

Practical introduction to machine learning

Part 3 : Supervised learning

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Overview of MAP654I

1. Data and Machine Learning problems

- ▶ Data properties and visualization
- ▶ Pre-processing
- ▶ Finding your Machine Learning problem

2. Unsupervised learning

- ▶ Clustering
- ▶ Density estimation and generative modeling
- ▶ Dictionary learning and collaborative filtering
- ▶ Dimensionality reduction and manifold learning

3. Supervised learning

- ▶ Bayesian decision and Nearest neighbors
- ▶ Linear models nonlinear methods for regression and classification
- ▶ Trees, forest and ensemble methods

4. Machine learning in practice

- ▶ Performance measures
- ▶ Models and parameter selection (validation)
- ▶ Interpretation of the methods

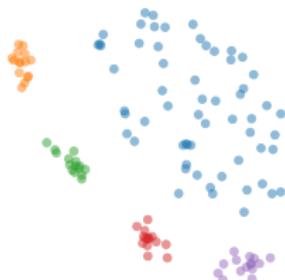
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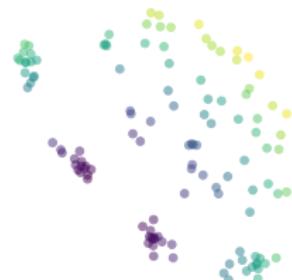
Supervised dataset

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_i^\top \\ \vdots \\ \mathbf{x}_n^\top \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_i \\ \vdots \\ y_n \end{bmatrix}$$

Classification



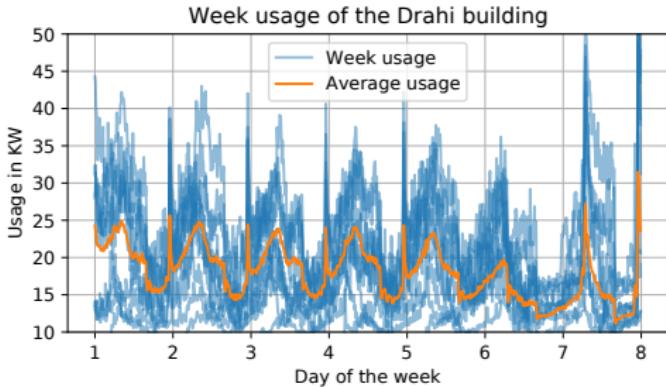
Regression



Supervised learning

- ▶ The dataset contains the samples $\{\mathbf{x}_i, y_i\}_{i=1}^n$ where \mathbf{x}_i is the feature sample and $y_i \in \mathcal{Y}$ its label.
- ▶ The values to predict (label) can be concatenated in a vector $\mathbf{y} \in \mathcal{Y}^n$
- ▶ Prediction space \mathcal{Y} can be:
 - ▶ $\mathcal{Y} = \{-1, 1\}$ or $\mathcal{Y} = \{1, \dots, p\}$ for classification problems.
 - ▶ $\mathcal{Y} = \mathbb{R}$ for regression problems (\mathbb{R}^p for multi-output regression).
 - ▶ Structured for structured prediction (graphs,...).
- ▶ Scatter plots for supervised data (`plt.scatter`) use color for the label.

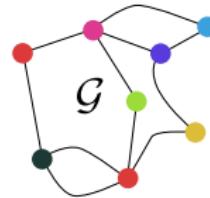
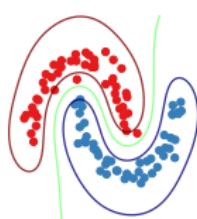
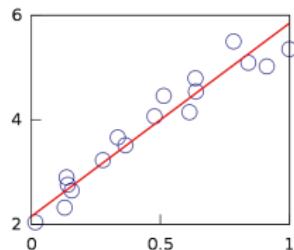
Example of real life dataset



Electrical usage of the Drahi X-Novation Center

- ▶ Demonstrator of Energy4Climate of IP Paris.
- ▶ Recording of the electrical usage of the building during 1.5 years.
- ▶ Each day of energy usage contains 144 measurements.
- ▶ Supervised learning problem from the measurements of the last two days ($d = 288$) predict:
 - ▶ If the energy usage will lower or increase on the next day (classification)
 - ▶ The energy usage for the next day (regression).

Supervised learning



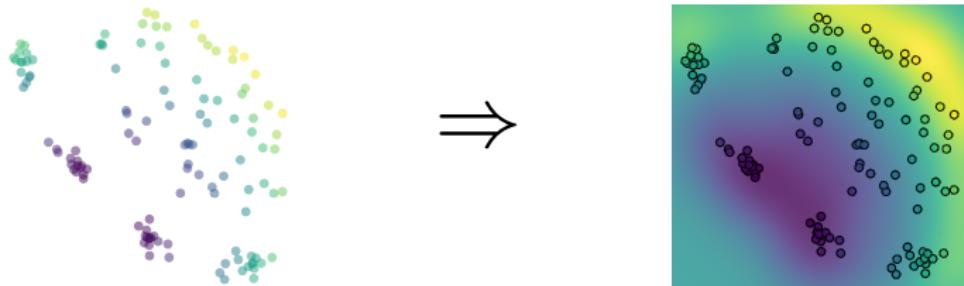
Objective

- ▶ Training dataset : $\{\mathbf{x}_i, y_i\}_{i=1}^n$ with observations $\mathbf{x}_i \in \mathbb{R}^d$ and labels $y_i \in \mathcal{Y}$.
- ▶ Train a function $f(\cdot) : \mathbb{R}^d \rightarrow \mathcal{Y}$ on the dataset.

Types of supervised prediction

- ▶ **Classification** $f(\cdot)$ predicts a class (discrete output) either binary $\mathcal{Y} = \{-1, 1\}$ or multiclass $\mathcal{Y} = \{1, \dots, p\}$.
- ▶ **Regression** $f(\cdot)$ predicts a continuous value ($\mathcal{Y} = \mathbb{R}$) or several ($\mathcal{Y} = \mathbb{R}^p$).
- ▶ **Structured prediction** $f(\cdot)$ predicts a structured object (graph, tree, molecule) (not discussed here).

Regression



Objective

$$\{\mathbf{x}_i, y_i\}_{i=1}^n \Rightarrow f : \mathbb{R}^d \rightarrow \mathbb{R}$$

- ▶ Train a function $f(\mathbf{x}) = y \in \mathcal{Y}$ predicting a continuous value ($\mathcal{Y} = \mathbb{R}$).
- ▶ Can be extended to multi-value prediction ($\mathcal{Y} = \mathbb{R}^p$).

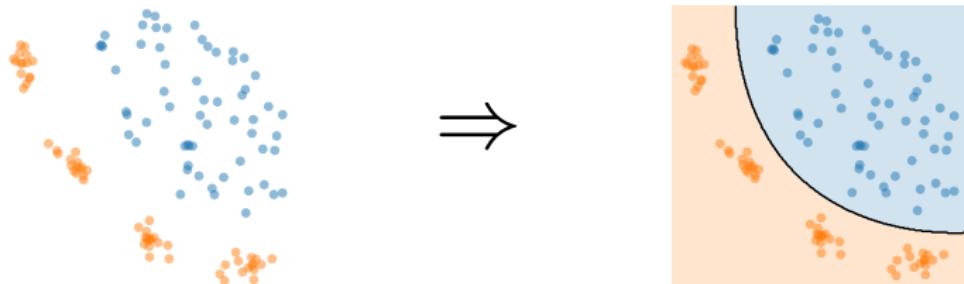
Parameters

- ▶ Type of function (linear, kernel, neural network).
- ▶ Performance measure.
- ▶ Regularization.

Methods

- ▶ Least Square (LS).
- ▶ Ridge regression, Lasso.
- ▶ Kernel regression.
- ▶ Deep learning.

Binary classification



Objective

$$\{\mathbf{x}_i, y_i\}_{i=1}^n \quad \Rightarrow \quad f : \mathbb{R}^d \rightarrow \{-1, 1\}$$

- ▶ Train a function $f(\mathbf{x}) = y \in \mathcal{Y}$ predicting a binary value ($\mathcal{Y} = \{-1, 1\}$).
- ▶ In practice, train a continuous function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ and predict with $\text{sign}(f)$.
- ▶ $f(\mathbf{x}) = 0$ defines the boundary on the partition of the feature space.
- ▶ Optional: provide uncertainty information such as probabilities of each class.

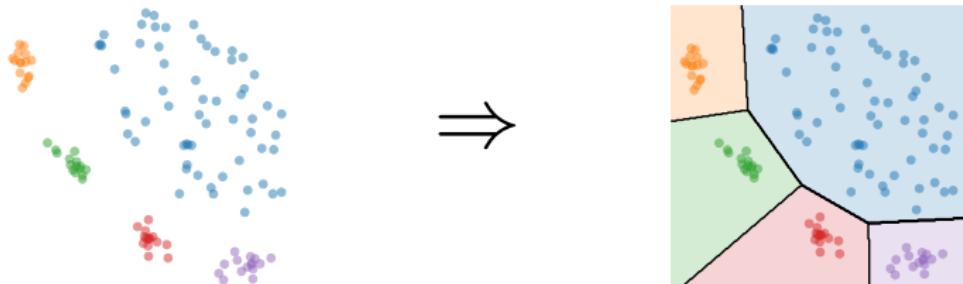
Parameters

- ▶ Type of function (linear, kernel, neural network).
- ▶ Performance measure.
- ▶ Regularization.

Methods

- ▶ Bayesian classifier (LDA, QDA)
- ▶ Linear and kernel discrimination
- ▶ Decision trees, random forests.
- ▶ Deep learning.

Multiclass classification



Objective

$$\{\mathbf{x}_i, y_i\}_{i=1}^n \Rightarrow f : \mathbb{R}^d \rightarrow \{1, \dots, p\}$$

- ▶ Train a function $f(\mathbf{x}) = y \in \mathcal{Y}$ predicting an integer value ($\mathcal{Y} = \{1, \dots, p\}$).
- ▶ In practice p continuous score functions f_k are estimated and the prediction is

$$f(\mathbf{x}) = \arg \max_k f_k(\mathbf{x}) \tag{1}$$

- ▶ Softmax can be used instead of argmax to get probability estimates.

Parameters

- ▶ Type of function (linear, kernel, neural network).
- ▶ Performance measure.
- ▶ Regularization.

Methods

- ▶ Bayesian classifier (LDA, QDA)
- ▶ Linear and kernel discrimination
- ▶ Decision trees, random forests.
- ▶ Deep learning.

Scikit-learn estimator for supervised learning

Scikit-learn object API

- ▶ Scikit-learn and its API became in recent years a standard for ML in Python.
- ▶ The estimator is usually used in 2 steps:
 1. Creation of the estimator :

```
est = Estimator(param='parameter value', param2=10)
```
 2. Fitting of the estimator to the data:

```
est.fit(X,y)
```
- ▶ After the fitting step, new attributes from the algorithms have been added to the object.

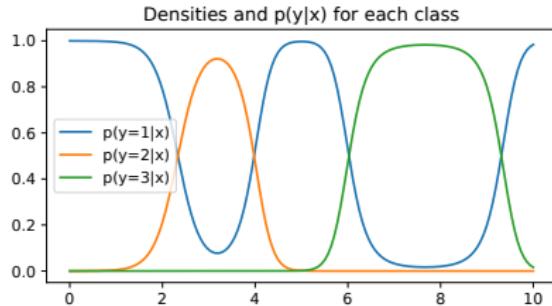
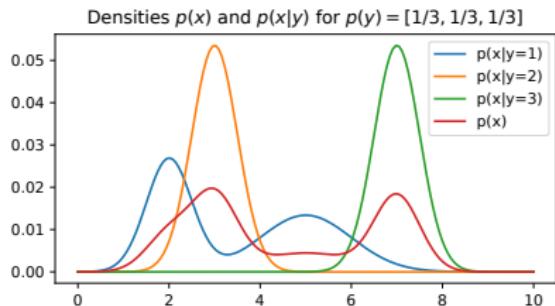
Using the estimator in supervised learning

- ▶ **Prediction**
Predict the labels (for regression and classification) with `est.predict(X)` or
`est.fit_predict(X)`
- ▶ **Probability prediction**
On some classification methods the probability of belonging to the classes is computed with `est.predict_proba(X)` (`predict_log_proba` also available).
- ▶ **Decision functions**
On some classification methods the score of belonging to the classes is computed by `est.decision_function(X)`.

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Probability distribution of the data



Probability distributions for classification problem

We suppose here that the data is generated following a joint feature/label distribution.

- ▶ $p(\mathbf{x}, y)$ is the joint feature/label probability.
- ▶ $p(\mathbf{x}) = \int p(\mathbf{x}, y) dy$ is the feature probability (marginal on the feature)
- ▶ $p(y) = \int p(\mathbf{x}, y) d\mathbf{x}$ is the discrete label probability (marginal on the labels)
- ▶ $p(\mathbf{x}|y) = \frac{p(\mathbf{x}, y)}{p(y)}$ is the conditional probability of \mathbf{x} for a given class.
- ▶ $p(y|\mathbf{x}) = \frac{p(\mathbf{x}, y)}{p(\mathbf{x})}$ is the conditional probability of y for a given observation \mathbf{x} .

Bayes Theorem : $p(x, y) = p(x|y)p(y) = p(y|x)p(x)$

Probability of error and Bayes risk

Error rate of a classifier

$$P_{err}(f) = E_{\mathbf{x}} \left[\sum_{k=1}^p (1_{f(\mathbf{x}) \neq k}) p(y = k | \mathbf{x}) \right] = 1 - \int \sum_{k=1}^p 1_{f(\mathbf{x}) = k} p(y = k | \mathbf{x}) p(\mathbf{x}) d\mathbf{x} \quad (2)$$

- ▶ 1_{cond} has value 1 when the condition $cond$ is true else 0.
- ▶ For a given classifier f the error rate is the probability that the classifier makes a mistake.
- ▶ Standard measure of performance for a classifier, often estimated empirically and called accuracy (`sklearn.metrics.accuracy_score`).

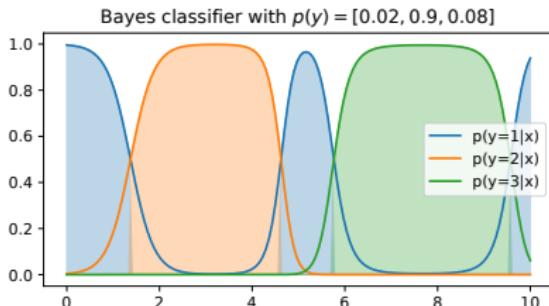
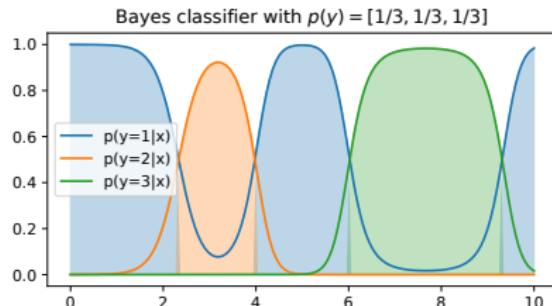
Bayes Risk

A more general expression of the error of a classifier is the Bayes risk expressed as

$$R(f) = E_{(\mathbf{x}, y)} [L(y, f(\mathbf{x}))] \quad (3)$$

- ▶ $L(i, j)$ is the cost of predicting class j when the true class is i .
- ▶ When $L(i, j) = 1_{i \neq j}$ we recover the error rate where all mistakes cost the same.
- ▶ The Bayes risk can be used to encode asymmetry between the errors of a classifier (some errors are more serious than others).

Bayesian decision



Bayes Classifier

- The Bayes classifier is the one minimizing the error rate

$$\min_f \quad 1 - \int \sum_{k=1}^K 1_{f(\mathbf{x})=k} p(y=k|\mathbf{x}) p(\mathbf{x}) d\mathbf{x}$$

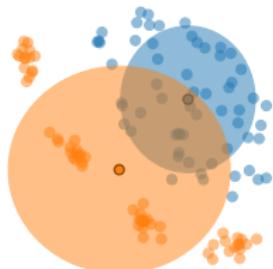
- We can see above that for a given \mathbf{x} the $f(\mathbf{x})$ that minimize the error is the one with maximum probability $p(y|\mathbf{x}) = p(y)p(\mathbf{x}|y)/p(\mathbf{x})$ ($p(\mathbf{x})$ indep. from y).
- The Bayes classifier minimizing the problem above is then

$$f^*(\mathbf{x}) = \arg \max_k p(y=k|\mathbf{x}) \tag{4}$$

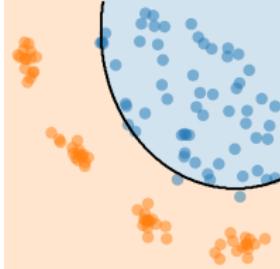
- This is exactly the multiclass classifier formula (1) with $f_k(\mathbf{x}) = p(y=k|\mathbf{x})$.
- In practice the probability distributions are unknown so they have to be estimated.

Naive Bayes Classifier (NB)

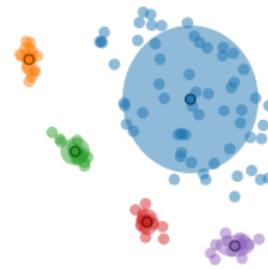
NB Gaussian distributions



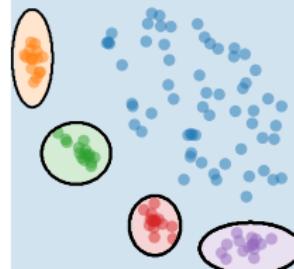
NB Gaussian classification



NB Gaussian distributions



NB Gaussian classification



Principle (Tutorial [Murphy et al., 2006])

- ▶ Assumption in NB Classification is that all variables are independent:

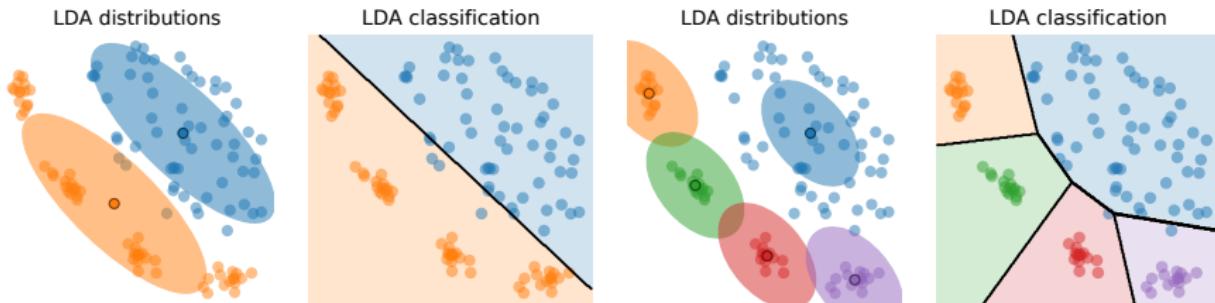
$$p(y|\mathbf{x}) = p(y) \prod_{i=1}^d p(x_i|y)$$

- ▶ Probabilities $\hat{p}(x_i|y)$ are estimated independently in 1D for each variable x_i with distributions depending on data prior (Gaussian, Bernoulli, Multinomial).
- ▶ Simple model that works very well on many applications [Zhang, 2004].
- ▶ Used a lot on textual data with bag of words (binary data for many spam filters)

Gaussian Naive Bayes (`sklearn.naive_bayes.GaussianNB`)

- ▶ Classes follow Gaussian distributions with diagonal covariances (indep. variables).
- ▶ The data is modeled as a GMM illustrated above for 2 and 5 classes.

Linear Discriminant Analysis (LDA)



Principle [Fisher, 1936]

- Model the conditional probabilities for each class as

$$p(\mathbf{x}|y = k) = \mathcal{N}(\boldsymbol{\mu}_k, \boldsymbol{\Sigma})$$

- The covariance matrix $\boldsymbol{\Sigma}$ is shared across all classes (Homoscedasticity).
- The proportions of classes are $\phi_k = p(y = k) \geq 0$ such that $\sum_k \phi_k = 1$.
- The Bayes decision function is taken as

$$f_k(\mathbf{x}) = \log(p(\mathbf{x}|y = k)p(y = k)).$$

- LDA is also known as Fisher Discriminant Analysis (FDA).
- Scikit-learn : `sklearn.discriminant_analysis.LinearDiscriminantAnalysis`

LDA discriminant functions

Score functions and simplifications

- The score function $f_k(\mathbf{x})$ can be expressed as

$$\begin{aligned}f_k(\mathbf{x}) &= \log(\phi_k) + \log(p(\mathbf{x}|y=k)) \\&= \log(\phi_k) - \frac{d}{2} \log(2\pi) - \frac{1}{2} \log \det(\boldsymbol{\Sigma}) - \frac{1}{2} (\mathbf{x} - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}_k)\end{aligned}$$

- Removing the terms that do not depend on k and do not change the decision we get the following equivalent score function

$$f_k(\mathbf{x}) = \boldsymbol{\mu}_k^T \boldsymbol{\Sigma}^{-1} \mathbf{x} + \log(\phi_k) - \frac{1}{2} \boldsymbol{\mu}_k^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_k = \mathbf{w}_k^T \mathbf{x} + b_k \quad (5)$$

- The decision function is linear because the quadratic terms are constant wrt k when the Gaussians have the same covariance $\boldsymbol{\Sigma}$.

LDA for binary classification

- Parameters for the Gaussian distributions are: $\phi, \boldsymbol{\Sigma}, \boldsymbol{\mu}_1, \boldsymbol{\mu}_{-1}$,
- Decision function f can be expressed as : $f(\mathbf{x}) = \text{sign}(f_1(\mathbf{x}) - f_{-1}(\mathbf{x}))$
- It can be expressed as $f(\mathbf{x}) = \text{sign}(\mathbf{w}^T \mathbf{x} + b) = \text{sign}(\sum_k w_k x_k + b)$ with

$$\mathbf{w} = \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_{-1}), \quad b = -\frac{1}{2} \mathbf{w}^T (\boldsymbol{\mu}_1 + \boldsymbol{\mu}_{-1}) + \log \phi_1 - \log \phi_{-1}$$

LDA in practice

LDA as dimensionality reduction [Rao, 1948]

- ▶ We want to find a subspace that maximizes the distance between the means of the classes in the projected space while minimizing the variance of each class.
- ▶ The optimization problem can be expressed as

$$\max_{\mathbf{D}, \mathbf{D}^\top \mathbf{D} = \mathbf{I}_{K-1}} \frac{\langle \boldsymbol{\Sigma}_b, \mathbf{DD}^\top \rangle}{\langle \boldsymbol{\Sigma}, \mathbf{DD}^\top \rangle}$$

where $\boldsymbol{\Sigma}_b = \sum_k \phi_k (\boldsymbol{\mu}_k - \bar{\boldsymbol{\mu}})(\boldsymbol{\mu}_k - \bar{\boldsymbol{\mu}})^\top$ with $\bar{\boldsymbol{\mu}} = \sum_k \phi_k \boldsymbol{\mu}_k$.

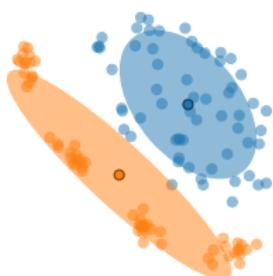
- ▶ The solution \mathbf{D}^* contains the eigenvector with largest eigenvalues for the generalized eigen-decomposition of $\boldsymbol{\Sigma}^{-1} \boldsymbol{\Sigma}_b$.

Estimating the parameters

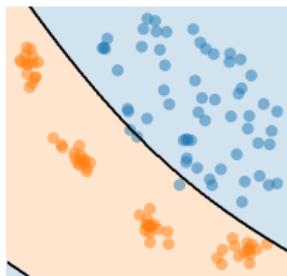
- ▶ Gaussian distributions for each class can be estimated by their empirical mean $\hat{\boldsymbol{\mu}}$ and covariance $\hat{\boldsymbol{\Sigma}}$ estimators.
- ▶ In high dimension good estimators for covariances require a large number of samples but still might lead to degenerate matrices (with numerical problems).
- ▶ In this case a good strategy is to perform a shrinkage of the matrix toward the identity by using $(1 - \alpha)\hat{\boldsymbol{\Sigma}} + \alpha \mathbf{I}_d$ instead of $\hat{\boldsymbol{\Sigma}}$.

Quadratic Discriminant Analysis (QDA)

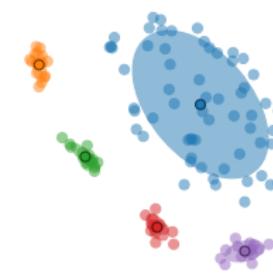
QDA distributions



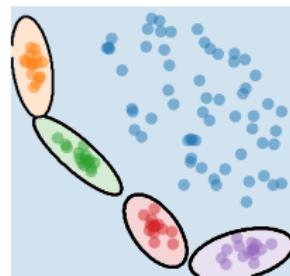
QDA classification



QDA distributions



QDA classification



Principle (Tutorial [Tharwat, 2016])

- Bayesian decision similar to LDA but where the conditional probabilities are :

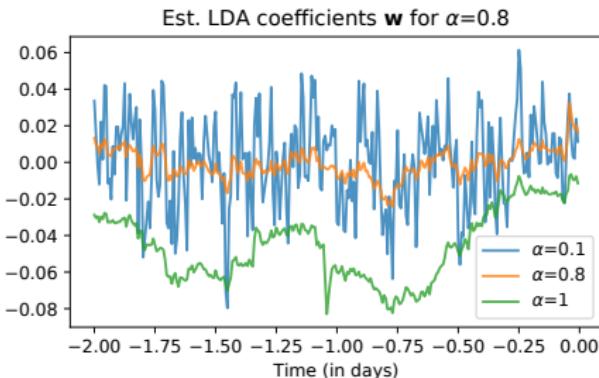
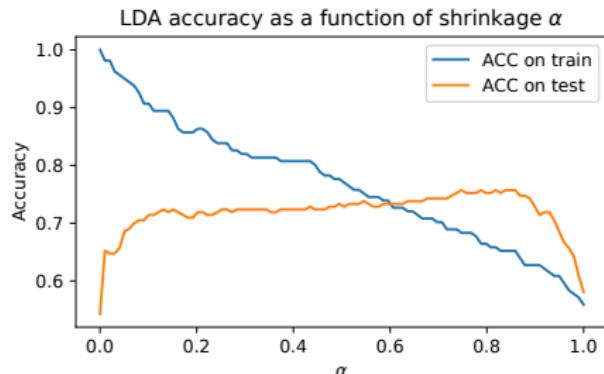
$$p(\mathbf{x}|y = k) = \mathcal{N}(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

- The score functions $f_k(\mathbf{x})$ can be expressed as

$$f_k(\mathbf{x}) = \log(\phi_k) - \frac{d}{2} \log(2\pi) - \frac{1}{2} \log \det(\boldsymbol{\Sigma}_k) - \frac{1}{2} (\mathbf{x} - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1} (\mathbf{x} - \boldsymbol{\mu}_k)$$

- When the covariances $\boldsymbol{\Sigma}_k$ are different the quadratic terms do not cancel each other and the final decision is quadratic.
- More sensitive to the curse of dimensionality than LDA.
- Scikit-learn : `sklearn.discriminant_analysis.QuadraticDiscriminantAnalysis`

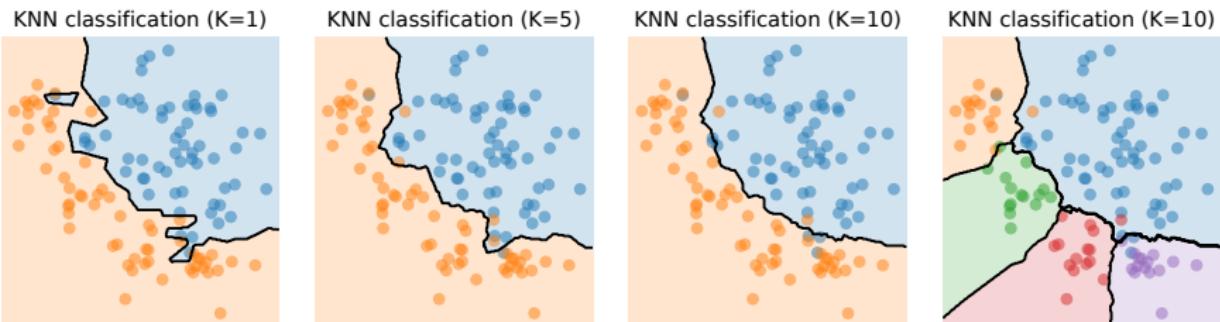
Bayesian decision on energy usage dataset



Application to energy usage classification

- ▶ Objective : predict if the energy usage will increase on the next day using the previous two days ($n = 161, d = 288$).
- ▶ Gaussian Naive Bayes classifier provided an accuracy on test data of : 0.59
- ▶ LDA with no shrinkage of the covariance gives an accuracy of : 0.54
- ▶ LDA with a shrinkage of $\alpha = 0.8$ gives an accuracy of : 0.75
- ▶ QDA with no shrinkage gives an accuracy of : 0.48
- ▶ QDA with a shrinkage of $\alpha = 0.8$ gives an accuracy of : 0.74
- ▶ Warning : in high dimension probability density estimation is hard, regularize/shrink your covariances.

K-nearest neighbors classification (KNN)



Principle [Fix and Hodges, 1989]

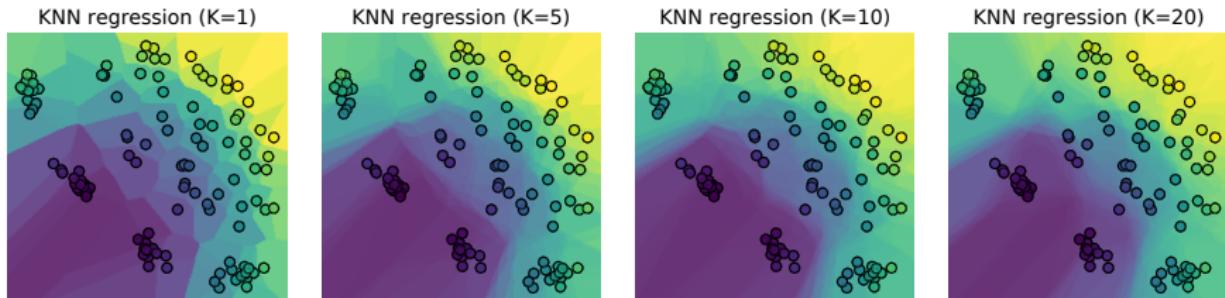
- ▶ Estimate locally the conditional densities $\hat{p}(\mathbf{x}|y = k)$ as

$$\hat{p}(\mathbf{x}|y = k) = \frac{1}{K} \sum_{i \in \mathcal{N}^K(\mathbf{x})} 1_{y_i=k} \quad (6)$$

where $\mathcal{N}^K(\mathbf{x})$ contains the index of the K nearest samples to \mathbf{x} in the dataset.

- ▶ The density estimation is a special case of KDE with adaptive kernel bandwidth.
- ▶ Instead of uniform voting one can use : $\hat{p}(\mathbf{x}|y = k) = \frac{\sum_{i \in \mathcal{N}^K(\mathbf{x})} \frac{1}{\|\mathbf{x} - \mathbf{x}_i\|} 1_{y_i=k}}{\sum_{i \in \mathcal{N}^K(\mathbf{x})} \frac{1}{\|\mathbf{x} - \mathbf{x}_i\|}}$
- ▶ Consistent estimator but requires the whole dataset for prediction (complexity).
- ▶ Scikit-learn implementation : `sklearn.neighbors.KNeighborsClassifier`

K-nearest neighbors for regression



Principle

- The predicted value for a given samples \mathbf{x} can be computed as:

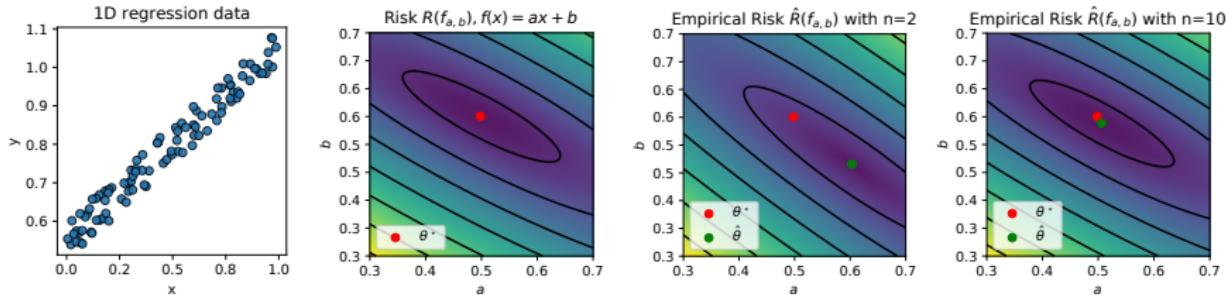
$$\hat{f}(\mathbf{x}) = \frac{1}{K} \sum_{i \in \mathcal{N}^K(\mathbf{x})} y_i \quad (7)$$

- This is the expected value of y on the distribution in the neighborhood \mathcal{N}^K
- For $K = 1$ the partition of the space is a Voronoi Diagram with prediction piecewise constant in each cell (for regression and classification).
- Smoother prediction using kernel or distance-based weighting similar to KNN classification with $\hat{f}(\mathbf{x}) = \frac{\sum_{i \in \mathcal{N}^K(\mathbf{x})} k(\mathbf{x}_i, \mathbf{x}) y_i}{\sum_{i \in \mathcal{N}^K(\mathbf{x})} k(\mathbf{x}_i, \mathbf{x})}$.
- Scikit-learn implementation : `sklearn.neighbors.KNeighborsRegressor`

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Empirical Risk Minimization



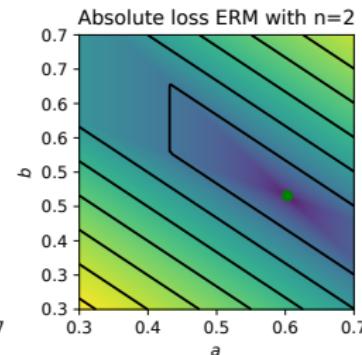
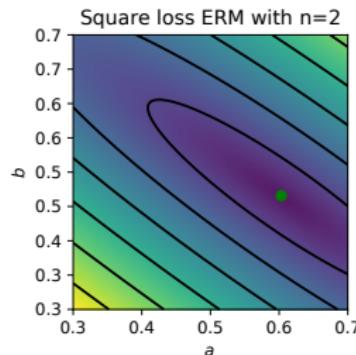
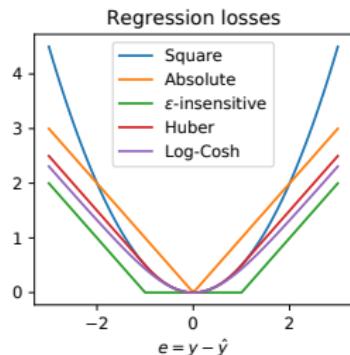
Principle

- ▶ In practice the Bayes risk is not known, we only have access to a sampling $\{\mathbf{x}_i, y_i\}_i$ of the true distribution.
- ▶ We search for a prediction function f that minimize the expected loss over the empirical distribution (training data):

$$\min_f \quad \left\{ \hat{R}(f) = \frac{1}{n} \sum_{i=1}^n L(y_i, f(\mathbf{x}_i)) \right\} \quad (8)$$

- ▶ L is a measure of discrepancy between the true and predicted values.
- ▶ The empirical risk $\hat{R}(f)$ is a good approximation of $R(f)$ for large n .
- ▶ Usually we use a parametric function f_θ and optimize its parameters θ .

Losses for regression

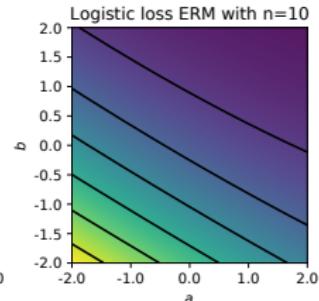
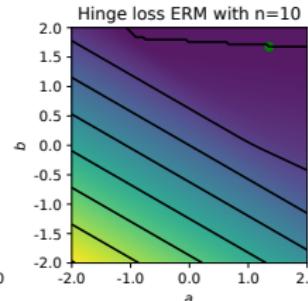
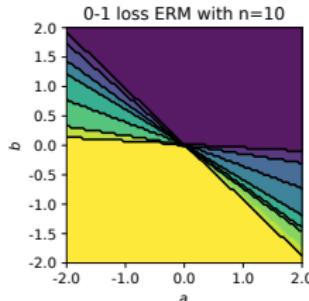
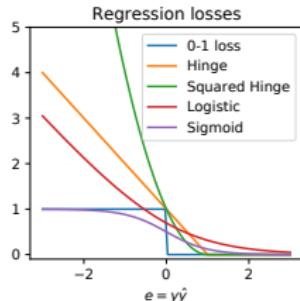


Penalizing prediction error

- For regression the error can be defined as : $e = y - f(\mathbf{x}) = y - \hat{y}$
- Typical losses :

Loss	$L(y, \hat{y})$	Smooth	Convex
Square loss (MSE, L2)	$\frac{1}{2}(y - \hat{y})^2$	++	++
Absolute deviation (MAE)	$ y - \hat{y} $	-	+
ϵ -insensitive	$\max(0, y - \hat{y} - \epsilon)$	-	+
Huber loss	$\begin{cases} \frac{1}{2}(y - \hat{y})^2 & \text{for } y - \hat{y} \leq \delta, \\ \delta(y - \hat{y} - \frac{1}{2}\delta), & \text{otherwise.} \end{cases}$	+	++
Log-Cosh	$\log(\cosh(y - \hat{y}))$	++	++

Losses for classification



Penalizing prediction error

- For binary classification ($\{-1, 1\}$) the error can be defined using : $e = yf(\mathbf{x}) = y\hat{y}$
- Typical losses are asymmetric wrt 0 :

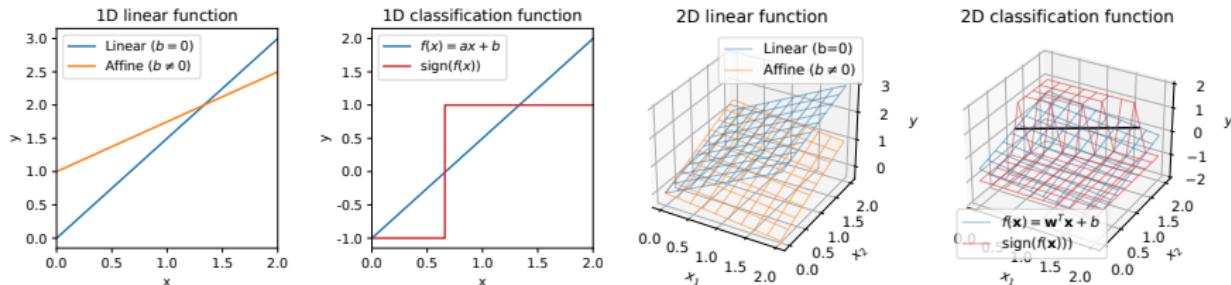
Loss	$L(y, \hat{y})$	Smooth	Convex
0-1 loss	$\frac{1}{2}(1 - \text{sign}(y\hat{y}))$	-	-
Hinge	$\max(0, 1 - y\hat{y})$	-	+
Squared Hinge	$\max(0, 1 - y\hat{y})^2$	+	+
Logistic	$\log(1 + \exp(-y\hat{y}))$	+	+
Sigmoid	$(1 - \tanh(y\hat{y}))/2$	+	-

- For multiclass classification the classical loss is the categorical cross-entropy :

$$L(y, f(\mathbf{x})) = - \sum_{k=1}^p \delta_{k=y} \log(f_k(\mathbf{x}))$$

where the output of f contains probability estimates (softmax).

Linear prediction model

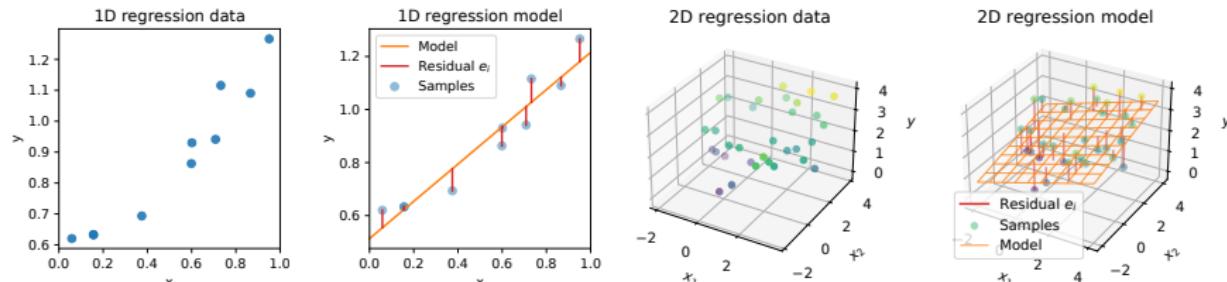


Linear (affine) function

$$f_{\boldsymbol{\theta}}(\mathbf{x}) = \sum_{i=1}^d w_i x_i + b = \mathbf{x}^\top \mathbf{w} + b = [\mathbf{x}^\top, 1] \boldsymbol{\theta} \quad (9)$$

- ▶ $\mathbf{w} \in \mathbb{R}^d$ a vector defining an hyperplane in \mathbb{R}^d (\mathbf{w} orthogonal to the hyperplane).
- ▶ $b \in \mathbb{R}$ a bias term displacing the function along the normal \mathbf{w} of the hyperplane.
- ▶ All the parameters can be stored in a unique vector $\boldsymbol{\theta}^\top = [\mathbf{w}^\top, b]$.
- ▶ Linear models are interpretable (look at the weights w_i and their sign).
- ▶ Estimating the bias b can be done using the data matrix $\tilde{\mathbf{X}} = [\mathbf{X}, \mathbf{1}_n]$.
- ▶ Linear models from `sklearn.linear_model` have the following attributes after fitting
 - ▶ `model.coef_` : contains the weight coefficients $\mathbf{w} \in \mathbb{R}^d$ of the variables.
 - ▶ `model.intercept_` : contains the bias b (also called the intersect).

Least Square regression (LS)



Principle

$$\min_{\mathbf{w}, b} \quad \frac{1}{n} \sum_{i=1}^n (y_i - \mathbf{w}^\top \mathbf{x}_i - b)^2 \quad (10)$$

- ▶ Also called Ordinary Least Squares Linear Regression (OLS).
- ▶ Minimize the mean of the squared prediction errors $e_i = y_i - \mathbf{w}^\top \mathbf{x}_i - b$ (MSE).
- ▶ Matrix and linear reformulation:

$$\min_{\mathbf{w}, b} \quad \frac{1}{n} \|\mathbf{y} - \mathbf{X}\mathbf{w} - b\mathbf{1}_n\|^2 \quad \equiv \quad \min_{\boldsymbol{\theta}} \quad \frac{1}{n} \|\mathbf{y} - \tilde{\mathbf{X}}\boldsymbol{\theta}\|^2 \quad (11)$$

where $\tilde{\mathbf{X}} = [\mathbf{X}, \mathbf{1}_n]$ is the data matrix with a concatenated column of ones.

- ▶ Scikit-learn : `sklearn.linear_model.LinearRegression`

Solving the least square

Minimum of a convex function

Let $J(\theta)$ be a smooth convex function $\mathbb{R}^{d+1} \rightarrow \mathbb{R}$. θ^* is a minimum $J(\theta)$ if and only if

$$\nabla J(\theta^*) = \mathbf{0} \quad (12)$$

where $\nabla J(\theta) \in \mathbb{R}^{d+1}$ is the gradient of the function $\nabla J(\theta)_i = \frac{\partial J(\theta)}{\partial \theta_i} \quad \forall i$

Gradient and solution for Least Square

- The objective function can be expressed as:

$$J(\theta) = \frac{1}{n} \|\mathbf{y} - \tilde{\mathbf{X}}\theta\|^2 = \frac{1}{n} \left(\mathbf{y}^\top \mathbf{y} - 2\theta^\top \tilde{\mathbf{X}}^\top \mathbf{y} + \theta^\top \tilde{\mathbf{X}}^\top \tilde{\mathbf{X}}\theta \right)$$

- The gradient of the function is

$$\nabla J(\theta) = \frac{2}{n} \left(-\tilde{\mathbf{X}}^\top \mathbf{y} + \tilde{\mathbf{X}}^\top \tilde{\mathbf{X}}\theta \right)$$

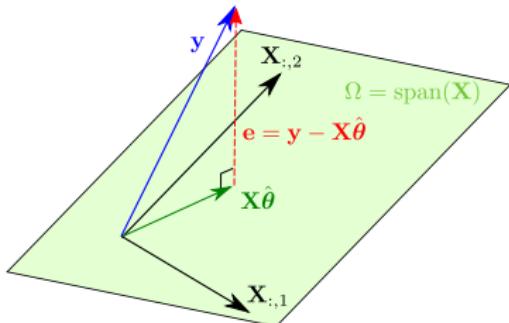
- Least Square estimator recovered by setting $\nabla J(\theta) = \mathbf{0}$

$$\tilde{\mathbf{X}}^\top \mathbf{y} = \tilde{\mathbf{X}}^\top \tilde{\mathbf{X}}\hat{\theta} \quad \rightarrow \quad \hat{\theta} = (\tilde{\mathbf{X}}^\top \tilde{\mathbf{X}})^{-1} \tilde{\mathbf{X}}^\top \mathbf{y} \quad (13)$$

- Warning : this solution requires that $\tilde{\mathbf{X}}$ be of rank $d + 1$ (at least $n \geq d + 1$).

Geometric interpretation of Ordinary Least Square

- ▶ We search for a vector $\tilde{\mathbf{X}}\hat{\theta} \in \mathbb{R}^n$ in the span $\Omega = \text{span}(\tilde{\mathbf{X}})$.
- ▶ Minimizing the norm of the error $e = \mathbf{y} - \tilde{\mathbf{X}}\hat{\theta}$ corresponds to finding the orthogonal projection on Ω .
- ▶ For an optimal solution $\hat{\theta}$, e is orthogonal to any vector in Ω .
- ▶ This means that the residual $e = \mathbf{y} - \tilde{\mathbf{X}}\hat{\theta}$ should be orthogonal to any of the columns in $\tilde{\mathbf{X}}$ which implies that



$$\tilde{\mathbf{X}}^\top (\mathbf{y} - \tilde{\mathbf{X}}\hat{\theta}) = \mathbf{0}$$

- ▶ This orthogonality conditions allows to recover geometrically the solution

$$\hat{\theta} = (\tilde{\mathbf{X}}^\top \tilde{\mathbf{X}})^{-1} \tilde{\mathbf{X}}^\top \mathbf{y}$$

that is the solution of the LS optimization problem (10).

Probabilistic interpretation of Least Square

Observation model and likelihood

- The model is supposed to be linear with Gaussian IID noise, that is

$$p(\mathbf{y}|\tilde{\mathbf{X}}) = \mathcal{N}(\tilde{\mathbf{X}}\boldsymbol{\theta}, \sigma^2 \mathbf{I}_n)$$

- The log-likelihood for parameters $\boldsymbol{\theta}$ and σ^2 can be expressed as

$$\mathcal{L}(\boldsymbol{\theta}, \sigma^2) = -\frac{n}{n} \log(2\pi) - \frac{n}{n} \log(\sigma^2) - \frac{1}{2\sigma^2} \|\mathbf{y} - \tilde{\mathbf{X}}\boldsymbol{\theta}\|^2$$

Maximum likelihood

- Estimating the parameters $\boldsymbol{\theta}$ and σ^2 is done by maximum likelihood that is by solving

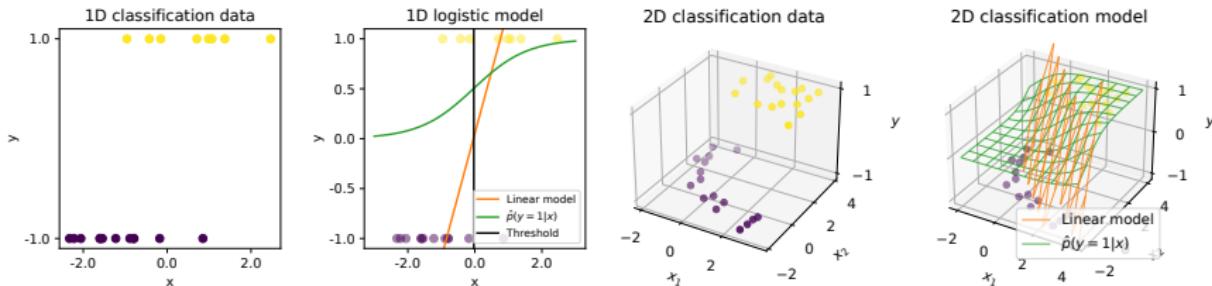
$$\max_{\boldsymbol{\theta}, \sigma^2} \mathcal{L}(\boldsymbol{\theta}, \sigma^2)$$

- The solution is recovered by computing the gradients w.r.t. $\boldsymbol{\theta}$ and σ^2 and setting them to 0 (and checking that it is a maximum with the Hessian). The optimal values are :

$$\hat{\boldsymbol{\theta}} = (\tilde{\mathbf{X}}^\top \tilde{\mathbf{X}})^{-1} \tilde{\mathbf{X}}^\top \mathbf{y}$$

$$\hat{\sigma}^2 = \frac{1}{n} \|\mathbf{y} - \tilde{\mathbf{X}}\hat{\boldsymbol{\theta}}\|^2$$

Logistic regression



Principle

$$\min_{\mathbf{w}, b} \quad \frac{1}{n} \sum_{i=1}^n \log(1 + \exp(-y_i(\mathbf{w}^\top \mathbf{x}_i - b))) \quad (14)$$

- Model the conditional probabilities for binary classes $\{-1, 1\}$ with

$$p(y = 1|\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^\top \mathbf{x} - b)}, \quad p(y = -1|\mathbf{x}) = \frac{1}{1 + \exp(\mathbf{w}^\top \mathbf{x} + b)} \quad (15)$$

- Bayes decision : $f(\mathbf{x}) = \text{sign}(p(y = 1|\mathbf{x}) - p(y = -1|\mathbf{x}))$ that is equivalent to
$$f(\mathbf{x}) = \text{sign}(\mathbf{w}^\top \mathbf{x} + b)$$
- Parameters $\hat{\mathbf{w}}, \hat{b}$ are optimized by maximum likelihood corresponding to the optimization problem (14).
- Scikit-learn : `sklearn.linear_model.LogisticRegression`

Solving the logistic regression

Recovering the MLE optimization problem

- The log-likelihood from the logistic regression can be expressed as:

$$\begin{aligned}\mathcal{L}(\mathbf{w}, b) &= \sum_{i, y_i=1} -\log(1 + \exp(-\mathbf{w}^\top \mathbf{x}_i - b)) + \sum_{i, y_i=-1} -\log(1 + \exp(\mathbf{w}^\top \mathbf{x}_i + b)) \\ &= -\sum_{i=1}^n \log(1 + \exp(-y_i(\mathbf{w}^\top \mathbf{x}_i - b)))\end{aligned}$$

- So maximizing the likelihood above is equivalent to minimizing its negative in Equation (14).

Gradient of the objective function

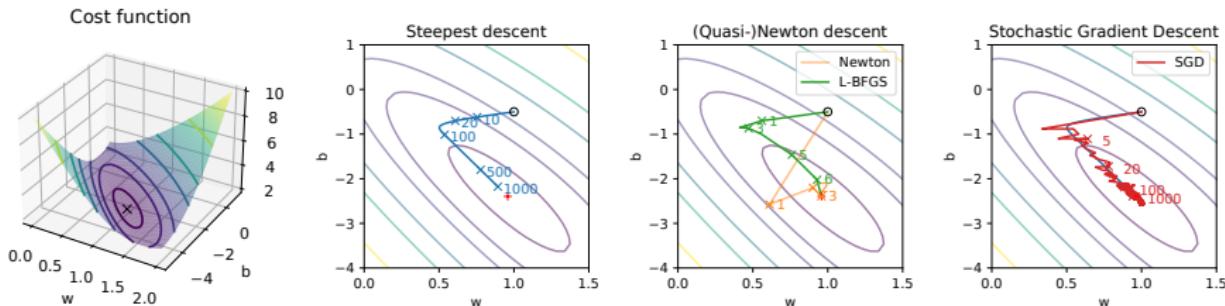
- The gradient of $J(\theta)$ defined in (14) can be expressed as

$$\nabla_{\theta} J(\theta) = -\frac{1}{n} \tilde{\mathbf{X}}^\top \mathbf{P} \mathbf{y} \quad (16)$$

where \mathbf{P} is a diagonal matrix of elements $\frac{p_i}{1+p_i}$ with $p_i = \exp(-y_i(\mathbf{w}^\top \mathbf{x}_i + b))$.

- Setting the gradients $\nabla_{\theta} J(\theta) = \mathbf{0}$ leads to a highly nonlinear equations so there is no close form solution as in LS.

Numerical optimization with gradient descent



Principle

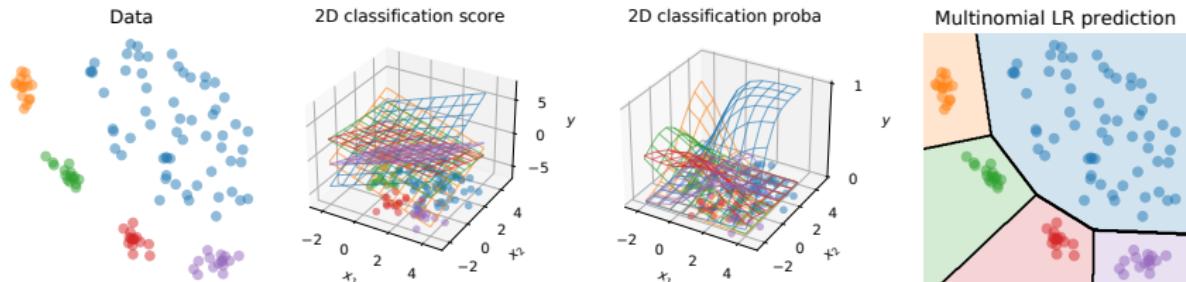
- ▶ Optimize a smooth function $J(\theta)$ using its gradient (or its approximation).
- ▶ Initialize a vector $\theta^{(0)}$ and update it at each iteration k as:

$$\theta^{(k+1)} = \theta^{(k)} + \mu_k \mathbf{d}_k \quad (17)$$

where μ_k is a step and \mathbf{d}_k is a descent direction ($\mathbf{d}_k^\top \nabla J(\theta^{(k)}) < 0$).

- ▶ Classical descent directions are :
 - ▶ **Steepest descent** : $\mathbf{d}_k = -\nabla J(\theta^{(k)})$
 - ▶ **Newton**: $\mathbf{d}_k = -(\nabla^2 J(\theta^{(k)}))^{-1} \nabla J(\theta^{(k)})$ where $\nabla^2 J(\theta^{(k)})$ is the Hessian.
 - ▶ **Quasi-Newton (QN)** : $\mathbf{d}_k = -\mathbf{B} \nabla J(\theta^{(k)})$ where \mathbf{B} is an approximation of the inverse of the Hessian.
 - ▶ **Stochastic Gradient Descent (SGD)** : $\mathbf{d}_k = -\nabla \tilde{J}(\theta^{(k)})$ with approx. gradient.

Multinomial logistic regression



Principle

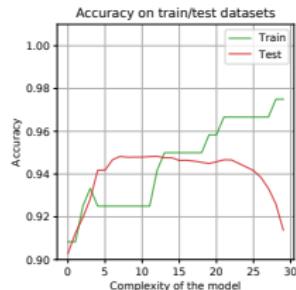
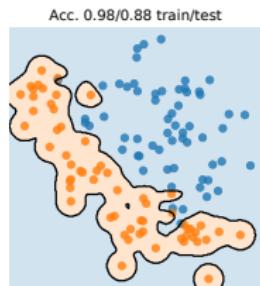
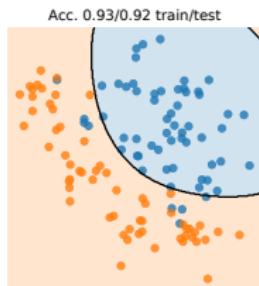
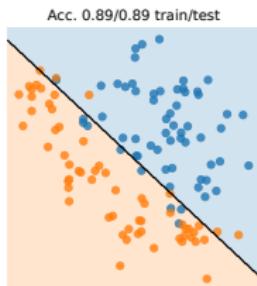
$$\min_{\mathbf{W}, \mathbf{b}} -\frac{1}{n} \sum_{i=1}^n \sum_{k=1}^p \delta_{y_i=k} \log(p_{\mathbf{W}, \mathbf{b}}(y = k | \mathbf{x}_i)) \quad (18)$$

- MLE of parameters where $\mathbf{W} = [\mathbf{w}_1, \dots, \mathbf{w}_p]$ and $\mathbf{b} = [b_1, \dots, b_p]^\top$ the linear parameters and the conditional probabilities are modeled as

$$p_{\mathbf{W}, \mathbf{b}}(y = k | \mathbf{x}) = \frac{\exp(\mathbf{w}_k^\top \mathbf{x} + b_k)}{\sum_{j=1}^p \exp(\mathbf{w}_j^\top \mathbf{x} + b_j)} \quad (19)$$

- The operator above is called the softmax of predictions $\mathbf{w}_k^\top \mathbf{x} + b_k$ per classes.
- Problem (18) is an ERM where the loss function is the Kullback-Leibler between the one-hot encoding of the labels and the softmax output.
- Scikit-learn : `sklearn.linear_model.LogisticRegression` (with multiclass labels)

Regularization for supervised learning



Empirical risk minimization with regularization

$$\min_f \quad \sum_{i=1}^n L(y_i, f(\mathbf{x}_i)) + \lambda \Omega(f) \quad (20)$$

- ▶ $L(\cdot \cdot \cdot)$ a loss function measure prediction performance on the training samples.
- ▶ $\Omega(\cdot)$ is a measure of complexity of the function weighted by $\lambda \geq 0$.
- ▶ For a given λ , (20) is an upper bound on the true expected risk.
- ▶ In practice the regularization is often applied on the parameters θ of the function f_θ leading to the following optimization problem

$$\min_{\theta} \quad \sum_{i=1}^n L(y_i, f_{\theta}(\mathbf{x}_i)) + \lambda \Omega(\theta) \quad (21)$$

Regularizing linear models

Complexity of a linear model

$$f_{\theta}(\mathbf{x}) = \sum_{i=1}^d w_i x_i + b = \mathbf{x}^\top \mathbf{w} + b$$

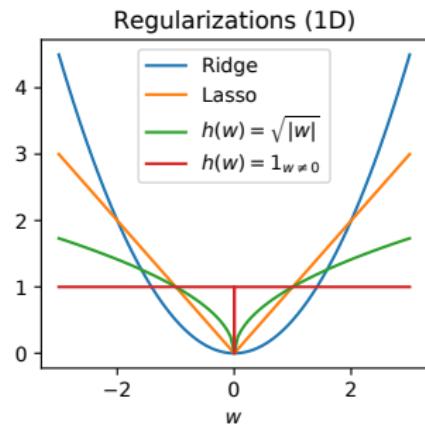
- ▶ A measure of complexity of a function is how quick it will change its value.
- ▶ This can be measured as the gradient of the function *w.r.t.* its input :

$$\nabla f_{\theta}(\mathbf{x}) = \mathbf{w}$$

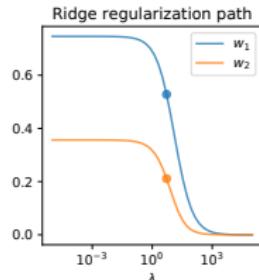
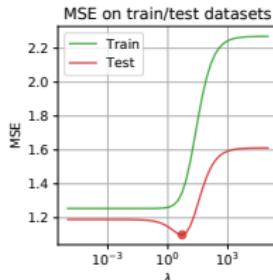
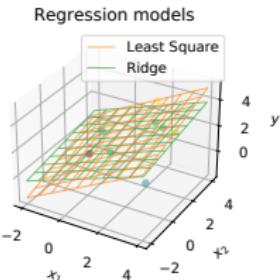
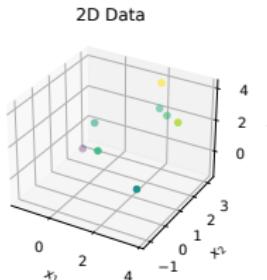
- ▶ One measure of complexity is then to use the norm of the linear parameters \mathbf{w} .

Common regularizations for linear models

- ▶ Ridge : $\Omega(\mathbf{w}) = \|\mathbf{w}\|^2 = \sum_j w_j^2$
- ▶ Lasso : $\Omega(\mathbf{w}) = \|\mathbf{w}\|_1 = \sum_j |w_j|$
- ▶ Mahalanobis : $\Omega(\mathbf{w}) = \mathbf{w}^\top \Sigma \mathbf{w}$
- ▶ Separable : $\Omega(\mathbf{w}) = \sum_j h(|w_j|)$
- ▶ Group-Lasso : $\Omega(\mathbf{w}) = \sum_{g \in \mathcal{G}} \|\mathbf{w}_g\|$
- ▶ L0 pseudo-norm : $\Omega(\mathbf{w}) = \|\mathbf{w}\|_0 = \sum_j 1_{w_j \neq 0}$



Ridge regression



Principle

$$\min_{\mathbf{w}, b} \quad \frac{1}{n} \sum_{i=1}^n (y_i - \mathbf{w}^\top \mathbf{x}_i - b)^2 + \lambda \|\mathbf{w}\|^2 \quad (22)$$

- Quadratic penalization limits the complexity of the model ($\lambda = 0$ is LS).
- Makes the optimization problem strictly convex even when $n < d$.
- Solutions without and with bias are

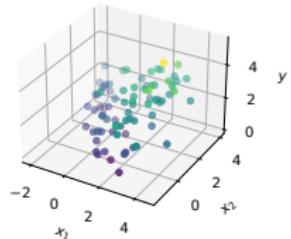
$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X} + n\lambda \mathbf{I}_d)^{-1} \mathbf{X}^\top \mathbf{y}, \quad \hat{\boldsymbol{\theta}} = (\tilde{\mathbf{X}}^\top \tilde{\mathbf{X}} + n\lambda \mathbf{S})^{-1} \mathbf{X}^\top \mathbf{y} \quad (23)$$

Where $\mathbf{S} \in \mathbb{R}^{d+1 \times d+1}$ is a matrix defined as $S_{i,j} = 1$ if $i = j \leq d$ else 0.

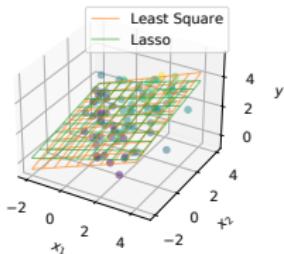
- Ridge with $\lambda = \frac{\sigma_n^2}{\sigma_w^2}$ is actually a MAP with a prior $p(\mathbf{w}) \sim \mathcal{N}(0, \sigma_w^2 \mathbf{I})$ and a known variance of the additive noise of σ_n^2 .
- Scikit-learn implementation (alpha is λ) : `sklearn.linear_model.Ridge(alpha=1)`

Lasso regression

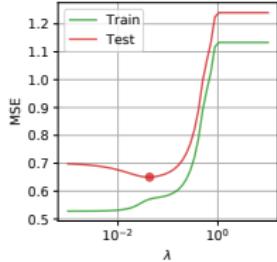
Data ($d = 2 + 8$ noisy features)



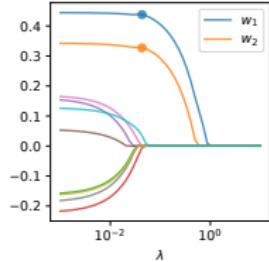
Regression models



MSE on train/test datasets



Lasso regularization path



Principle [Tibshirani, 1996]

$$\min_{\mathbf{w}, b} \quad \frac{1}{n} \sum_{i=1}^n (y_i - \mathbf{w}^\top \mathbf{x}_i - b)^2 + \lambda \sum_{j=1}^d |w_j| \quad (24)$$

- ▶ L1 norm $\|\mathbf{w}\|_1 = \sum_j |w_j|$ regularization is non-smooth in $w_j = 0, \forall j$.
- ▶ For a large enough λ the solution of the problem is sparse (some components \hat{w}_j of $\hat{\mathbf{w}}$ are exactly equal to 0).
- ▶ Under some conditions, when the true model \mathbf{w}^* is sparse the true support of \mathbf{w}^* can be recovered [Zhao and Yu, 2006].
- ▶ Lasso regularization can be used for classification [Koh et al., 2007].
- ▶ Scikit-learn implementation ($\text{alpha}=\lambda$) : `sklearn.linear_model.Lasso`
- ▶ Efficient solver for large/sparse problems : `celer.Lasso` [Massias et al., 2020]

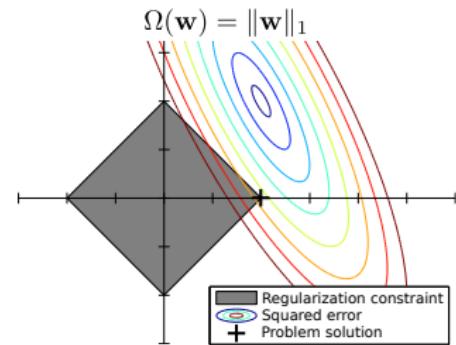
Solution for the Lasso

Why is the Lasso sparse?

- ▶ L1 regularization is non-smooth in $w_j = 0, \forall j$ which creates attraction points toward sparsity.
- ▶ Lasso Problem (24) is equivalent to

$$\min_{\mathbf{w}, b, \|\mathbf{w}\|_1 \leq \tau} \frac{1}{n} \sum_{i=1}^n (y_i - \mathbf{w}^\top \mathbf{x}_i - b)^2 \quad (25)$$

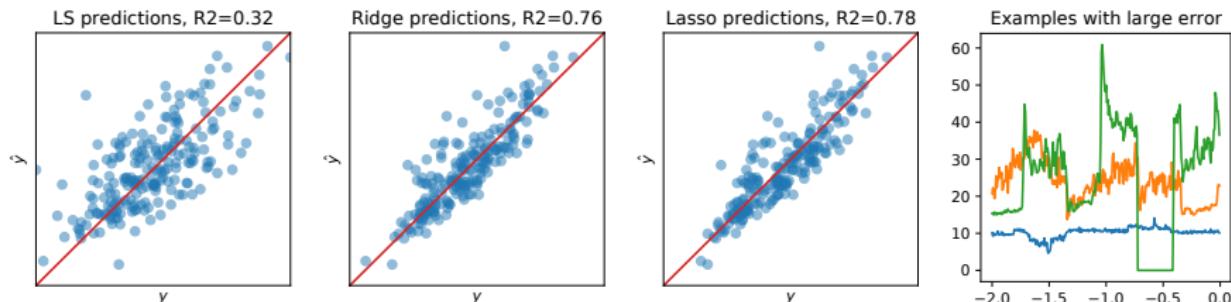
- ▶ The geometrical constraints promotes sparse \mathbf{w} on the axis.



Optimization algorithms

- ▶ **Coordinate descent** Optimize iteratively each w_j independently (sklearn).
- ▶ **Homotopy Methods** Create iteratively solutions along the regularization path using the fact that it is piece-wise linear (`sklearn.linear_model.lasso_path`).
- ▶ **Proximal algorithms** Extension of gradient descent to non-smooth optimization with stochastic solver for large scale datasets (`sklearn.linear_model.SGDRegressor`).

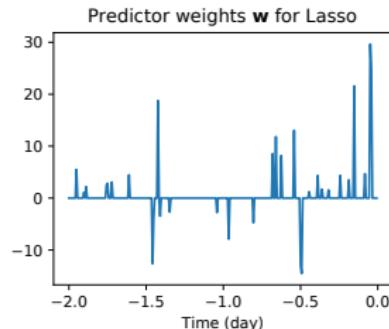
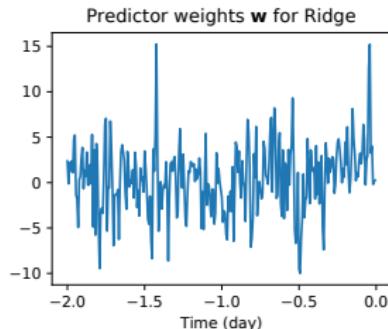
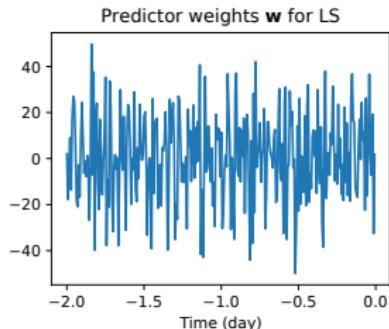
Application on energy usage data



Application to energy usage prediction

- ▶ Learn to predict total energy usage for the next day using recordings of usage from the last two days.
- ▶ Prediction performance measured with the coefficient of determination R^2 (1 is perfect, 0 is random).
- ▶ Comparison for Least Square ($R^2 = 0.32$), Ridge ($R^2 = 0.76$) and Lasso ($R^2 = 0.78$), Ridge and Lasso are far better on large data ($d = 288$).
- ▶ Parameters λ selected through cross validation (see next course).
- ▶ Plot the predictions and true values (perfect prediction on the red line).
- ▶ Plot the linear models w for all the methods (lasso selects 31/288 features).

Application on energy usage data



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- ▶ Parameters λ selected through cross validation (see next course).
- ▶ Plot the predictions and true values (perfect prediction on the red line).
- ▶ Plot the linear models \mathbf{w} for all the methods (lasso selects 31/288 features).

Learning nonlinear models

Optimization problem

$$\min_{\theta} \sum_{i=1}^n L(y_i, f_{\theta}(\mathbf{x}_i)) + \lambda \Omega(f_{\theta}) \quad (26)$$

- ▶ where f_{θ} is a nonlinear function parametrized by θ .
- ▶ Optimization problem can become non-convex and/or non-smooth.
- ▶ Different approaches depend on the modeling of the non-linear function f_{θ} .

What kind of nonlinearity ?

- ▶ **Non-linear basis** : $\phi_j(\mathbf{x})$ are nonlinear functions and the model is expressed as

$$f_{\theta}(\mathbf{x}) = \sum_{j=1}^{d'} \phi_j(\mathbf{x}) w_j + b \quad (27)$$

that can be seen as pre-processing of the data (all linear methods can be applied).

- ▶ **Kernel methods** : prediction function lies in a Reproducible Kernel Hilbert Space (RKHS) and non-linearity depends on the choice of the kernel.
- ▶ **Neural network** : design the non-linear function as a combination of linear operators and nonlinear transformations. Allows for learning complex feature extraction and taking account the structure of the data.

Representation theorem for kernel methods

Theorem (simplified from [Schölkopf et al., 2001, Boser et al., 1992])

Let \mathcal{H} be a Reproducible Kernel Hilbert Space (RKHS) associated to the positive definite kernel k defined on $\mathbb{R}^d \times \mathbb{R}^d$ and a sampling $\{\mathbf{x}_i, y_i\}_i$. Minimizing the following optimization problem

$$\min_{f \in \mathcal{H}} \sum_{i=1}^n L(y_i, f(\mathbf{x}_i)) + h(\|f\|_{\mathcal{H}}) \quad (28)$$

where h is a monotonically increasing function leads to an optimal solution that can be expressed as

$$\hat{f}(\mathbf{x}) = \sum_{i=1}^n \hat{\alpha}_i k(\mathbf{x}, \mathbf{x}_i) + \hat{b} \quad (29)$$

where $\hat{\alpha} \in \mathbb{R}^n$ and \hat{b} are the parameters of the function.

Discussion on Support Vector Machines (SVM)

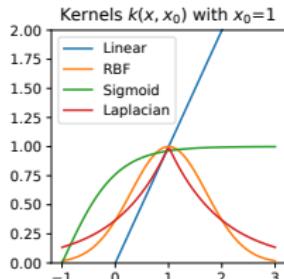
- ▶ The "kernel trick" used in RKHS allows us to have a non-linear implicit feature extraction $\phi(\mathbf{x}) = k(\mathbf{x}, \cdot)$.

- ▶ The norm $\|f\|_{\mathcal{H}}$ in the RKHS can be expressed for a given $f \in \mathcal{H}$ as

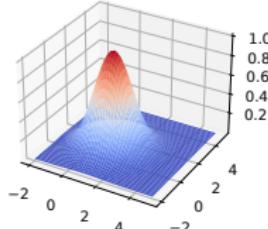
$$\|f\|_{\mathcal{H}}^2 = \sum_{i,j}^{n,n} \alpha_i \alpha_j k(\mathbf{x}_i, \mathbf{x}_j)$$

- ▶ The function f is described through its weight on $k(\mathbf{x}, \mathbf{x}_i)$ the similarity measure with the training samples denoted as support vectors when $\alpha_i \neq 0$.

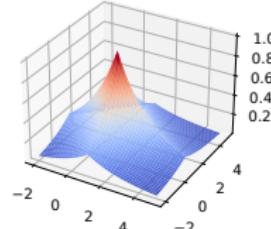
Kernels as feature extraction



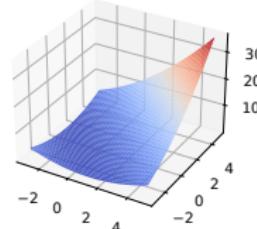
RBF Kernel $k(\mathbf{x}, \mathbf{x}_0), \mathbf{x}_0=[1,1]$



Laplacian Kernel $k(\mathbf{x}, \mathbf{x}_0), \mathbf{x}_0=[1,1]$



Polynomial Kernel $k(\mathbf{x}, \mathbf{x}_0), \mathbf{x}_0=[1,1]$

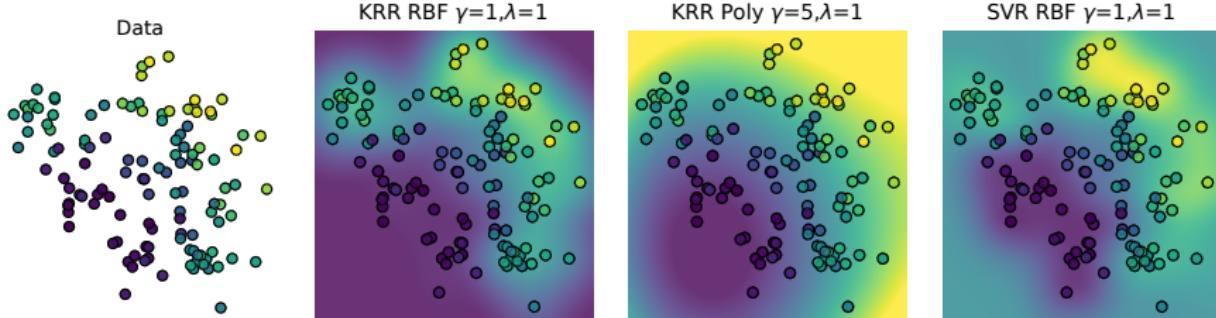


Common kernels (`sklearn.metrics.pairwise`)

- ▶ **Linear** : $k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^\top \mathbf{x}'$ (recover linear models where $\mathbf{w} = \sum_i \alpha_i \mathbf{x}_i$)
- ▶ **Radial Basis Function (RBF) or Gaussian** : $k(\mathbf{x}, \mathbf{x}') = \exp(-\gamma \|\mathbf{x} - \mathbf{x}'\|^2)$
- ▶ **Polynomial** : $k(\mathbf{x}, \mathbf{x}') = (\gamma \mathbf{x}^\top \mathbf{x}' + c_0)^d$
- ▶ **Laplacian** : $k(\mathbf{x}, \mathbf{x}') = \exp(-\gamma \|\mathbf{x} - \mathbf{x}'\|)$
- ▶ **Cosine** : $k(\mathbf{x}, \mathbf{x}') = \frac{\mathbf{x}^\top \mathbf{x}'}{\|\mathbf{x}\| \|\mathbf{x}'\|}$
- ▶ **Sigmoid** : $k(\mathbf{x}, \mathbf{x}') = \tanh(\gamma \mathbf{x}^\top \mathbf{x}' + c_0)$

Numerous kernels have been designed by domain experts for specific applications.

Kernel methods for regression (KRR, SVR)



Kernel Ridge Regression (KRR) ([Murphy, 2012, Chap 14.3])

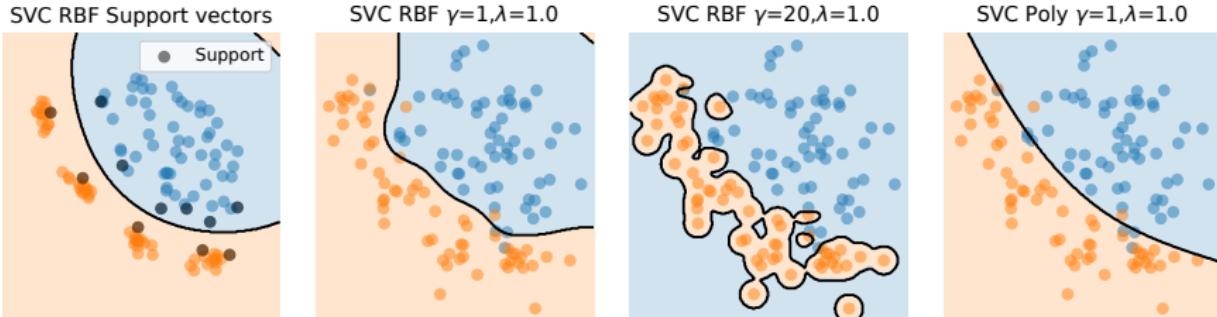
$$\min_{f \in \mathcal{H}} \quad \frac{1}{n} \sum_{i=1}^n (y_i - f(\mathbf{x}_i))^2 + \lambda \|f\|_{\mathcal{H}}^2 \quad (30)$$

- Optimal parameters $\hat{\alpha} = (\mathbf{K} + n\lambda \mathbf{I}_n)^{-1} \mathbf{y}$ with \mathbf{K} the kernel matrix.
- There exist a Lasso counterpart for sparse $\hat{\alpha}$ [Guigue et al., 2005].
- Scikit-learn implementation (`alpha=λ`) : `sklearn.kernel_ridge.KernelRidge`

Support Vector Regression (SVR) [Drucker et al., 1997]

- Similar to KRR but using the ϵ -invariant loss $L(y, \hat{y}) = \max(0, |y - \hat{y}| - \epsilon)$.
- Solution $\hat{\alpha}$ is sparse (weight on support vectors) and less sensitive to outliers.
- Scikit-learn implementation ($c=\frac{1}{\lambda}$): `sklearn.svm.SVR`

Support Vector Classification (SVC)



Principle [Boser et al., 1992]

$$\min_{f \in \mathcal{H}} \quad \frac{1}{n} \sum_{i=1}^n \max(1 - y_i f(\mathbf{x}_i), 0) + \lambda \|f\|_{\mathcal{H}}^2 \quad (31)$$

- The optimization will promote a large margin between the classes.
- The problem (31) can be reformulated as the following convex Quadratic Program

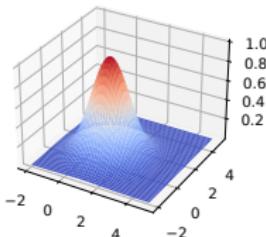
$$\max_{\mathbf{0} \leq \boldsymbol{\beta} \leq \frac{1}{2n\lambda}, \boldsymbol{\beta}^\top \mathbf{y} = 0} \quad \sum_j^n \beta_j - \frac{1}{2} \sum_{i,j}^{n,n} \beta_i \beta_j y_i y_j k(\mathbf{x}_i, \mathbf{x}_j) \quad (32)$$

with the solution $\hat{f}(\mathbf{x})$ using the weights $\hat{\alpha}_i = \hat{\beta}_i y_i$.

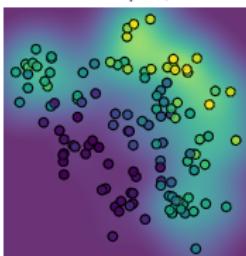
- Consistent estimator (converges to Bayes for large n) [Steinwart, 2005].
- Scikit-learn implementation: `sklearn.svm.SVC`

Support Vector Machines

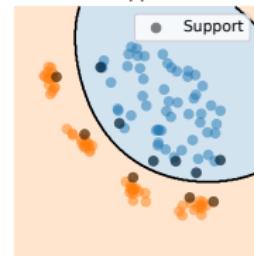
RBF Kernel $k(\mathbf{x}, \mathbf{x}_0)$, $\mathbf{x}_0=[1,1]$



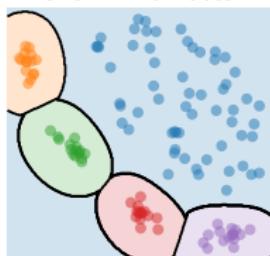
KRR RBF $\gamma=1, \lambda=1$



SVC RBF Support vectors



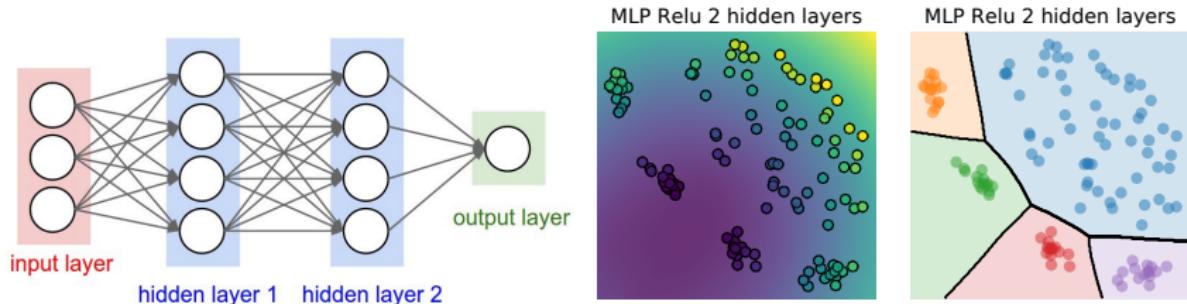
SVC RBF multi-class



SVM and extensions

- ▶ Multi-class classification [Weston and Watkins, 1998] or One-Against-All strategy [Hsu and Lin, 2002] (default in Scikit-learn).
- ▶ Estimation of probability of classes done with a logistic regression on the prediction function f [Platt et al., 1999].
- ▶ Squared SVM (squared hinge loss) lead to a differentiable problem can be solved with gradient descent [Chapelle, 2007].
- ▶ Multiple Kernel Learning allows for learning the feature extraction and selecting the kernel parameter [Bach et al., 2004, Rakotomamonjy et al., 2008].
- ▶ Kernels can be approximated using Nyström method [Williams and Seeger, 2001] or Random Fourier Features (RFF) [Rahimi et al., 2007] for learning on large scale datasets (`sklearn.kernel_approximation`).

Neural Networks



Multi-Layer Perceptron (MLP) [Goodfellow et al., 2016, Chapter 6]

$$\min_{\theta} \sum_{i=1}^n L(y_i, f_{\theta}(\mathbf{x}_i)) + \lambda \Omega(\theta) \quad (33)$$

- Where the function f_{θ} is expressed as

$$f_{\theta}(\mathbf{x}) = f_K(f_{K-1}(\dots(f_1(\mathbf{x})))), \quad \text{with} \quad f_k(\mathbf{x}) = \sigma_k(\mathbf{W}_k \mathbf{x} + \mathbf{b}_k) \quad (34)$$

- The parameters are $\theta = \{\mathbf{W}_k, \mathbf{b}_k\}_k$ and σ_k are non-linear activations.
- Highly non-convex and non-smooth optimization problem in general.
- MLP are universal approximators [Hornik et al., 1989].
- Scikit-learn : `sklearn.neural_network.MLPClassifier / MLPRegressor`
- Implementation faster with GPU-compatible toolboxes (Pytorch/tensorflow).

Neural Networks design

Major architectures

- ▶ **Convolutional layers** [LeCun et al., 1998] for signal and images use a convolution of the signal \mathbf{x} instead of a general linear operator :

$$f_k(\mathbf{x}) = \sigma_k(\mathbf{w}_k * \mathbf{x} + \mathbf{b}_k)$$

- ▶ **Fully convolutional network (U-Nets)** proposed for image segmentation and processing [Long et al., 2015, Ronneberger et al., 2015].
- ▶ **Residual Layers** [He et al., 2016] help train deeper network and avoid vanishing gradients (also facilitates recovering the identity function) :

$$f_k(\mathbf{x}) = \sigma_k(\mathbf{W}_k \mathbf{x} + \mathbf{b}_k) + \mathbf{x}$$

- ▶ **Recurrent Neural Nets (RNN)** [Rumelhart et al., 1986] and Long short-term memory (LSTM) [Hochreiter and Schmidhuber, 1997] for modeling sequences in signals and Natural Language Processing.
- ▶ **Attention models** (transformers) is pointwise product in the layers to focus on some features/parts of the embedding [Vaswani et al., 2017].

Practical implementation

- ▶ ReLU activation $\sigma(x) = \max(0, x)$ allows for deeper networks [Glorot et al., 2011, He et al., 2015]
- ▶ Initialization of the parameters is important [Glorot and Bengio, 2010].

Optimization of deep neural networks

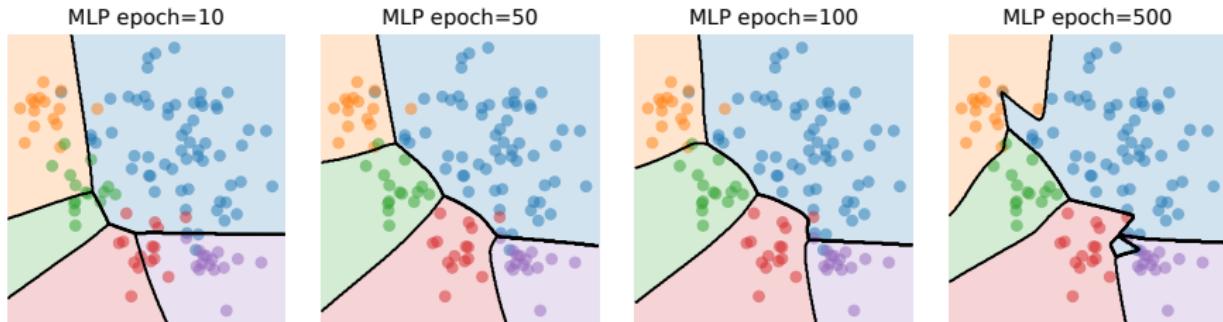
Stochastic Gradient Descent (SGD) on large scale datasets

- ▶ Principle : Never compute the full gradient, only on samples (1 or minibatch).
- ▶ Going through the whole dataset is called an epoch (numerous gradient steps).
- ▶ Fast convergence with averaging (SAG, SRVG, SAGA)
[Johnson and Zhang, 2013, Roux et al., 2012, Defazio et al., 2014].
- ▶ State of the art algorithm for linear SVM, logistic regression, least square.
- ▶ Classification (SVM, Logistic) : `sklearn.linear_model.SGDClassifier`.
- ▶ Regression (least square, huber) : `sklearn.linear_model.SGDRegressor`.

Gradient descent for deep learning

- ▶ Stochastic Gradient Descent and variants work very well on continuous, non-smooth non-convex problems [Bottou, 2010].
- ▶ Use fixed step or change of step size along iterations.
- ▶ Several momentum, averaging and adaptive step size strategies:
 - ▶ Momentum and Accelerated gradients [Nesterov, 1983]
 - ▶ RMSPROP [Tieleman and Hinton, 2012].
 - ▶ Adaptive gradient step ADAGRAD [Duchi et al., 2011].
 - ▶ Adaptive Moment estimation ADAM [Kingma and Ba, 2014].
- ▶ Most optimization strategies implemented in Pytorch/tensorflow.

Regularization of deep neural networks



Regularization strategies [Goodfellow et al., 2016, Chapter 7]

- ▶ Ridge (weight decay) or Lasso on the parameters \mathbf{W}_k for smooth prediction.
- ▶ Early stopping along the epochs (using validation set) [Yao et al., 2007].
- ▶ Dropout shuts down some neurons during training [Srivastava et al., 2014].
- ▶ Data Augmentation uses transformation of data (signals) to create new samples and promote invariance [Shorten and Khoshgoftaar, 2019].
- ▶ Adversarial regularization penalize the classification error of (virtual) adversarial examples [Miyato et al., 2018].

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Ensemble methods

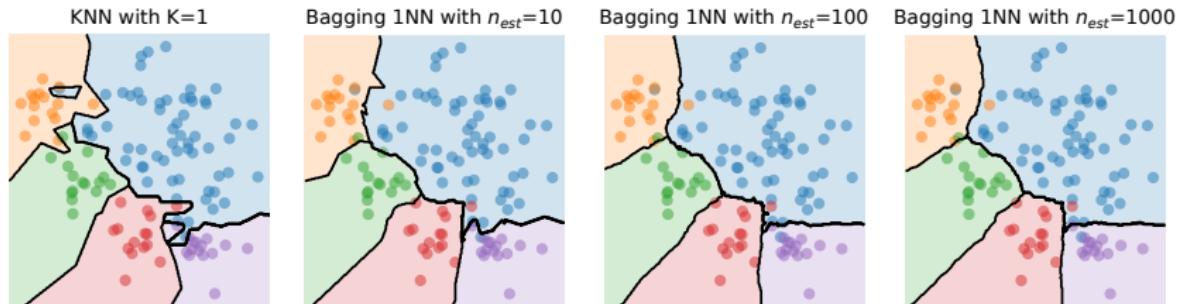
Principle of ensemble methods

- ▶ Generalization of a unique predictor is hard to estimate.
- ▶ Strength in number (and different opinions).
- ▶ Estimate a number of predictors f_k (with some variability).
- ▶ Use the predictions of those predictors to reach a consensus that is more robust.
- ▶ Theoretical result show that merging prediction from "weak" classifiers can minimize the variance and better generalize.
- ▶ Ensemble methods are meta-estimators : they can use existing "black box" estimators.

Two main approaches

- ▶ **Averaging methods** Several predictors f_k are build independently and they are averaged for a prediction (Bagging, Random Forests).
- ▶ **Boosting** Several predictors f_k are build sequentially to reduce the bias/error of their combination (Adaboost, Gradient Boosting)

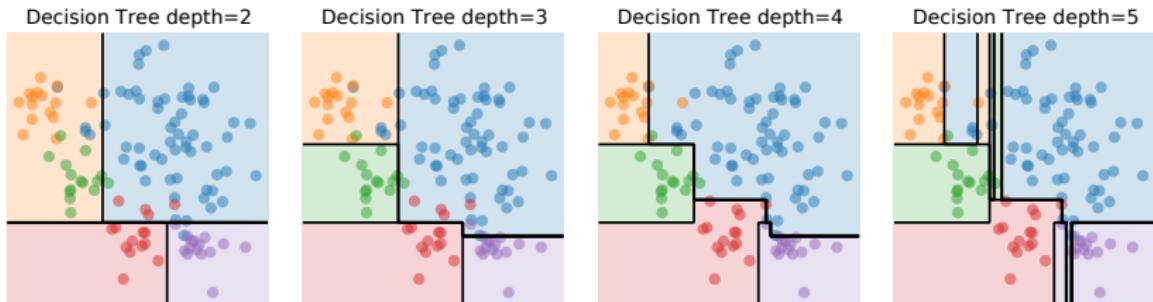
Bagging



Principle [Breiman, 1996]

- ▶ Select a supervised estimation method (any supervised predictor).
- ▶ Train several predictors on random selection of the train data.
- ▶ Sampling subset of samples with replacement is also called **Bootstraping**.
- ▶ Predict using majority voting (classification) or average value (regression).
- ▶ Several variants where predictors are trained on random subsets :
 - ▶ of the features **Random subspaces** [Ho, 1998].
 - ▶ of features and samples **Random Patches** [Louppe and Geurts, 2012].
- ▶ General implementations can select proportion of selected samples and features.
- ▶ Scikit-learn : `sklearn.ensemble.BaggingClassifier / BaggingRegressor`

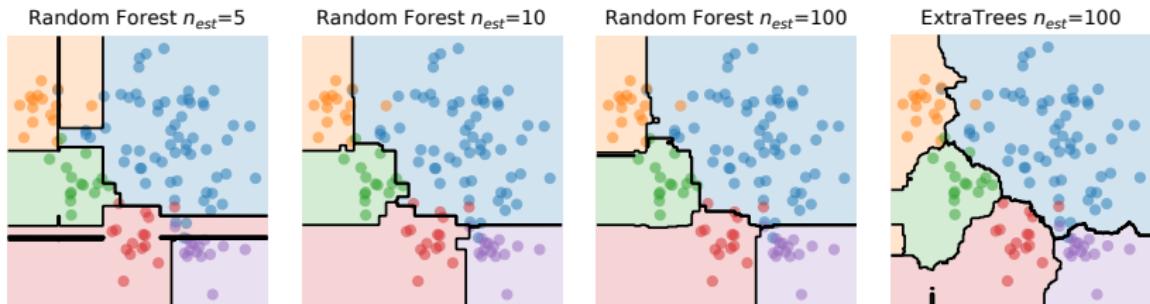
Decision Tree



Principle [Breiman et al., 2017]

- ▶ Predictor modeled as a binary tree where each node is a decision based on a threshold of the value of one of the features.
- ▶ Standard algorithms are ID3 [Quinlan, 1986] and C4.5 [Quinlan, 1993] and CART that use information entropy to select the variable that will be used on each node.
- ▶ Complexity of the tree depends on the depth of the tree.
- ▶ Model is very interpretable and explainable : you can express all the reasons for a given decision.
- ▶ Rarely used alone in high dimension due to low generalization ability.
- ▶ Scikit-learn : `sklearn.tree.DecisionTreeClassifier / DecisionTreeRegressor`

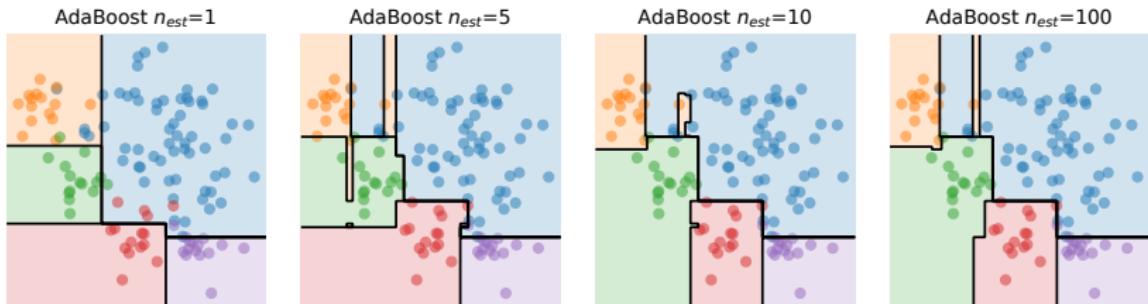
Random Forests (RF)



Principle [Ho, 1995, Breiman, 2001]

- ▶ Perform Bagging using Decision Trees as weak classifiers.
- ▶ Select only from a random subset of features on each node (similar to random subspaces but on each node).
- ▶ Loose some interpretability of the trees but gain generalization performance.
- ▶ Similar adaptive neighborhood with RF and KNN [Lin and Jeon, 2006].
- ▶ Extremely randomized trees (ExtraTrees) use random thresholds in the trees instead of optimal thresholds as in Decision Trees [Geurts et al., 2006].
- ▶ Scikit-learn : `sklearn.tree.RandomForestClassifier / RandomForestRegressor`
`sklearn.ensemble.ExtraTreesClassifier / ExtraTreesRegressor`

Adaboost



Principle [Freund and Schapire, 1997]

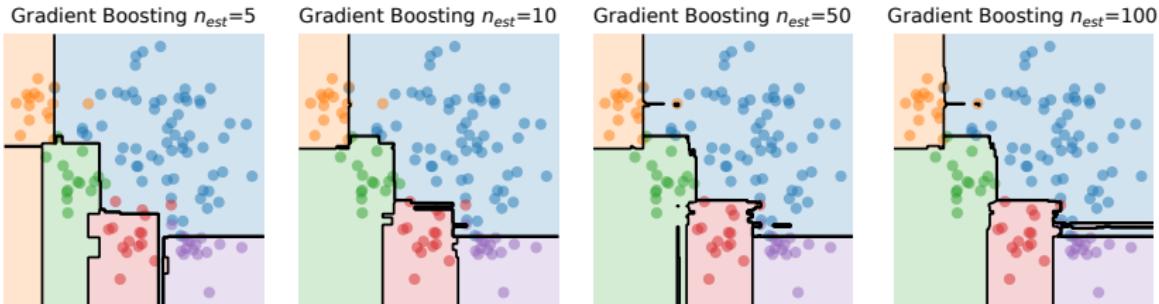
- ▶ The predictor is a weighted sum $F_k(\mathbf{x}) = \sum_k \alpha_k f_k$.
- ▶ Estimated predictors f_k trained sequentially on weighted training samples.
- ▶ At each step k a new predictor is estimated by minimizing :

$$f_k, \alpha_k = \arg \min_{f, \alpha} \sum_{i=1}^n e^{-y_i(F_{k-1}(\mathbf{x}) + \alpha f(\mathbf{x}))} = \sum_{i=1}^n w_i^k e^{-y_i \alpha f(\mathbf{x})} \quad (35)$$

For binary classification with $f(\mathbf{x}) \in \{-1, 1\}$.

- ▶ The weights are updated at each iteration to favor samples miss-predicted by the previous predictors.
- ▶ Scikit-learn : `sklearn.ensemble.AdaBoostClassifier / AdaBoostRegressor`

Gradient Boosting (GB)



Principle [Friedman, 2001]

- ▶ Generalization of AdaBoost to any differentiable loss L .
- ▶ Estimate a predictor $F_k(\mathbf{x}) = \sum_k f_k$ by minimizing iteratively the ERM:

$$f_k = \arg \min_f \sum_{i=1}^n L(y_i, F_{k-1}(\mathbf{x}) + f(\mathbf{x})) \quad (36)$$

- ▶ This is approximated by a gradient descent in the functional space with

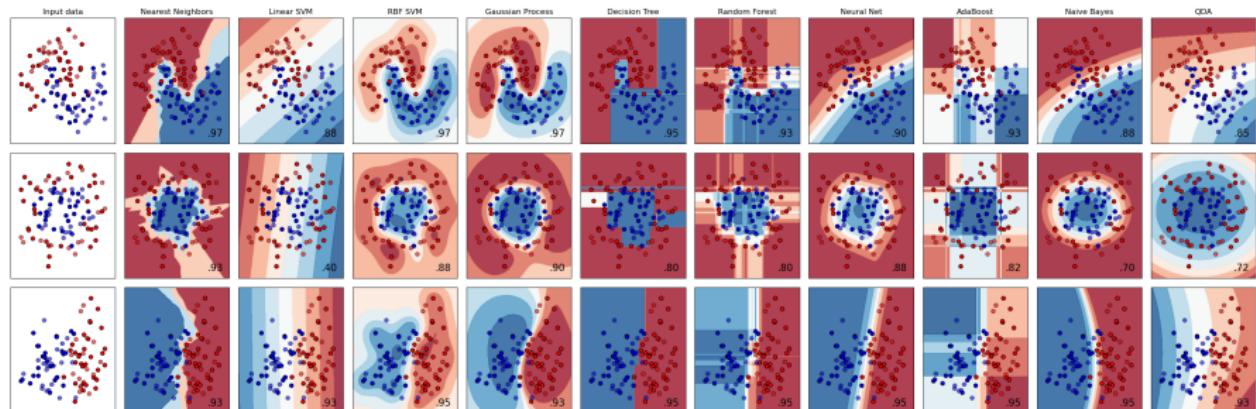
$$F_k(\mathbf{x}) = F_{k-1}(\mathbf{x}) - \gamma_m \sum_{i=1}^n \nabla_f L(y_i, F_{k-1}(\mathbf{x}) + f(\mathbf{x})) \quad (37)$$

- ▶ Stochastic Gradient Boosting use random subsets of samples [Friedman, 2002].
- ▶ XGBoost, GB variant, won numerous competitions [Chen and Guestrin, 2016].
- ▶ Sklearn : `sklearn.ensemble.GradientBoostingClassifier / GradientBoostingRegressor`

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Conclusion



Supervised learning

- ▶ Bayesian methods lead to probabilistic predictions but densities can be hard to estimate in high dimension.
- ▶ Always try linear models first! They are harder to overfit but use regularization with Ridge or Lasso especially in high dimension.
- ▶ For small datasets with nonlinear prediction functions use SVM with hand-crafted kernels (large datasets can use kernel approximation).
- ▶ Neural Network can estimate complex functions on large datasets. The different layers can benefit from the structure of the data (convolution on image or signal).
- ▶ Gradient Boosting (XGBoost) works in many cases when good features available.

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