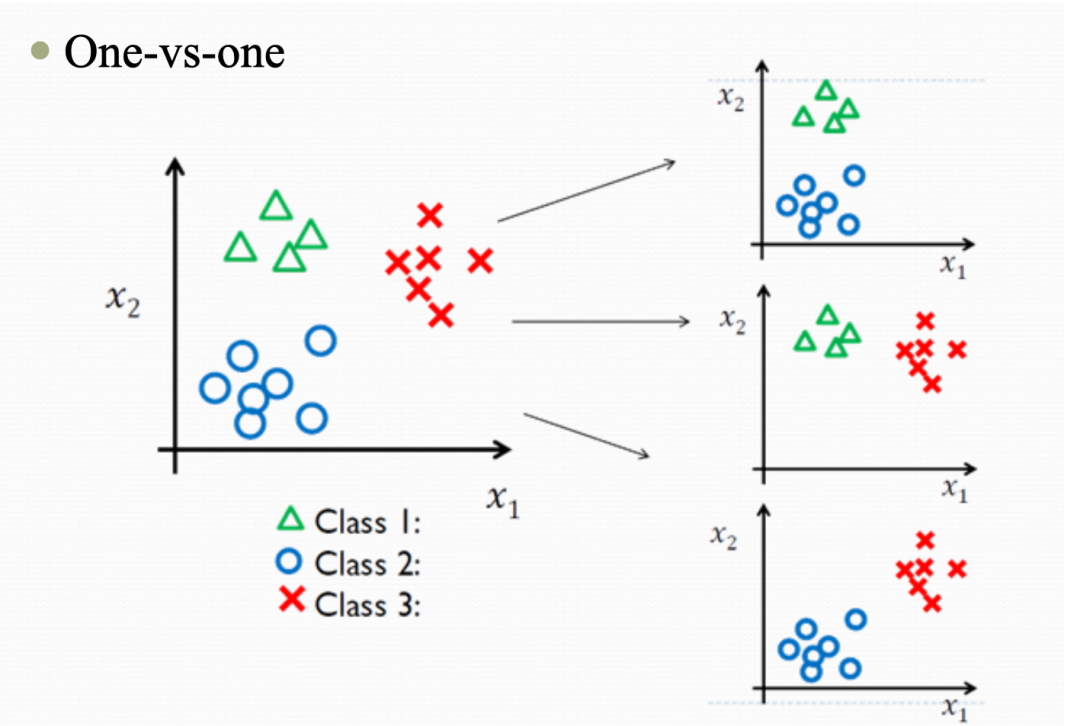
- One-vs-all (one-vs-rest)



Multi-class classification= one-versus-one

$$\omega^* = \arg \max_{k=1,\dots,K} S_k(\boldsymbol{x}) \text{ with } S_k(\boldsymbol{x}) = \sum_{j \neq k} \text{sign}\left[g_{ij}(\tilde{\boldsymbol{x}})\right]$$

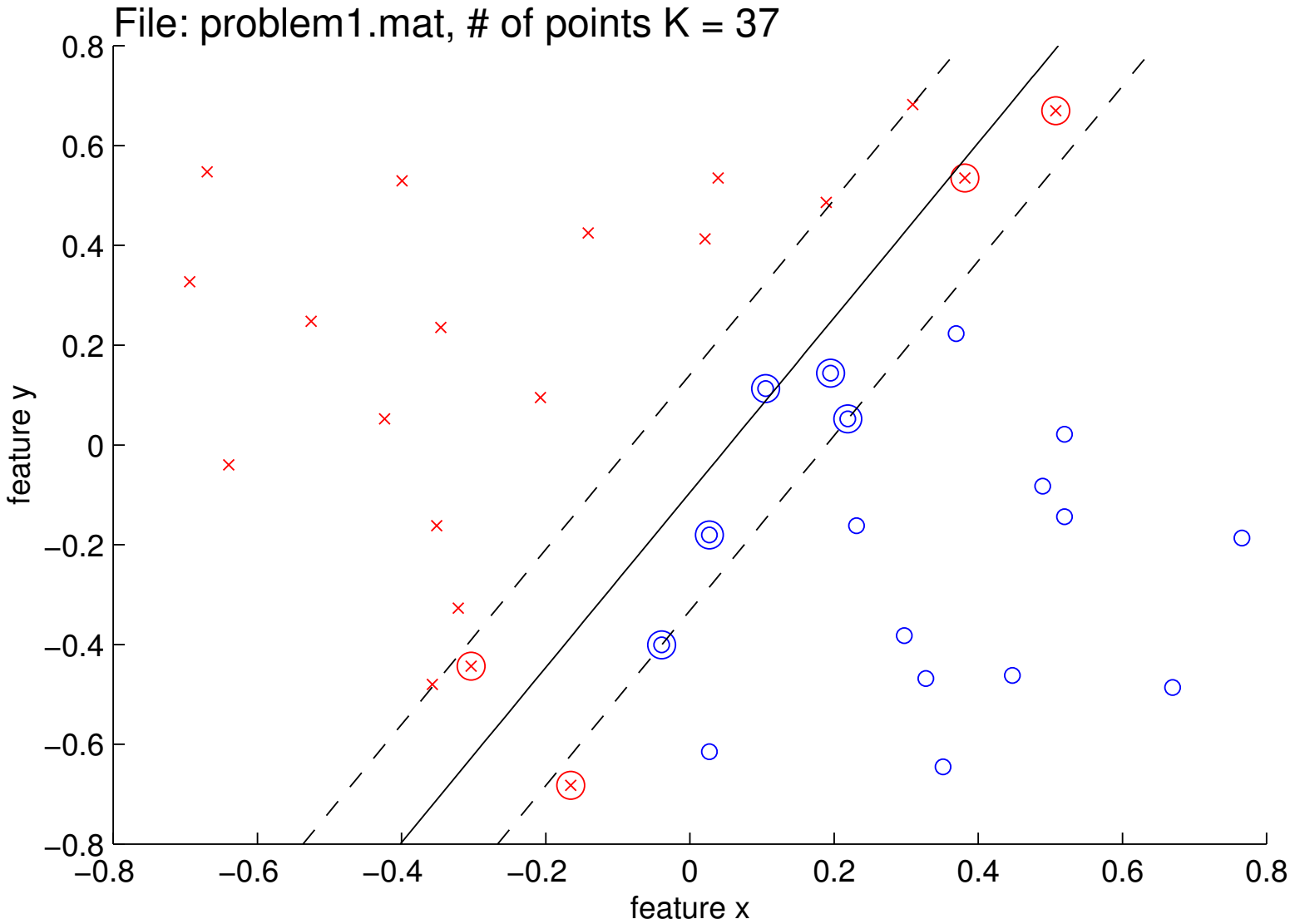
with g_{ij} the decision function between classes ω_i and ω_j.



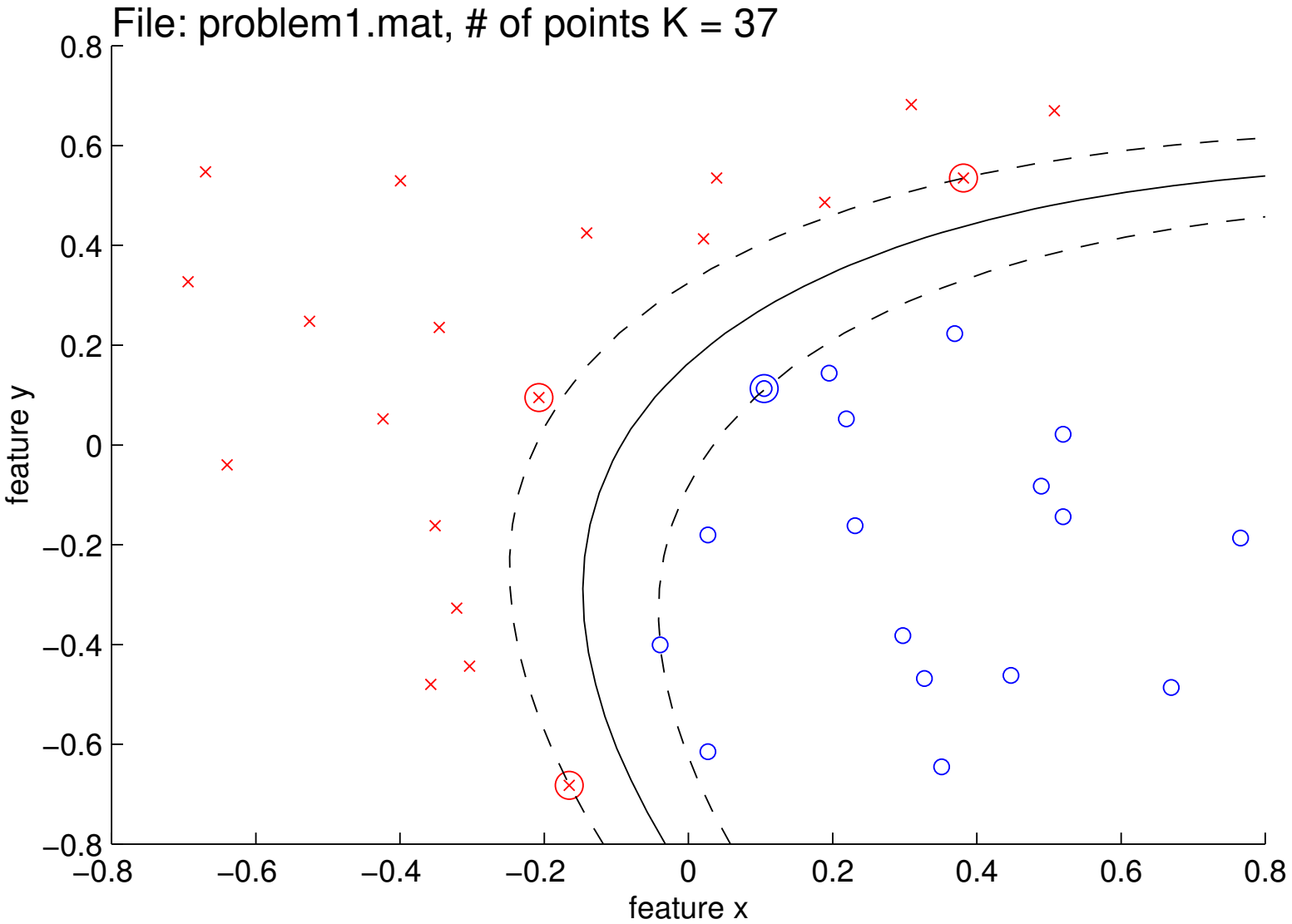
In conflictual situations (same score for different classes), one can select the class with the highest prior probability.

Summary

Example of linear SVMs



Example of non-linear SVMs



Equalization of non-linear communication channels

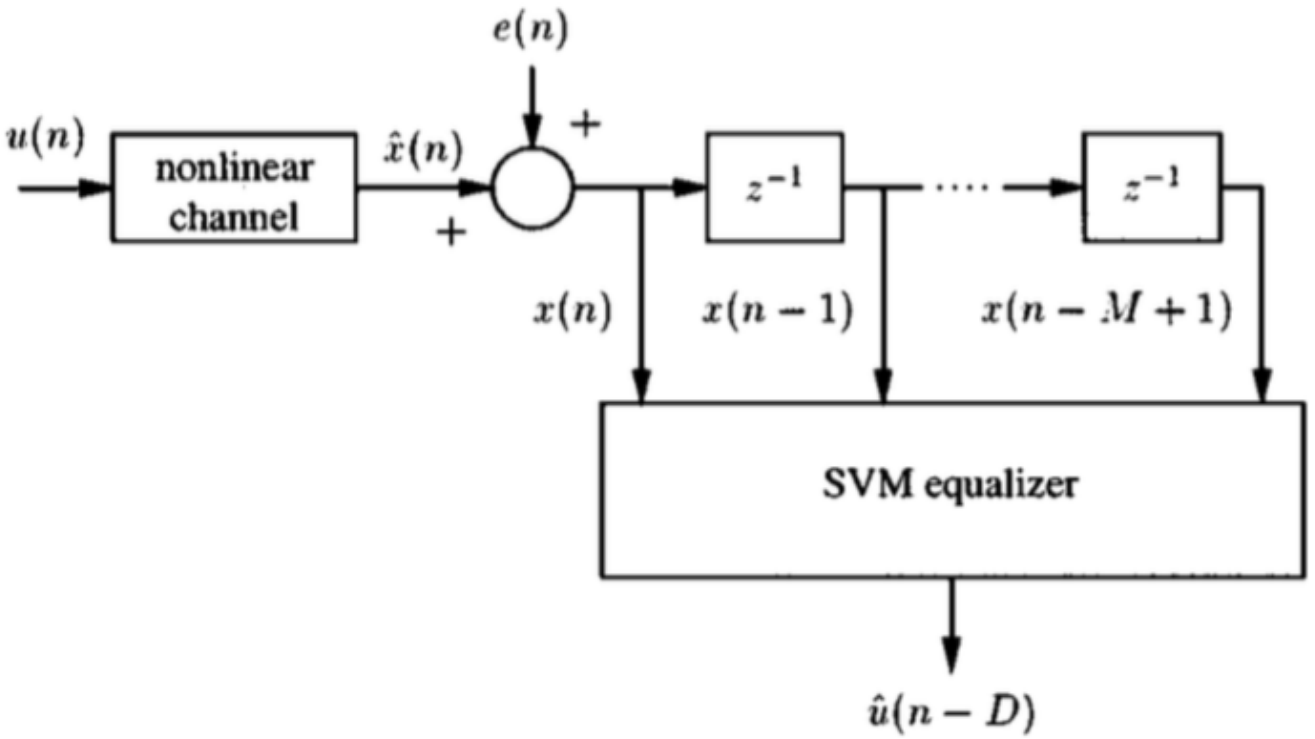


Fig. 2. Model of the nonlinear transmission system originating from Chen *et al.* [12].

Equalization of non-linear communication channels

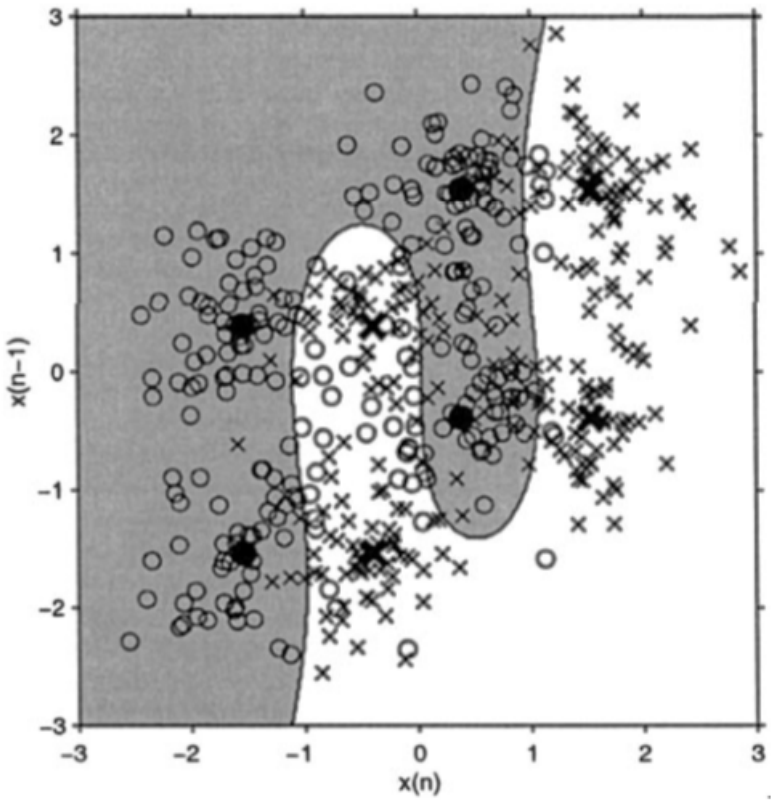


Fig. 3. Example of typical classification regions of an SVM and associated training points with channel $\hat{x}(n) = \tilde{x}(n) - 0.9\ \tilde{x}^3(n)$, $\tilde{x}(n) = u(n) + 0.5u(n-1)$, and Gaussian white noise of power $\sigma_e^2 = 0.2$ and equalizer dimension $M = 2$, polynomial kernel order $d = 3$, constraint $C = 5$, and lag $D = 0$.

Equalization of non-linear communication channels

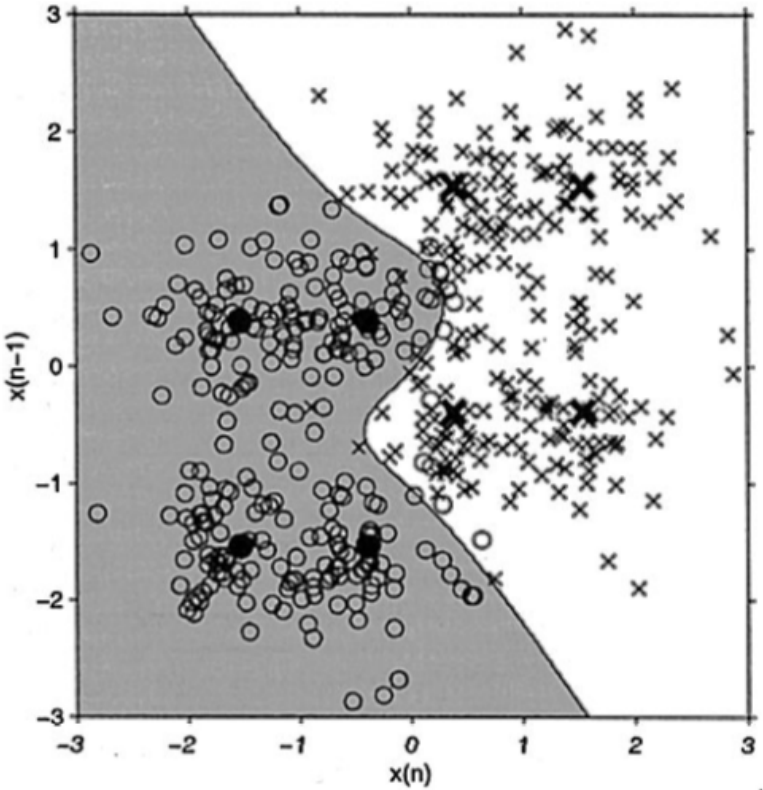


Fig. 4. Example of typical classification regions of an SVM and associated training points with the channel described in Fig. 3, except the equalizer lag is now $D = 1$.

Equalization of non-linear communication channels

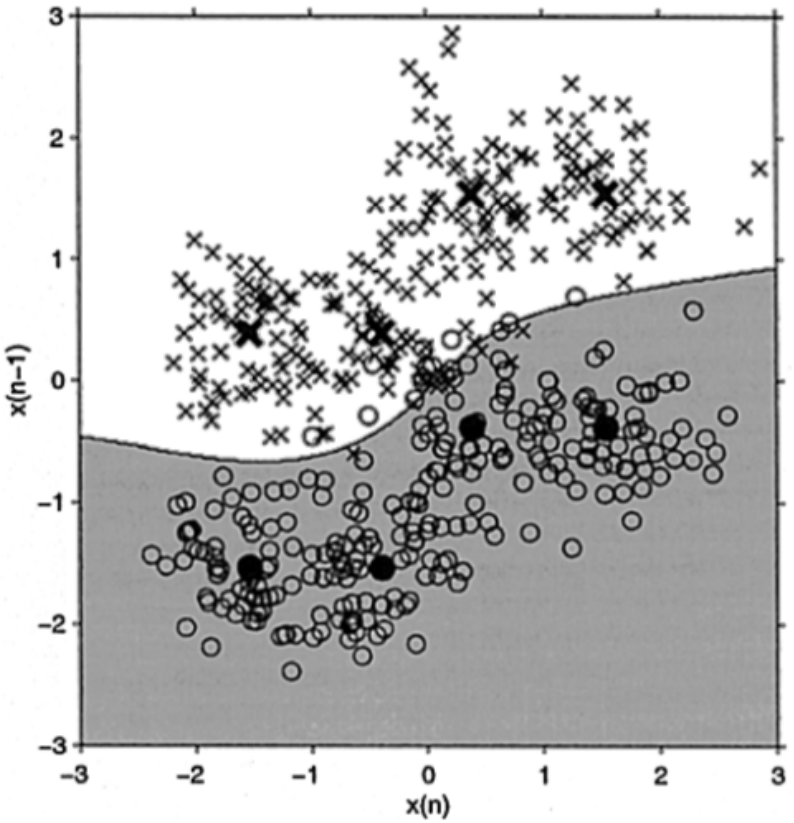


Fig. 5. Example of typical classification regions of an SVM and associated training points with the channel described in Fig. 3, except the equalizer lag is now $D = 2$.

Summary

Example of decision tree

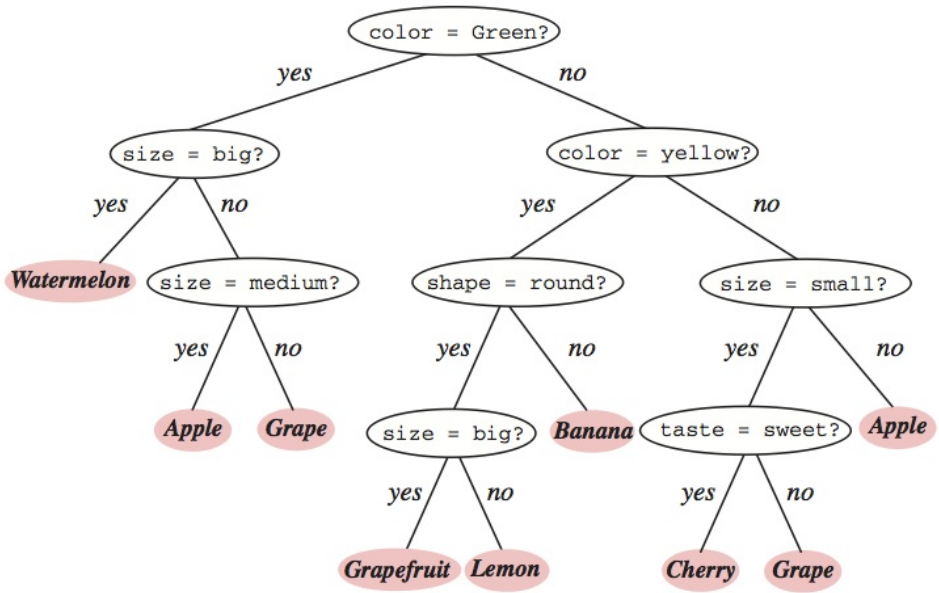


FIGURE 8.2. A tree with arbitrary branching factor at different nodes can always be represented by a functionally equivalent binary tree—that is, one having branching factor $B = 2$ throughout, as shown here. By convention the "yes" branch is on the left, the "no" branch on the right. This binary tree contains the same information and implements the same classification as that in Fig. 8.1. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.

- Construction of the tree
- Classification rule

Splitting Rules

Inhomogeneity or impurity of the data

- Entropy (Algorithm C4.5)

$$i_n = -\sum_j \frac{n_j}{n} \log_2 \left(\frac{n_j}{n} \right)$$

- Gini Index (CART)

$$i_n = \sum_j \frac{n_j}{n} \left(1 - \frac{n_j}{n} \right) = 1 - \sum_j \left(\frac{n_j}{n} \right)^2$$

Drop of Impurity

$$\Delta i_n = i_n - P_L i_L - P_R i_R$$

where $P_L = \frac{n_L}{n}, P_R = \frac{n_R}{n}$ are the proportions of the sets D_L, D_R.

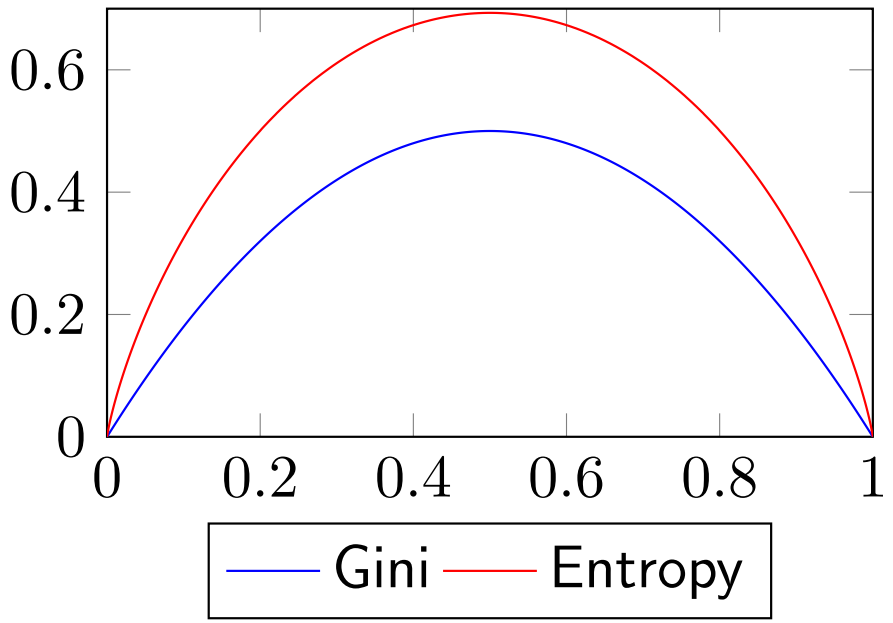
Choose the split associated with the maximum drop of impurity!

Gini Index or Entropy?

Example of 2 classes ($x = n_1/n$)

$$\text{Gini}(S) = 2x(1-x)$$

$$\text{Entropy}(S) = -x\log(x) - (1-x)\log(1-x)$$



Summary

Implementation by default

Algorithm CART (`Matlab`: ClassificationTree)

- All variables are considered for each split
- All splits are considered
- Stopping rule: pure node or number of elements less than $n_{\min}$ (specified by the user)
- Splitting rule: Gini index

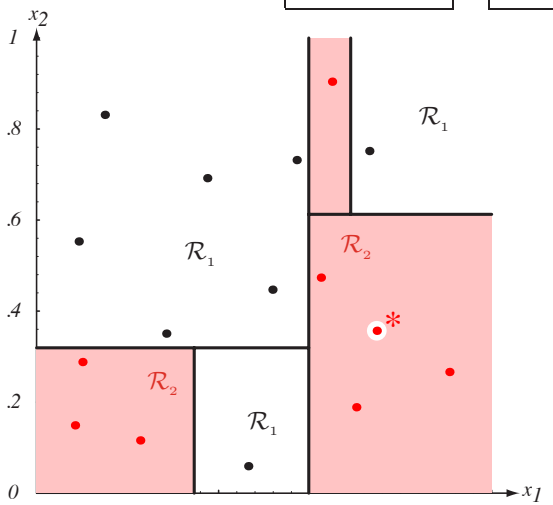
CART algorithm (example #1 for vectors in $\mathbb{R}^2$)

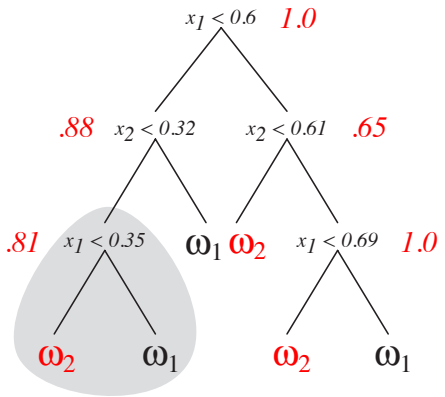
Example 1: A simple tree classifier

Consider the following $n = 16$ points in two dimensions for training a binary CART tree ($B = 2$) using the entropy impurity (Eq. 1).

ω_1 (black)	
x_1	x_2
.15	.83
.09	.55
.29	.35
.38	.70
.52	.48
.57	.73
.73	.75
.47	.06

ω_2 (red)	
x_1	x_2
.10	.29
.08	.15
.23	.16
.70	.19
.62	.47
.91	.27
.65	.90
.75	.36* (.32†)



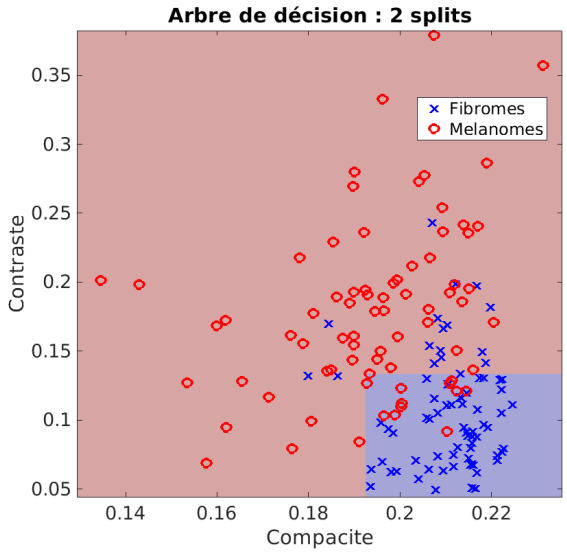


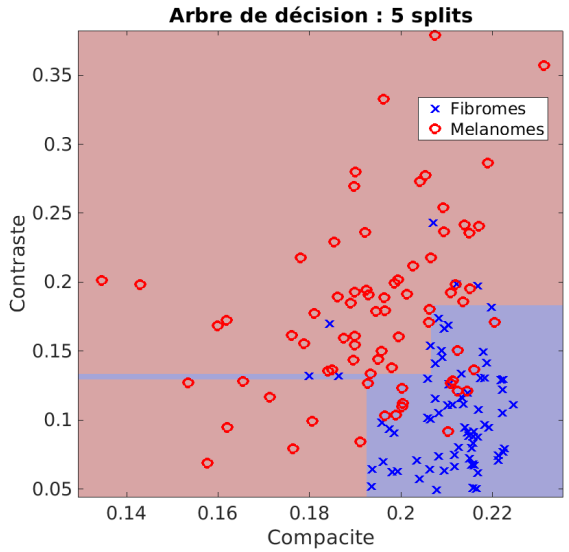
CART algorithm (example #2 for qualitative data)

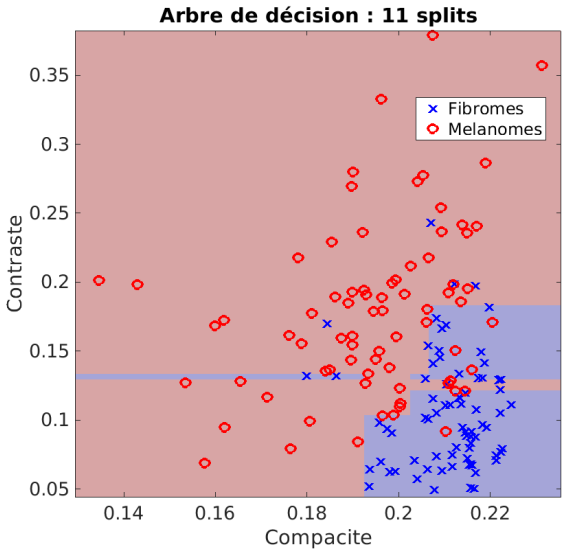
	Weight	Size	Age	Result
$\boldsymbol{x}_1$	Light	Small	Young	Pass
$\boldsymbol{x}_2$	Light	Small	Young	Pass
$\boldsymbol{x}_3$	Light	Tall	Young	Pass
$\boldsymbol{x}_4$	Light	Tall	Old	Fail
$\boldsymbol{x}_5$	Light	Tall	Old	Pass
$\boldsymbol{x}_6$	Light	Tall	Old	Fail
$\boldsymbol{x}_7$	Heavy	Small	Old	Fail
$\boldsymbol{x}_8$	Heavy	Small	Young	Fail
$\boldsymbol{x}_9$	Light	Small	Old	Pass
$\boldsymbol{x}_{10}$	Heavy	Tall	Old	Pass

- First branch (Gini Index)
  - Weight $\Rightarrow 2(1/7 + 1/15) \sim 0.42$
  - Size $\Rightarrow 12/25 \sim 0.48$
  - Age $\Rightarrow 2(3/40 + 3/20) \sim 0.45$

Lab example

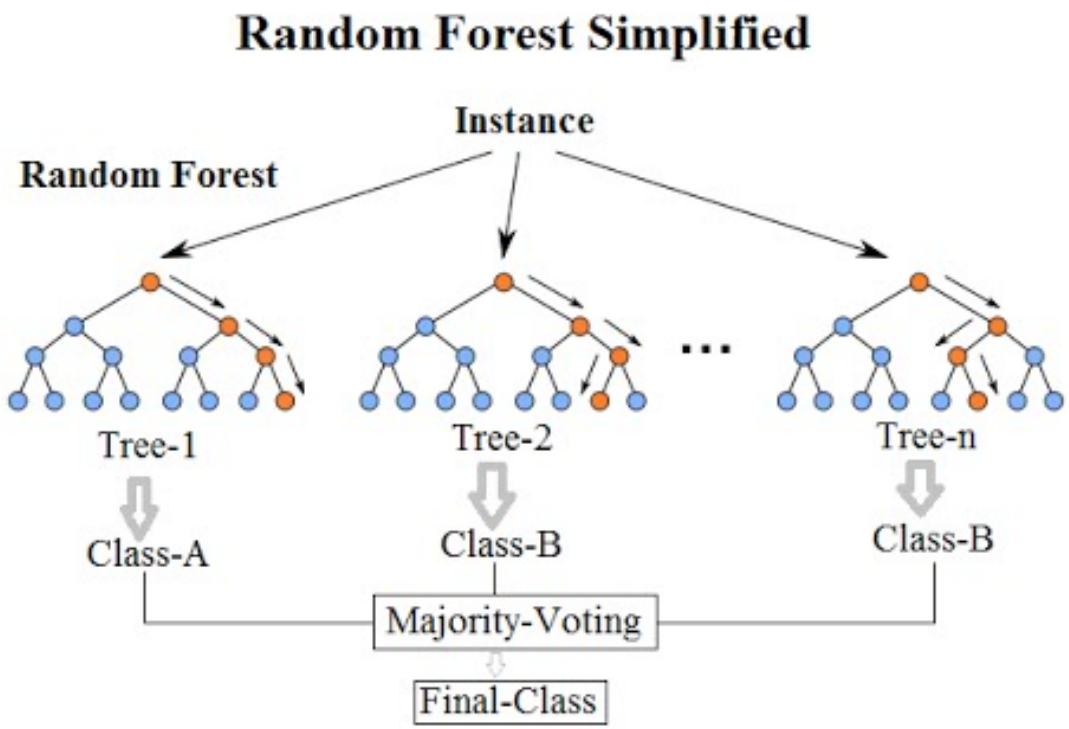

Arbre de décision : 2 splits
Fibromes
Melanomes
Contraste
Compacite
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.14
0.16
0.18
0.2
0.22


Arbre de décision : 5 splits
Fibromes
Melanomes
Contraste
Compacite
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.14
0.16
0.18
0.2
0.22


Arbre de décision : 11 splits
Fibromes
Melanomes
Contraste
Compacite
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.14
0.16
0.18
0.2
0.22

Summary

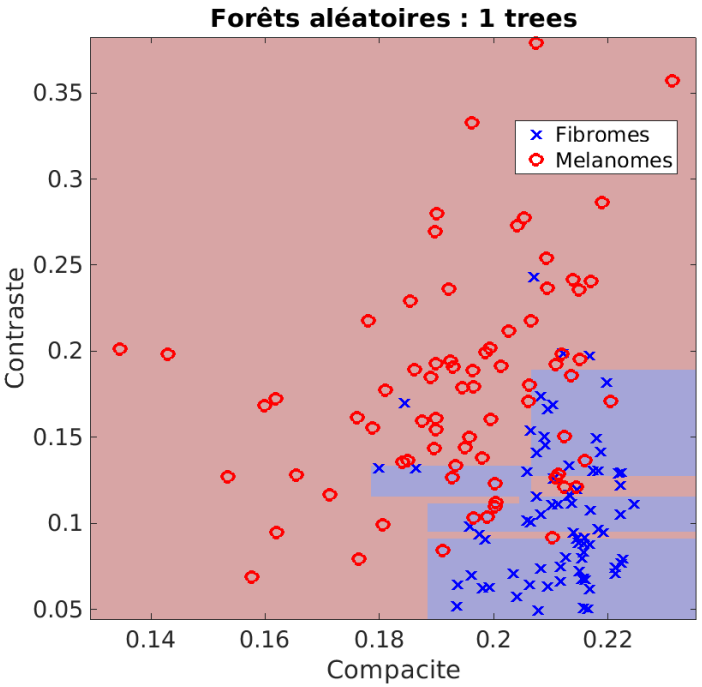
Random Forests



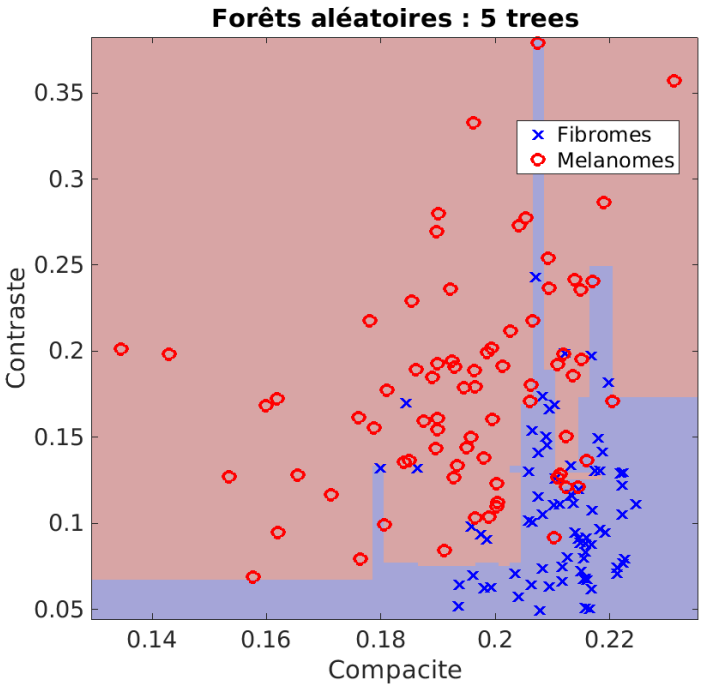
Matlab: TreeBagger (options by default)

- Resampling all the data in the training set by bootstrap (and not a subset)
- Number of variables to select at random for each decision split: $\sqrt{n_{\text{var}}}$

Lab example: number of trees (fraction of data per tree: 70%)

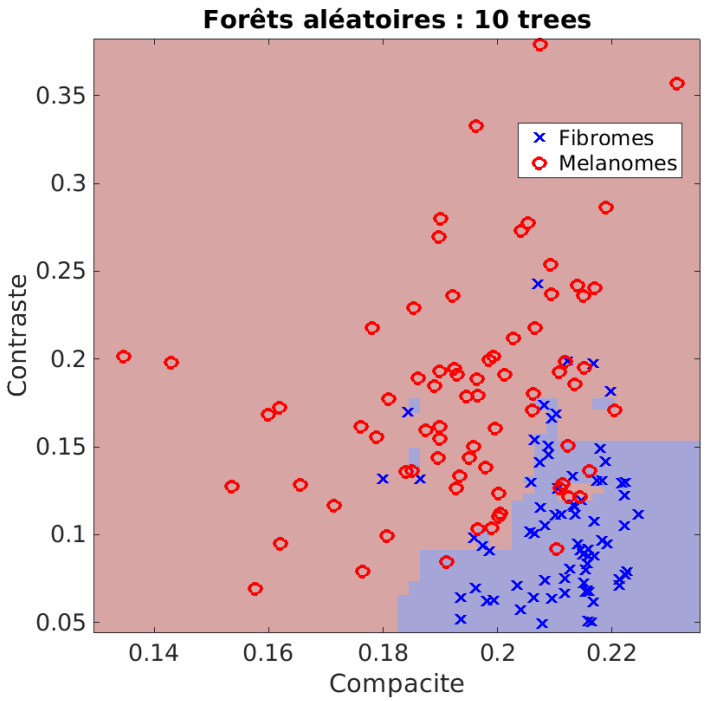


1 tree

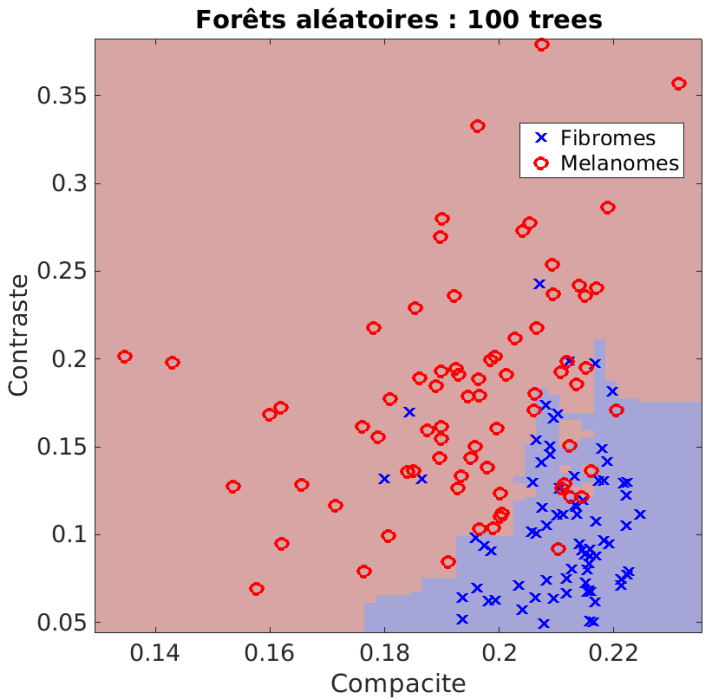


5 trees

Lab example: number of trees (fraction of data per tree: 70%)

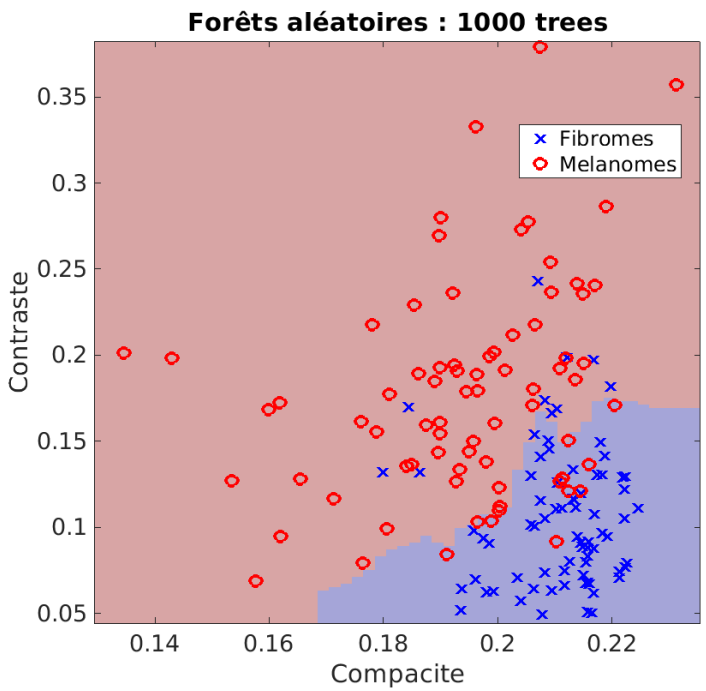


10 trees

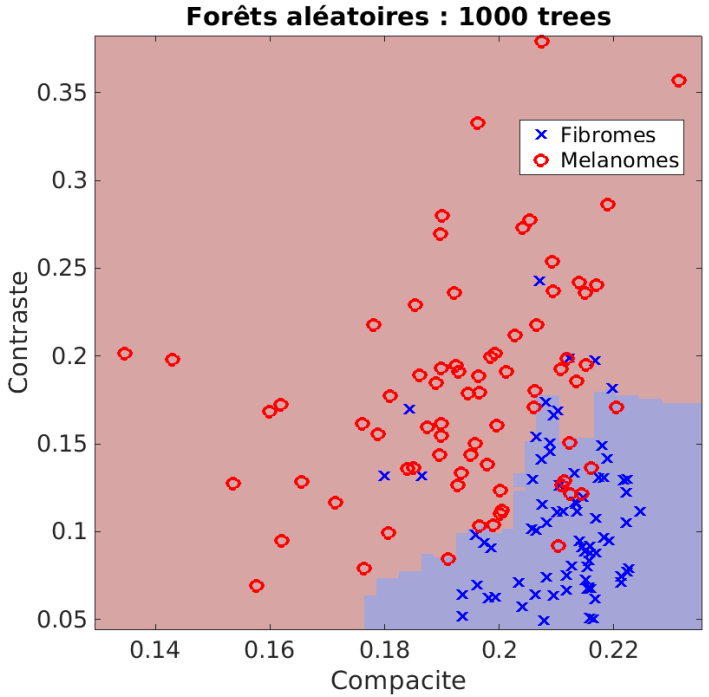


100 trees

Lab example: influence of the fraction of data per tree

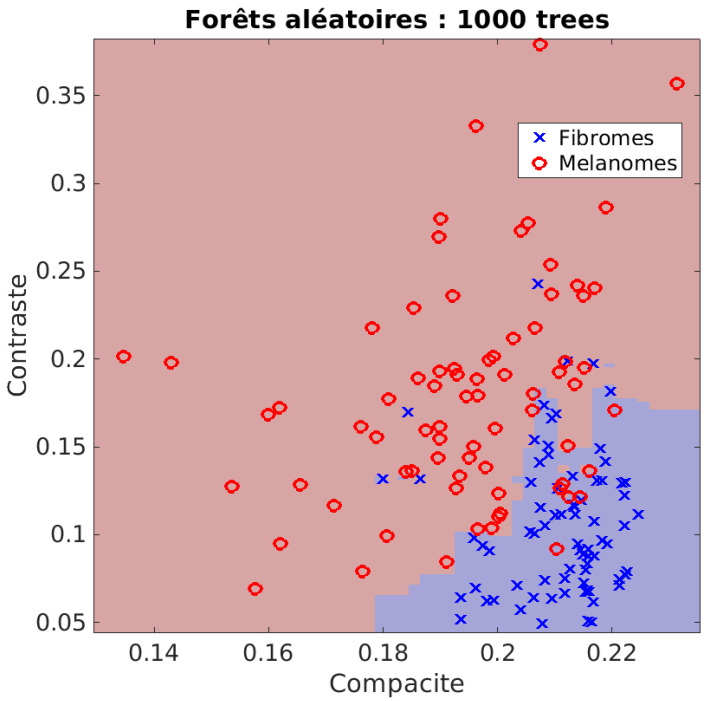


10%

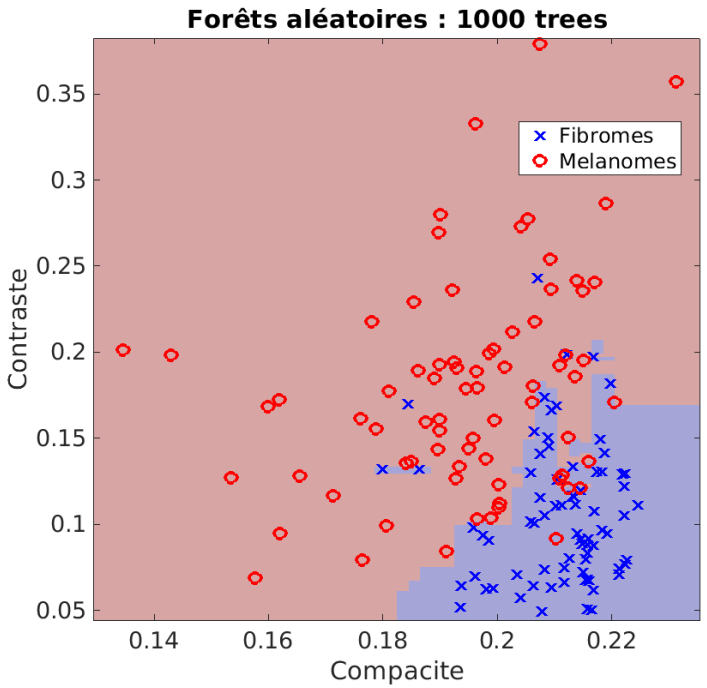


30%

Lab example: influence of the fraction of data per tree



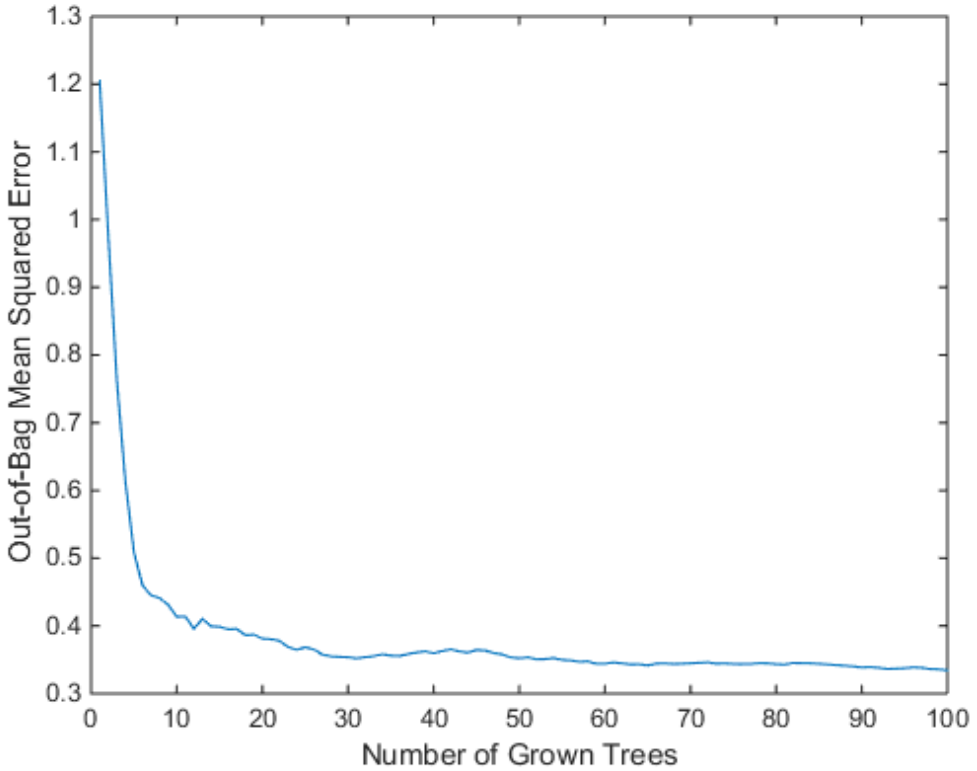
50%



70%

Out-of-bag error

Matlab example



Comparison between CART and Random Forests

Book by G. James, D. Witten, T. Hastie and R. Tibshirani

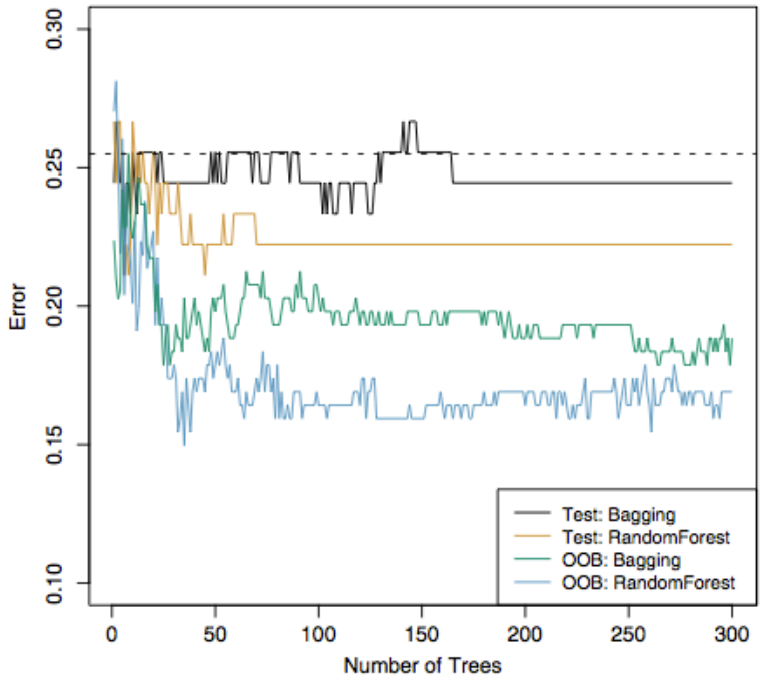


FIGURE 8.8. *Bagging and random forest results for the* `Heart` *data. The test error (black and orange) is shown as a function of* B*, the number of bootstrapped training sets used. Random forests were applied with* $m = \sqrt{p}$*. The dashed line indicates the test error resulting from a single classification tree. The green and blue traces show the OOB error, which in this case is considerably lower.*

Importance of the different variables

Mean decrease in Gini index

Average of decreases of the Gini index when the attribute has been used for splitting

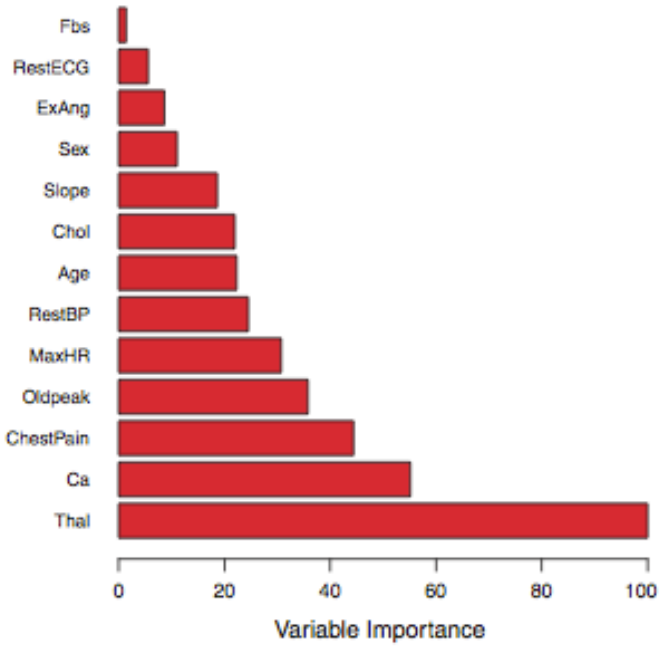


FIGURE 8.9. *A variable importance plot for the* `Heart` *data. Variable importance is computed using the mean decrease in Gini index, and expressed relative to the maximum.*

References

CART and Random Forests

- L. Breiman, J. H. Friedman, R. A. Olshen and C. J. Stone, Classification and Regression Trees, Chapman & Hall, New-York, 1993.
- L. Breiman, Random Forests, Machine Learning, vol. 45, no. 1, pp. 5-32, 2001.
- R. O. Duda, P. E. Hart and D. G. Stork, Pattern Classification, 2nd edition, Wiley, 2000.
- G. James, D. Witten, T. Hastie and R. Tibshirani, An Introduction to Statistical Learning with Applications in R, Springer, New-York, 2013.

Summary

Unsupervised learning

N unlabelled data vectors of $\mathbb{R}^p$ denoted as $\boldsymbol{X} = \{\boldsymbol{x}_1, ..., \boldsymbol{x}_N\}$ which should be split into K classes $\omega_1, ..., \omega_K$.

Motivations

- Supervised learning is costly
- The classes can change with time
- Provide some information about the data structure

Optimal solution

Number of partitions of $\boldsymbol{X}$ in K subsets

$$P(N, K) = \frac{1}{K!} \sum_{k=0}^{K} k^N (-1)^{K-k} C_K^k \qquad K < N$$

Example: $P(100, 5) \approx 10^{68}$!

Partition with minimum mean square error

Mean square error of a partition

Mean square error (MSE) of the class ω_i and of the partition $\boldsymbol{X}$

$$E_i^2 = \sum_{k=1}^{N_i} d^2\left(\boldsymbol{x}_k, \boldsymbol{g}_i\right), \qquad E^2 = \sum_{i=1}^{K} E_i^2$$

where $\boldsymbol{g}_i = \frac{1}{N_i}\sum_{k=1}^{N_i} \boldsymbol{x}_k$ is the centroid of the class ω_i

Properties

$$\sum_{k=1}^{N_i} d^2\left(\boldsymbol{x}_k, \boldsymbol{y}\right) = \sum_{k=1}^{N_i} d^2\left(\boldsymbol{x}_k, \boldsymbol{g}_i\right) + N_i d^2\left(\boldsymbol{g}_i, \boldsymbol{y}\right)$$

In particular, for $\boldsymbol{y} = \boldsymbol{g}$ (data centroid), we obtain

$$\sum_{i=1}^{K}\sum_{k=1}^{N_i} d^2\left(\boldsymbol{x}_k, \boldsymbol{g}\right) = \underbrace{\sum_{i=1}^{K}\sum_{k=1}^{N_i} d^2\left(\boldsymbol{x}_k, \boldsymbol{g}_i\right)}_{E^2} + \sum_{i=1}^{K} N_i d^2\left(\boldsymbol{g}_i, \boldsymbol{g}\right)$$

MSE of $\boldsymbol{X}$ = within-class MSE + between-class MSE

K-means Algorithm (ISODATA)

Search a partition of $\boldsymbol{X}$ ensuring a local minimum of E^2

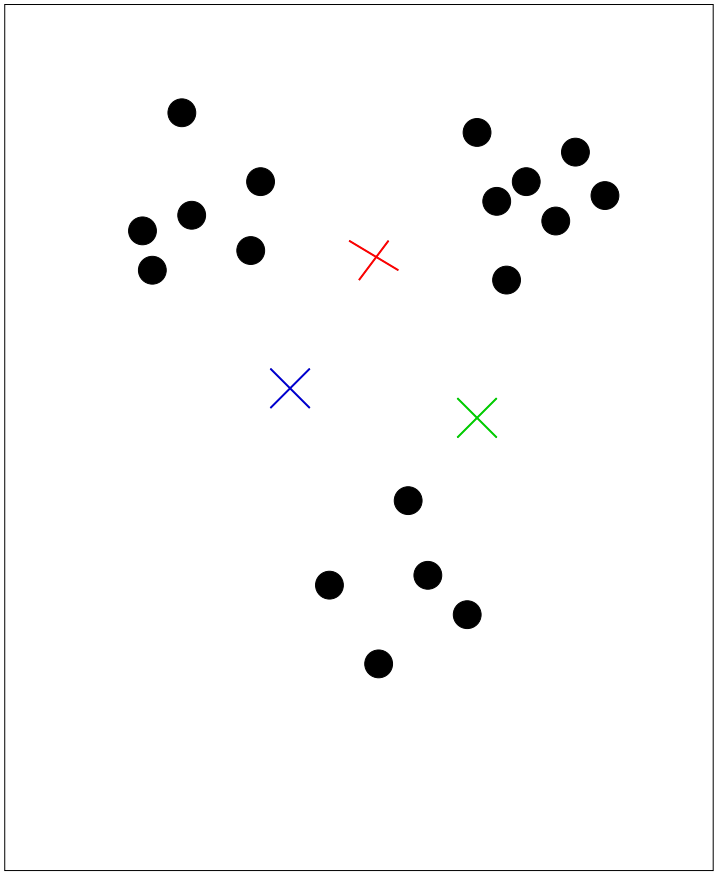
1. Initial choice of the number of classes and the class centroids
2. Assign each vector $\boldsymbol{x}_i$ to ω_j (using the centroid distance rule) such that

$$d(\boldsymbol{x}_i, \boldsymbol{g}_j) = \inf_k d(\boldsymbol{x}_i, \boldsymbol{g}_k)$$

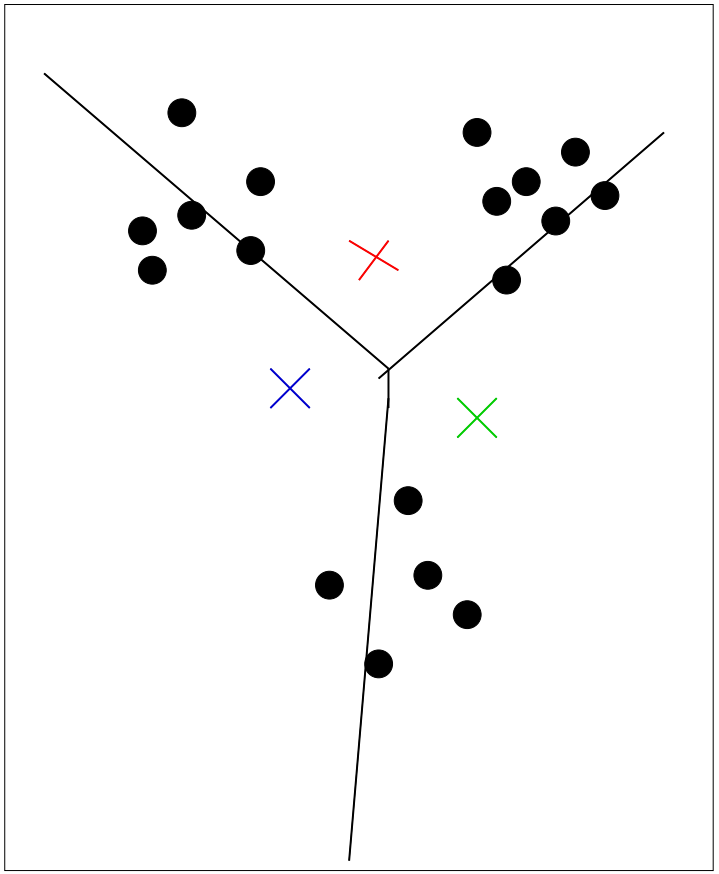
3. Compute the centroids $\boldsymbol{g}_k^*$ of the new classes ω_k^*
4. Repeat steps 2) and 3) until convergence

- *Improved version of ISODATA*
  - Two classes are merged if their centroids are close
  - A class is split if it contains too many vectors x_i or if its mean square error is too large
- *Convergence*: see notes or textbooks
- Example: `https://tmalon.github.io/k-means/`

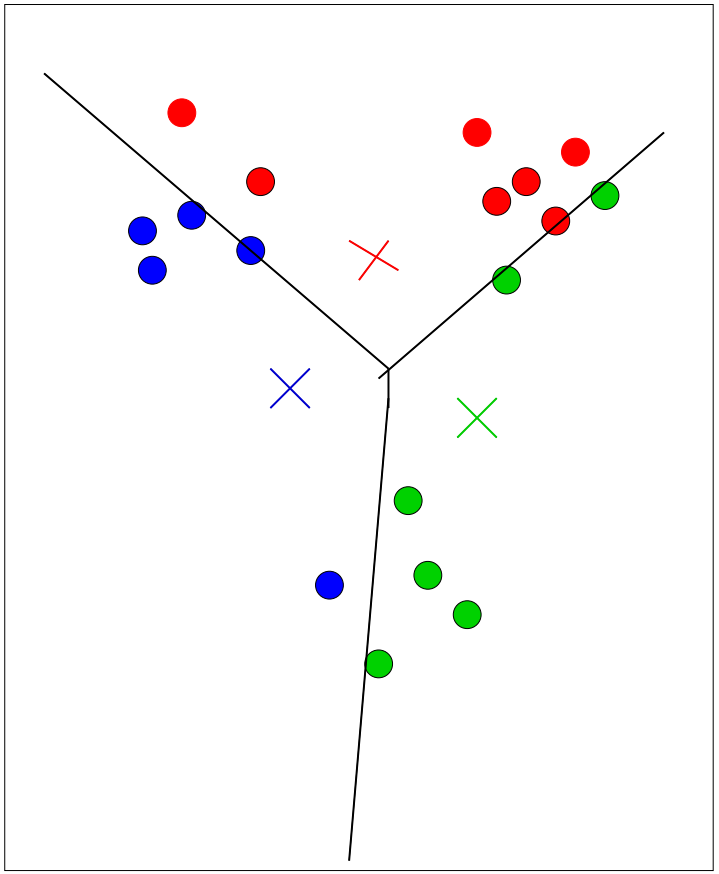
K-means



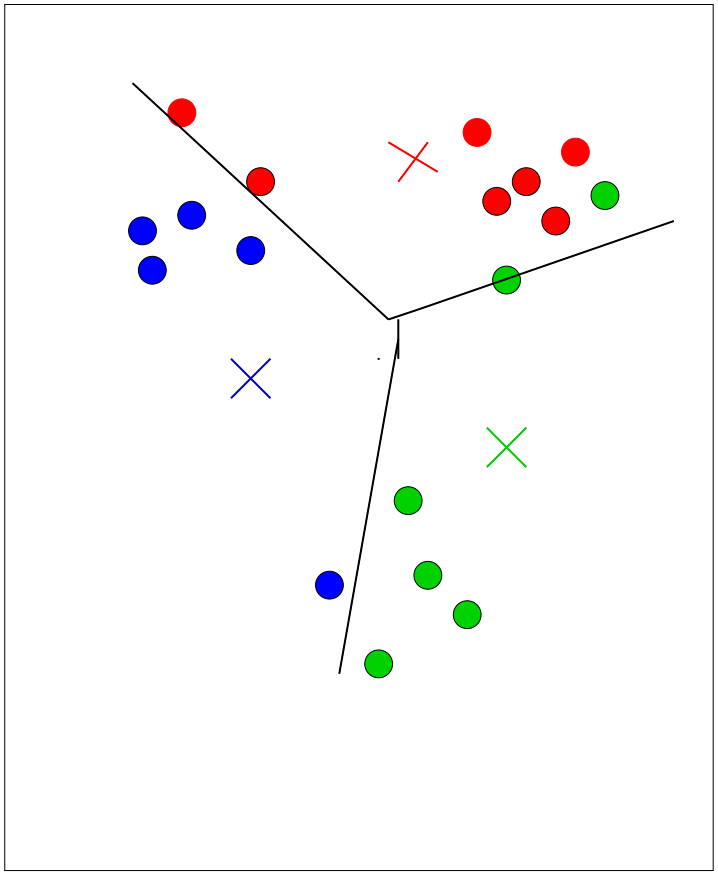
K-means



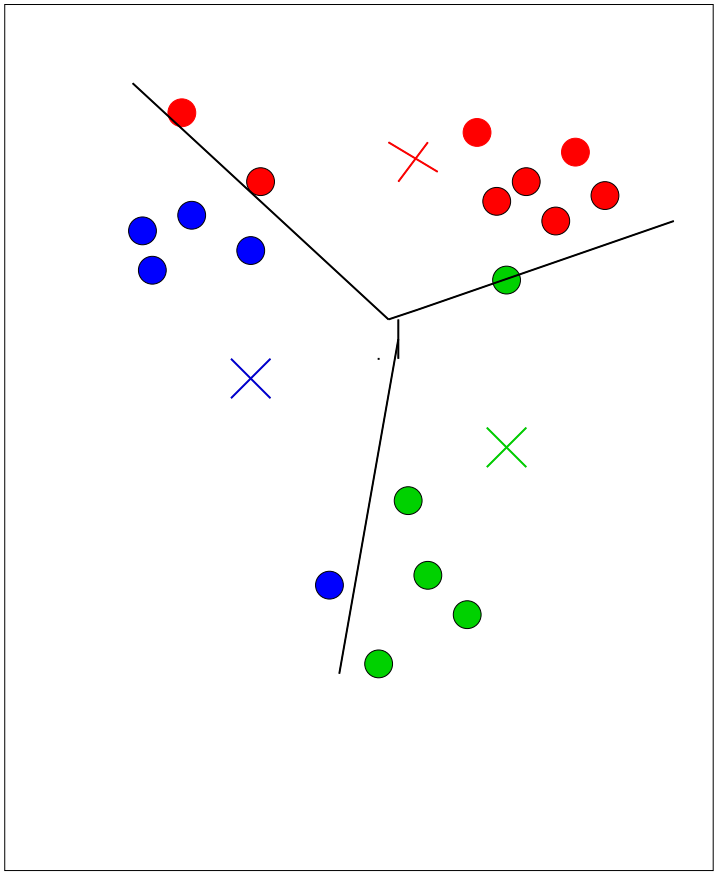
K-means



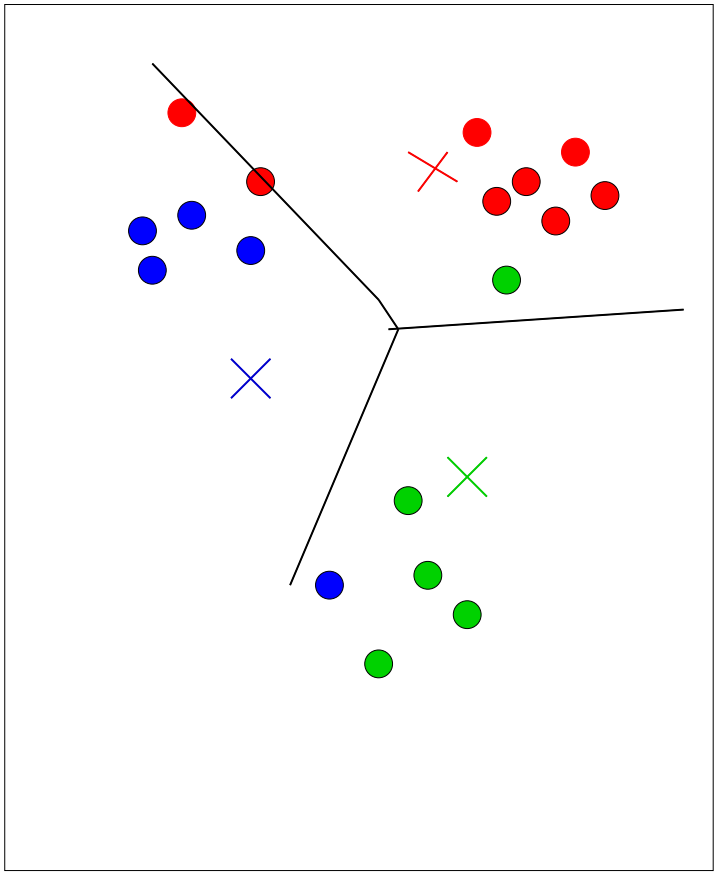
K-means



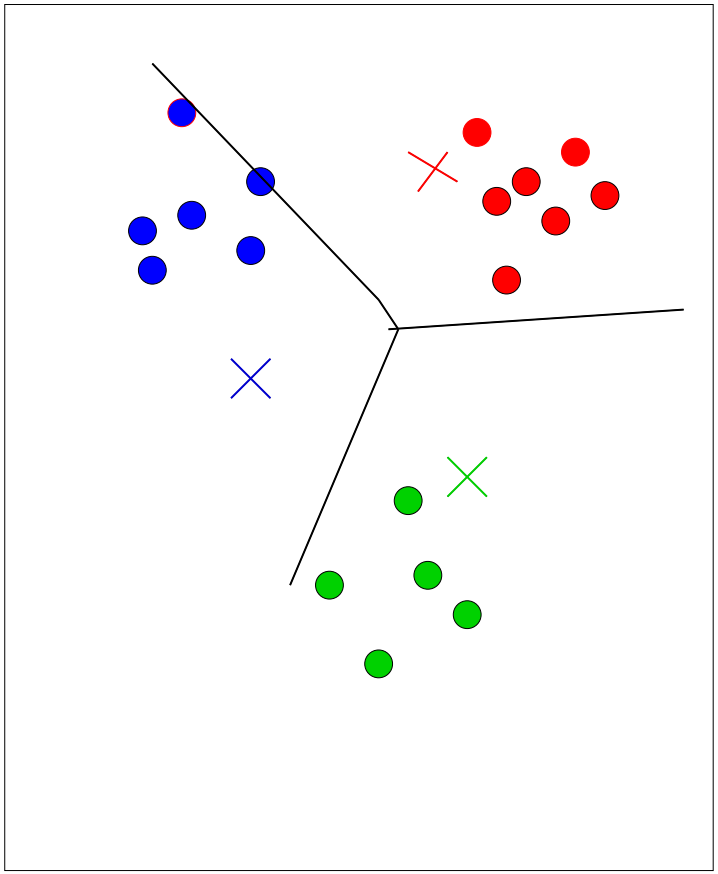
K-means



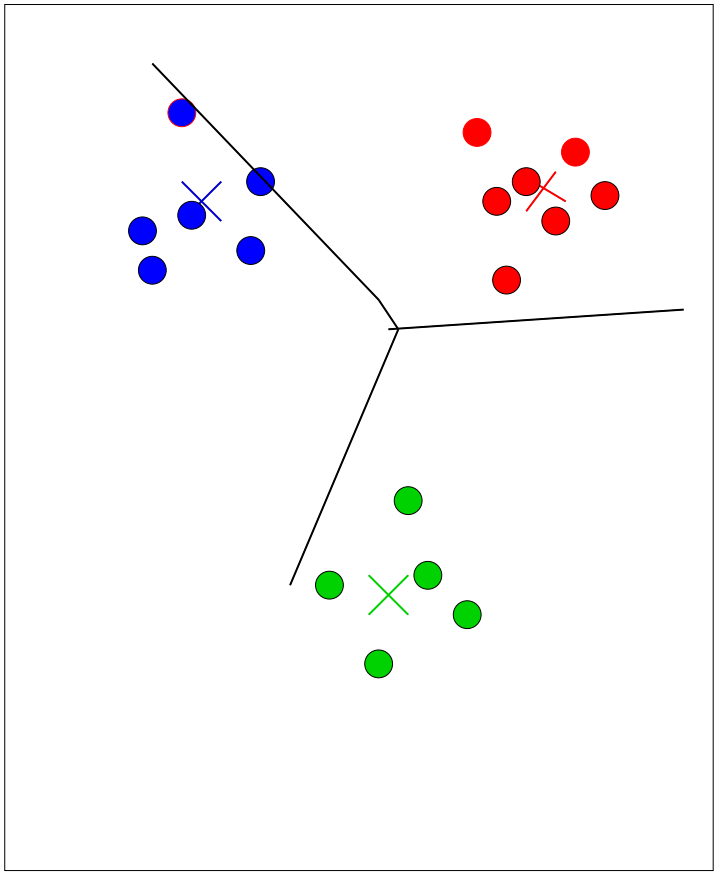
K-means



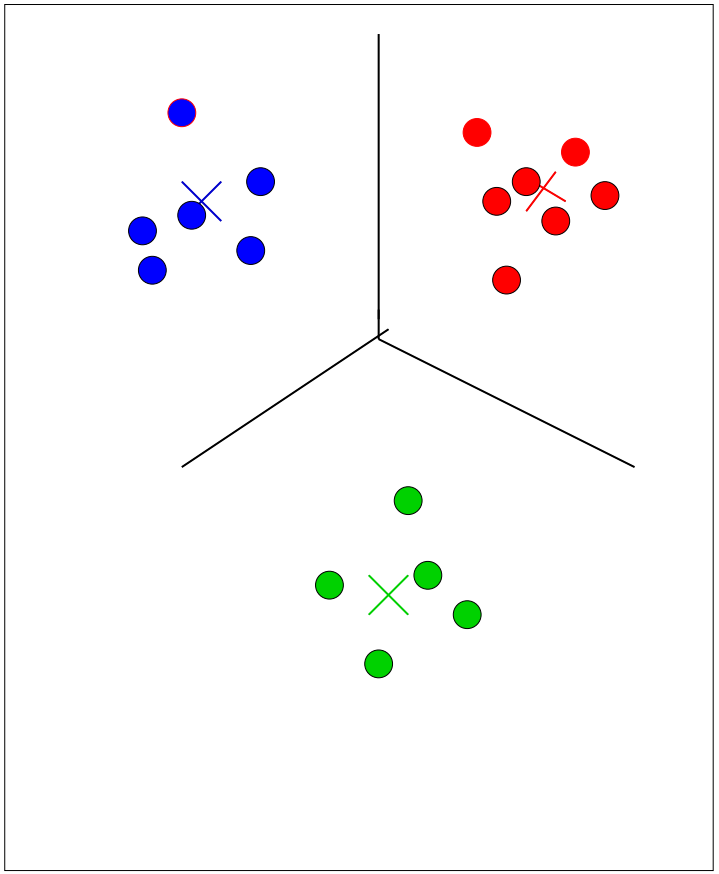
K-means



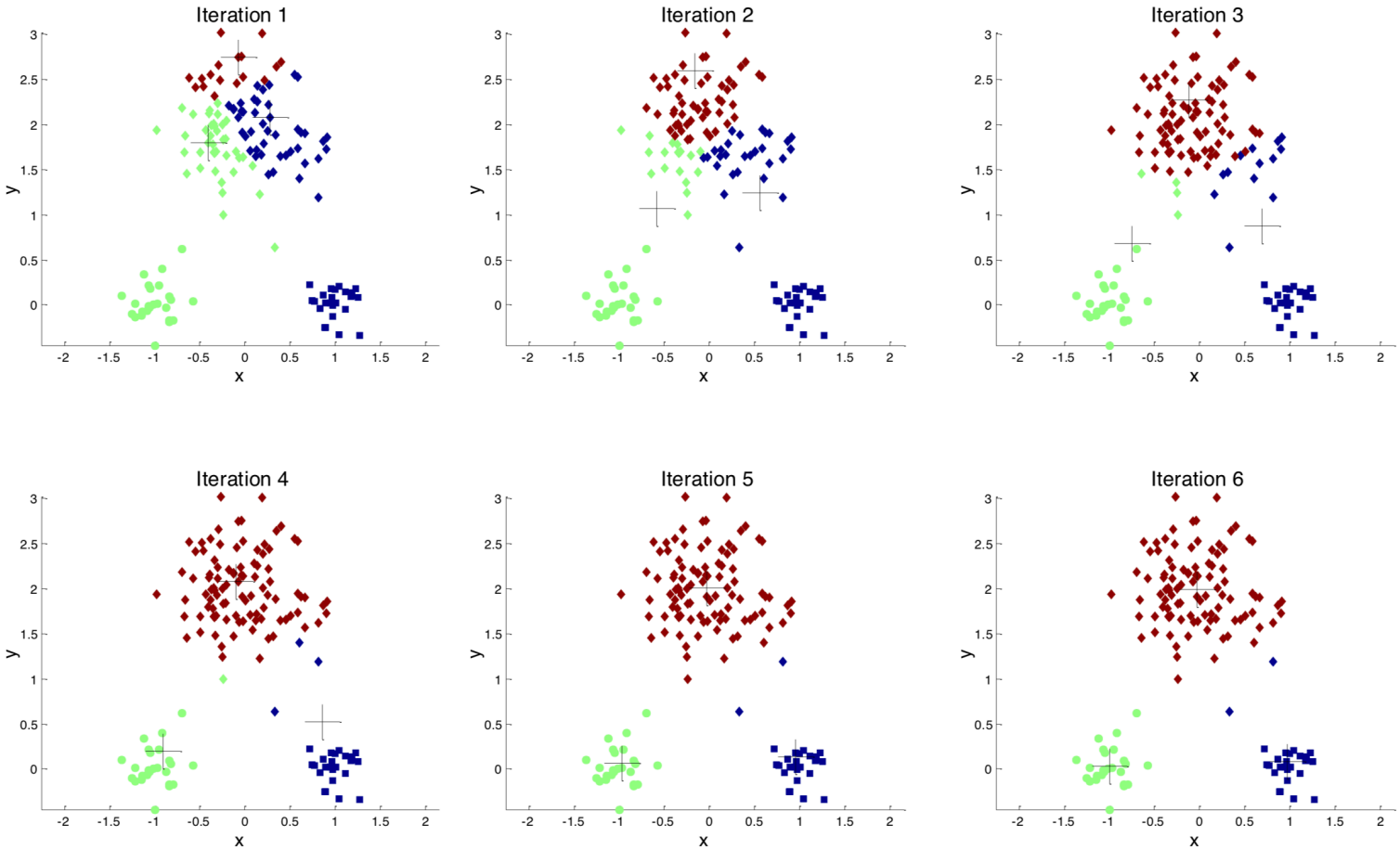
K-means



K-means

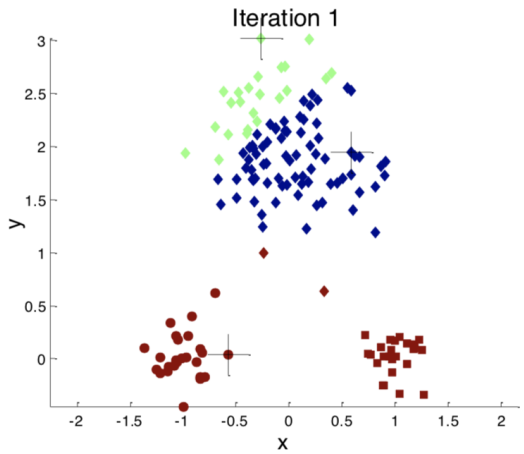


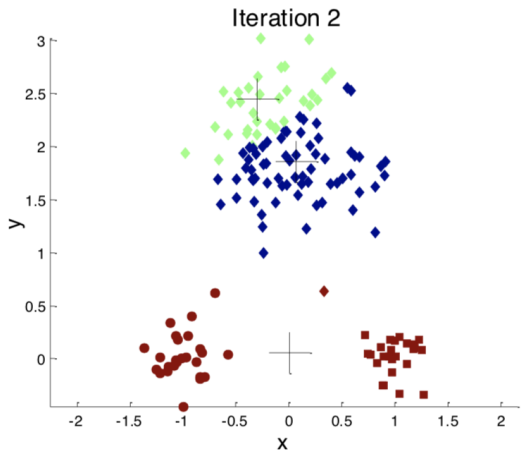
Initialization Problems

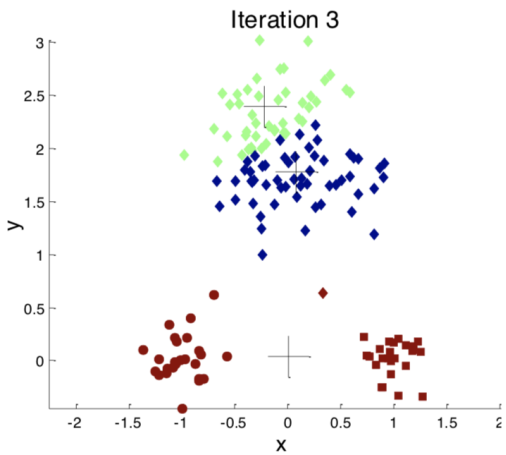


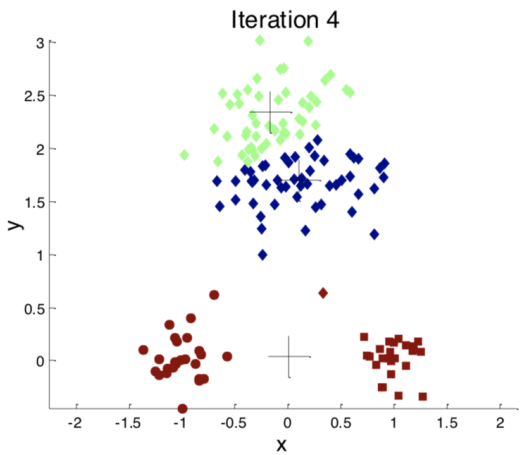
Thanks to Jing Gao from SUNY Buffalo university for her slides!!

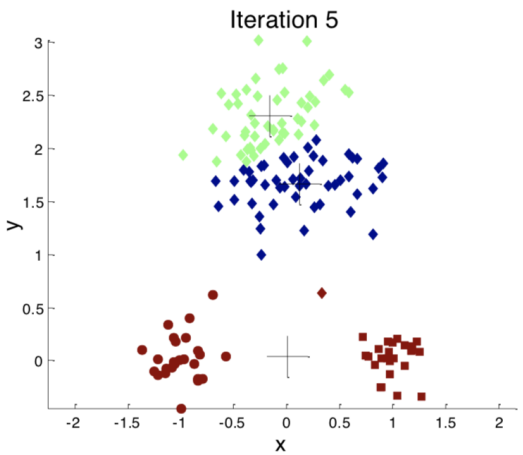
Initialization Problems



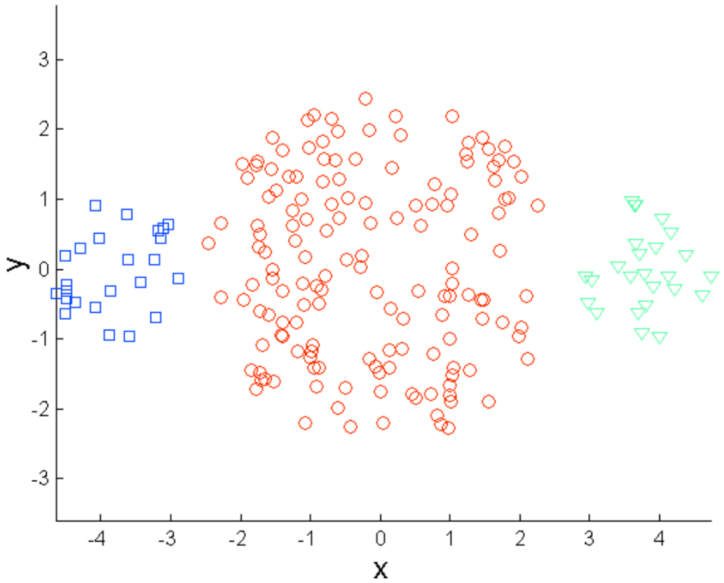




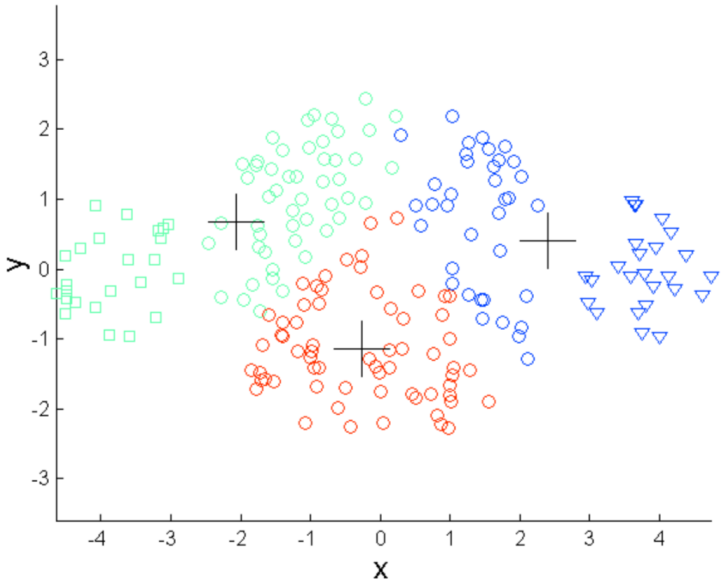




Limitations of K-means: Differing Sizes

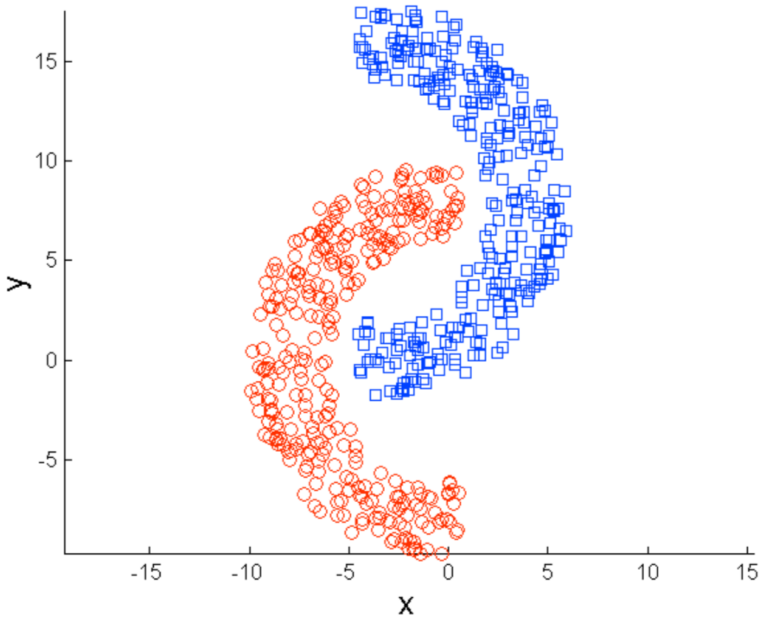


Original Points

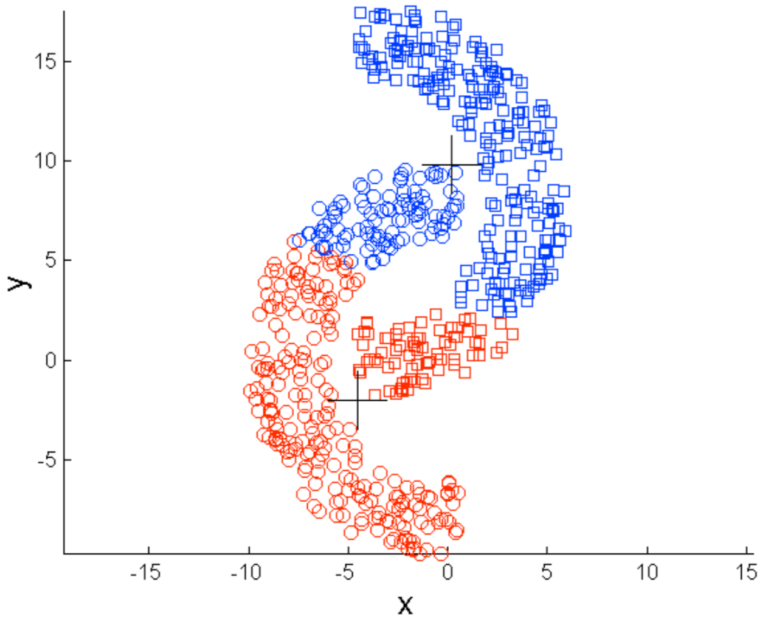


K-means (3 Clusters)

Limitations of K-means: Irregular Shapes

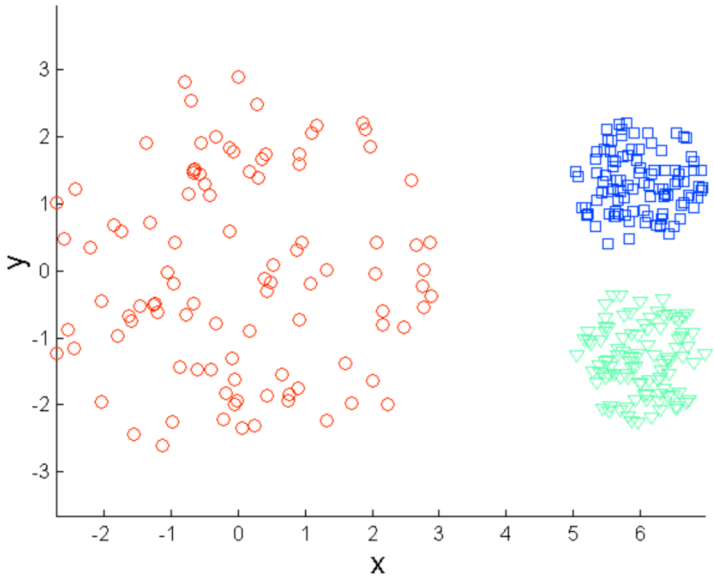


Original Points

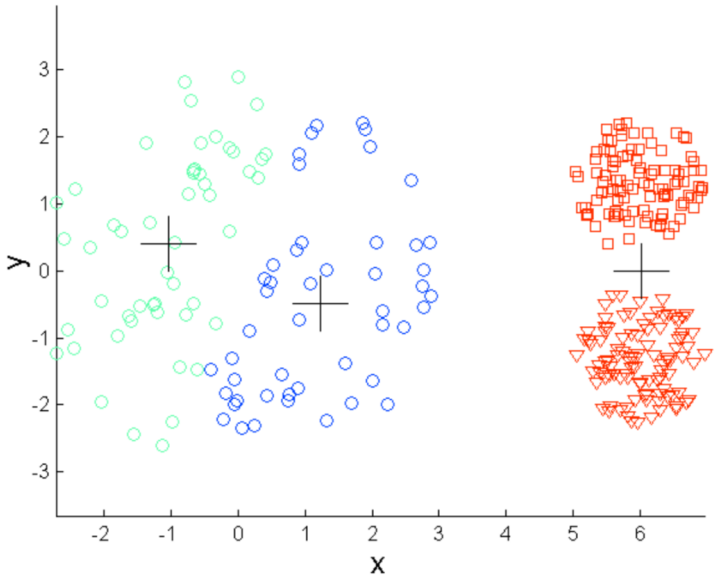


K-means (2 Clusters)

Limitations of K-means: Differing Density



Original Points



K-means (3 Clusters)

Summary

Hierarchical classification

Ascending hierarchy: method of distances

- Distance *Min* (single linkage algorithm)

$$d(X_i, X_j) = \min d(\boldsymbol{x}, \boldsymbol{y}) \qquad \boldsymbol{x} \in X_i, \boldsymbol{y} \in X_j$$

  This distance favors elongated classes

- Distance *Max* (complete linkage algorithm)

$$d(X_i, X_j) = \max d(\boldsymbol{x}, \boldsymbol{y}) \qquad \boldsymbol{x} \in X_i, \boldsymbol{y} \in X_j$$

- Average linkage algorithm

$$d(X_i, X_j) = \frac{1}{N_i N_j} \sum_{\boldsymbol{x} \in X_i, \boldsymbol{y} \in X_j} d(\boldsymbol{x}, \boldsymbol{y})$$

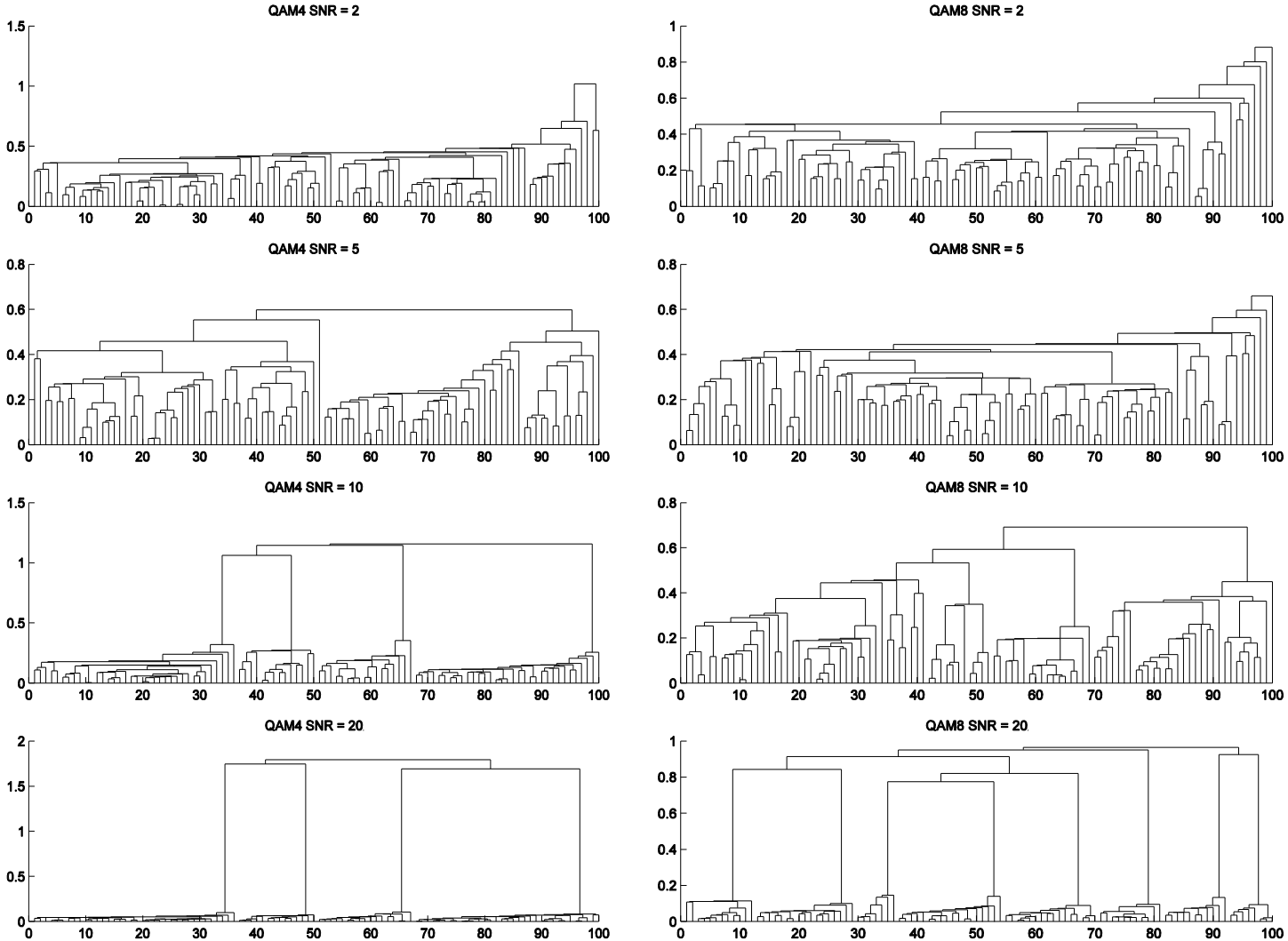
- Distance between the means

$$d(X_i, X_j) = d(\boldsymbol{g}_i, \boldsymbol{g}_j)$$

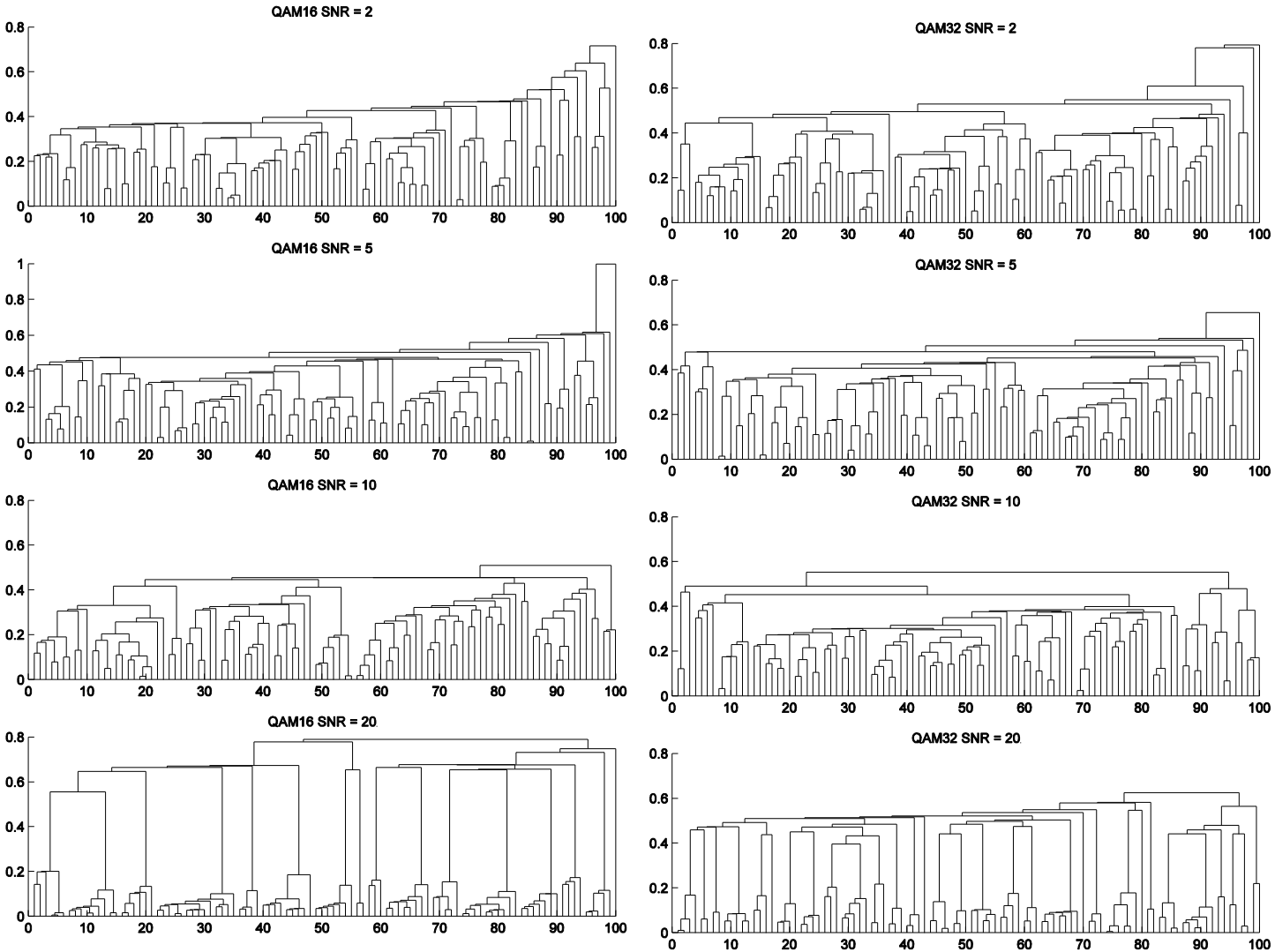
  where X_i and X_j have cardinals N_i and N_j and centroids $\boldsymbol{g}_i$ and $\boldsymbol{g}_j$.

Representation using a tree whose nodes indicate the different groups

Classification of Modulations



Classification of Modulations



Summary

Density-based clustering methods

Definitions

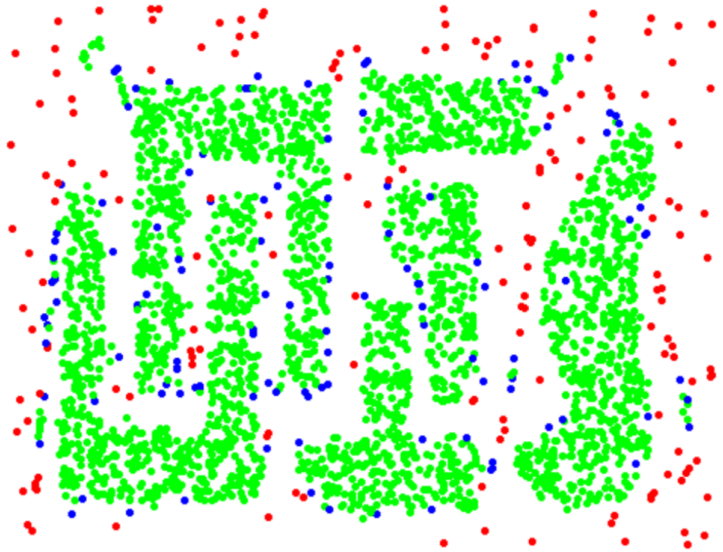
- Neighborhood of a point $p \in \boldsymbol{X}$

$$N_\epsilon(p) = \{q \in \boldsymbol{X} | d(p,q) \leq \epsilon\}$$

- Core point: a point p is a core point if it has more than MinPts neighbors in $N_\epsilon(p)$.
- Border point: a point p is a border point if it has less than MinPts neighbors in $N_\epsilon(p)$ and if it is in the neighborhood of a core point
- Noise point: a noise point is a point that is not a core point nor a border point

Core, border and noise points

Original Points



Point types: core, border and outliers

$\varepsilon = 10$, MinPts = 4

Thanks to Jing Gao from SUNY Buffalo university for her slides!!

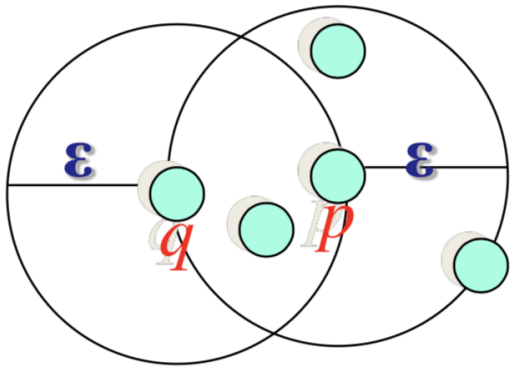
Relationships between different points

Directly density-reachable points

A point q is directly reachable from p for $(\epsilon, \mathrm{MinPts})$ if

- $q \in N_\epsilon(p)$
- p is a core point, i.e., $N_\epsilon(p)$ contains more than MinPts points.

Example



$\mathrm{MinPts} = 4$

- q is directly density-reachable from p
- p is not directly density-reachable from q (q is not a core point)

It is an asymmetric relationship!

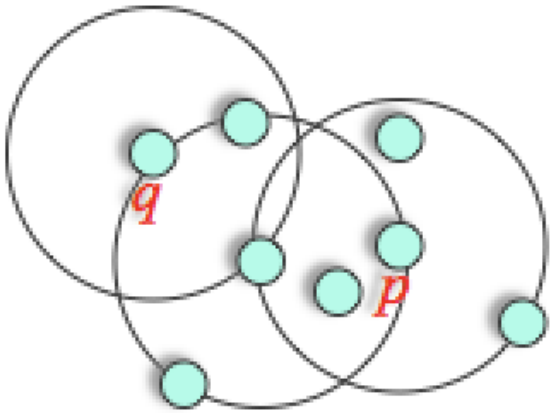
Relationships between different points

Density-reachable points

A point q is density-reachable from p for $(\epsilon, \mathrm{MinPts})$ if there is chain of points p_i such that

- $p_1 = p$ and $p_N = q$
- each point p_{i+1} is directly density-reachable from p_i.

Example



- q is directly density-reachable from p
- p is not directly density-reachable from q (q is not a core point)

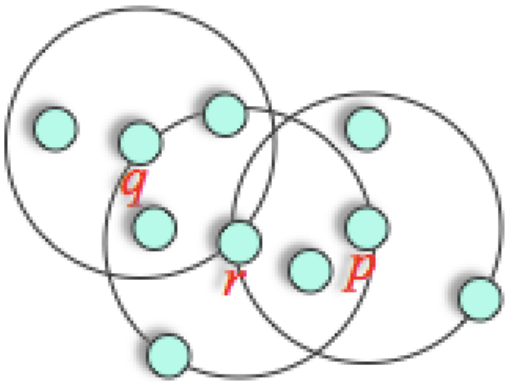
It is an asymmetric relationship!

Relationships between different points

Density-connectivity

Points p and q are density-connected for $(\epsilon, \mathrm{MinPts})$ if there is an object r such that both p and q are density reachable from r.

Example



It is a symmetric relationship!

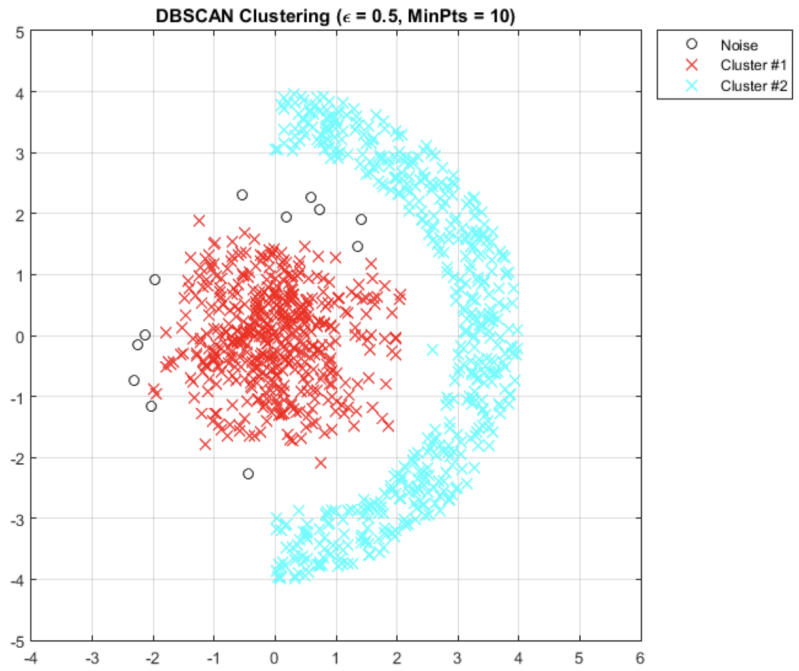
Density-Based Spatial Clustering of Applications with Noise (DBSCAN)

Cluster definition

A cluster C is defined as a maximal set of density-connected points

- Maximality: if $p \in C$ and if q is density-reachable from p, then $q \in C$.
- Connectivity: for all $(p, q) \in C$, p and q are density-connected.

Example



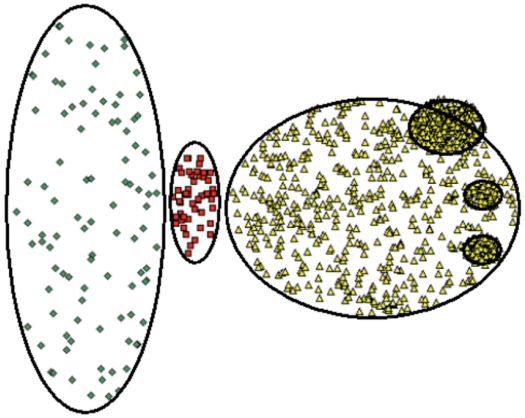
DBSCAN

A simple algorithm

- Select a point p
- Determine all density-reachable points from p for $(\epsilon, \mathrm{MinPts})$.
- If p is a core point, i.e., if the cardinal of $N_\epsilon(p)$ is larger than MinPts, a cluster is formed
- If p is a border point, DBSCAN visits the next point
- Continue the procedure until all points have been visited

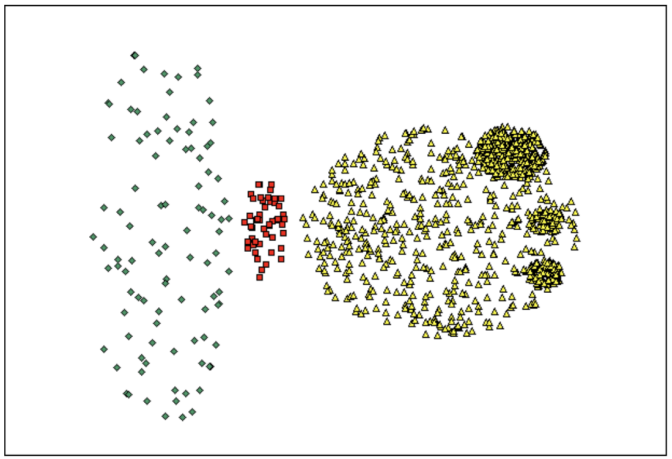
The DBSCAN algorithm generally provides a result independent of the order the points have been processed.

How can we choose ϵ and MinPts?

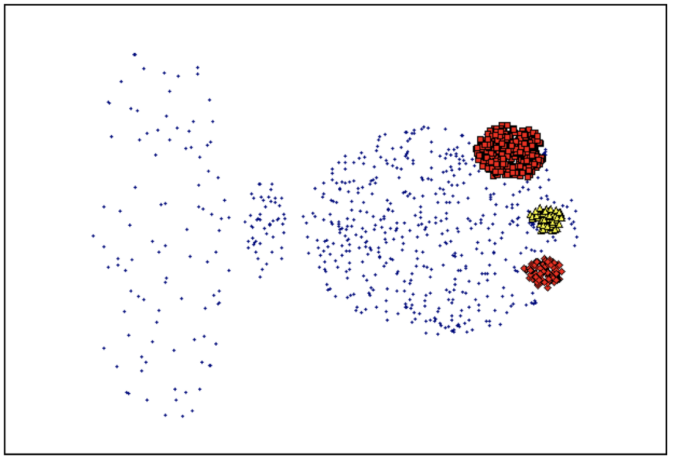


Original Points

- **Cannot handle varying densities**
- **sensitive to parameters—hard to determine the correct set of parameters**



(MinPts=4, Eps=9.92).



(MinPts=4, Eps=9.75)

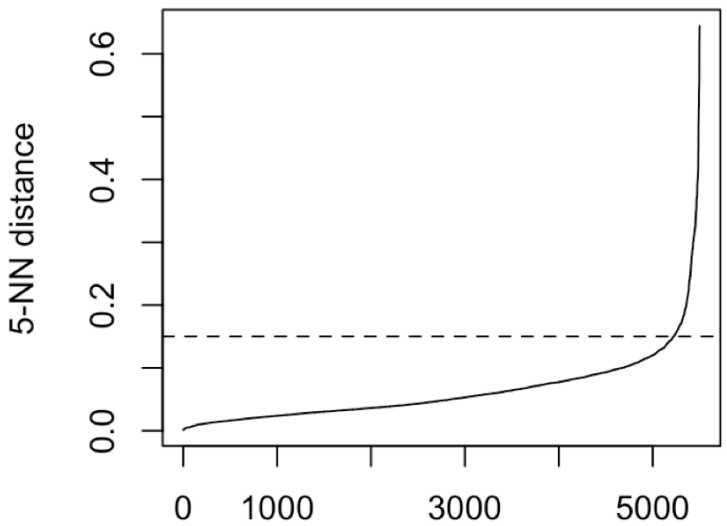
Thanks to Jing Gao from SUNY Buffalo university for her slides!!

How can we choose ϵ and MinPts?

Some ideas

- Points belonging to a cluster have a distance to their k-nearest neighbor (denoted as k-dist) smaller than noise points
- Compute all the k-dist values and sort them in increasing order
- Choose ϵ as the value of k-dist associated with a sharp change in the curve (this value does not vary significantly with the value of k)

Example



Conclusions

Pros

- Clusters of arbitrary shapes
- Robustness to noise

Cons

- Problems with clusters of different densities
- Parameter determination can be difficult

Some references (related to DBSCAN)

- M. Ester, H.-P. Kriegel, J. Sander and X. Xu, "A density-based algorithm for discovering clusters in large spatial databases with noise," in Proc. Int. Conf. Knowledge Discovery and Data Mining (KDD'96), Portland, Oregon, Aug. 1996.
- J. Gao, Slides on Data Mining and Bioinformatics, University at Buffalo, https://www.cse.buffalo.edu/ jing/cse601/fa13/.

Summary

Gaussian mixture (unsupervised learning)

Idea: N unlabelled data vectors of $\mathbb{R}^p$ denoted as $\boldsymbol{X} = \{\mathbf{x}_1, ..., \mathbf{x}_n\}$ emerge from K Gaussian components/classes denoted as $\omega_1, \ldots, \omega_K$.

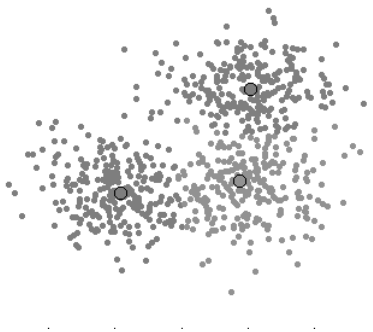
Gaussian mixture model (GMM)

- Definition

$$p(\mathbf{x}|\theta) = \sum_{k=1}^{K} \pi_k p(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \tag{3}$$

- $\boldsymbol{\theta} = (\pi_1, \ldots, \pi_K, \boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K, \boldsymbol{\Sigma}_1, \ldots, \boldsymbol{\Sigma}_K)$ contains all the parameters of the mixture model.

Example: $K = 3$ seems reasonable ($\boldsymbol{\theta}$ is unknown)



Gaussian mixture (supervised learning)

When the N data $\boldsymbol{X} = \{\mathbf{x}_1, ..., \mathbf{x}_n\}$ are *complete* (i.e. labelled, assigned to classes), the parameter estimation problem is straightforward (each Gaussian can be estimated separately). Besides the data, we also have their labels: $\{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\}$ where $y_i \in \{\omega_1, \ldots, \omega_K\}$.

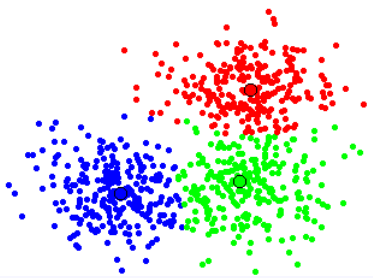
Gaussian mixture model (GMM)

- Definition

$$p(\mathbf{x}|\boldsymbol{\theta}) = \sum_{k=1}^{K} \pi_k p(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \tag{4}$$

- Assignments: binary variable $\delta(k|i)$ assigns data $\mathbf{x}_i$ to the kth Gaussian (class ω_k) if $\delta(k|i) = 1$ ($\delta(k|i) = 0$ otherwise).

Example: $K = 3$ is now given (along with data assignments).



Gaussian mixture (supervised learning)

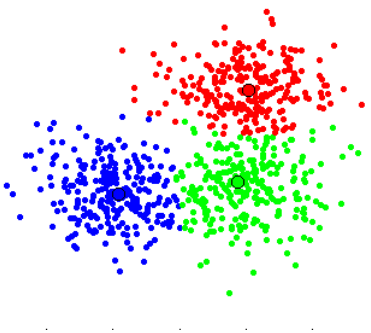
When the N data $\boldsymbol{X} = \{\mathbf{x}_1, ..., \mathbf{x}_N\}$ are *complete* (i.e., labelled or assigned to classes), the parameter estimation problem is straightforward (each Gaussian density can be estimated separately).

Estimation of the Gaussian mixture model

- $\widehat{\pi}_j \leftarrow \frac{\widehat{n}_j}{n}$ with $\widehat{n}_j = \sum_{i=1}^{n} \delta(j|i)$
- $\widehat{\boldsymbol{\mu}}_j \leftarrow \frac{1}{\widehat{n}_j} \sum_{i=1}^{n} \delta(j|i) \boldsymbol{x_i}$
- $\widehat{\boldsymbol{\Sigma}}_j \leftarrow \frac{1}{\widehat{n}_j} \sum_{i=1}^{n} \delta(j|i)(\mathbf{x_i} - \widehat{\boldsymbol{\mu}}_j)(\mathbf{x_i} - \widehat{\boldsymbol{\mu}}_j)^T$

  where $\delta(j|i) = 1$ assigns data $\mathbf{x}_i$ to the jth Gaussian density

Example: $K = 3$ is now given (along with data assignments).



Gaussian mixture (back to unsupervised case)

Without assignment (unsupervised learning), we start from an initial setting of the parameters $\boldsymbol{\theta}$: $\boldsymbol{\theta}^0 = (\pi_1^0, \ldots, \pi_K^0, \boldsymbol{\mu}_1^0, \boldsymbol{\Sigma}_1^0, \ldots, \boldsymbol{\mu}_K^0, \boldsymbol{\Sigma}_K^0)$ and compute

$$P(y_i = \omega_j | \boldsymbol{x_i}, \boldsymbol{\theta}^0) = \frac{p(\boldsymbol{x_i} | y_i = \omega_j, \boldsymbol{\theta}^0) P(\omega_j)}{\sum_{k=1}^K p(\boldsymbol{x_i} | y_i = \omega_k, \boldsymbol{\theta}^0) P(\omega_k)} \tag{5}$$

$$P(y_i = \omega_j | \boldsymbol{x_i}, \boldsymbol{\theta}^0) = \frac{\pi_j^0 p(\boldsymbol{x_i} | \boldsymbol{\mu}_j^0, \boldsymbol{\Sigma}_j^0)}{\sum_{k=1}^K \pi_k^0 p(\boldsymbol{x_i} | \boldsymbol{\mu}_k^0, \boldsymbol{\Sigma}_k^0)} \tag{6}$$

Soft assignment

- $\widehat{\delta}(j|i) = P(y_i = \omega_j | \boldsymbol{x_i}, \boldsymbol{\theta}^0)$
- $\sum_{j=1}^K \widehat{\delta}(j|i) = 1.$

Expectation-Maximization (EM-Algorithm for GMM estimation)

Without assignment (unsupervised case), we start from $\boldsymbol{\theta}^0$ and iterate soft-assignments that "complete the incomplete data" (Expectation-step) and parameter refinement (Maximisation-step). We can show that the new setting of the parameters $\boldsymbol{\theta}^{(k+1)}$ increases the log-likelihood of the "completed" data.

EM-algorithm:

1. **Initialization** Specify $\boldsymbol{\theta}^{(k=0)}$.
2. **Repeat**

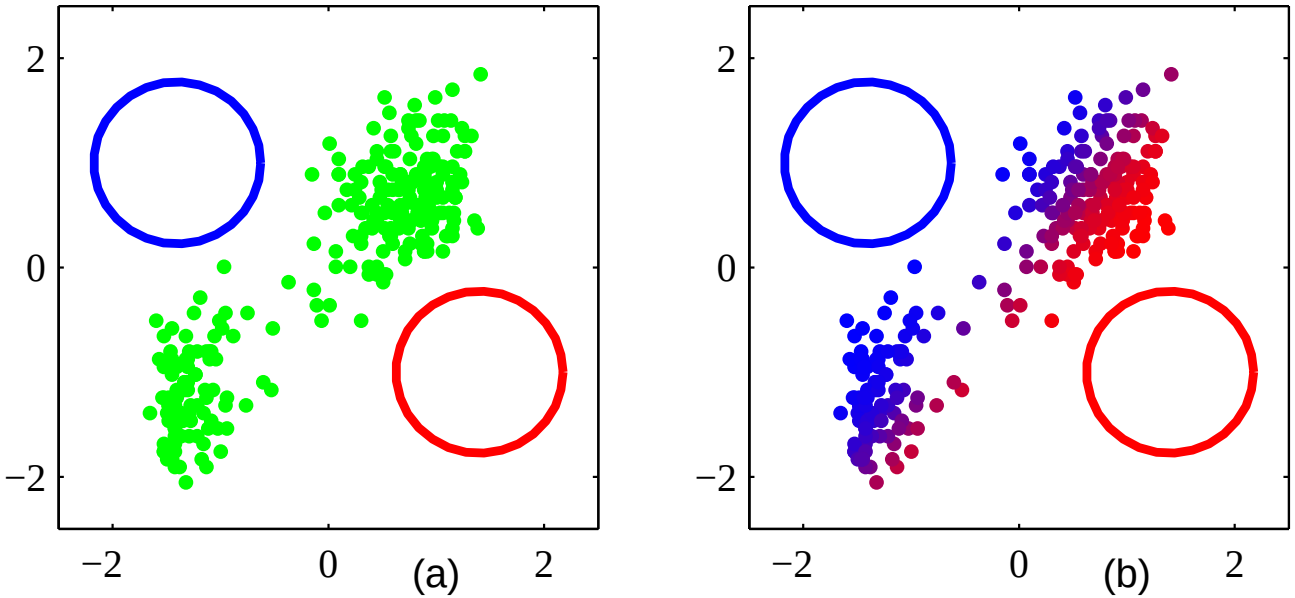
(E-step) soft-assignments of $\mathbf{x_i}$ $\forall i$

$$\widehat{\delta}(j|i) \leftarrow P(y_i = \omega_j | \mathbf{x_i}, \boldsymbol{\theta}^{(k)}) \tag{7}$$

(M-step) Refine $\theta^{(k+1)}$:

- $\widehat{\pi}_j \leftarrow \frac{\widehat{n}_j}{n}$ with $\widehat{n}_j = \sum_{i=1}^{n} \widehat{\delta}(j|i)$
- $\widehat{\boldsymbol{\mu}}_j \leftarrow \frac{1}{\widehat{n}_j} \sum_{i=1}^{n} \widehat{\delta}(j|i) \mathbf{x_i}$
- $\widehat{\boldsymbol{\Sigma}}_j \leftarrow \frac{1}{\widehat{n}_j} \sum_{i=1}^{n} \widehat{\delta}(j|i)(\mathbf{x_i} - \widehat{\boldsymbol{\mu}}_j)(\mathbf{x_i} - \widehat{\boldsymbol{\mu}}_j)^T$
- $k \leftarrow k + 1$

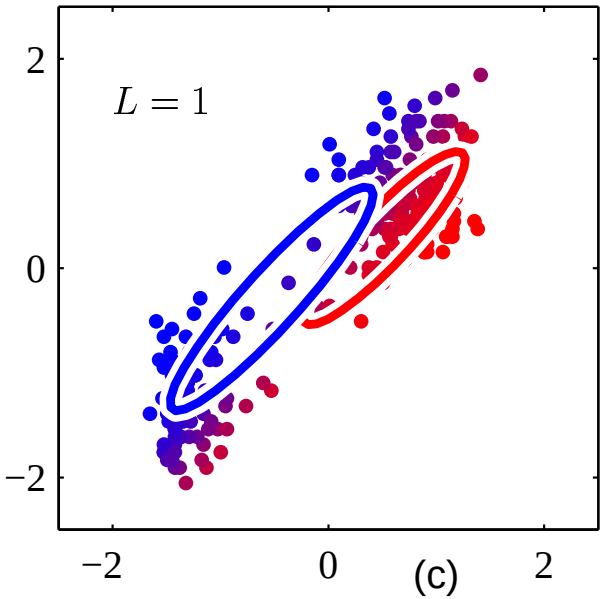
EM-Algorithm for GMM estimation (demo from book by Bishop*)



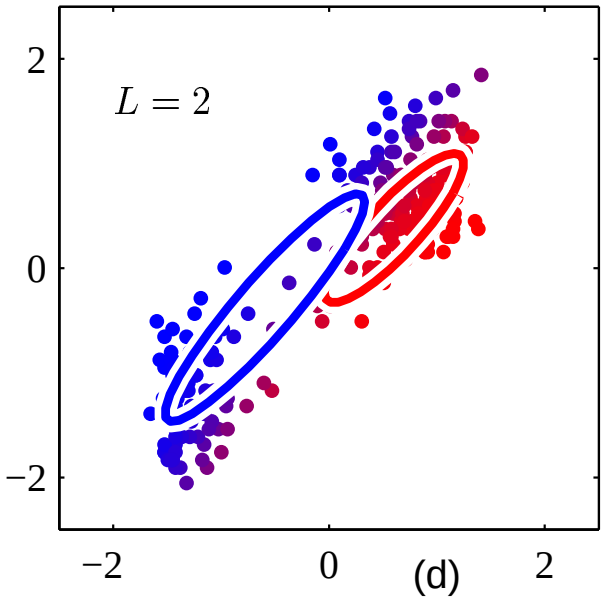
(Initialisation) (E)

* Christopher Bishop, *Pattern Recognition and Machine Learning*. New-York: Springer Verlag, 2006.

EM-Algorithm for GMM estimation (demo 2/3)

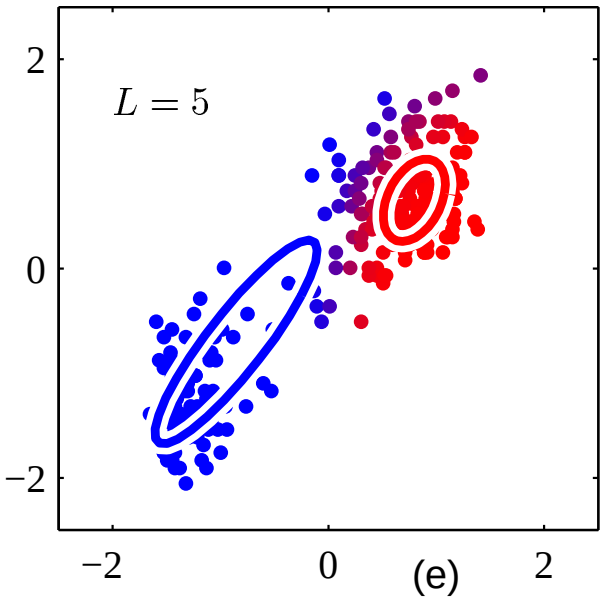


(M)

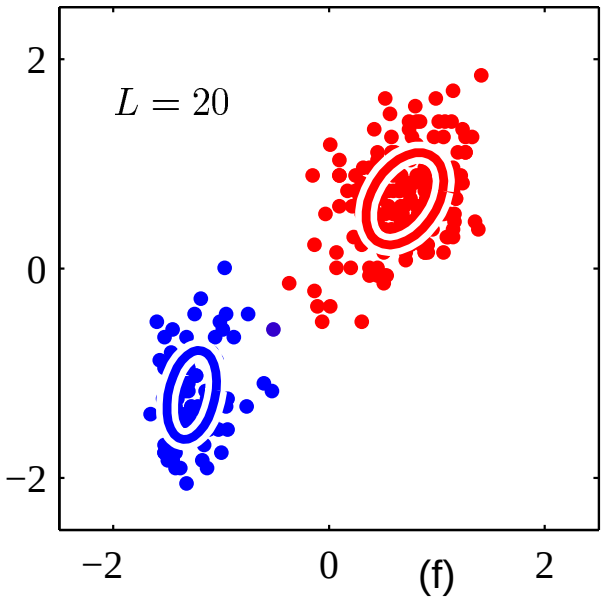


(Iteration $k = 2$)

EM-Algorithm for GMM estimation (demo 3/3)



(Iteration $k = 5$)



(Iteration $k = 20$)

Convergence

- The EM algorithm monotonically increases the log-likelihood of the data.
- We have $l(\boldsymbol{\theta}^0) < l(\boldsymbol{\theta}^1) < ... < l(\boldsymbol{\theta}^k)$ with $l(\boldsymbol{\theta}^k) = \sum_{i=1}^{n} \ln\, p(\boldsymbol{x_i}|\boldsymbol{\theta}^k)$

Mélange de lois AGGD

Vraisemblance du mélange

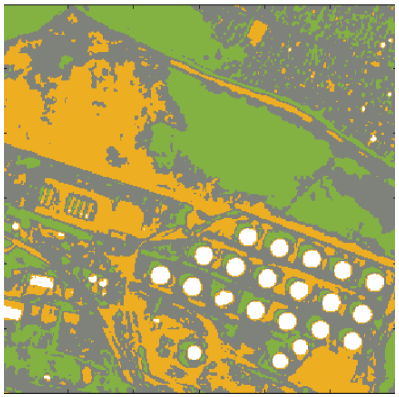
$$p(x|\theta) = \sum_{j=1}^{M} p_j p(x|\theta_j)$$

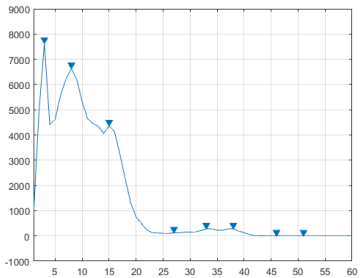
avec

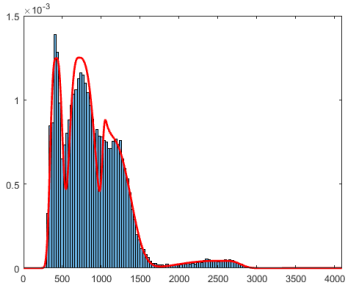
$$p(x|\theta_j) = \begin{cases} \dfrac{\delta_j^{1/\lambda_j}}{\gamma_j^{1/\lambda_j}\Gamma(1+1/\lambda_j)} \exp\left(-\dfrac{\delta_j}{\gamma_j}\left(\dfrac{\mu_j - x}{\alpha_j}\right)^{\lambda_j}\right) & \text{si } x < \mu_j \\ \dfrac{\delta_j^{1/\lambda_j}}{\gamma_j^{1/\lambda_j}\Gamma(1+1/\lambda_j)} \exp\left(-\dfrac{\delta_j}{\gamma_j}\left(\dfrac{x - \mu_j}{1-\alpha_j}\right)^{\lambda_j}\right) & \text{si } x \geq \mu_j \end{cases}$$

- α_j : paramètre d'asymétrie
- μ_j : paramètre de décalage
- γ_j : paramètre d'échelle
- λ_j : paramètre de forme
- $\delta_j = \dfrac{2\alpha_j^{\lambda_j}(1-\alpha_j)^{\lambda_j}}{\alpha_j^{\lambda_j} + (1-\alpha_j)^{\lambda_j}}$
- M : nombre de composantes

Algorithme 2







Summary

Examples of Applications

Bayes classifier

- Document classification
- Detection of SPAMS in emails

SVM

- Face detection
- Object detection and recognition

Neural networks

- Image recognition
- Natural language processing
- Object detection and recognition

CART and Random Forests

- Medical applications