Machine Learning

Model Selection

Alberto Maria Metelli - Francesco Trovò

Definition of different models

What to do in the case the model you are considering is not performing well even by tuning properly the parameters (cross-validation)?

We have two opposite options:

- simplify the model $\rightarrow$ **model selection** (today)
- increase its complexity (next time)

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How to Select a Model

We already discussed how to evaluate a specific model (bias/variance dilemma)

- Model Selection
  - Feature selection: choose only a subset of significant features to use
  - Feature extraction (Dimensionality reduction): project the features in another (lower) dimensional space
  - Regularization (shrinkage): introduce some penalization for complex models in the loss function
- Ensemble model
  - Bagging
  - Boosting

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- Feature Selection
  - **Filter methods**
  - Embedded methods (e.g., Lasso)
  - Wrapper methods
    - Brute force
    - Forward Step-wise selection
    - **Backward step-wise selection**
- Feature Extraction
  - **PCA**
  - ICA
- Regularization (e.g., Ridge)

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Feature Selection: Filter method

Correlation filter

- We have no hypothesis space of models as input
- For each feature $j \in \{1, \dots, M\}$ compute the **Pearson correlation coefficient** between x_k and the target y:

$$\hat{\rho}(x_j, y) = \frac{\sum_{n=1}^{N}(x_{j,n} - \overline{x}_j)(y_n - \overline{y})}{\sqrt{\sum_{n=1}^{N}(x_{j,n} - \overline{x}_j)^2}\sqrt{\sum_{n=1}^{N}(y_n - \overline{y})^2}}, \qquad \overline{x}_j = \frac{1}{N}\sum_{n=1}^{N} x_{j,n}, \quad \overline{y} = \frac{1}{N}\sum_{n=1}^{N} y_n.$$

- Select the features with **higher** Pearson correlation coefficient
- Captures only **linear** relationships between features and target
- There exist approaches for non-linear relationships (e.g., mutual information)

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Feature Selection: Wrapper Methods

Brute force

- We have a hypothesis space of models $\mathcal{H}$ as input
- For each k number of features $k \in \{1, \ldots, M\}$
  - Learn all the possible $\binom{M}{k}$ possible models within $\mathcal{H}$ with k inputs
  - Select the model with the smallest loss
- Select the number of features k providing the model with the smallest loss
- Warning: model selection should be done appropriately (e.g., cross-validation)
- Problem: if M is large enough the computation of all the models is **unfeasible** (combinatorial complexity)

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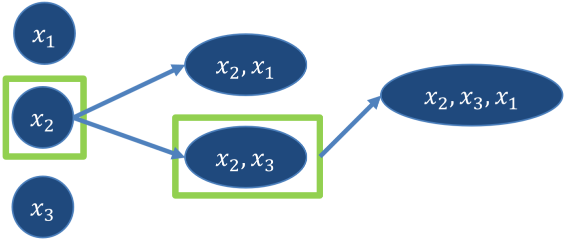
Step-wise selection

We evaluate only a subset of the possible models

Forward step-wise selection



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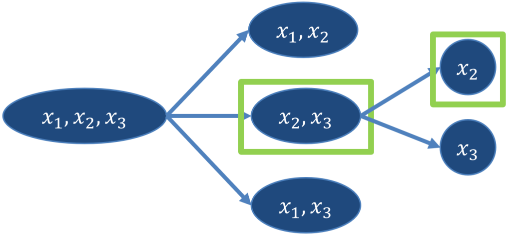

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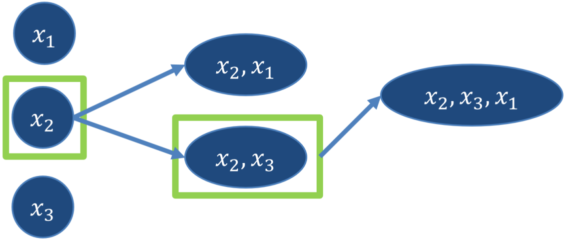

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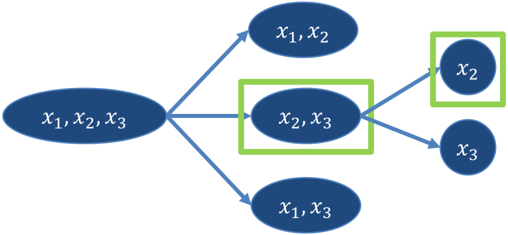

Backward step-wise selection on the Iris Dataset (1)

- Assume the problem is to discriminate between Virginica and Non-Virginica iris
- We select a performance index: validation accuracy on 20% of the data
- Train a model on the full data $(x_1, x_2, x_3, x_4)^\top$: Logistic regression
- Remove one of the features and check the error:
  - Model with $(x_1, x_2, x_3)^\top$: accuracy 1
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- Removing a single feature does not change the model performance

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Backward Feature selection on the Iris Dataset (2)

- Let us remove one of the features at random x_4
- Remove another feature and check the error:
  - Model with $(x_1, x_2)^\top$: accuracy 0.96
  - Model with $(x_1, x_3)^\top$: accuracy 0.96
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- The model with (x_2, x_3) is performing better than the others
- Iterate *one more time*

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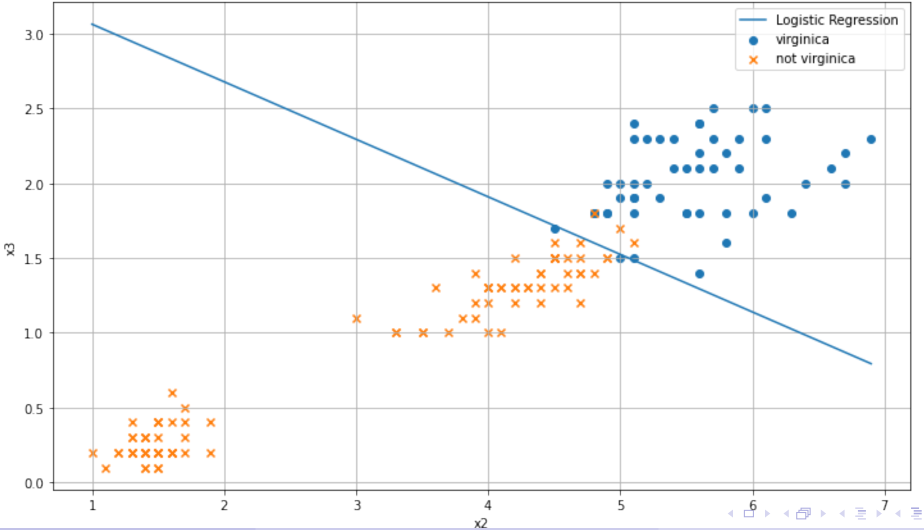
Results on the Iris Dataset



Feature Extraction: Principal Component Analysis (PCA)

- unsupervised **dimensionality reduction** technique
    - extract some low dimensional features from a dataset
- perform a **linear transformation** of the original data $\mathbf{X}$
    - the largest variance lies on the first transformed feature
    - the second largest variance on the second transformed feature
    - ...
- At last, we only keep some of the features we extract

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Procedure

- Translate the original data $\mathbf{X}$ to $\tilde{\mathbf{X}}$ s.t. they have zero mean
- Compute the covariance matrix of $\tilde{\mathbf{X}}$, $\mathbf{C} = \tilde{\mathbf{X}}^\top \tilde{\mathbf{X}}$
- The eigenvectors of $\mathbf{C}$ are the **principal components**
  - The eigenvector $\mathbf{e}_1$ corresponding to the largest eigenvalue λ_1 is the first principal component
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- Compute the covariance matrix of $\tilde{\mathbf{X}}$, $\mathbf{C} = \tilde{\mathbf{X}}^\top \tilde{\mathbf{X}}$
- The eigenvectors of $\mathbf{C}$ are the **principal components**
    - The eigenvector $\mathbf{e}_1$ corresponding to the largest eigenvalue λ_1 is the first principal component
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$$\mathbf{T} = \tilde{\mathbf{X}}\mathbf{W}$$

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How Many Features

There are a few different methods to determine how many feature to choose

- Keep all the principal components until we have a **cumulative variance** of 90%-95%

$$\text{cumulative variance with } k \text{ components} = \frac{\sum_{j=1}^{k} \lambda_i}{\sum_{j=1}^{M} \lambda_i}$$

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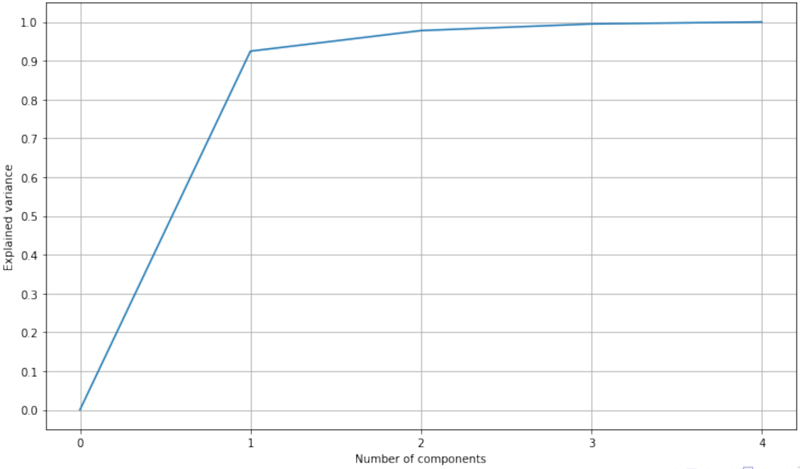
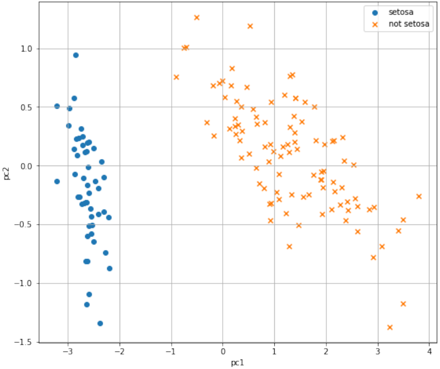
Cumulated Variance Plot

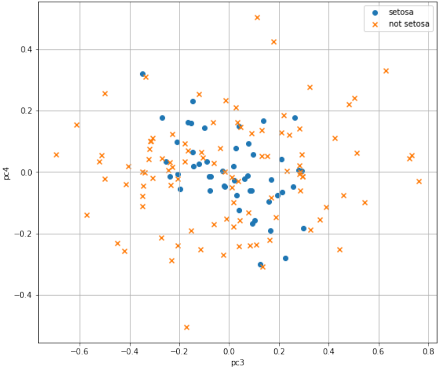
Using the Iris dataset inputs:



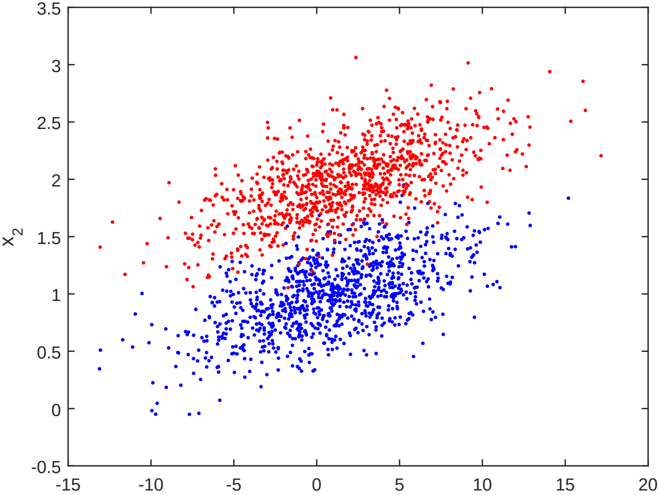
Principal Components

If we separate the first two components from the second twos:





Simpson's Paradox



PCA Different Purposes

- **Feature Extraction**: reduce the dimensionality of the dataset by selecting only the number of principal components retaining information about the problem
- **Compression**: keep the first k principal components and get $\mathbf{T}_k = \tilde{\mathbf{X}}\mathbf{W}_k$. The linear transformation $\mathbf{W}_k$ minimizes the **reconstruction error**:

$$\min_{\mathbf{W}_k \in \mathbb{R}^{M \times k}} \|\mathbf{T}\mathbf{W}_k^\top - \tilde{\mathbf{X}}\|_2^2$$

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Regularization

Already known regularization procedure:

- Ridge:

$$L(\mathbf{w}) = \frac{1}{2}\mathrm{RSS}(\mathbf{w}) + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$$

- Lasso:

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- They can be applied to the linear regression techniques, it can be extended for other methods
- For classification we will see some specific methods

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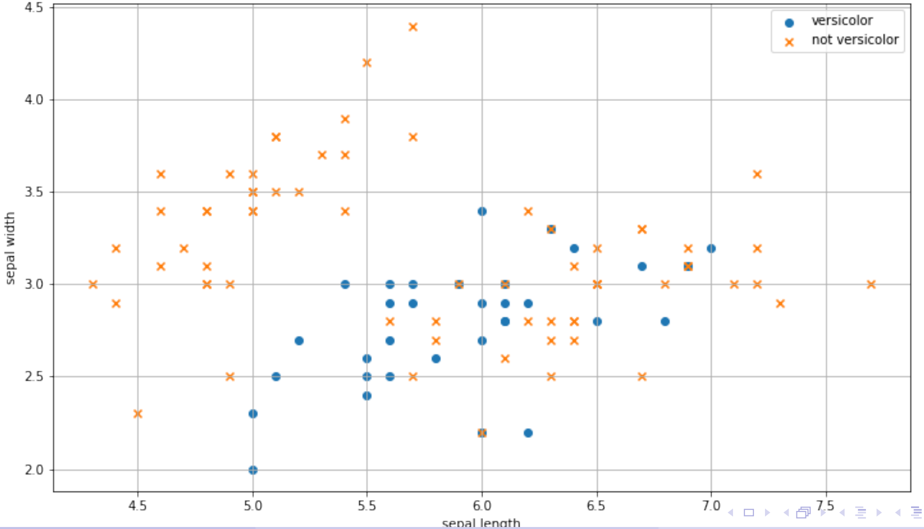
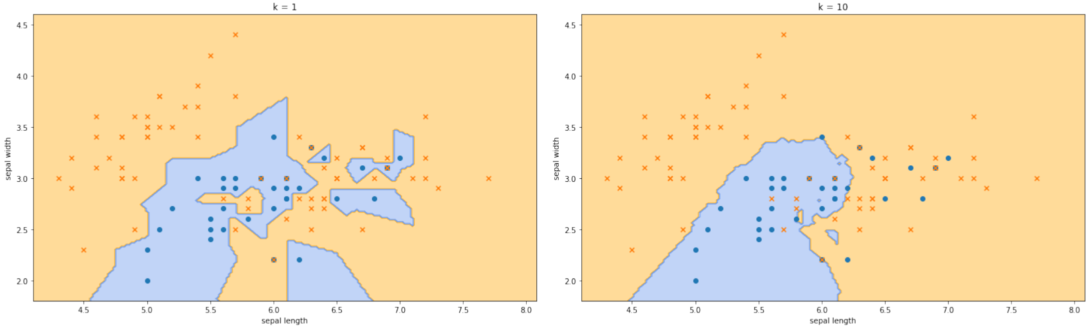
A hard problem



K-Nearest Neighbour

Different values of the K parameter



The larger the value of K, the more the model is regularized ($1/K$ acts as a regularization hyperparameter)

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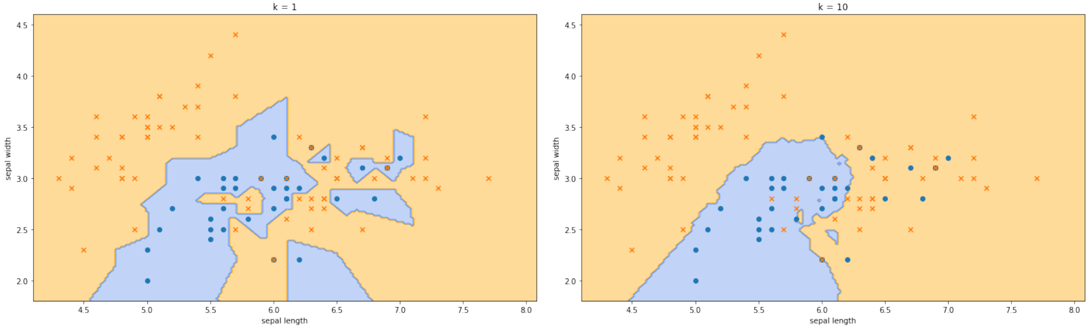

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Ensemble Methods

Bagging

- **Goal**: achieve a **small variance** without increasing the bias
- This is achieved by **training (possibly) in parallel** N learners:
  1. Generate a dataset applying random sampling with replacement (**bootstrapping**)
  2. Train the model on the dataset
- To compute the **prediction** for new samples, apply all the trained models and combine the outputs with **majority voting** (classification) or **averaging**
- Bagging is generally helpful and reduce the variance, although the **sampled datasets are not independent**
- It helps with **unstable learners**, i.e., learners that change significantly with even small changes in the dataset (low bias and high variance) (regression)

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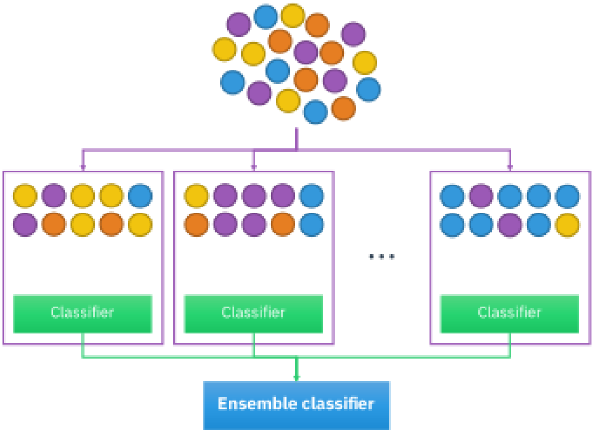

Boosting

- **Goal**: achieve a **small bias** by using on simple (**weak**) learners
- At the same time, using simple learners, aims at keeping a **small variance**
- This is achieved by **sequentially training** weak learners:
  1. Give an **equal weight** to all the samples in the training set
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  3. Compute the error of the trained model on the **weighted training set**
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- The ensemble of models learned can be applied on new samples by computing the **weighted prediction** of each model (more accurate models weight more)

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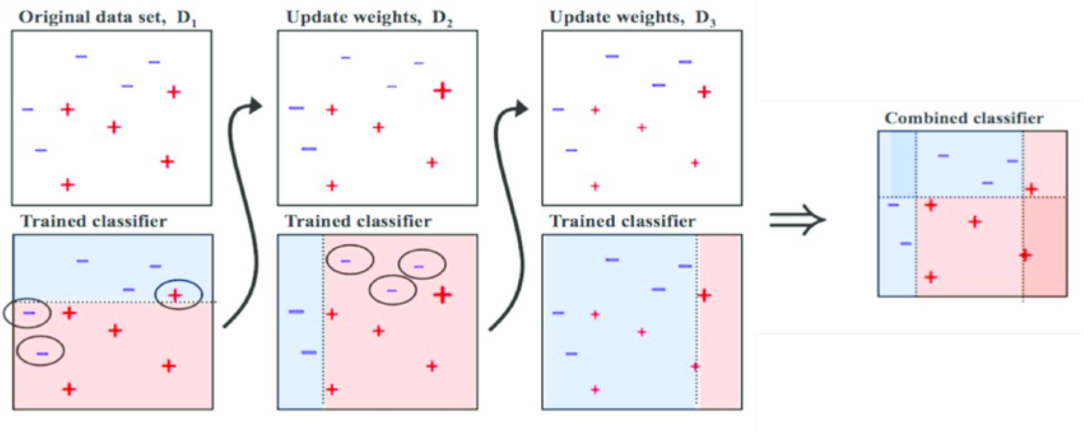
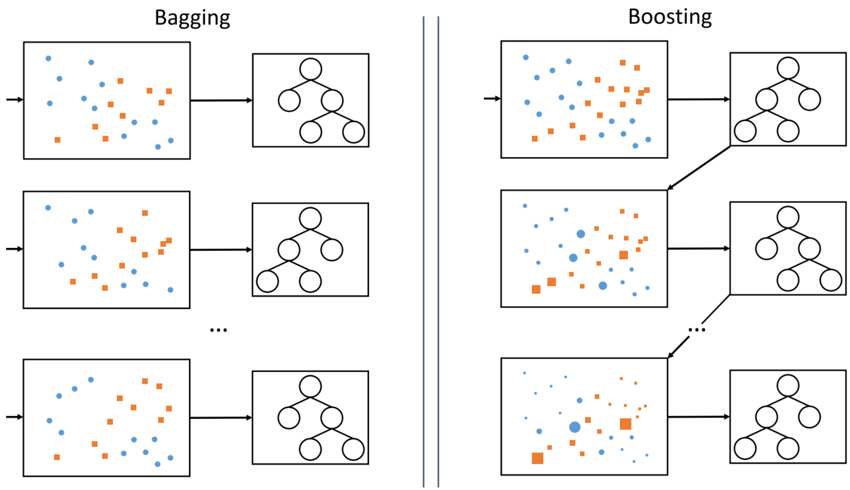

Original data set, D1
Update weights, D2
Update weights, D3
Trained classifier
Trained classifier
Trained classifier
Combined classifier

Bagging vs Boosting



Bagging vs Boosting

Bagging

- Reduces variance
- Not good for stable learners
- Can be applied with noisy data
- Usually helps but the difference might be small
- Parallel

Boosting

- Reduces bias (generally without overfitting)
- Works with stable learners
- Might have problem with noisy data
- Not always helps but it can makes the difference
- Sequential