Inferential statistics

Applied Data Analysis (ADA) - October 2025

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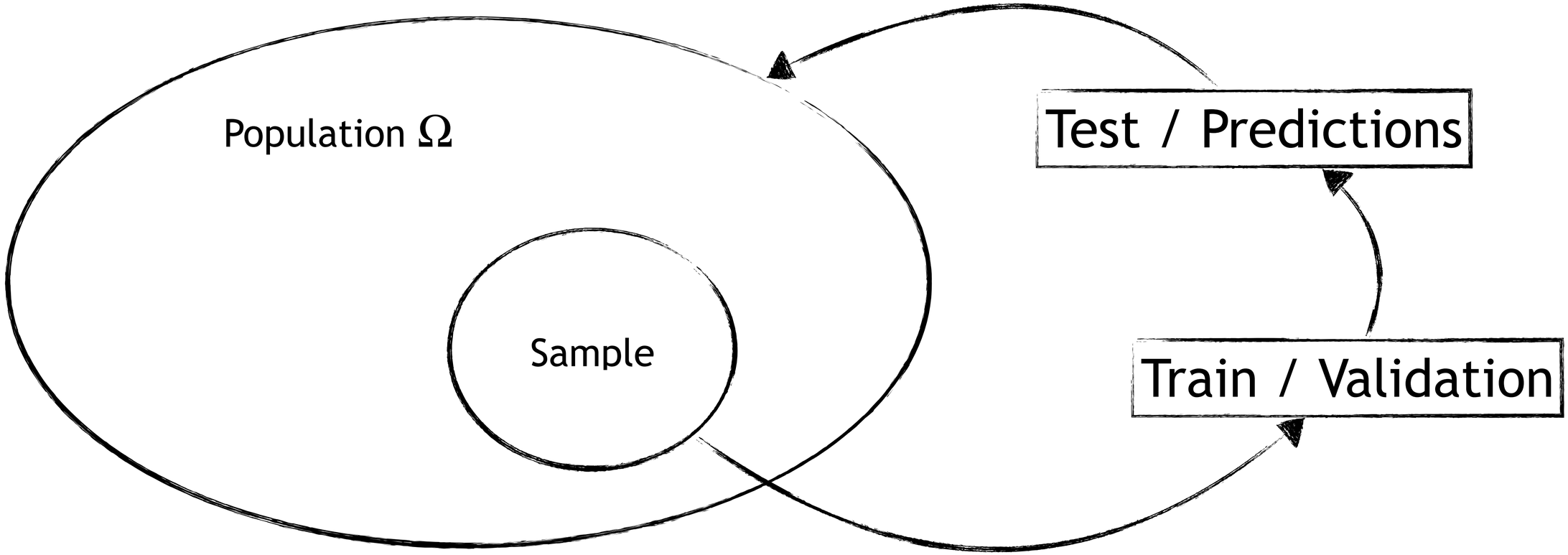
- Monday : Metrics and training process
  - Supervised & Unsupervised learning
  - Evaluation metrics
  - Training process
- Tuesday : Linear models
- Wednesday : Support Vector Machine models
- Thursday : Decision trees
- Friday : Time series analysis

Inferential statistics

Definition : Inferential statistics is the idea of drawing conclusions about a population base on data from a sample.



Underfitting

Definition : The model is too simple to capture underlying patterns. It can be visualised by a poor performance both on training and validation sets.

=> Make the model more complex by modifying its parameters or completely change the model.

Overfitting

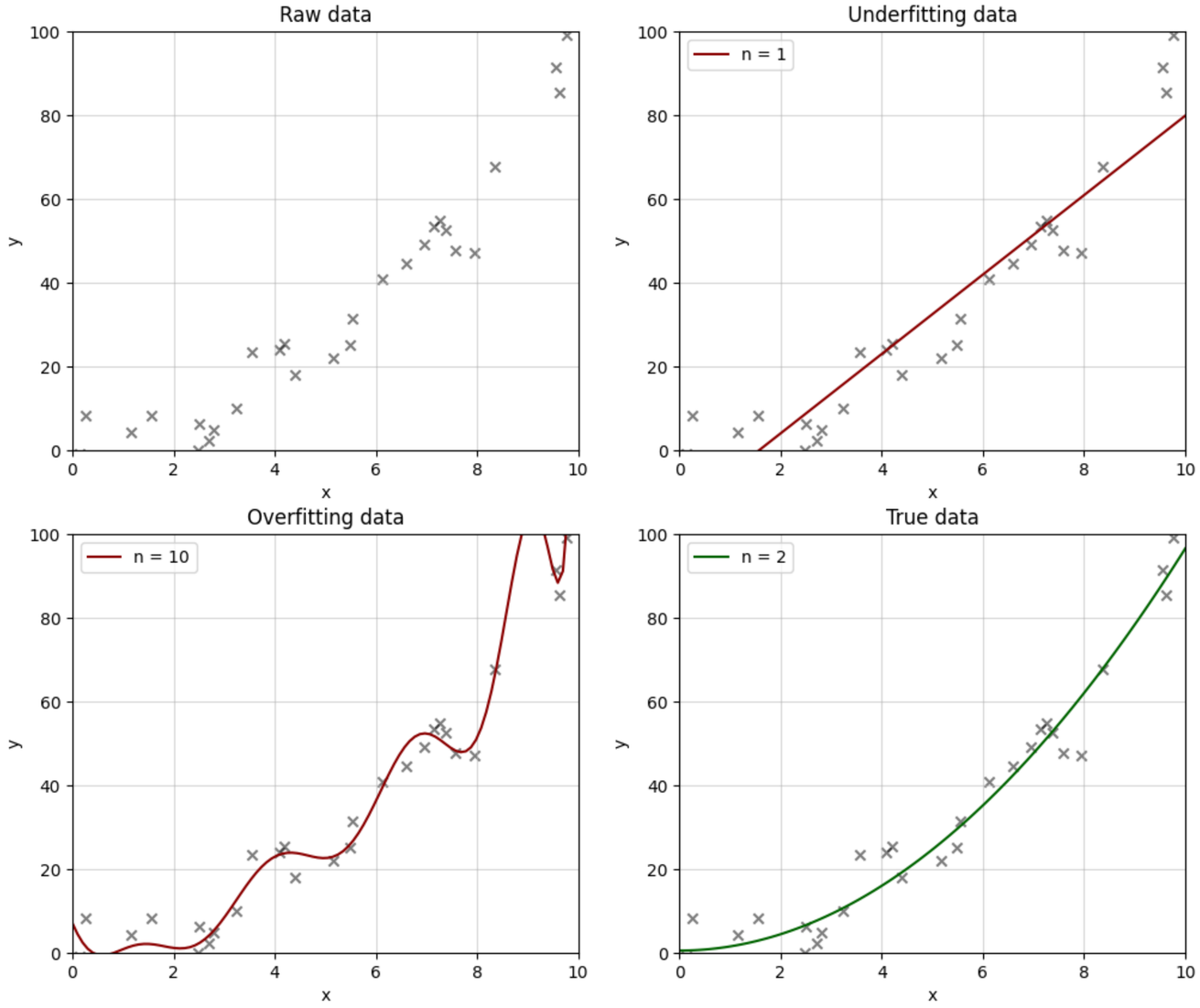
Definition : The model learns noise and details from the training data. It can be visualised by a good performance on training set but poorly on validation set.

=> Simplify the model, regularisation or training data set not well defined regarding the validation set (split to redo).

Underfitting / Overfitting

Practice : Use the data set `overfitting_data.csv`, train a Polynomial Regression model on it and plot the results. Do it for $n = 1, 2$ and 10.

Underfitting / Overfitting



Supervised learning

Definition : Supervised learning is a type of machine learning where the model is trained on a labeled dataset, meaning each input data point is paired with the correct output (target).

=> The goal is for the model to learn the mapping from inputs to outputs and make predictions on new unseen data.

Supervised learning
- Example -

- Spam detection in mails => Input : email text / Label : spam or not spam
- Prediction of house prices => Input : number of rooms, area, location / Label : price.
- Medical diagnosis => Input : patient symptoms and test results / Label : disease present or not.
- Image classification => Input : image pixels / Label : “cat”, “dog”, etc…

Unsupervised learning

Definition : Unsupervised learningn is a type of machine learning where the model is given unlabeled data.

=> The goal is to find patterns, groupings, or structures within the data without knowing the “correct” answers.

Unsupervised learning
- Example -

- Customer segmentation => Task : grouping customers by purchasing behaviour.
- Anomaly detection => Task : Finding fraudulent transactions in banking data.
- Topic modelling => Task : discovering themes in a collection of new articles.
- Dimensionality reduction => Task : visualizing high-dimensional data (e.g., genetics, images) using PCA.

Supervised learning
- Regression methods -

Definition : It models the relationship between one or more independent variables (features) and a continuous dependent variable (target).

=> It’s a supervised learning method.

Regression methods
- Illustration of some models -

- *Simple linear regression :* single feature vs target.
- *Multiple linear regression :* multiples features to predict the target.
- *Polynomial regression :* Useful for modelling non-linear trends.
- *Regularized regression :* Penalizes weights to prevent overfitting and manage multicollinearity => Improves generalisation.

Supervised learning
- Classification methods -

Definition : It models the relationship between one or more independent variables (features) and a categorical dependent variable (target).

=> It’s also a supervised learning method.

Classification methods
- Example -

- *Logistic regression :* Probability model for binary tasks.
- *Decicision tree :* Tree based model, interpretable model.
- *Random forest :* multiple random trees.
- *Support Vector Machines (SVM) :* Find optimal separating hyperplane.
- *Neural Networks :* Flexible and powerful (especially for high-dimensional inputs).

Evaluation of models
- Metrics -

How do you know you model is working better than the others ?

➡ You define metrics to evaluate the model’s performance.

Evaluation of models
- Metrics -

How do you know you model is working better than the others ?

➡ You define metrics to evaluate the model’s performance.

➡ But can you use the same metrics for regression and classification tasks ?
➡ How do you chose your metric ?

Evaluation of models
- Metrics for regression -

Goal : We need to have a metric that evaluate how close predictions of continuous variables are to the actual target variables.

1 - Error terms : Let y_i be the true value and $\hat{y}_i$ the predicted value:

$$\epsilon_i = y_i - \hat{y}_i$$

$$\Rightarrow \text{ Error} = \sum_{i=1}^{n} \epsilon_i$$

Evaluation of models
- Metrics for regression -

2 - Mean Absolute Error (MAE) : It measures average absolute difference.

$$\text{MAE} = \frac{1}{n}\sum_{i=1}^{n} |y_i - \hat{y}_i|$$

Remark : Easy to interpret but doesn't penalise large errors.

Evaluation of models
- Metrics for regression -

3 - Mean Squared Error (MSE) : It measures the square of errors.

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \hat{y}_i\right)^2$$

Remark : Commonly used in optimisation!

Evaluation of models
- Metrics for regression -

4 - Root Mean Squared Error (RMSE) : Its measure has the same units as the target variable.

$$\text{RMSE} = \sqrt{\text{MSE}}$$

Remark : More sensitive to outliers than MAE.

Evaluation of models
- Metrics for regression -

5 - R-Squared (R^2) : It measures a proportion of variance explained.

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2}$$

Remark : 0 means that the prediction is not better than the mean as a naïve prediction.

Evaluation of models
- Metrics for regression -

6 - Mean Average Percentage Error (MAPE) : It measures a prediction accuracy of the models.

$$\text{MAPE} = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{y_i - \hat{y}_i}{y_i}\right|$$

Remark : Very intuitive error interpretation in terms of relative error.

Evaluation of models
- Metrics for classification -

Goal : We need to have a metric that evaluate the quality of the prediction given by a specific model.

0 - Basic concepts:

- *True Postive (TP) :* true value = 1, predicted value = 1
- *True Negative (TN) :* true value = 0, predicted value = 0
- *False Postive (FP) :* true value = 0, predicted value = 1
- *False Negative (FN) :* true value = 1, predicted value = 0

Evaluation of models
- Metrics for classification -

1 - Accuracy: It measures the proportion of correct predictions.

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

Remark : Issues when facing imbalanced classes.

Evaluation of models
- Metrics for classification -

2 - Precision : It measures how many predicted positives were correct.

$$\text{Precision} = \frac{???}{???}$$

Remark : Useful for imbalanced classes.

Evaluation of models
- Metrics for classification -

2 - Precision : It measures how many predicted positives were correct.

$$\text{Precision} = \frac{TP}{TP + FP}$$

Remark : Useful for imbalanced classes.

Evaluation of models
- Metrics for classification -

3 - Recall : It measures how many actual positives were captured.

$$\text{Recall} = \frac{???}{???}$$

Remark : Useful for imbalanced classes.

Evaluation of models
- Metrics for classification -

3 - Recall : It measures how many actual positives were captured.

$$\text{Recall} = \frac{TP}{TP + FN}$$

Remark : Useful for imbalanced classes.

Evaluation of models
- Metrics for classification -

4 - F1-score : It measures harmonic mean of precision and recall.

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

Remark : Useful for imbalanced classes.

Evaluation of models
- Metrics for classification -

5 - Confusion matrix : It shows all 4 outcomes (TP, TN, FP, FN) in a 2x2 table.

		Prediction	
		0	**1**
Truth	**0**	TN	FP
	1	FN	TP

Evaluation of models
- Metrics for classification -

6 - Log-loss (cross-entropy loss) : It measures probabilistic confidence in predictions.

$$\text{Log-loss} = -\frac{1}{n}\sum_{i=1}^{n}\left[y_i \log(p_i) + (1-y_i)\log(1-p_i)\right]$$

Remark : Commonly used in optimisation!

Practice
- Cross-validation using sklearn -

Training process
- General overview -

- ***Data preprocessing :*** Cleaning, normalisation, encoding, split, etc… (EDA)
- ***Model selection :*** Chose one or multiples model types.
- ***Loss function definition :*** Quantify how wrong the model is (not performance!)
- ***Optimization :*** Algorithms to minimize loss such as gradient descent.
- ***Evaluation :*** Measure performance on training and validation sets.

Practice
- KNN -

- Monday : Metrics and training process
- Tuesday : Linear models
  - Linear regression
  - Polynomial & Interaction terms regression
  - Ridge & Lasso regression
- Wednesday : Support Vector Machine models
- Thursday : Decision trees
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Correction of the exercises

Linear Models

Linear regression

Definition : It's a classic model for regression task, the idea is to predict a continuous target variable with a linear combination of the features (categorical or continuous).

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_n x_n + \epsilon$$

Assumptions : Linearity, independence, normality of errors.

Linear regression
- How it trained technically ? -

To compute the « right » parameters of the model, we are aiming to minimise a loss. This loss can be MSE like:

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \hat{y}_i\right)^2$$

How to minimise it ?

Linear regression
- Gradient descent -

We start from a random parameter β and we iterate from it until convergence of the method. More formally it gives a iteration n the following:

$$\beta_{n+1} = \beta_n - \alpha \nabla_\beta \text{MSE}$$

$$= \beta_n - \alpha \frac{2}{n} X^T (X\beta - y)$$

Linear regression
- Practice -

Exercise : Load the data set `load_diabetes` from sklearn library, and train and test a linear regression model on this data set.

Polynomial and interaction terms regression

Definition : We stick to a linear regression architecture but adding new feature to our data set. We add features combinations (e.g. x_i^2 or $x_i x_j$) to our set of features and do the same as before.

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \beta_4 x_2^2 + \epsilon$$

Remark : The main work here is done in EDA to determine which interaction should be included in your set of features

Ridge regression

Definition : We face overfitting with linear regression and there is no inside parameters to play with to compensate this. Then, we use « regularizers ». Here we use L2-regularization, also called **Ridge regression :**

$$\text{loss} = \text{MSE} + \lambda \sum_i \beta_i^2$$

Specificities : Encourage small weights (but not zero) which helps keeping features when they are all important, keep the model smooth and reduce sensitivity to individual features.

Lasso regression

Definition : Same situation as before but instead we use L1-regularization:

$$\text{loss} = \text{MSE} + \lambda \sum_i |\beta_i|$$

Specificities : Encourage weights to zero (sparsity), useful for feature selection, model robust when only few features matter.

Ridge and Lasso regressions
- Practice -

Exercise : Still on the data set `load_diabetes`, train and test Ridge and Lasso regression models and cross-validate the best parameter to use for λ.

- Monday : Metrics and training process
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  - Logistic regression
  - Support Vector Machine
  - Support Vector Regression
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Correction of the exercises

Logistic regression

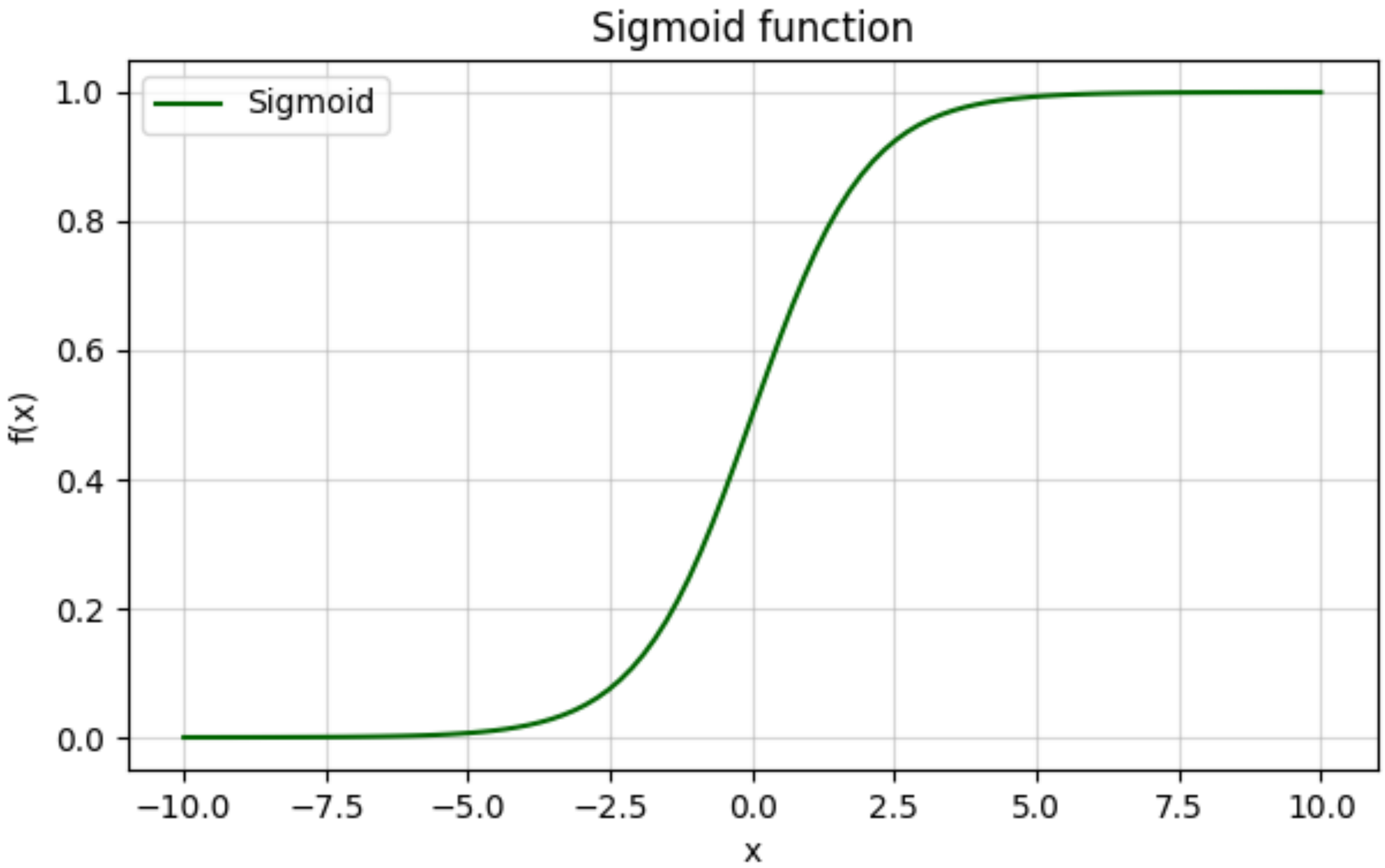
Definition : The logistic regression method is not for regression tasks but for classification tasks. The idea is to start from logistic function defined as:

$$\sigma(t) = \frac{1}{1 + e^{-t}}$$

And we define t as a linear combination of the exploratory variable such as $t = \beta_0 + \beta_1 x$ inducing (probability x belongs to class 1):

$$\mathbb{P}[y = 1 \,|\, x] = p_x = \sigma(\beta_0 + \beta_1 x) = \frac{1}{1 + e^{-\beta_0 - \beta_1 x}}$$

Sigmoid function



Logistic regression

Then, we use the log-loss (or cross-entropy loss) to train the logistic regression model. It can be defined as follow :

$$\mathscr{L}(\beta) = -\frac{1}{n}\sum_{i=1}^{n}\left[y_i \log(p_i) + (1-y_i)\log(1-p_i)\right]$$

Remark : Commonly used when face to binary classification.

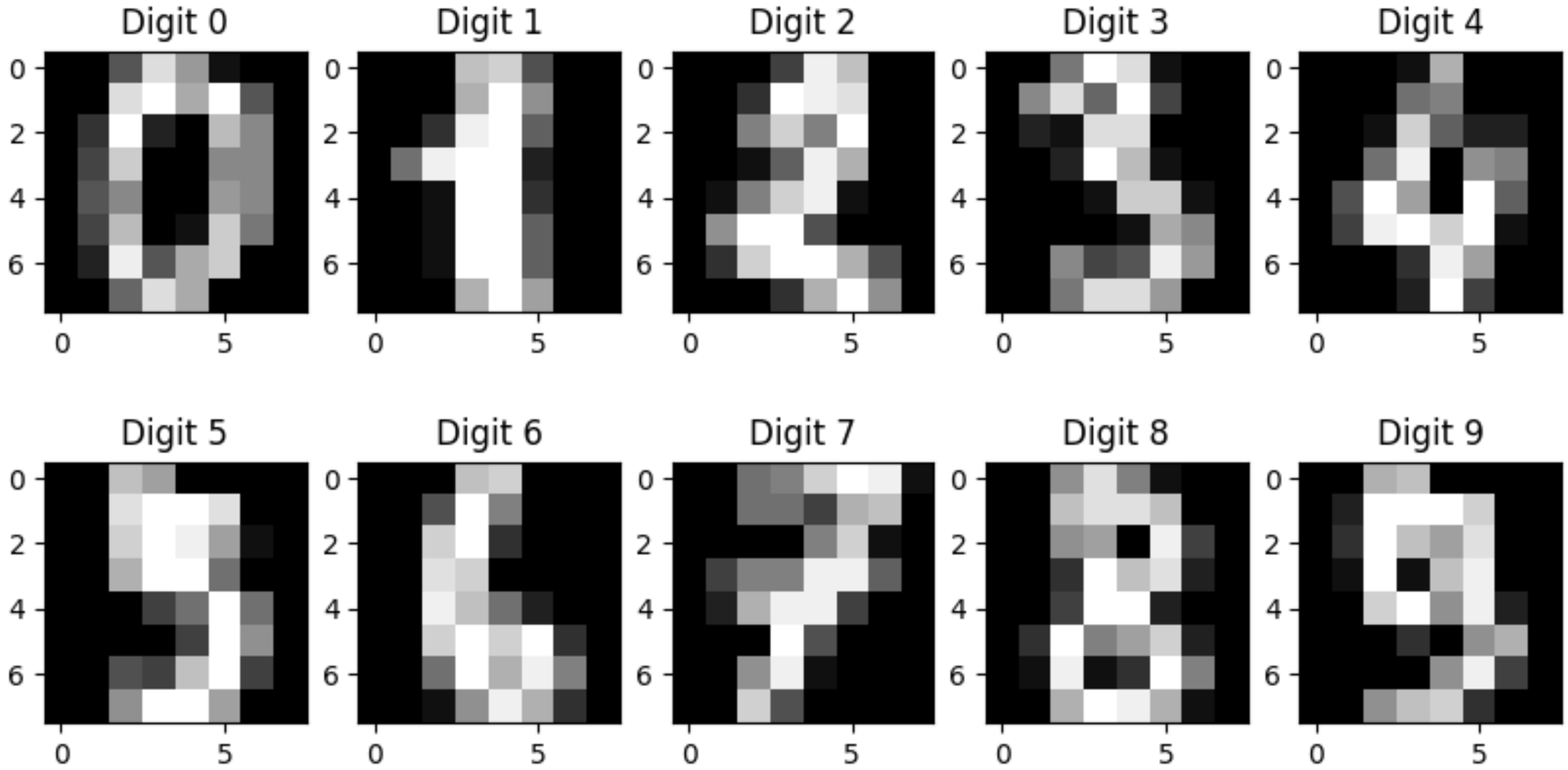
Multinomial logistic regression

We follow the same idea as logistic regression but we are facing multi-class target instead of binary, i.e. $y \in \{0,1,\ldots,K\}$ and we note:

$$p_{ij} = \mathbb{P}\left[y_i = j \,|\, x\right]$$

for each class $j \in \{0,1,\ldots,K\}$ and element $i = 1,\ldots,n$.

Some practice
- What model do you use ? -



Support Vector Machines
- SVM -

Definition : Intuitively, you have a set of points with different labels you want to classify. The Support Vector Machine (SVM) models are looking for an hyperplane that separates the classes.

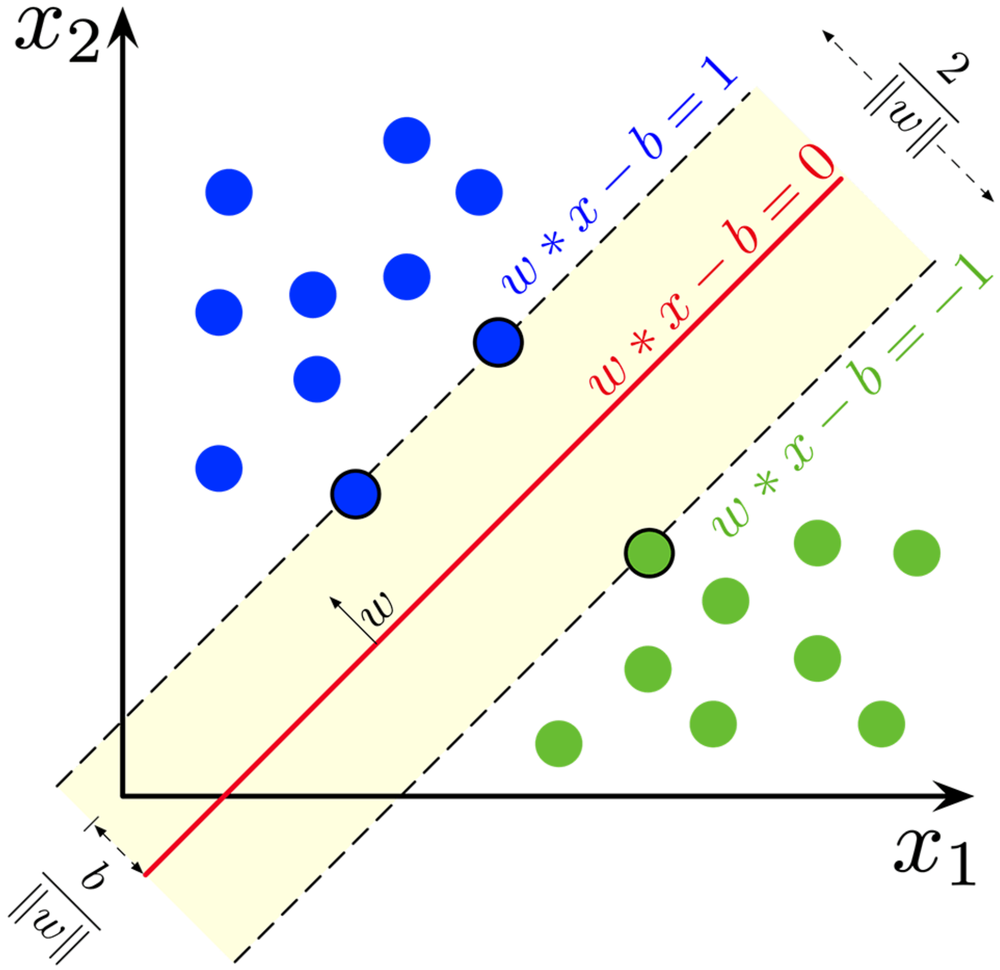
Remark : Here we consider binary classification with target variable $y \in \{-1,1\}$.

Support Vector Machines
- SVM -

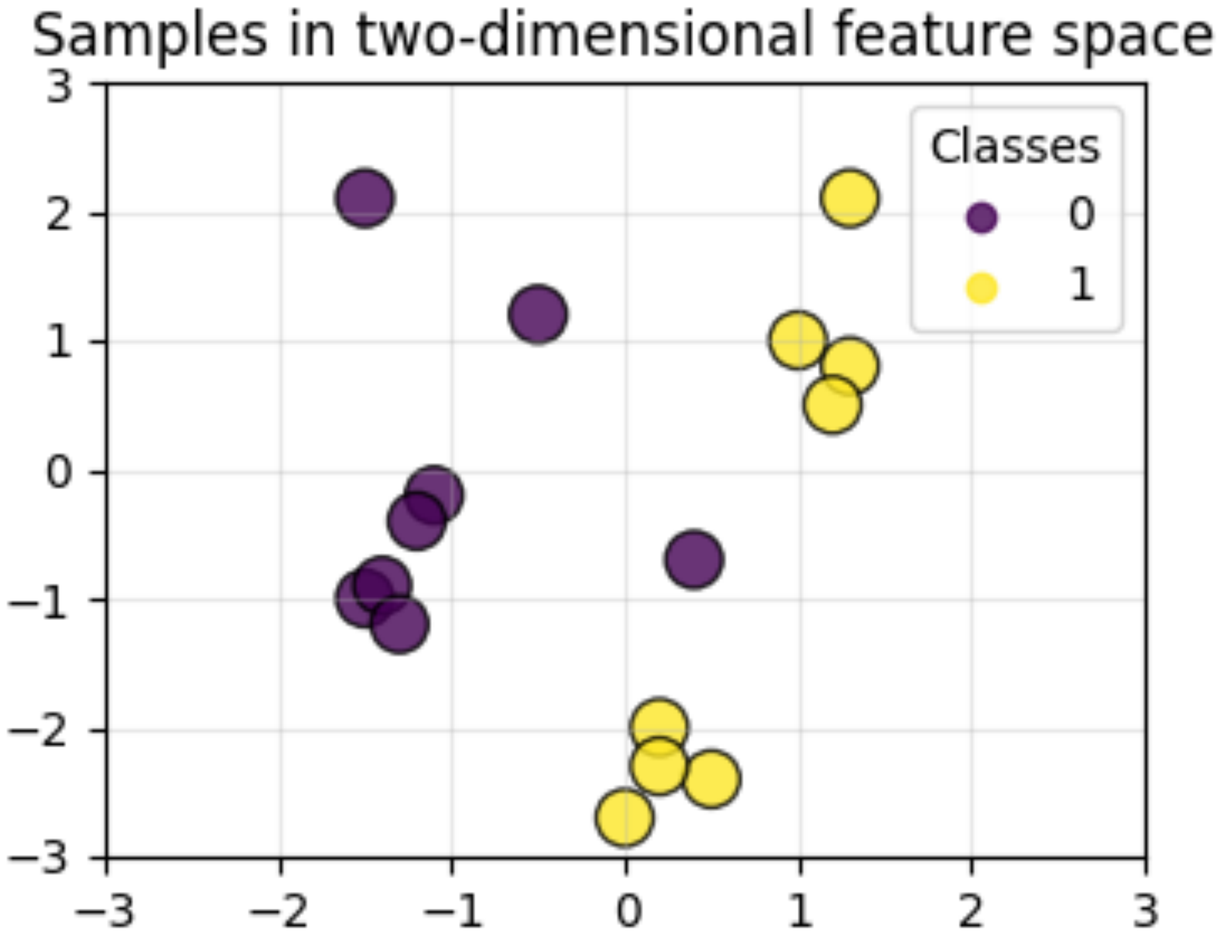
The formula to minimise for the SVM process is given by the following:

$$\min_{w,b} \frac{1}{2}\|w\|^2, \text{ such that } y_i(w^T x_i - b) \geq 1 \text{ for all } i.$$

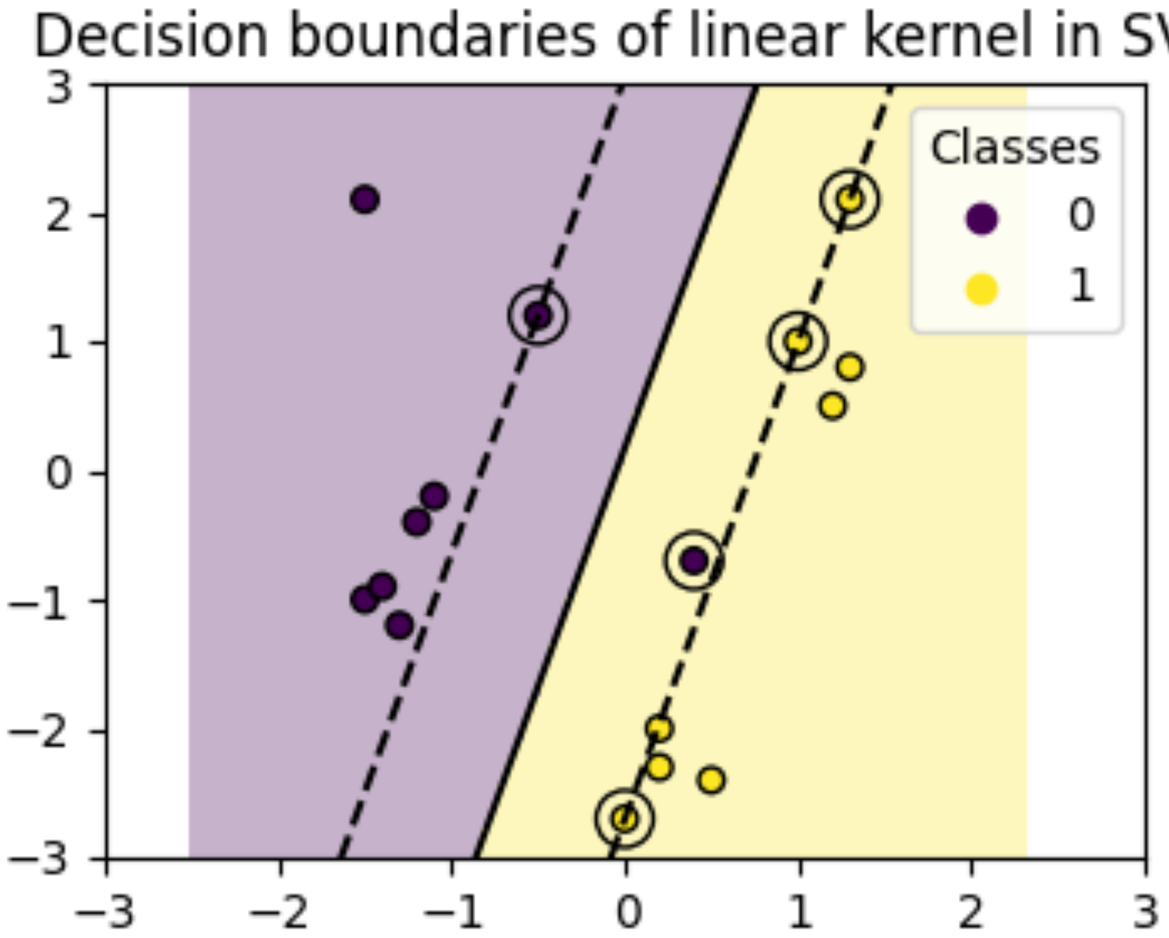
Support Vector Machines
- SVM -



SVM
- Example -


Samples in two-dimensional feature space
Classes
0
1
3
2
1
0
−1
−2
−3
−3
−2
−1
0
1
2
3

SVM
- Example -


Decision boundaries of linear kernel in SVC
Classes
0
1
3
2
1
0
−1
−2
−3
−3
−2
−1
0
1
2
3

SVM
- Slack variables -

In real world data set, there is not perfect plane separating the classes, then we have to accept the fact that some of the points violates the margin constraint :

$$\min_{w,b,\xi} \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n} \xi_i$$

such that $\xi_i = \max\left(0, 1 - y_i(w^T x_i - b)\right)$ for all i.

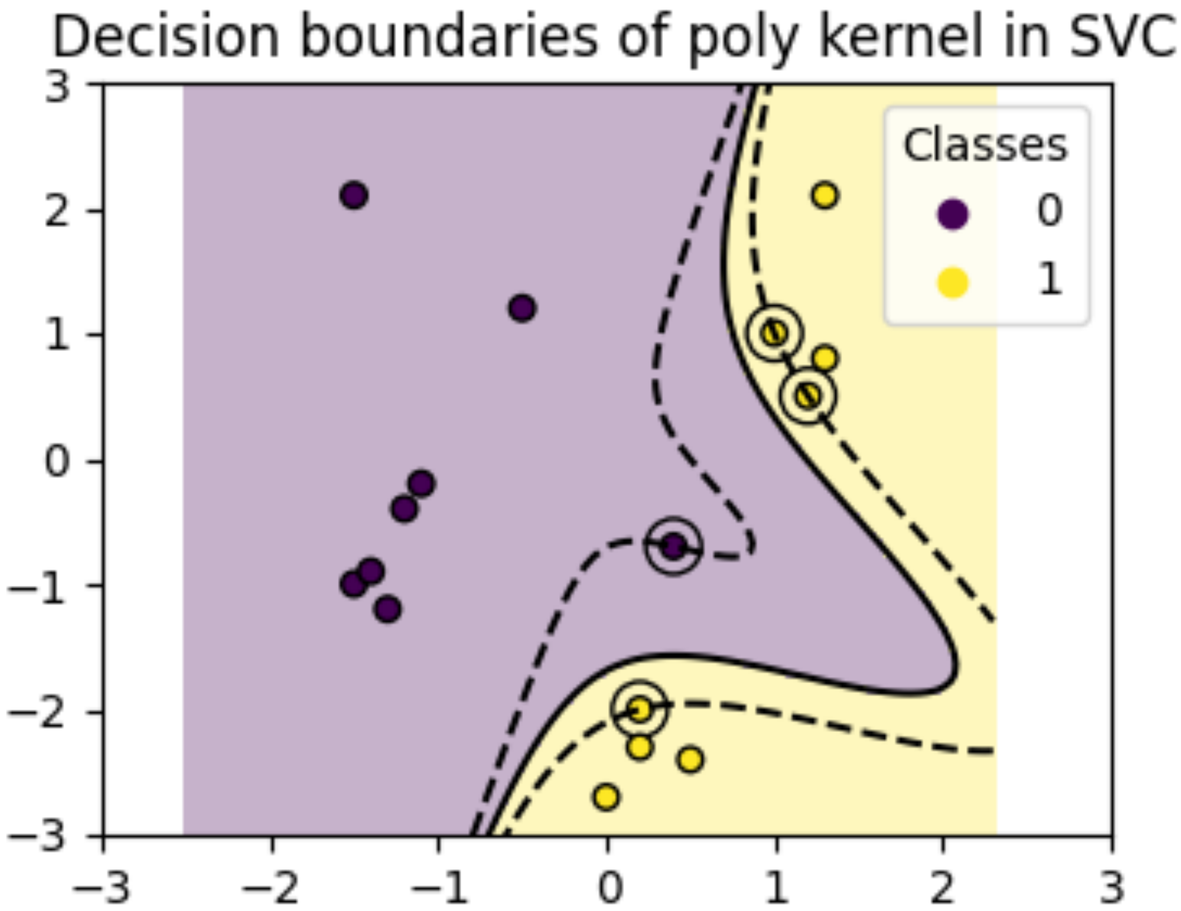
Remark : Large value of C => overfitting /vs/ low value of C => underfitting.

SVM
- Kernels -

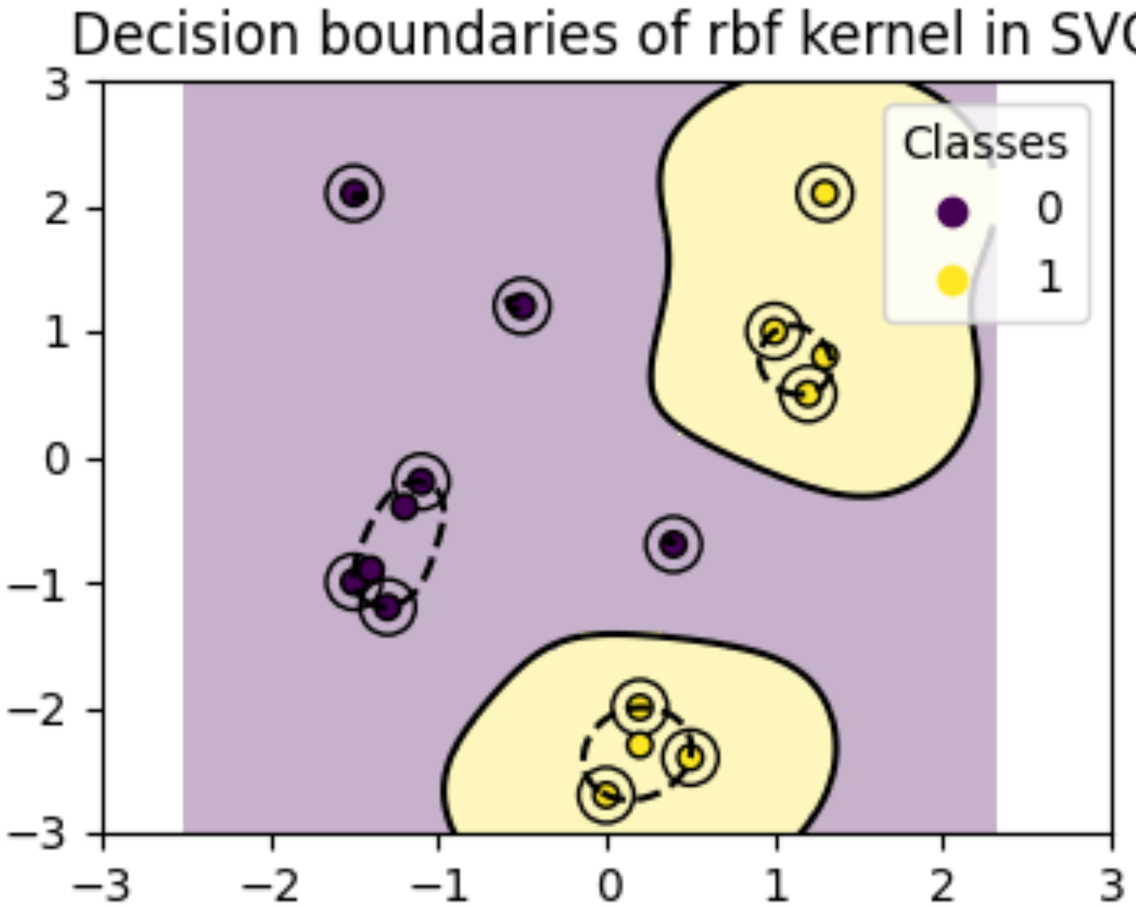
SVM can model non-linear decision boundaries using kernels. Some common kernels are used for SVM such as:

- Linear : $K(x, x') = x^T x'$
- Polynomial : $K(x, x') = (x^T x' + c)^d$
- RBF (Gaussian) kernel : $K(x, x') = \exp\left(-\frac{\|x - x'\|^2}{2\sigma^2}\right)$
- Sigmoid kernel : $K(x, x') = \tanh(\kappa x^T x' + c)$

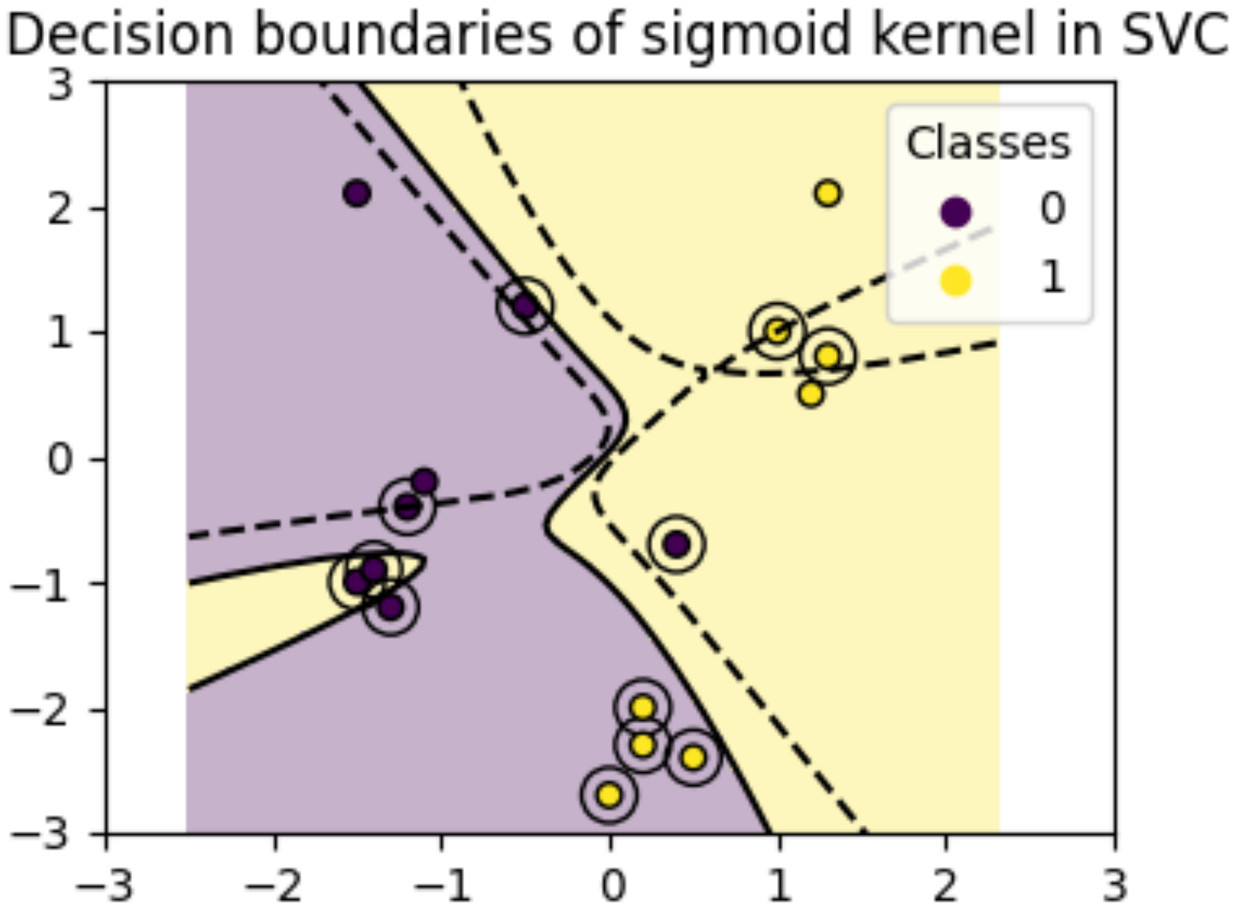
SVM
- Example -


Decision boundaries of poly kernel in SVC
Classes
0
1
3
2
1
0
−1
−2
−3
−3
−2
−1
0
1
2
3

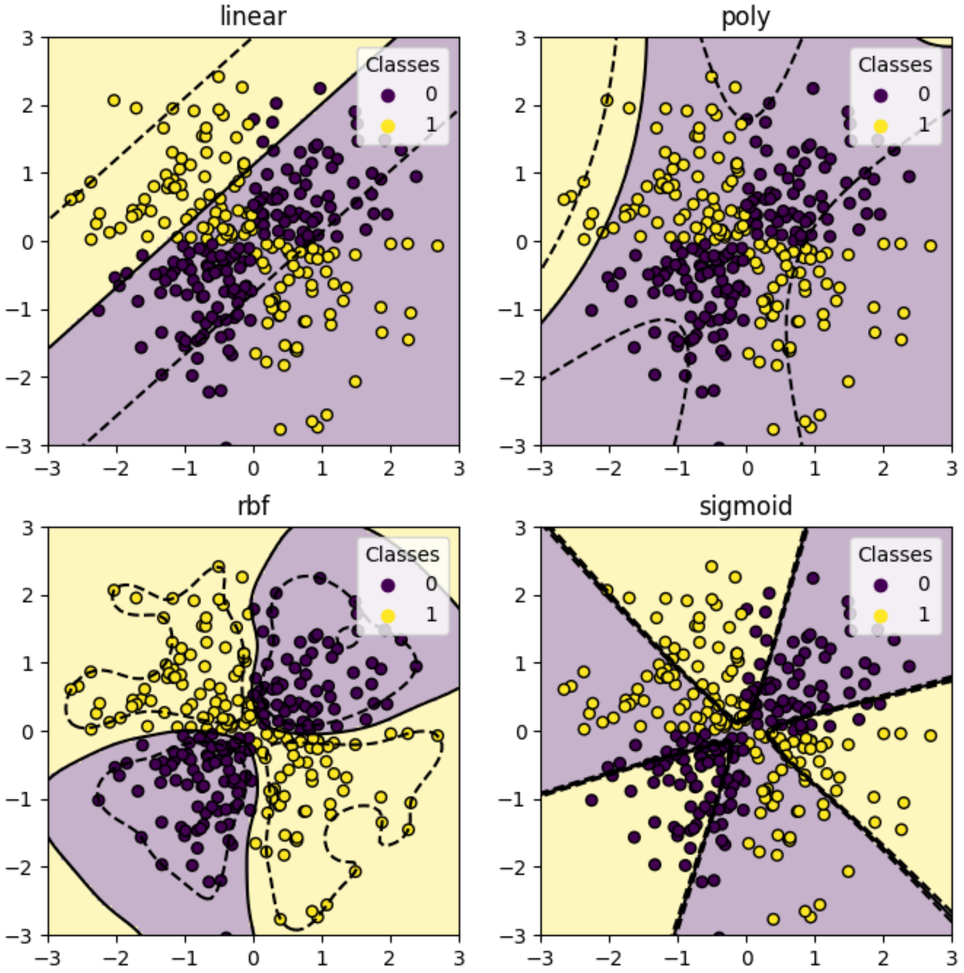
SVM
- Example -


Decision boundaries of rbf kernel in SVC
Classes
0
1
3
2
1
0
−1
−2
−3
−3
−2
−1
0
1
2
3

SVM
- Example -


Decision boundaries of sigmoid kernel in SVC
Classes
0
1
3
2
1
0
−1
−2
−3
−3
−2
−1
0
1
2
3

SVM
- Example -



SVM
- Practice -

Exercice : Train and validate the best kernel with the best parameters on the data set `load_digits` from sklearn. Compare your results with the ones found with logistic regression.

Support Vector Regression
- SVR -

Support Vector Regression is the regression counterpart of SVM. Instead of classifying data points, SVR predicts a continuous value.

Remark : It uses the same principles as SVM: maximizing margin, kernel trick, and regularisation.