Introduction to Supervised Learning

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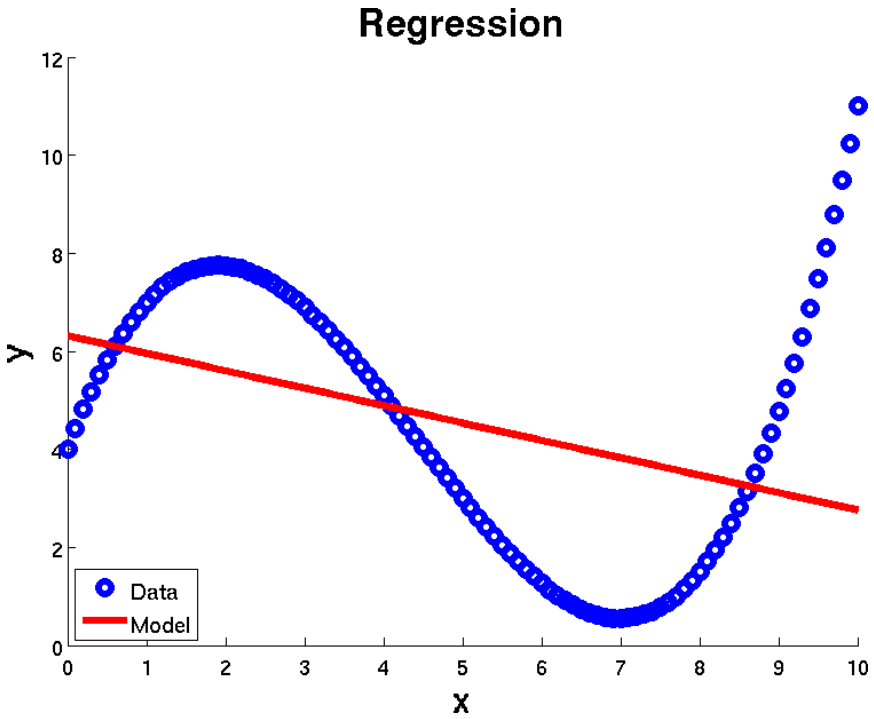
Summary

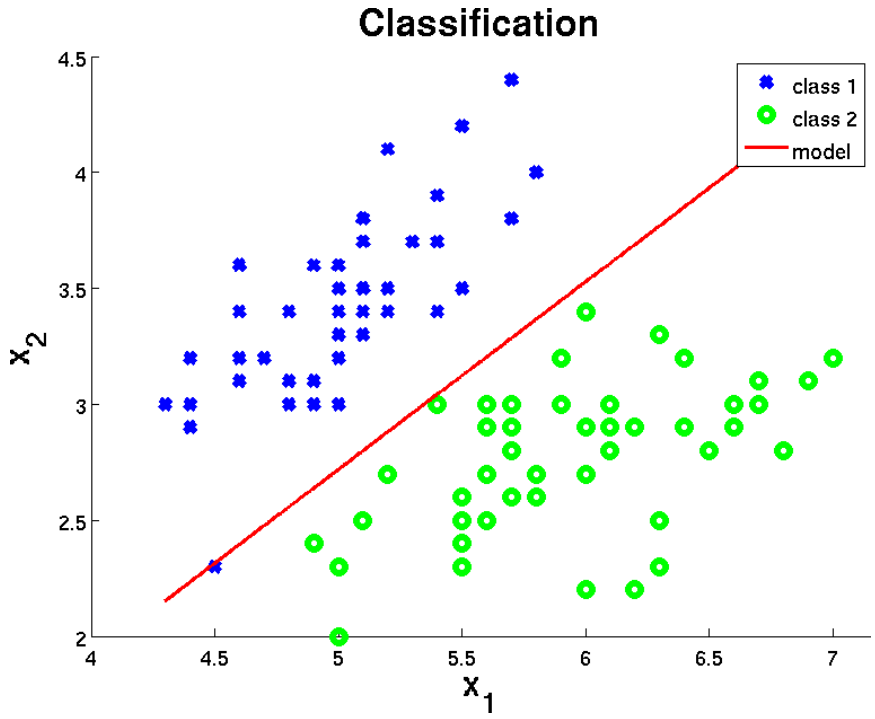
Statistical Machine Learning

- **Supervised Learning**: inferring a rule f from a labeled training set $(X,Y)=\{(x_1,y_1),...,(x_N,y_N)\}$ such that x_i is the vector of features describing the i-th observation and y_i is its label. The rule f will map any new observation t described by x_t to its corresponding y_t.
  - **Regression**: y_i is a set of continuous variables (e.g., $y_i \in \mathbb{R}$)
  - **Classification**: y_i is a set of discrete categories/classes

- **Unsupervised Learning**: No labels are given, we only have X. Possible goals are:
  - **Clustering**: divide X into homogeneous groups
  - **Dimensionality reduction**: simplify X by mapping it into a lower dimensional-space (e.g., PCA)
  - **Outlier detection**

Supervised Learning



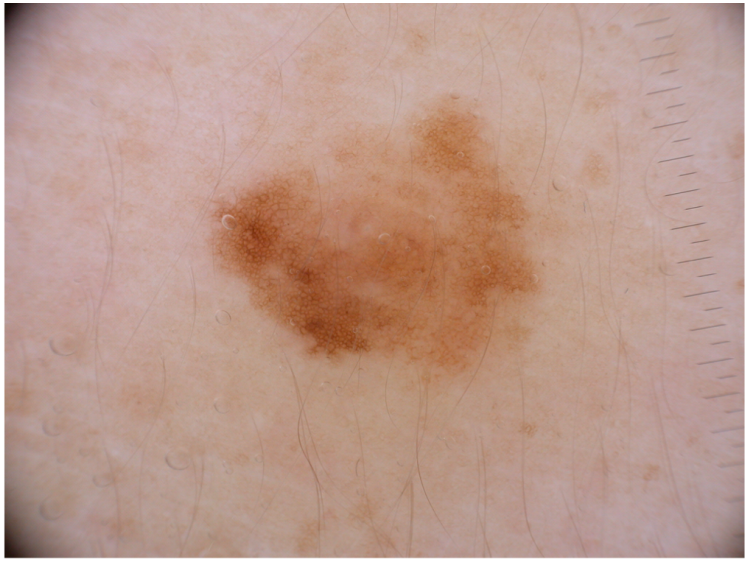


- Every blue dot is an observation described by a scalar feature $x_i \in \mathbb{R}$ and a scalar *continuous* output $y_i \in \mathbb{R}$
- The goal is to model the relationship between y and x

- Every dot is an observation described by a vector feature $x_i \in \mathbb{R}^2$ and a binary *class* y_i
- The goal is to estimate a model f that divides the input space into two classes

Supervised Learning - Binary Classification

Observation 1



$$x_1 = \begin{cases} Asimmetry \\ Border \\ Color \\ Dimension \end{cases} \qquad y_1 = Nevus$$

$\vdots$

Observation N

$$x_N = \begin{cases} Asimmetry \\ Border \\ Color \\ Dimension \end{cases} \qquad y_N = Melanoma$$

Supervised Learning - Regression

Subject 1

$$x_1 = \begin{cases} Atrophy\ hyppocampus \\ Temporal\ lobe\ thickness \\ Volume\ ventricles \\ Thickness\ Corpus\ Callosum \end{cases} \qquad y_1 = Age\ subject\ 1$$

Subject N

$$x_N = \begin{cases} Atrophy\ hyppocampus \\ Temporal\ lobe\ thickness \\ Volume\ ventricles \\ Thickness\ Corpus\ Callosum \end{cases} \qquad y_N = Age\ subject\ N$$

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- $f(x_t) : \mathcal{X} \to \mathcal{Y}$: function estimated from $\mathcal{D}_n$ to predict the output y_t of a new observation t described by x_t
- $L(y, f(x)) : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}^+$: loss function which measures the prediction error, namely the difference between y and $f(x)$

Supervised Learning - Practical point of view

- From a practical point of view, we usually have a set of n images characterized by one or more channels (c) with p pixels and one vector of classes/outputs $\mathbf{y}$ of size $[n \times 1]$. Images can then be stored as an array $\mathbf{x}$ of size $[n \times p \times c]$ or $[n \times pc]$ depending on the problem.

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  - '**One-vs-all**': we estimate K binary classifiers, one for each class. The classification score might be seen as a probability.
  - '**One-vs-one**': we estimate K(K-1)/2 binary classifiers, one for each pair. We choose the class that wins most of the 'duels' (or based on other rules).

Summary

Features

In many occasions, we want to use both images and categorical scores to solve a problem. How to use both of them within the same machine learning method ?
There are two kinds of features (variables):

- Numerical (quantitative) features. Examples are: image intensities, volumes, surfaces, temperatures, distances, etc.
- Categorical (qualitative) features. Examples are: citizenship, colors, types, sex, cities, perfumes, etc.

As a rule of thumb, if you can add it, it's a numerical variable !

But if we can not add, multiply, divide categorical features. How can we use them ?

Categorical features

Ordinal Encoder

- A first naive solution would be to code them as integers
- If we take the example of citizenship: 'European' could be coded as '0', 'American' as '1' and 'Asian' as '2' $\rightarrow$ function `OrdinalEncoder` in scikit-learn
- **Problem**: why 'European' is more distant from 'Asian' than 'American' ? $\rightarrow$ Some models would interpret them as ordered even if they are not !

One Hot Encoder

- A better solution is to transform each categorical feature with K possible values into a binary features with K values where one would be 1 and all others 0 $\rightarrow$ function `OneHotEncoder` in scikit-learn

Categorical features - One Hot Encoder

- Taking the same example as before, using the 'One Hot Encoder' strategy, we would obtain:

Subject	Citizenship
1	American
2	European
3	Asian
4	Asian
5	American

$\rightarrow$

European	American	Asian
0	1	0
1	0	0
0	0	1
0	0	1
0	1	0

Numerical features - Standardization

- Standardization means centering the data (i.e. remove the mean value of each feature) and then scale them by the standard deviation
- **Why ?** : Because many models assume that all features are centered around zero and have similar variance. If a feature is way bigger than the others, it might dominate the objective function and the gradient descent and make the model unable to correctly learn from the other features.
- This is very important and common in machine learning $\rightarrow$ function `StandardScaler` in scikit-learn

Numerical features - Normalization

- Normalization (or Min-Max scaling) scales the data to a fixed range, usually $[0, 1]$ by doing:

$$\mathcal{X}_N = \frac{X - X_{min}}{X_{max} - X_{min}} \tag{1}$$

- **Why ?** : It is very common in image processing where data pixel intensities should lie within a certain range (i.e. between 0 and 255 or between 0 and 1)
- **Cons** : More sensitive to the presence of outliers
- Function `MinMaxScaler` in scikit-learn
- Other scalers at `https://scikit-learn.org`

Features - Missing values

- When we do not know the value for a variable, it is *very important* to indicate it. We usually write 'NaN' (i.e. Not a Number)

Subject	**Citizenship**
1	American
2	-
3	Asian

$\rightarrow$

Subject	**Citizenship**
1	American
2	**NaN**
3	Asian

- Possible solutions:
  - **Remove** the entire observation (even if it lacks of only one variable)
  - **Attribute** a value using simple statistics such as the average or the most common value (usually used for categorical variables)
  - Use **advanced techniques**: clustering, interpolation, robust methods, etc.

Summary

Function space

First question: Which model f should we use ? We do not usually know it a priori. We need to do an assumption, constraining it to a function space $\mathcal{F}$. We can divide existing algorithms into two categories:

- **Parametric models**: f depends on a set of *fixed* parameters θ: $\mathcal{F} = \{f(X;\theta), \theta \in \Theta\}$. An example is linear regression.
- **Non-parametric models**: the form of f is not specified. They are more flexible. They use the training data to locally estimate the best f. An example is the k-nearest neighbors algorithm. It estimates f based on the k most similar training data. It only assumes that samples that have a similar x value should also have a similar y value. In this case, the number of parameters is *not fixed* beforehand but it grows with the number of samples (N/k)!

Function space

- **Parametric models**
  - *Benefits*: Simple, Easy to interpret, Fast, Less data
  - *Limitations*: Constrained, Accuracy not guaranteed
- **Non-parametric models**
  - *Benefits*: Flexibility, Not constrained (more general), more Accurate (if enough data)
  - *Limitations*: Many data, Slow, Not always easy to interpret

Risk function

Second question: How do we choose the best f ? We look for the f in the restricted space $\mathcal{F}$ that minimizes the average loss that is called the **risk function** or **expected prediction error** associated to f:

$$\tilde{f}(x) = \arg\min_{f \in \mathcal{F}} R(f) \tag{2}$$

where $R(f)$ is defined as:

$$\begin{aligned} R(f) =& E_{XY}[L(Y, f(X))] = \int_{\mathcal{X}} \int_{\mathcal{Y}} L(y, f(x)) p_{X,Y}(x, y) dx dy \\ =& \int_{\mathcal{X}} \left[\int_{\mathcal{Y}} L(y, f(x)) p_{Y|X}(y|x) dy \right] p_X(x) dx \\ =& E_X[E_{Y|X}[L(Y, f(X))|X]] \end{aligned} \tag{3}$$

Examples of loss functions

Third question: how do we choose $L(y, f(x))$? This is the loss function which measures the error of the classifier/model.

It depends on the application (classification or regression), on the data (presence of outliers) and on the goal (is interpretability important ?)

Here are some examples:

- Squared error loss (L_2-loss): $L(y, f(x)) = (y - f(x))^2$
- Absolute error loss (L_1-loss): $L(y, f(x)) = |y - f(x)|$
- L_q-loss: $L(y, f(x)) = (y - f(x))^q \quad q > 0$
- Zero-one loss: $L(y, f(x)) = I(y \neq f(x))$, where I is the Indicator function, namely it is equal to 0 if $y = f(x)$ and 1 otherwise.

Question: Which is the one for classification ?

Risk function - Theory

We look for the function f which minimizes the risk function $R(f)$:

$$f^* = \arg\min_f R(f) = E_X[E_{Y|X}[L(Y, f(X))|X]] \tag{4}$$

In the discrete case, this can be seen as a sum: $R(f) = \sum_{x_j \in \mathcal{X}} \left(E_{Y|X}[L(Y, f(X))|X] \right) P(X = x_j)$. We can thus minimize every summand individually, which means solving for every $x_j \in \mathcal{X}$:

$$f^*(x_j) = \arg\min_f E_{Y|X}[L(Y, f(x_j))|X = x_j] \tag{5}$$

Risk function - L2-loss

For L_2-losses we obtain:

$$\begin{aligned} f^*(x_j) &= \arg\min_f E_{Y|X}[L(Y, f(x_j))|X = x_j] \\ &= \arg\min_f E_{Y|X}[(Y - f(x_j))^2|X = x_j] \\ &= E_{Y|X}[Y|X = x_j] \end{aligned} \tag{6}$$

That is, under the squared error loss, the best function f^* at every point $X = x_j$ is the conditional expectation $E_{Y|X}[Y|X = x_j]$, which is also called the *regression function*. This is the conditional average of Y ($\int_{y \in \mathcal{Y}} y p_{Y|X}(y|x_j) dy$) at every point $X = x_j$.

Risk function - Zero-one loss

The Zero-one loss is usually used in classification where $\mathcal{Y} = \{C_1, \ldots, C_K\}$. In this case, we can rewrite the risk function:

$$R(f) = E_X[\sum_{k=1}^{K} L(C_k, f(X))P(Y = C_k|X)] \tag{7}$$

Solving again for every $x_j \in \mathcal{X}$, we obtain:

$$f^*(x_j) = \arg\min_{f \in \mathcal{Y}} \sum_{k=1}^{K} L(C_k, f(x_j))P(Y = C_k|X = x_j) \tag{8}$$

Being a sum, we want $f(x_j)$ to be equal to the C_k with the greatest $P(Y = C_k|X = x_j)$, so that to minimize the cost function.
That is, under the Zero-one loss, the best function f^* at every point $x = x_j$, is the most probable class C_k. This is known as the *Bayes classifier*.

Bayes classifier

We can rewrite the Bayes classifier in the following way:

$$f^*(x_j) = \arg\max_{f \in \mathcal{Y}} P(Y = f(x_j)|X = x_j) = \arg\max_{C_k} P(X = x_j|Y = C_k)\pi_{C_k} \tag{9}$$

where $P(X = x_j|Y = C_k) = P_k(X)$ and π_{C_k} is the prior of class C_k.

Example: We have two classes $k \in 1, 2$ and we suppose that $P_1(X) = \mathcal{N}(-1, 1)$ and $P_2(x) = \mathcal{N}(1, 1)$ and that the two classes have equal priors $\pi_1 = \pi_2 = 0.5$.

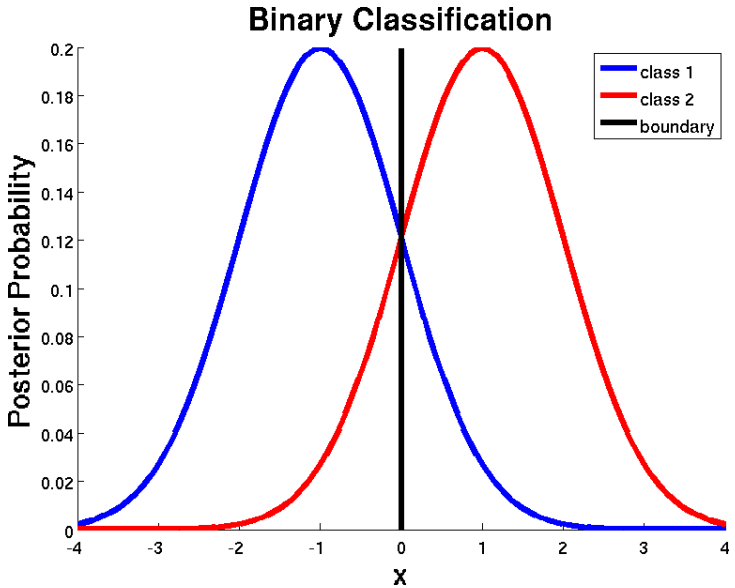
Bayes classifier

How do we classify a new observation $x_j = 0.5$?

$$f^*(x_j) = \arg\max_{C_k} P_k(x_j)\pi_{C_k} \tag{10}$$

With

- $P_1(x_j) \sim \exp(-\frac{(x_j-(-1))^2}{2})$
- $P_2(x_j) \sim \exp(-\frac{(x_j-1)^2}{2})$
- $\pi_1 = \pi_2 = 0.5$



Empirical risk minimization

Problem: Since we usually do not know the joint distribution p_{XY}, we can either make assumptions, for instance on $P_k(x_j)$ as in LDA, or compute an approximation of $R(f)$ called *empirical risk* $R_{emp}(f)$ by averaging the loss function L over the training set $\mathcal{D}_n$:

$$R_{emp}(f) = \frac{1}{n} \sum_{i=1}^{n} L(y_i, f(x_i)) \tag{11}$$

The *empirical risk minimization principle*[1] states that we should choose the $f \in \mathcal{F}$ that minimizes $R_{emp}(f)$:

$$\hat{f}(x) = \arg\min_{f \in \mathcal{F}} R_{emp}(f) \tag{12}$$

[1] Vapnik - Principles of Risk Minimization for Learning Theory - 1992

Empirical risk minimization

Let $\mathcal{F}$ be the restricted space of f:

- f^* is the theoretical optimal model
- $\tilde{f}$ is the theoretical best model in the restricted space $\mathcal{F}$
- $\hat{f}$ is the best model in the restricted space $\mathcal{F}$ based on the limited data $\mathcal{D}_n$

We can notice that:

$$\text{err}\{f^* - \hat{f}\} = \text{err}\{\underbrace{f^* - \tilde{f}}_{\text{approximation error}}\} + \text{err}\{\underbrace{\tilde{f} - \hat{f}}_{\text{estimation error}}\} \tag{13}$$

- The *approximation error* is due to the restriction of f to $\mathcal{F}$ since it is possible that $f^* \notin \mathcal{F}$.
- The *estimation error* is due to the limited training data. This tends to 0 when $n \to \infty$, e.g. we observe all possible cases.

Summary

The Bias-Complexity tradeoff

Depending on the choice of $\mathcal{F}$ it can happen that the model f is:

- **Too Rich** (many parameters)
  - Approximation error gets smaller (*lower bias*)
  - Estimation error gets larger (*higher statistical complexity*)
  - *Overfitting*
- **Too simple** f (few parameters)
  - Approximation error gets larger (*higher bias*)
  - Estimation error is likely to reduce (*lower statistical complexity*)
  - *Underfitting*

We should look for a "simple" f suitable for our problem ! How to choose f ?

Training, Validation and Test Set

Let $\{f_i\} \in \mathcal{F}$ be an ensemble of models that we want to test. We first divide the available data into three sets, Training, Validation and Test, which we use in the following way:

- **Training Set** $\mathcal{T}$: we use it to fit all the models $f_i \in \mathcal{F}$ (i.e. estimate the parameters)
- **Validation Set**: we use it to compare the performances of all f_i and choose the best one $\hat{f}_i$
- **Test Set**: we use it to test the performance of the best $\hat{f}_i$ using an *evaluation measure* on previously unseen, namely not used, data.

As rule of thumb, the available data are usually split into 50% for training, 25% for validation and 25% for testing.

Evaluation measures

Regression - The performance of a regression model $\hat{f}_i$ can be evaluated using $R_{emp}(\hat{f}_i)$ computed on the *test samples*. This is called *expected prediction error*.

Classification - Suppose that every test sample s is a subject described by some features x_s (e.g., blood pressure, weight, height, etc.). The output y_s can belong to two classes: healthy or sick. The performance of the classifier $\hat{f}_i$ can be evaluated using:

- *sensitivity* (or recall) $\frac{TP}{TP+FN}$
- *specificity* (or selectivity): $\frac{TN}{FP+TN}$
- *precision* : $\frac{TP}{TP+FP}$
- *accuracy*: $\frac{TP+TN}{TP+FP+FN+TN}$
- *F1 score*: $\frac{2TP}{2TP+FP+FN}$

Where TP=correctly identified, FP = incorrectly identified, TN = correctly rejected, FN = incorrectly rejected.

Confusion matrix

- It is a matrix showing whether the system mislabels one class as another one. With $K = 3$ with 10 European, 50 American and 90 Asian, one might obtain:

		Predicted classes		
		European	**American**	**Asian**
True class	**European**	7	3	0
	American	20	20	10
	Asian	10	30	50

- If we only have two classes (e.g. European and Asian), the matrix displays TP, TN, FP and FN:

		Predicted classes	
		European	**Asian**
True class	**European**	0 (TN)	10 (FP)
	Asian	0 (FN)	90 (TP)

		Predicted classes	
		European	**Asian**
Trues class	**European**	0 (TN)	10 (FP)
	Asian	0 (FN)	90 (TP)

- Using the previous example, we can see that the two classes are imbalanced $\rightarrow$ classifying all subjects as 'Asian' produces an accuracy score of 0.9 (max is 1)
- Balanced accuracy (like other metrics) overcomes this issue by taking into account the size of each class. In the previous example it would give a score of 0.45 (max is 1):

  balanced accuracy: $\frac{1}{2}(\frac{TP}{TP+FN} + \frac{TN}{TN+FP})$
- For other metrics available in scikit-learn, please refer to: `https://scikit-learn.org/stable/modules/model_evaluation.html`

Evaluation measures - Multi-class Classification

- Another evaluation measure used in multi-class classification (especially when classes are imbalanced) is the **weighted (categorization) accuracy** WA.
- Let $G = G_1, ..., G_K$ be the K classes the data-set is dived into. We define it as:

$$WA = \frac{1}{N} \sum_{s=1}^{N} w_s I(y_s = \hat{y}_s) \quad \text{s.t.} \sum_{s=1}^{N} w_s = N \tag{14}$$

- Here, I is the indicator function, N the number of observations, $\hat{y}_s$ the prediction of the model f for sample s and w_s its weight. Weights are constraint so that the maximum of WA is equal to 1. Please note that without w_s this would be exactly equal to the Accuracy.
- Weights can be used to give more importance to specific samples or classes.

Evaluation measures - Multi-class Classification

- If we decide to give the same weight to the samples belonging to the same class, we obtain:

$$\sum_{s=1}^{N} w_s = \sum_{t=1}^{K} \sum_{s \in G_t} w_s = \sum_{t=1}^{K} w_t |G_t| = N \tag{15}$$

- where w_t is the weight assigned to class t and $|G_t|$ is the number of elements of class G_t. We can notice that if w_t is equal to $w_t = \frac{N}{K|G_t|}$ then the constraint is fulfilled.
- By plugging it into the WA definition, we obtain:

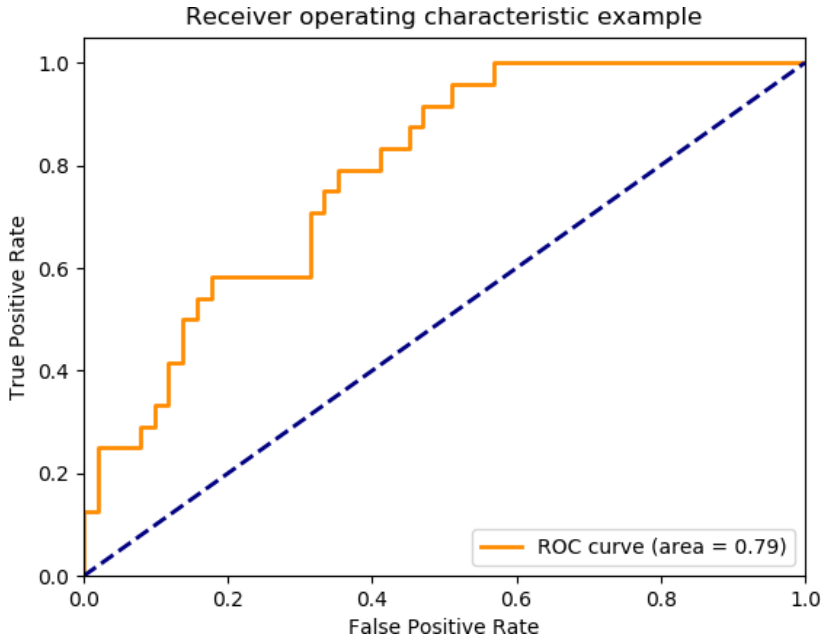
$$WA = \frac{1}{K} \sum_{t=1}^{K} \sum_{s \in G_t} \frac{I(y_s = \hat{y}_s)}{|G_t|} \tag{16}$$

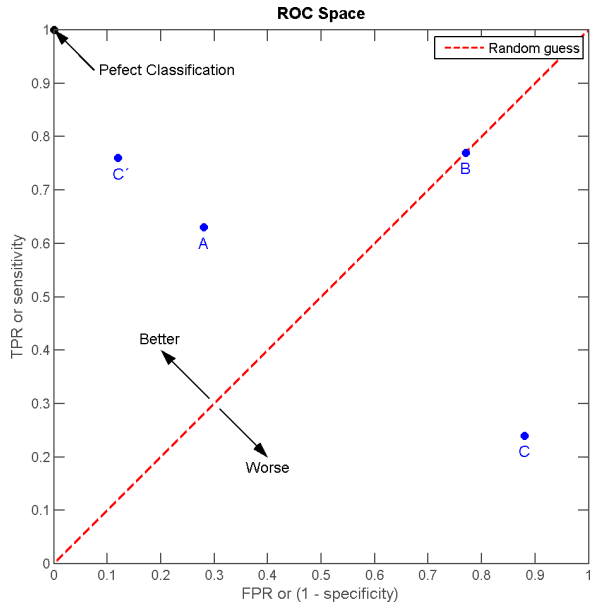
- WA thus becomes the average across classes of the proportion of correct predictions within each class. This is exactly equal to the Balanced accuracy when $K = 2$.

Evaluation measures - ROC curves

- In a **binary** classification problem, we may predict directly the class or the probability P for each class
- Then, we can choose a threshold T on the probability to discriminate between the two classes ($P < T \rightarrow$ class 0, $P \geq T \rightarrow$ class 1)
- A receiver operating characteristic (ROC) curve shows the classification ability of a binary classifier as we vary the threshold
- It plots the True Positive Rate (TPR) or sensitivity against the False Positive Rate (FPR) or (1-specificity)
- Good model has only points in the top-left corner of the plot
- To compare two models, one could compute the **Area Under the Curve** (AUC) which varies between 0 (worst) and 1 (best)
- In case of class imbalance, Precision-Recall curves are more adapted.

Evaluation measures - ROC curves





Summary

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Example - Linear model

In a linear model, we assume that the output random variable Y and the input random variable X have a linear relationship:

$$f(x;\theta) = \beta_0 + \sum_{j=1}^{d} \beta_j x_j \quad \text{with } \theta = \{\beta_j\}_{j=0,\ldots,d} \tag{17}$$

By defining a dummy variable $x_0 = 1$ we can rewrite the previous Eq. as:

$$f(x;\theta) = \sum_{j=0}^{d} \beta_j x_j = x^T \beta \tag{18}$$

where $\beta = (\beta_0, ..., \beta_d)^T$ and $x = (x_0, ..., x_d)^T$ are two $(d+1) \times 1$ vectors.

Ordinary Least Squares

Let n be the number of samples in the training set, for every sample i we can write:

$$y_i = f(x_i; \theta) + \epsilon_i = x_i^T \beta + \epsilon_i \tag{19}$$

where ϵ_i is a random variable called *residual* which accounts for the prediction error.
Let $\mathbf{x}$ be the $n \times (d+1)$ matrix containing the x_i, $\mathbf{y}$ the $n \times 1$ vector containing the y_i and $\boldsymbol{\epsilon}$ the $n \times 1$ vector containing the ϵ_i, we can write the previous Eq. in matrix notation:

$$\mathbf{y} = \mathbf{x}\beta + \boldsymbol{\epsilon} \tag{20}$$

In **ordinary least squares** (OLS) we look for the β coefficients that minimize the residual sum of squares (RSS), that is $R_{emp}(f)$ with a L2-loss.

Ordinary Least Squares

The goal of OLS is:

$$\begin{aligned}\beta^* &= \arg\min_{\beta} \mathsf{RSS} = \sum_{i=1}^{n} (y_i - x_i^T \beta)^2 \\ &= \arg\min_{\beta} (\mathbf{y} - \mathbf{x}\beta)^T (\mathbf{y} - \mathbf{x}\beta)\end{aligned} \tag{21}$$

Differentiating with respect to β, we obtain:

$$\begin{aligned}\frac{\partial \mathsf{RSS}}{\partial \beta} &= -2\mathbf{x}^T(\mathbf{y} - \mathbf{x}\beta) = 0 \\ \beta^* &= (\mathbf{x}^T\mathbf{x})^{-1}\mathbf{x}^T\mathbf{y}\end{aligned} \tag{22}$$

Ordinary Least Squares - Geometry

From the previous equations we can notice that we choose β^* such that the residuals $\mathbf{y} - \mathbf{x}\beta$ are orthogonal to the subspace given by the columns of $\mathbf{x}$, that is $\mathbf{x}^T(\mathbf{y} - \mathbf{x}\beta) = 0$.
Furthermore we can see that:

$$f(\mathbf{x}; \beta) = \mathbf{x}\beta^* = \mathbf{x}(\mathbf{x}^T\mathbf{x})^{-1}\mathbf{x}^T\mathbf{y} \tag{23}$$

Thus, the resulting estimate $\mathbf{x}\beta^*$ is the orthogonal projection of $\mathbf{y}$ onto the columns of $\mathbf{x}$.

Ordinary Least Squares - Geometry

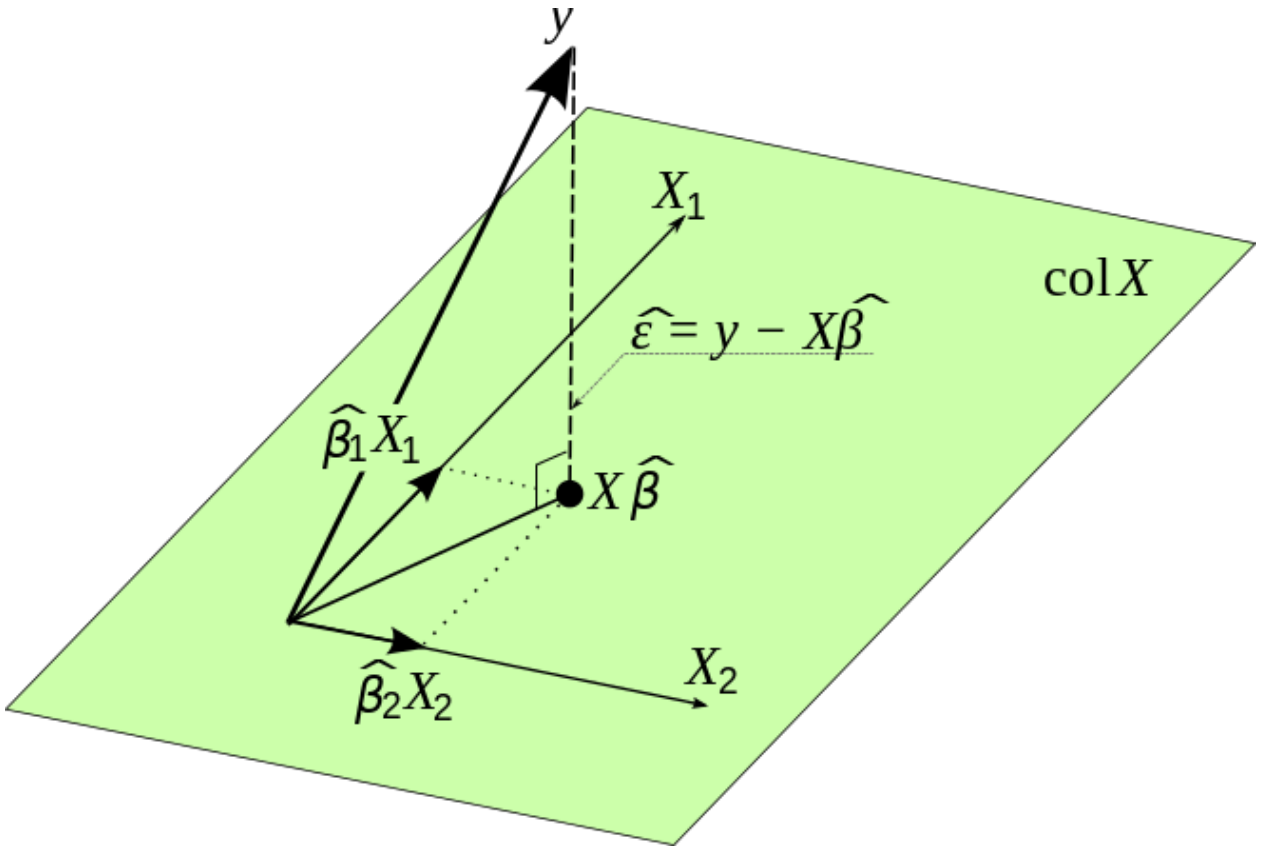


Figure 1: The OLS estimate $\mathbf{x}\beta^*$ is the orthogonal projection of $\mathbf{y}$ onto the columns of $\mathbf{x}$. Image from Wikipedia.

Ordinary Least Squares - Assumptions

Under the following assumptions, the **Gauss–Markov theorem** states that the best linear unbiased estimator (BLUE) is the OLS estimator.

Assumptions:

- $\mathcal{D}_n$ is composed of n i.i.d.samples drawn from p_{XY}
- **Linearity**: linear relationship in the parameters β, not necessarily between y and x. This means that $y = \beta_0 + \beta_1 x^2$ is still valid ! We also assume that we have chosen the proper functional space $\mathbf{F}$.
- $\mathbf{x}$ **must have full column rank**: columns of $\mathbf{x}$ are linearly independent, namely $\mathbf{E}[\mathbf{x}^T\mathbf{x}]$ must be finite and positive semi-definite.
- $\mathbf{x}$ must be non-stochastic or at least independent of $\boldsymbol{\epsilon}$: $\mathbf{E}[\mathbf{x}^T\boldsymbol{\epsilon}] = 0$
- **Exogeneity**: $\mathbf{E}[\epsilon_i|\mathbf{x}] = 0$ for all i.
- **Homoscedasticity**: $\text{Var}[\epsilon_i|\mathbf{x}] = \sigma^2 < \infty$ for all i
- **Uncorrelated errors**: $\text{Cov}(\epsilon_i, \epsilon_j|x_i, x_j) = 0$ for $i \neq j$
- (Optional) Normal distribution $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \sigma^2\mathbf{I})$

Ordinary Least Squares - Assumptions

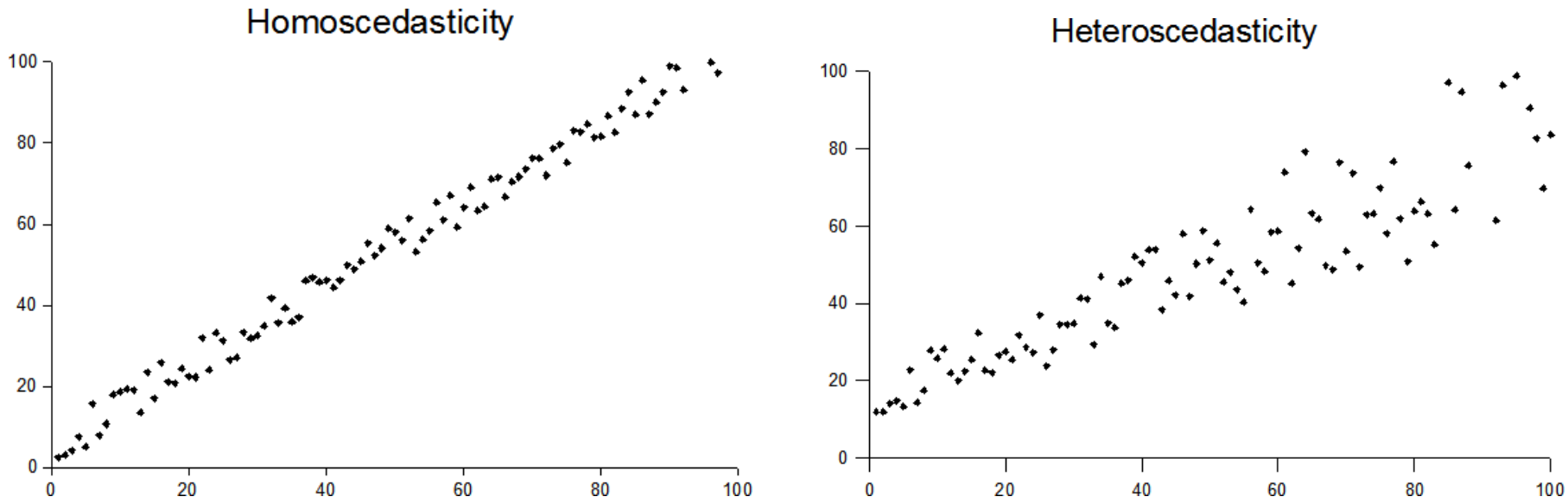


Figure 2: Difference between homoscedasticity (constant variability of the residuals) and heteroscedasticity. Image from Wikipedia.

Ordinary Least Squares

$$\begin{aligned}\beta^* &= (\mathbf{x}^T\mathbf{x})^{-1}\mathbf{x}^T\mathbf{y} \\ &= (\mathbf{x}^T\mathbf{x})^{-1}\mathbf{x}^T(\mathbf{x}\beta + \boldsymbol{\epsilon}) \\ &= \beta + (\mathbf{x}^T\mathbf{x})^{-1}\mathbf{x}^T\boldsymbol{\epsilon}\end{aligned} \tag{24}$$

From this we can see that OLS is unbiased $\mathbf{E}[\beta^*] = \beta$ only if $\mathbf{x}$ is deterministic and $\mathbf{E}[\boldsymbol{\epsilon}] = 0$, or at least if $\mathbf{E}[\mathbf{x}^T\boldsymbol{\epsilon}] = 0$.
Furthermore, "best linear unbiased estimator" means that β^* has the smallest variance among all linear unbiased estimators (to prove in the TP...). Using $\mathbf{E}[\boldsymbol{\epsilon}\boldsymbol{\epsilon}^T] = \sigma^2\mathbf{I}$:

$$\begin{aligned}\mathbf{E}[(\beta^* - \beta)(\beta^* - \beta)^T] &= \mathbf{E}[((\mathbf{x}^T\mathbf{x})^{-1}\mathbf{x}^T\boldsymbol{\epsilon})((\mathbf{x}^T\mathbf{x})^{-1}\mathbf{x}^T\boldsymbol{\epsilon})^T] \\ &= (\mathbf{x}^T\mathbf{x})^{-1}\mathbf{x}^T\mathbf{E}[\boldsymbol{\epsilon}\boldsymbol{\epsilon}^T]\mathbf{x}(\mathbf{x}^T\mathbf{x})^{-1} \\ &= \sigma^2(\mathbf{x}^T\mathbf{x})^{-1}\end{aligned} \tag{25}$$

Ordinary Least Squares

It is important to notice that if the normality assumption holds (that is $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \sigma^2 \mathbf{I})$) it follows that

$$\beta^* \sim \mathcal{N}(\beta, \sigma^2 (\mathbf{x}^T \mathbf{x})^{-1}) \tag{26}$$

and in this case, the OLS estimator is also **efficient**, that is to say has the smallest variance among all unbiased, linear and non-linear, estimators. (Cramér–Rao inequality)

Bias-Complexity tradeoff - revisited

Let (x_0, y_0) be a test sample, $y_0 = x_0^T\beta + \epsilon_0$ the true model and $x_0^T\beta^*$ the OLS estimate. The expected prediction error, that is the mean squared error (MSE) when using a L2-norm, of OLS at (x_0, y_0) is equal to:

$$
\begin{aligned}
\text{MSE} &= \mathbf{E}[(y_0 - x_0^T\beta^*)^2] \\
&= \mathbf{E}[(x_0^T\beta + \epsilon_0 - x_0^T\beta^*)^2] \\
&= \mathbf{E}[\epsilon_0^2] + (x_0^T\beta)^2 + \mathbf{E}[(x_0^T\beta^*)^2] - 2(x_0^T\beta)\mathbf{E}[(x_0^T\beta^*)] \\
&+ \mathbf{E}[(x_0^T\beta^*)]^2 - \mathbf{E}[(x_0^T\beta^*)]^2 \\
&= \sigma^2 + \Big(\mathbf{E}[(x_0^T\beta^*)^2] - \mathbf{E}[(x_0^T\beta^*)]^2\Big) + \Big(\mathbf{E}[(x_0^T\beta^*)] - (x_0^T\beta)\Big)^2 \\
&= \underbrace{\sigma^2}_{\text{irreducible error}} + \text{Var}(x_0^T\beta^*) + \text{Bias}^2(x_0^T\beta^*) \\
&= \sigma^2 + \sigma^2(x_0^T(\mathbf{x}^T\mathbf{x})^{-1}x_0) + 0
\end{aligned}
\tag{27}
$$

Bias-Complexity tradeoff - revisited

The first term σ^2 is beyond our control. It is the inherent error in the data that we can not remove. The other two terms are exactly what we have seen before:

- *Bias* is the *approximation error*, namely the difference between the true model and the theoretical best model in $\mathcal{F}$.
- *Variance* is the *estimation error*, namely the difference between the theoretical best model in $\mathcal{F}$ and the estimated model in $\mathcal{F}$ using a limited amount of data $\mathcal{D}_n$.

The Bias will most likely decrease if we enrich $\mathcal{F}$, namely if we increase d. At the same time, if we increase d, the variance will also increase ! This is the **bias-variance tradeoff** !

Bias-variance tradeoff

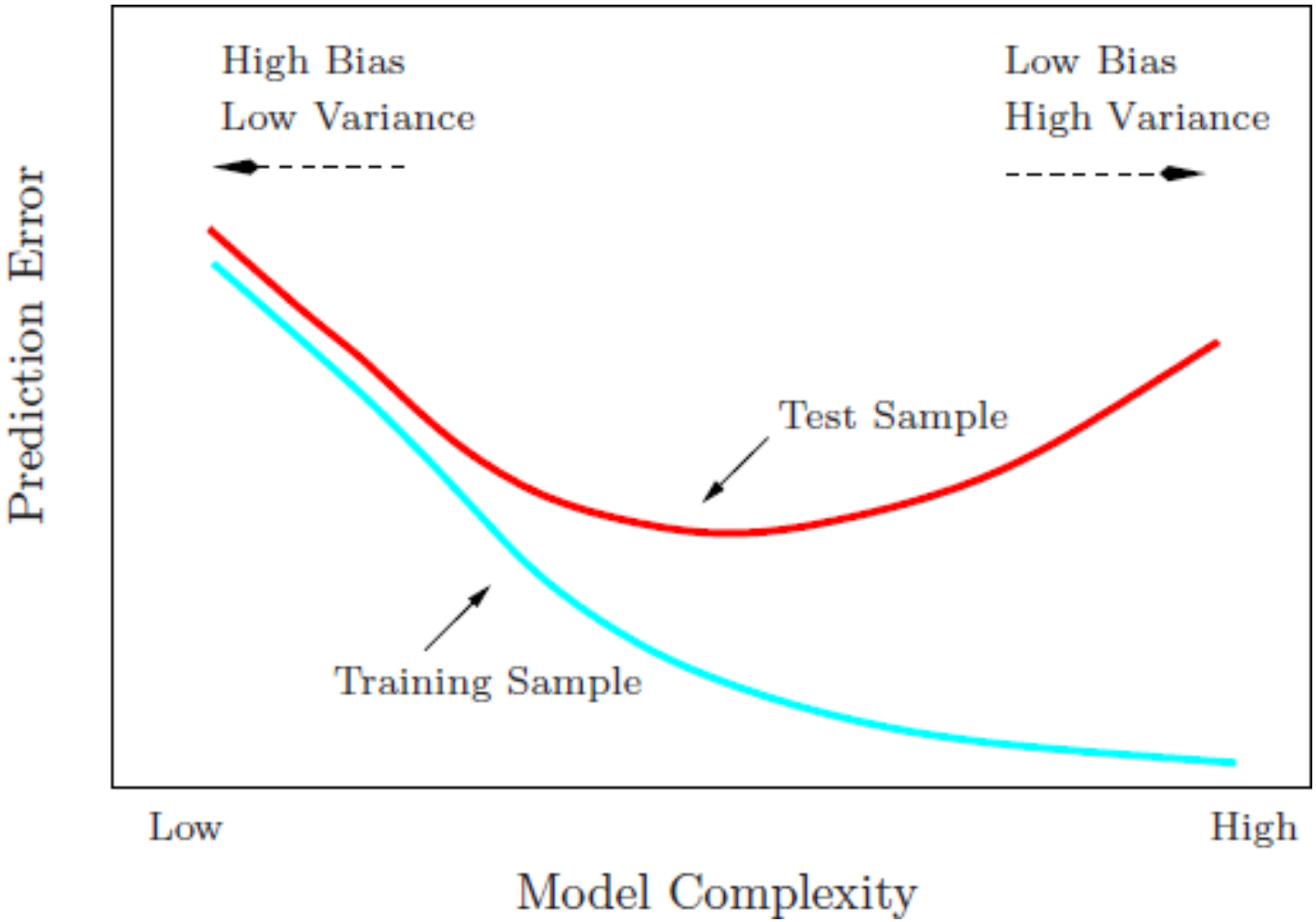
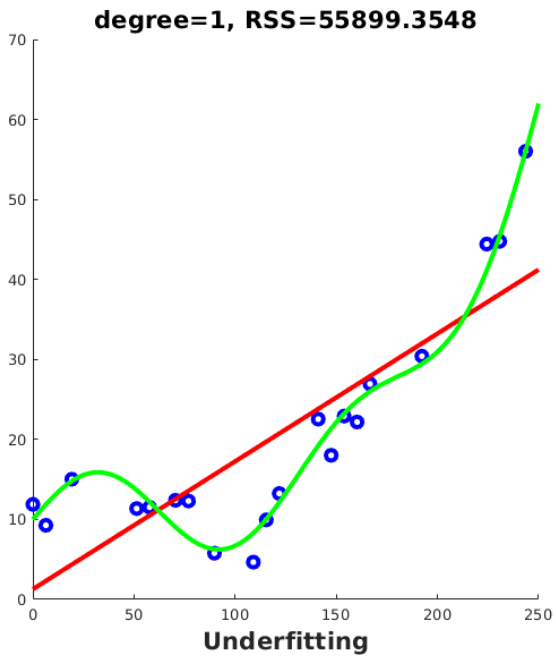
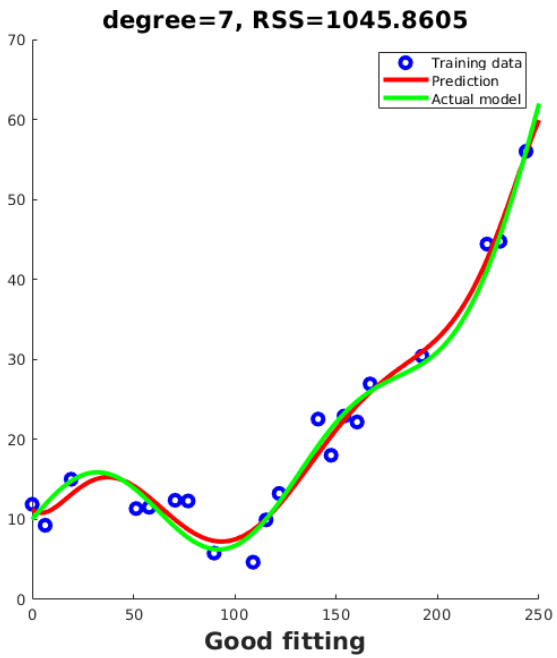
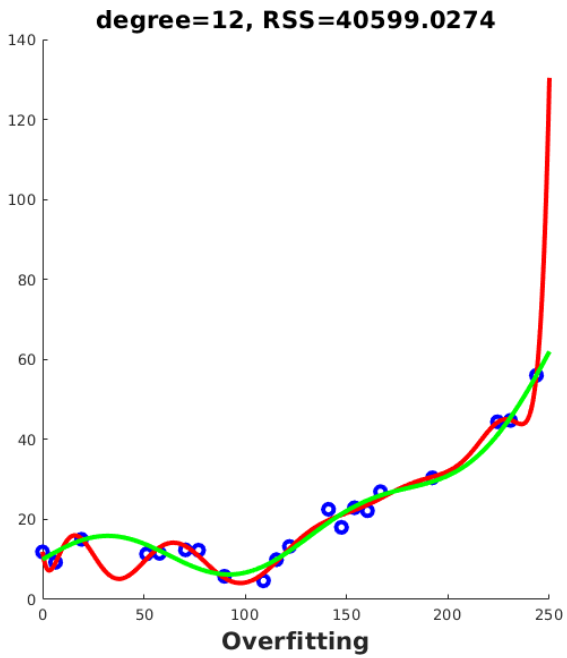


Figure 3: Test and training error as a function of the model complexity. We go from underfitting (left) to overfitting (right).

Bias-variance tradeoff - Overfitting Regression

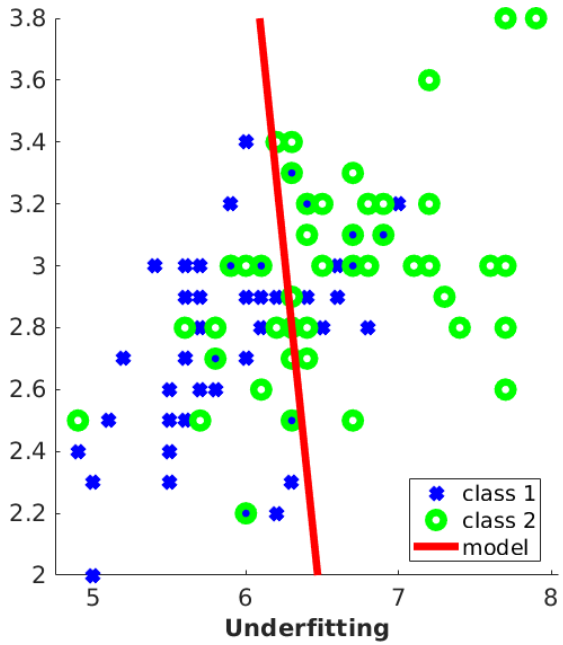


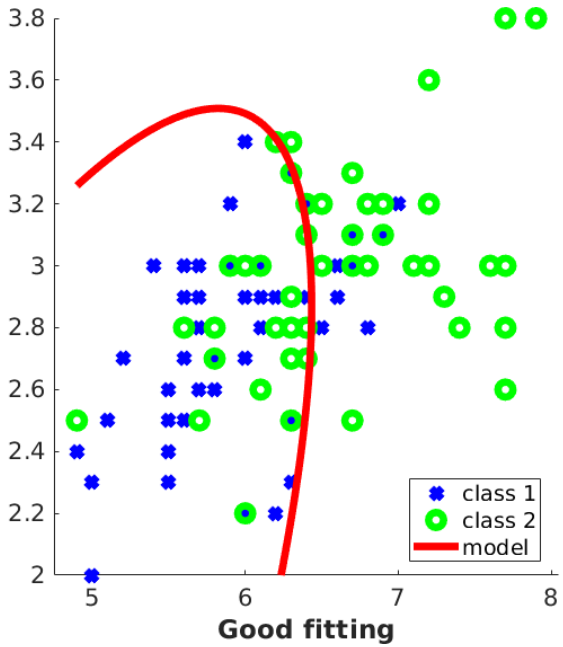


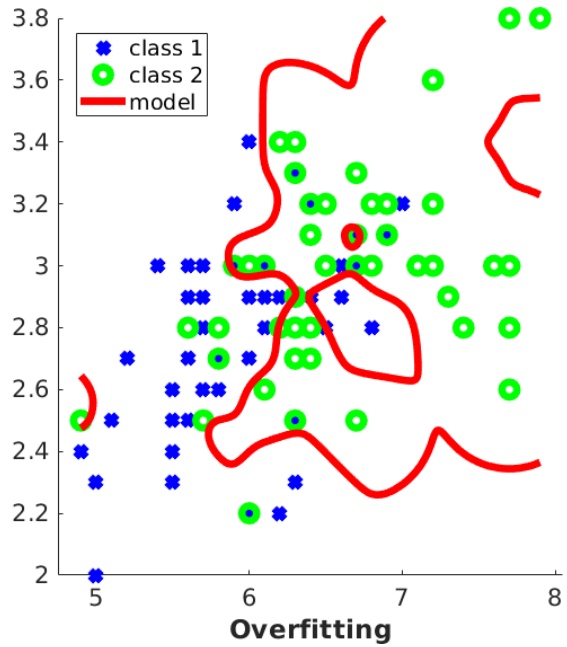


- Here, we use a polynomial regression model:
  $y = \beta_0 + \beta_1 x + \beta_2 x^2 + ... + \beta_q x^q$
- Please note that this is still a linear function in the unknown parameters β !

Bias-variance tradeoff - Overfitting Classification







- Here, we have used LDA, QDA and non-linear SVM

Extending Linear Model

OLS is the best linear unbiased estimator, namely it is the estimator that has the lowest variance with a zero bias. However, the MSE is equal to a sum between *Bias* (squared) and *Variance*. Linear regression may suffer from high variance, So it may be worth sacrificing some bias to achieve a lower variance (**better prediction accuracy**).

Furthermore, we might also have a large number of regression coefficients β which can make **difficult the interpretation** of the results. We often would like to determine a smaller subset of coefficients that exhibit the strongest effect.

We will see two methods:

- Ridge regression
- LASSO

Summary

Ridge regression

Ridge regression shrinks the regression coefficients β by imposing a penalty on their size. We force the coefficients to lie in a ball around the origin with radius $\sqrt{t}$. We have:

$$\beta^*_{ridge} = \arg\min_{\beta} \underbrace{\sum_{i=1}^{n}(y_i - x_i^T\beta)^2}_{f(\beta)} \quad \text{subject to} \quad \underbrace{\sum_{j=1}^{d}\beta_j^2}_{g(\beta)} \leq t \tag{28}$$

From the first KKT equation we have: $\Delta_\beta \left[f(\beta) + \lambda(g(\beta) - t)\right] = 0$ which is equivalent to solving $\arg\min_\beta f(\beta) + \lambda g(\beta)$ for the same choice of λ.

Ridge regression

$$\beta^*_{ridge} = \arg\min_{\beta} \underbrace{\sum_{i=1}^{n}(y_i - x_i^T\beta)^2}_{Loss} + \lambda \underbrace{\sum_{j=1}^{d}\beta_j^2}_{Penalty} \tag{29}$$

Here the Lagrange multiplier $\lambda \geq 0$ can be seen as a **tuning parameter**, which controls the strength of the penalty term.
Note that:

- When $\lambda = 0$, what do we have ?

Ridge regression

$$\beta^*_{ridge} = \arg\min_{\beta} \underbrace{\sum_{i=1}^{n}(y_i - x_i^T\beta)^2}_{Loss} + \lambda \underbrace{\sum_{j=1}^{d}\beta_j^2}_{Penalty} \tag{29}$$

Here the Lagrange multiplier $\lambda \geq 0$ can be seen as a **tuning parameter**, which controls the strength of the penalty term.
Note that:

- When $\lambda = 0$, what do we have ? OLS solution

Ridge regression

$$\beta^*_{ridge} = \arg\min_{\beta} \underbrace{\sum_{i=1}^{n}(y_i - x_i^T\beta)^2}_{Loss} + \lambda \underbrace{\sum_{j=1}^{d}\beta_j^2}_{Penalty} \tag{29}$$

Here the Lagrange multiplier $\lambda \geq 0$ can be seen as a **tuning parameter**, which controls the strength of the penalty term.
Note that:

- When $\lambda = 0$, what do we have ? OLS solution
- When $\lambda = \infty$, what do we have ?

Ridge regression

$$\beta^*_{ridge} = \arg\min_{\beta} \underbrace{\sum_{i=1}^{n}(y_i - x_i^T\beta)^2}_{Loss} + \lambda \underbrace{\sum_{j=1}^{d}\beta_j^2}_{Penalty} \tag{29}$$

Here the Lagrange multiplier $\lambda \geq 0$ can be seen as a **tuning parameter**, which controls the strength of the penalty term.
Note that:

- When $\lambda = 0$, what do we have ? OLS solution
- When $\lambda = \infty$, what do we have ? $\beta^*_{ridge} = 0$

Ridge regression

$$\beta^*_{ridge} = \arg\min_{\beta} \underbrace{\sum_{i=1}^{n}(y_i - x_i^T\beta)^2}_{Loss} + \lambda \underbrace{\sum_{j=1}^{d}\beta_j^2}_{Penalty} \tag{29}$$

Here the Lagrange multiplier $\lambda \geq 0$ can be seen as a **tuning parameter**, which controls the strength of the penalty term.
Note that:

- When $\lambda = 0$, what do we have ? OLS solution
- When $\lambda = \infty$, what do we have ? $\beta^*_{ridge} = 0$
- We look for the best trade-off. When λ increases from 0 to ∞ the bias also increases whereas the variance decreases

Ridge regression

$$\beta^*_{ridge} = \arg\min_{\beta} \underbrace{\sum_{i=1}^{n}(y_i - x_i^T\beta)^2}_{Loss} + \lambda \underbrace{\sum_{j=1}^{d}\beta_j^2}_{Penalty} \tag{30}$$

Note that:

- We do not penalize the intercept β_0 otherwise, adding a constant c to each y_i, it would not result in a shift of the predictions ($x_i^T\beta$) by the same amount c.
- If we center the columns of $\mathbf{x}$ then the OLS intercept β_0 is simply the average of y_i. Thus, we could also center both $\mathbf{y}$ and $\mathbf{x}$ and do not include the intercept in our linear model.
- If the predictor variables x_j (columns of $\mathbf{x}$) are not on the same scale (same measurement units), we should scale them to have sample variance equal to 1 (very important !)

Ridge regression

- We can rewrite the ridge regression in vector notation:

$$\beta^*_{ridge} = \arg\min_{\beta} \mathsf{RSS} = (\mathbf{y} - \mathbf{x}\beta)^T(\mathbf{y} - \mathbf{x}\beta) + \lambda||\beta||_2^2 \tag{31}$$

- It is convex and hence has unique solution:

$$\begin{aligned} \frac{\partial \mathsf{RSS}}{\partial \beta} &= -2\mathbf{x}^T(\mathbf{y} - \mathbf{x}\beta) + 2\lambda\beta = 0 \\ \beta^*_{ridge} &= (\mathbf{x}^T\mathbf{x} + \lambda I_d)^{-1}\mathbf{x}^T\mathbf{y} \end{aligned} \tag{32}$$

- Even if $(\mathbf{x}^T\mathbf{x})$ is singular (not invertible) the addition of λI_d makes it invertible ! (original motivation)

Summary

LASSO

The LASSO (least absolute shrinkage and selection operator) estimate is defined as:

$$\begin{aligned}\beta^*_{lasso} &= \arg\min_{\beta} \sum_{i=1}^{n}(y_i - x_i^T\beta)^2 \quad \text{subject to } \sum_{j=1}^{d}|\beta_j| \leq t \\ &= \arg\min_{\beta} \underbrace{\sum_{i=1}^{n}(y_i - x_i^T\beta)^2}_{Loss} + \lambda \underbrace{\sum_{j=1}^{d}|\beta_j|}_{Penalty}\end{aligned} \tag{33}$$

The only difference between ridge regression and lasso is the penalty. The former uses a L2 penalty whereas the latter a L1 penalty.

The minimization of the L1 penalty **brings some coefficients to zero** ! The L2 penalty decreases the value of all coefficients at the same time !

LASSO

$$\beta^*_{lasso} = \arg\min_{\beta} \underbrace{\sum_{i=1}^{n}(y_i - x_i^T\beta)^2}_{Loss} + \lambda \underbrace{\sum_{j=1}^{d}|\beta_j|}_{Penalty} \tag{34}$$

$$\beta^*_{lasso} = \arg\min_{\beta} \underbrace{(\mathbf{y} - \mathbf{x}\beta)^T(\mathbf{y} - \mathbf{x}\beta)}_{Loss} + \lambda \underbrace{||\beta||_1}_{Penalty}$$

The LASSO is able to perform **variable selection**. As λ increases more coefficients are set to zero. We keep only the most "important" ones !

In the following courses you will see "black box" methods which can achieve impressive prediction accuracy but which may also be difficult to interpret (i.e. deep learning) !

LASSO

$$\beta^*_{lasso} = \arg\min_{\beta} \underbrace{(\mathbf{y} - \mathbf{x}\beta)^T(\mathbf{y} - \mathbf{x}\beta)}_{Loss} + \lambda \underbrace{||\beta||_1}_{Penalty} \tag{35}$$

Note that:

- When $\lambda = 0$, what do we have ?

LASSO

$$\beta^*_{lasso} = \arg\min_{\beta} \underbrace{(\mathbf{y} - \mathbf{x}\beta)^T(\mathbf{y} - \mathbf{x}\beta)}_{Loss} + \lambda \underbrace{||\beta||_1}_{Penalty} \tag{35}$$

Note that:

- When $\lambda = 0$, what do we have ? OLS solution

LASSO

$$\beta^*_{lasso} = \arg\min_{\beta} \underbrace{(\mathbf{y} - \mathbf{x}\beta)^T(\mathbf{y} - \mathbf{x}\beta)}_{Loss} + \lambda \underbrace{||\beta||_1}_{Penalty} \tag{35}$$

Note that:

- When $\lambda = 0$, what do we have ? OLS solution
- When $\lambda = \infty$, what do we have ?

LASSO

$$\beta^*_{lasso} = \arg\min_{\beta} \underbrace{(\mathbf{y} - \mathbf{x}\beta)^T(\mathbf{y} - \mathbf{x}\beta)}_{Loss} + \lambda \underbrace{||\beta||_1}_{Penalty} \tag{35}$$

Note that:

- When $\lambda = 0$, what do we have ? OLS solution
- When $\lambda = \infty$, what do we have ? $\beta^*_{lasso} = 0$

LASSO

$$\beta^*_{lasso} = \arg\min_{\beta} \underbrace{(\mathbf{y} - \mathbf{x}\beta)^T(\mathbf{y} - \mathbf{x}\beta)}_{Loss} + \lambda \underbrace{||\beta||_1}_{Penalty} \tag{35}$$

Note that:

- When $\lambda = 0$, what do we have ? OLS solution
- When $\lambda = \infty$, what do we have ? $\beta^*_{lasso} = 0$
- The difference between ridge and lasso is "in between", that is to say how the coefficients β go to zero when varying λ.

LASSO

$$\beta^*_{lasso} = \arg\min_{\beta} \underbrace{(\mathbf{y} - \mathbf{x}\beta)^T(\mathbf{y} - \mathbf{x}\beta)}_{Loss} + \lambda \underbrace{||\beta||_1}_{Penalty} \tag{36}$$

Note that:

- Unlike Ridge regression, Lasso does not have a closed form solution
- Different algorithms have been proposed such as: quadratic programming ($O(n2^d)$), LARS (least angle regression) ($O(nd^2)$) and coordinate descent ($O(nd)$)

Note that, if $\mathbf{x}^T\mathbf{x} = I_d$, then:

$$\begin{aligned}
\beta^*_{lasso} &= \arg\min_{\beta} \mathsf{RSS} = (\mathbf{y} - \mathbf{x}\beta)^T(\mathbf{y} - \mathbf{x}\beta) + \lambda||\beta||_1 \\
\beta^*_{lasso} &= \arg\min_{\beta} -2\beta^T\mathbf{x}^T\mathbf{y} + \beta^T\beta + \lambda\sum_{j=1}^{d}|\beta_j| \\
\beta^*_{lasso} &= \arg\min_{\beta} -2\beta^T\beta^*_{OLS} + \beta^T\beta + \lambda\sum_{j=1}^{d}|\beta_j| \\
\beta^*_{lasso} &= \arg\min_{\beta} \sum_{j=1}^{d}\Big(-2\beta_j(\beta^*_{OLS})_j + \beta_j^2 + \lambda|\beta_j|\Big)
\end{aligned} \tag{37}$$

We can work with each index j separately (we remove the index in the following for clarity purpose):

$$\beta^*_{lasso} = \arg\min_{\beta} -2\beta\beta^*_{OLS} + \beta^2 + \lambda|\beta|$$

$$\beta^*_{lasso} = \arg\min_{\beta} \begin{cases} \text{if } \beta \geq 0 & -2\beta\beta^*_{OLS} + \beta^2 + \lambda\beta \\ \text{if } \beta < 0 & -2\beta\beta^*_{OLS} + \beta^2 - \lambda\beta \end{cases}$$

$$\beta^*_{lasso} = \begin{cases} \text{if } \beta \geq 0 & \beta^*_{OLS} - \frac{\lambda}{2} \\ \text{if } \beta < 0 & \beta^*_{OLS} + \frac{\lambda}{2} \end{cases} \tag{38}$$

$$\beta^*_{lasso} = \begin{cases} \beta^*_{OLS} - \frac{\lambda}{2} & \text{if } \beta^*_{OLS} \geq \frac{\lambda}{2} \\ \beta^*_{OLS} + \frac{\lambda}{2} & \text{if } \beta^*_{OLS} < -\frac{\lambda}{2} \\ 0 & \text{otherwise} \end{cases}$$

Ridge Regression Vs LASSO

Using $\mathbf{x}^T\mathbf{x} = I_d$, we obtain:

$$\beta^*_{ridge} = \frac{\beta^*_{OLS}}{1+\lambda}$$

$$\beta^*_{lasso} = \begin{cases} \beta^*_{OLS} - \frac{\lambda}{2} & \text{if } \beta^*_{OLS} \geq \frac{\lambda}{2} \\ \beta^*_{OLS} + \frac{\lambda}{2} & \text{if } \beta^*_{OLS} < -\frac{\lambda}{2} \\ 0 & \text{otherwise} \end{cases} \tag{39}$$

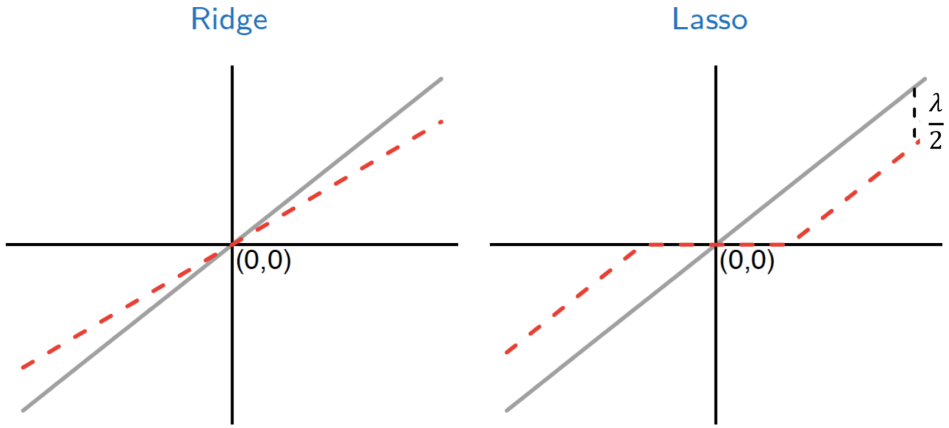


Figure 4: β^* and β^*_{OLS} are shown in the y-axis and x-axis respectively. The gray line shows β^*_{OLS}. The red lines represent the Ridge and Lasso estimators.

Ridge Regression Vs LASSO

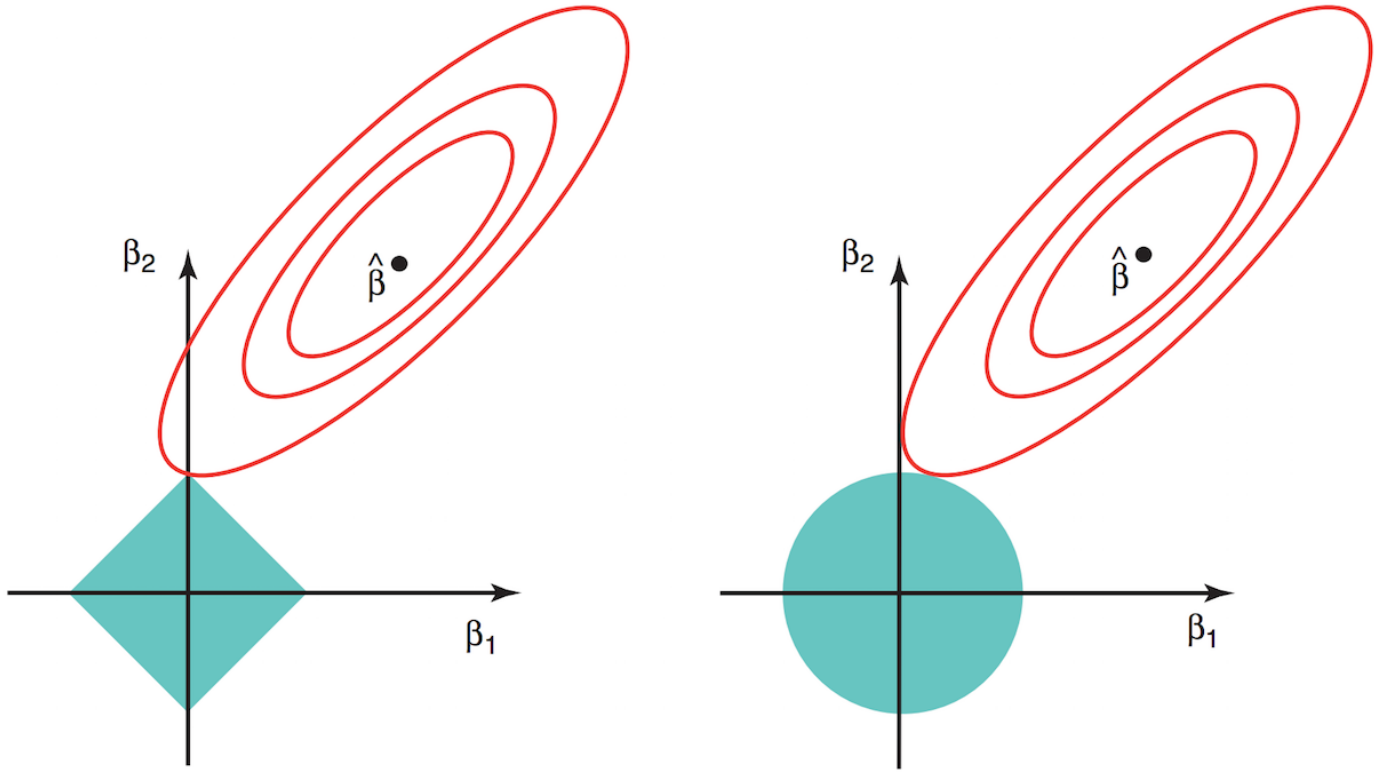


Figure 5: LASSO on the left and Ridge on the right. We suppose we have two β: β_1 and β_2. In red are shown the elliptical contours of the OLS RSS ($\hat{\beta} = \beta^*_{OLS}$). In blue are shown the constraint regions: $|\beta_1| + |\beta_2| \leq t$ for LASSO and $\beta_1^2 + \beta_2^2 \leq t$ for Ridge.

Ridge Regression Vs LASSO

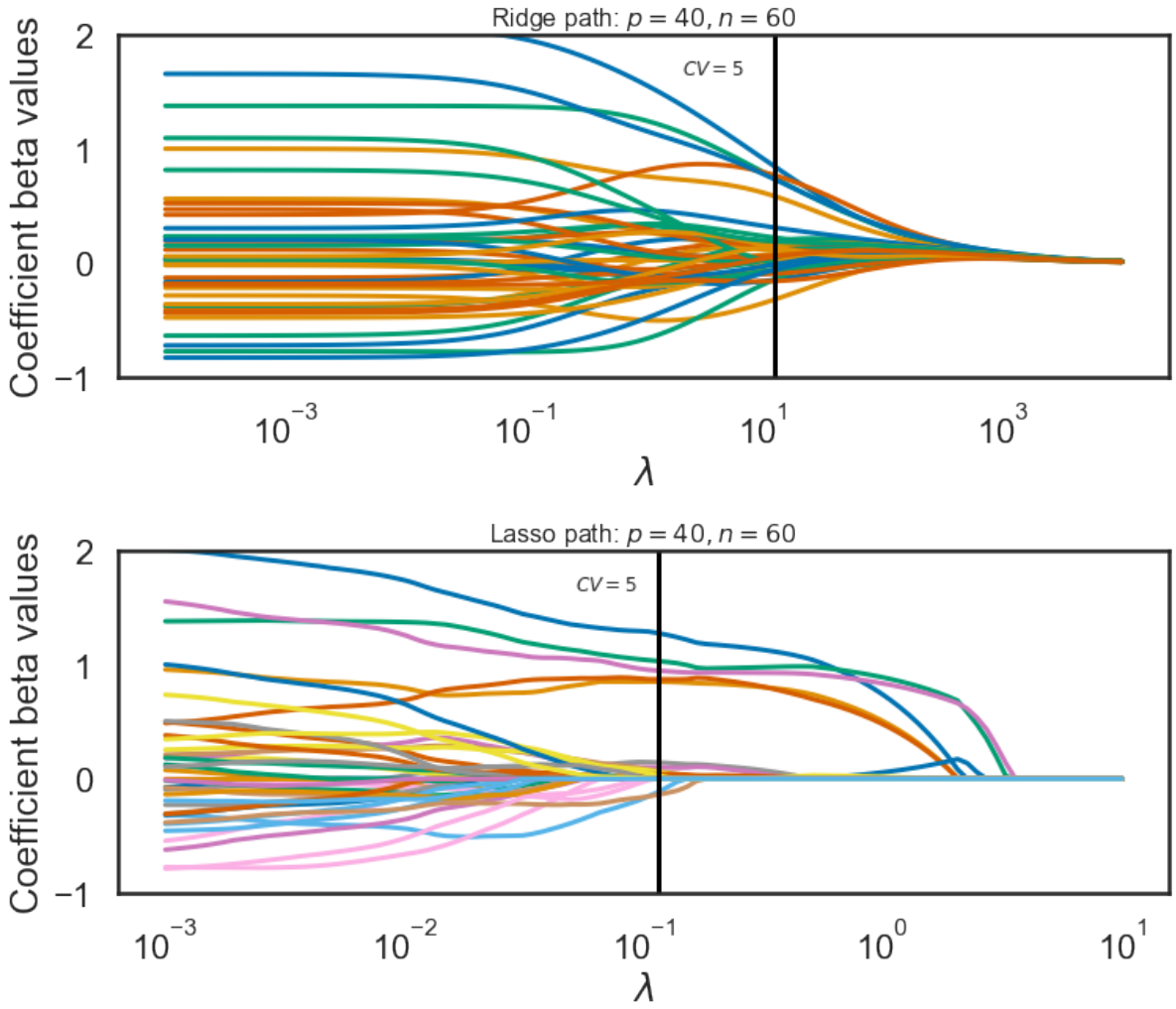


Figure 6: Trends of β when varying λ for Ridge and Lasso. In Ridge all β tends to 0 in the same way. In Lasso β go to 0 at different times.

Degrees of freedom

- The number of degrees of freedom df can be seen as the number of linearly independent parameters. However, what does it mean in Ridge and Lasso ?
- A more useful definition is: $df(\mathbf{y}^*) = \frac{1}{\sigma^2} \sum_{i=1}^{N} \mathsf{Cov}(y_i^*, y_i)$ which means that the harder we fit to the data, the larger $\mathsf{Cov}(y_i^*, y_i)$ and hence $df(\mathbf{y}^*)$ [1]
- $df(\mathbf{y}^*_{OLS}) = d$
- $df(\mathbf{y}^*_{ridge}) = \mathsf{Tr}[\mathbf{x}(\mathbf{x}^T\mathbf{x} + \lambda I_d)^{-1}\mathbf{x}^T]$
- $df(\mathbf{y}^*_{lasso}) =$ number of predictors (non-zero coefficients in β^*_{lasso})

Summary

Model assessment

- If we have no hyper-parameters (like in OLS) to fix, namely we only have one model f, we do not need a Validation set. We only need a Training set to fit the model (i.e. estimate the best parameters) and a Test set to compute the prediction error (generalization error). The test set is used for **Model assessment**.

  Recipe:

  - Randomize and, if necessary, standardize/normalize the data $\mathcal{D}_n$
  - Split $\mathcal{D}_n$ into, for instance, 70% for Training set and 30% for Test set
  - Choose a class of models $\mathcal{F}$ without hyper-parameters, like OLS
  - Fit the model $f \in \mathcal{F}$ to the Training set (i.e. estimate the best parameters β^*)
  - Evaluate the generalization error of the model f using the Test set

Model selection and assessment

- If we do have hyper-parameters, like the λ in Ridge and LASSO, we also need a Validation set for **Model selection**. Each value of λ corresponds to a different model f_i.
  - Randomize and, if necessary, standardize/normalize the data $\mathcal{D}_n$
  - Split $\mathcal{D}_n$ into, for instance, 70% for Training set, 20% for Validation set and 10% for Test set
  - Choose a class of models $\mathcal{F}$ with one hyper-parameter λ, like Ridge or LASSO
  - Choose a set of values L for the hyper-parameter $\{\lambda_l\}_{l=1,\dots,L}$
  - **Loop** ($l = 1$ to L)
    - Fit the model f_{λ_l} to the Training set (i.e. estimate the best parameters β^* using λ_l)
    - Evaluate the performance of the model f_{λ_l} using the Validation set
  - Select as best model f^* the one, among $\{f_{\lambda_l}\}$, with the best performance on the Validation set (i.e. lowest prediction error)
  - Evaluate the generalization error of the model f^* using the Test set

Model selection

- If the data-set $\mathcal{D}_n$ is very rich (i.e. N is big), we can randomly divide it into three subsets (Training, Validation and Test). But what if $\mathcal{D}_n$ is small ?
- We need to find a way to estimate the best model $\hat{f}$ with few data. In the case of Ridge and Lasso this means finding the best hyper-parameter λ
- Two possible ways are:
  - Information criteria: AIC and BIC
  - Cross-validation

Summary

Information criteria: AIC

- We can use an information criterion (or more than one) to select the "best" model $\hat{f}$
- The model $\hat{f}$ should not be too much complex (high df) in order not to over-fit the data but at the same time it should not be too simple (low df) in order not to under-fit the data !
- The **Akaike information criterion (AIC)** finds the best model $\hat{f}$ among a collection of models $\{f_i\}$ by balancing the goodness of fit with the complexity of the model: $\text{AIC}_{f_i} = 2k_{f_i} - 2\ln(\hat{L_{f_i}})$
  - k_{f_i} is the number of effective parameters of the model f_i (i.e. degrees of freedom)
  - $\hat{L_{f_i}}$ is the maximum likelihood estimate of the model f_i
- A further refinement to correct for small data-sets is: $\text{AICc}_{f_i} = \text{AIC} + \frac{2k(k+1)}{N-k-1}$ where N is the number of samples
- The best model $\hat{f}$ is the one with the lowest AIC or AICc

Information criteria: BIC

- Another criterion for model selection is the **Bayesian information criterion (BIC)**: $\text{BIC}_{f_i} = \ln(N)k_{f_i} - 2\ln(\hat{L}_{f_i})$
- The only difference between the two criteria is the penalty for the number of effective parameters ($2k_{f_i}$ Vs $\ln(N)k_{f_i}$) $\rightarrow$ BIC penalizes model complexity more heavily !
- Main differences:
  - BIC will select the "true optimal model" (if it is present in the list of candidates) with probability 1 when $N \rightarrow \infty$. The probability for AIC/AICc can be less than 1.
  - If the "true optimal model" is not present in the list of candidates and/or if N is small, AIC and AICc may select a better model than BIC

Information criteria - OLS

- If all residuals are i.i.d.normally distributed (with zero mean) $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$ then the log-likelihood is equal to
  $\ln(L_{f_i}) = \ln\left(\prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \exp(\frac{-\epsilon_i^2}{2\sigma^2})\right) = -\frac{N}{2}\ln(2\pi) - \frac{N}{2}\ln(\sigma^2) - \frac{RSS}{2\sigma^2}$
- The maximum likelihood estimate for σ^2 is equal to: $\sigma^2 = \frac{RSS}{N}$
- Thus, $\ln(\hat{L}_{f_i}) = -\frac{N}{2}\ln(RSS) + C$ where C is a constant which depends on the data (so it's the same for all models f_i)
- Thus we obtain:
  - $\text{AIC}_{f_i} = 2k_{f_i} + N\ln(RSS)$
  - $\text{BIC}_{f_i} = \ln(N)k_{f_i} + N\ln(RSS)$

Information criteria

Pros

- Easy to interpret
- Fast to compute

Cons

- Need proper estimation of degrees of freedom (may be difficult like in Lasso)
- Asymptotic results (true only when $N \to \infty$)
- Assume that data are actually generated by the model f_i
- Tend to have bad results when $k > N$

Summary

Prediction error

- Given a data-set $\mathcal{D}_n$ divided into Training set $\mathcal{T}$ and Test set $((X_T, Y_T))$, what we actually measure is the **empirical generalization error** on the Test set given $\mathcal{T}$, which is defined as $\text{Err}_{\mathcal{T}} = \text{E}[L(Y_T, \hat{f}(X_T))|\mathcal{T}]$
- For statistical analysis, it would be better suited the **expected empirical generalization error** defined as $\text{Err} = \text{E}[L(Y, \hat{f}(X))] = \text{E}[\text{Err}_{\mathcal{T}}]$ where we would average over all possible Training sets $\mathcal{T}$. This means that we should have many data-sets $\mathcal{D}_n$ sampled from the same theoretical distribution, divided into Training and Test sets.

Prediction error

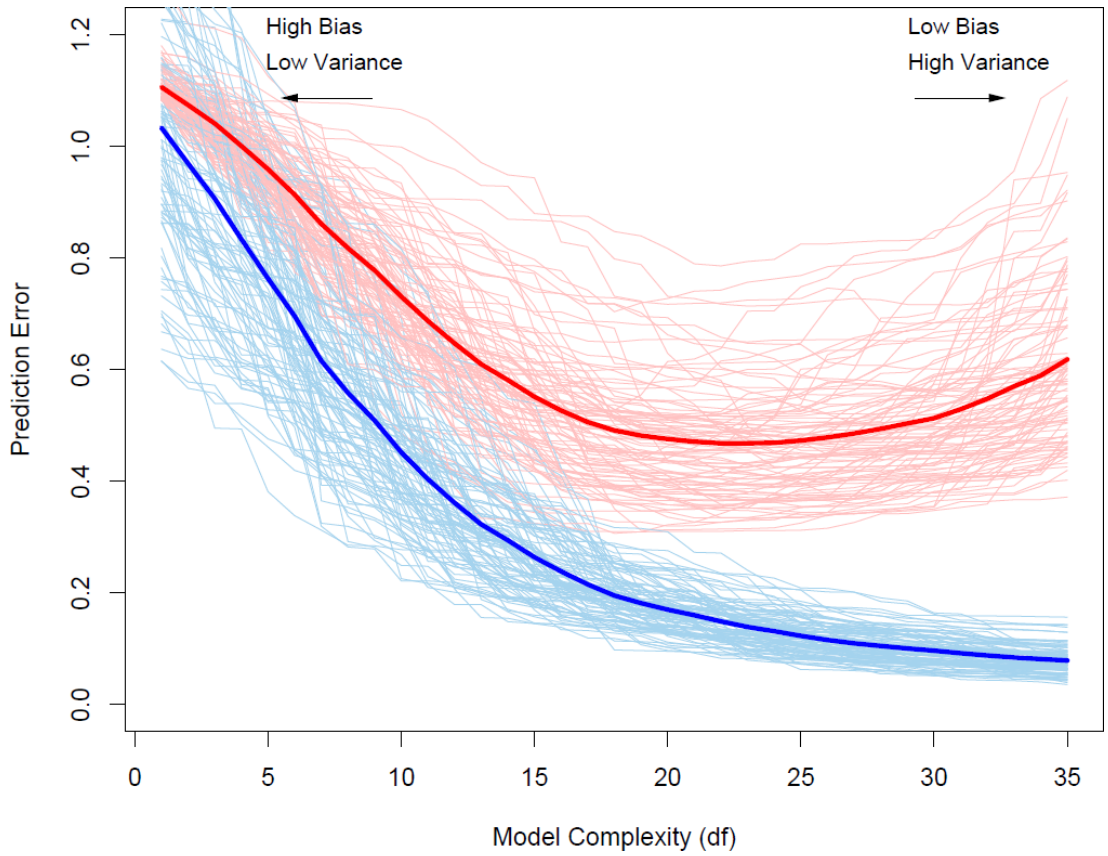


Figure 7: Behavior of training and test error as the model complexity is varied. Light curves refer to the errors given a training set. Solid curves show the averages error. Image taken from [1]

Cross-validation (CV)

- Unfortunately, we usually have only one data-set set $\mathcal{D}_n \rightarrow$ the solution of cross-validation is to divide the data-set into Training and Test sets not only once but several times, combining then (i.e. averaging) the test performances. This should reduce the variability of the generalization error.

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- **Exhaustive cross-validation**: It uses all possible splits into Training and Test sets of the original data $\mathcal{D}_n \rightarrow$ usually computationally infeasible even for small n
- **K-fold cross-validation**: $\mathcal{D}_n$ is randomly partitioned into K equal sized parts or "folds". We then train on all but the k-th part which is used as Test set. We then iterate over all K parts and average the test error over all folds. All observations are used for both training and testing. It is computationally feasible.

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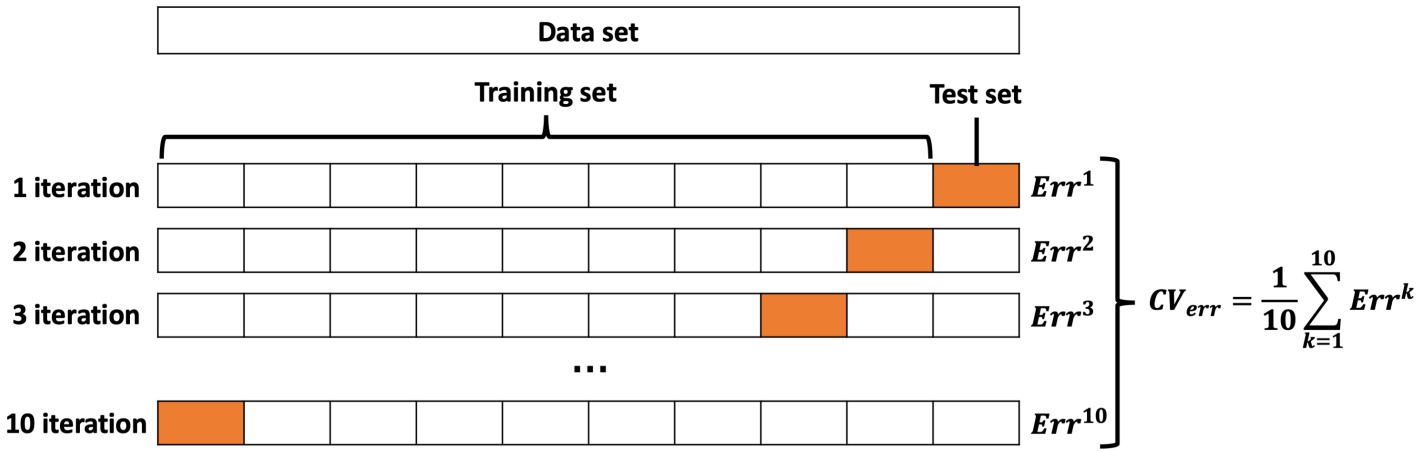
- In classification, we usually use **stratified K-fold cross-validation** where each fold contains roughly the same proportion of observations from the different classes

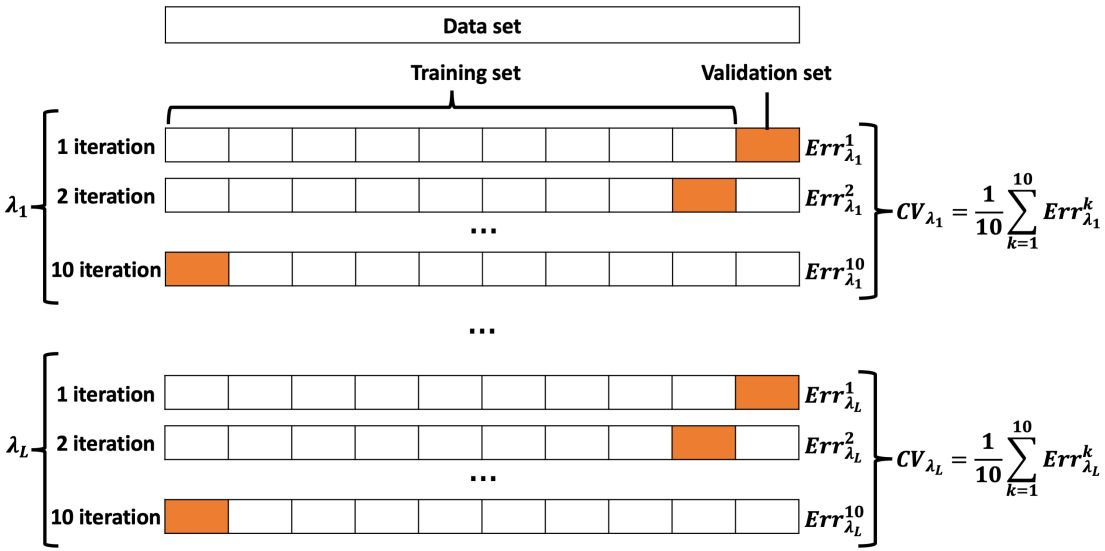
K-fold cross validation - Model Assessment

- Split the training N samples into K disjoint sets $\{S_k\}_{k=1,\ldots,K}$ of size N/K
- **Loop** ($k = 1$ to K):
  - Fit the model f^k using all samples $\notin S_k$, that is estimate the optimal parameters of the model without the k-th part
  - Record the error on the k-th (test) fold $\text{Err}^k = \sum_{i \in S_k} L(y_i, f^k(x_i))$
- Compute the average error over all K folds: $\text{CV}_{\text{err}} = \frac{1}{N} \sum_{k=1}^{K} \text{Err}^k$



K-fold cross validation - Model Validation

- Given a set of tuning hyper-parameters $\{\lambda_l\}_{l=1,\dots,L}$, split the training N samples into K disjoint sets $\{S_k\}_{k=1,\dots,K}$ of size N/K
- **Loop** ($l = 1$ to L):
  - **Loop** ($k = 1$ to K):
    - Fit the model $f^k_{\lambda_l}$ using all samples $\notin S_k$, that is estimate the optimal parameters of the model without the k-th part and using λ_l
    - Record the error on the validation set $\text{Err}^k_{\lambda_l} = \sum_{i \in S_k} L(y_i, f^k_{\lambda_l}(x_i))$
  - Compute the average error over all K folds: $CV_{\lambda_l} = \frac{1}{N} \sum_{k=1}^{K} \text{Err}^k_{\lambda_l}$



K-fold cross validation - Model Validation

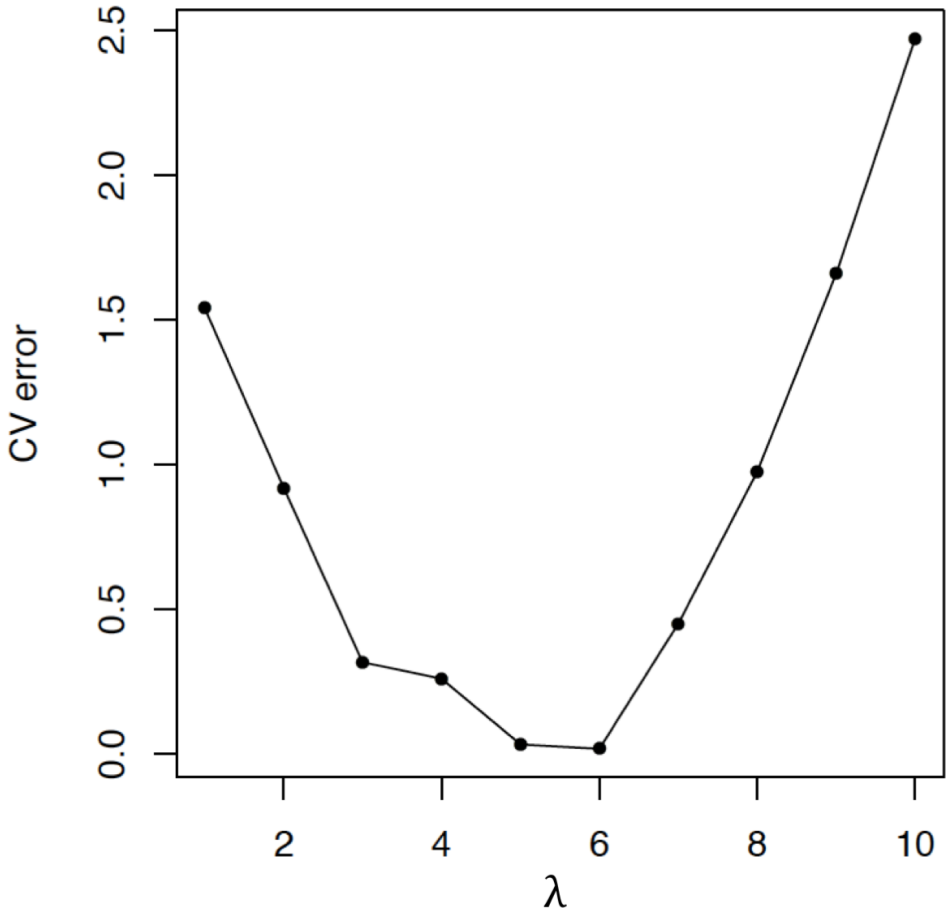


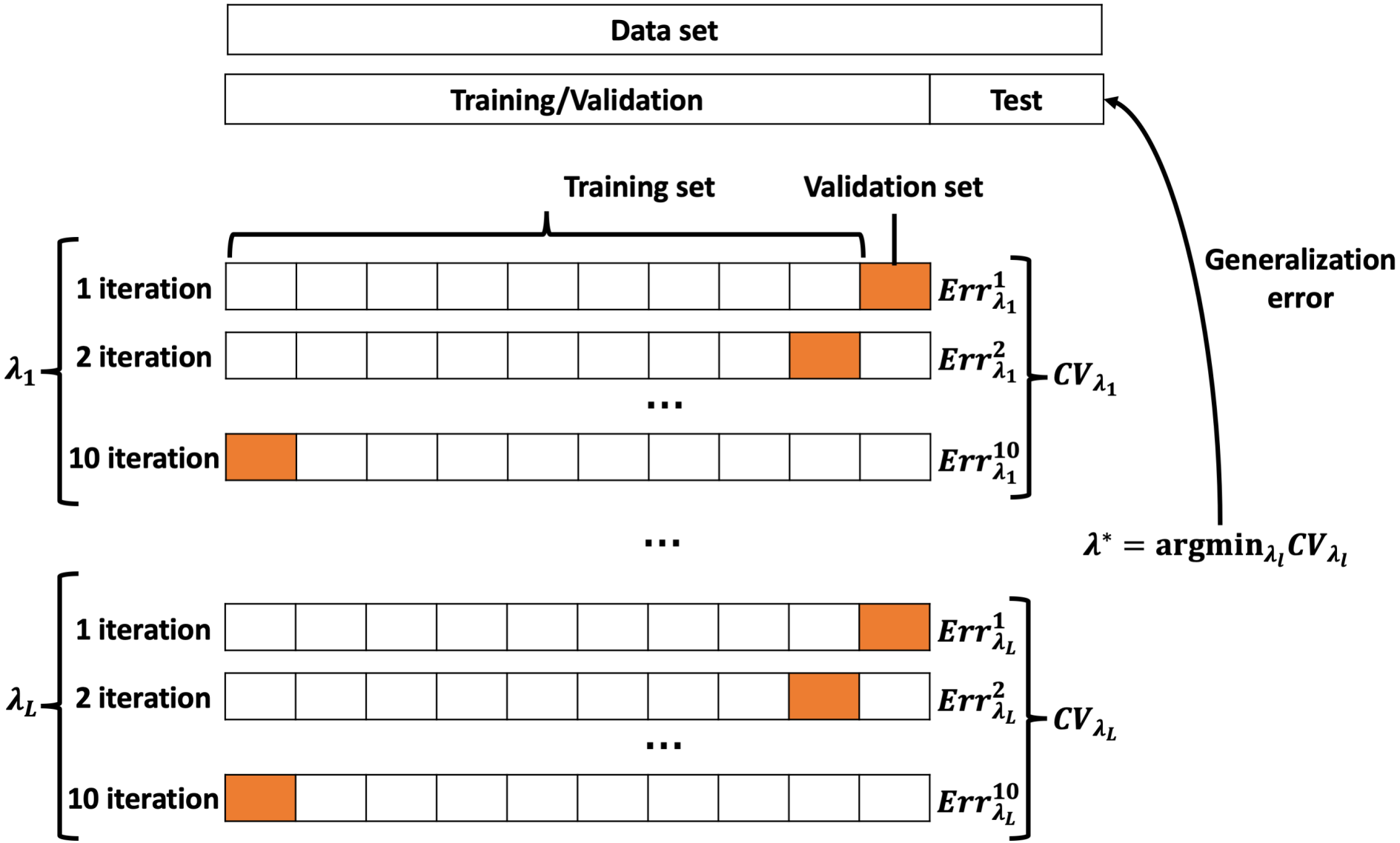
Figure 8: Curve of the CV error which is a function of λ. Image taken from [1]

We then choose the best λ as: $\lambda^* = \arg\min_{\lambda_l} CV_{\lambda_l}$

K-fold cross validation - Model Validation and Assessment

- Divide $\mathcal{D}_n$ into two parts, one for training/validation and one for test
- Given a set of tuning hyper-parameters $\{\lambda_l\}_{l=1,\dots,L}$, split the training/validation samples into K disjoint sets $\{S_k\}_{k=1,\dots,K}$
- **Loop** ($l = 1$ to L):
  - **Loop** ($k = 1$ to K):
    - Fit the model $f^k_{\lambda_l}$ using all samples $\notin S_k$, that is estimate the optimal parameters of the model without the k-th part and using λ_l
    - Record the error on the validation set $\mathsf{Err}^k_{\lambda_l} = \sum_{i \in S_k} L(y_i, f^k_{\lambda_l}(x_i))$
  - Compute the average error over all K folds: $CV_{\lambda_l} = \frac{1}{N} \sum_{k=1}^{K} \mathsf{Err}^k_{\lambda_l}$
- Choose as best model f_{λ^*} the one with the smallest error CV_{λ_l}
- Recompute the parameters of the best model over all $K - 1$ sets
- Compute the generalization error on the test set $\mathsf{Err}_{\lambda^*} = \sum_{i \in \mathsf{Test}} L(y_i, f_{\lambda^*}(x_i))$

K-fold cross validation - Model Validation and Assessment



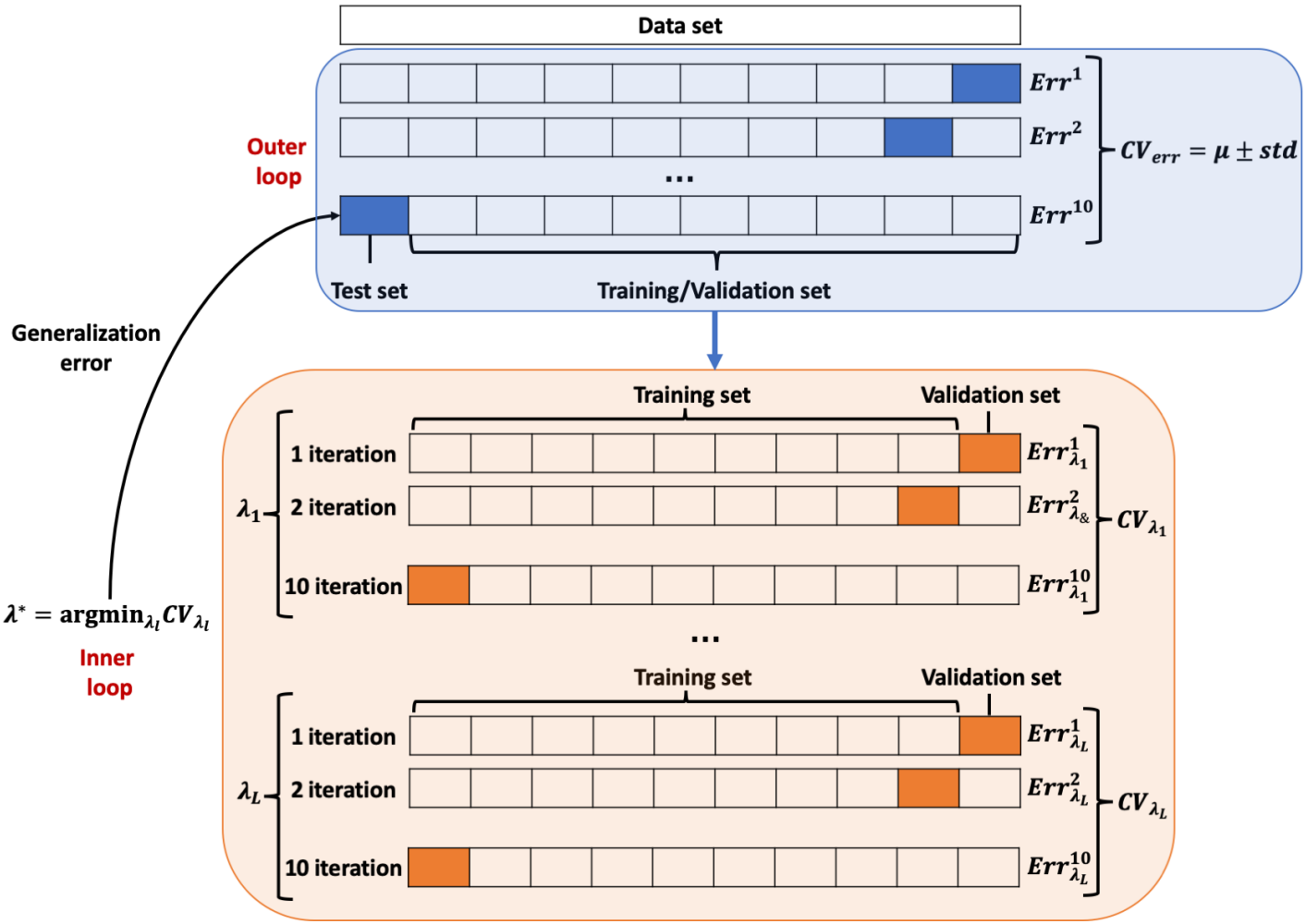
K-fold cross validation

- Be careful, once estimated the best tuning parameter λ^*, we fit our model to the **entire training/validation set** ! We can then use the estimated best parameters β^* to compute the generalization error in the test set
- The choice of K is important
  - $K = 2$: high bias since we will train on only half of the data
  - $K = N$ (leave-one-out): high variance (big overlap between the training sets of each fold)
  - $K = 5, 10$: seems to be a good trade-off between bias and variance (no theory behind)
- Using the previous technique, there was only one test set $\rightarrow$ **nested cross-validation** (more computationally demanding)

k*t-fold nested cross-validation

- Split all the available n samples into K disjoint sets S_i of size n/K
- Here each model corresponds to a different value of the hyper-parameter λ
  - **Outer loop** (i=1 to K):
  - For every i, use S_i as test set and all the other $K-1$ sets as training + validation set
  - Divide the training + validation set into t disjoint sets S_j of equal size
    - **Inner loop** (j=1 to t):
    - For every j, train the model in $t-1$ sets (training set) and evaluate it (validation set) in the left out j-th set
  - Choose the model with the best average performance over all t runs
  - Recompute the parameters of the best model over all $K-1$ sets
  - Compute the error in the left-out S_i set
- Compute the average and standard deviation of the CV error as the mean$\pm$std of the errors over all K runs.

k*t-fold nested cross-validation



Implementation using scikit-learn: https://scikit-learn.org/stable/auto_examples/model_selection/plot_nested_cross_validation_iris.html

Summary

Summary

Linear discriminant analysis (LDA)

Remember that in a classification task, with a 0-1 loss, the optimal procedure is to estimate the most probable class of a test sample x_j (i.e. maximize the posterior probability):

$$f^*(x_j) = \arg\max_{f \in \mathcal{Y}} P(Y = f(x_j)|X = x_j) = \arg\max_{C_k} P(X = x_j|Y = C_k)\pi_{C_k} \tag{40}$$

where we have used the Bayes' theorem ($P(A|B) \propto P(B|A)P(A)$).
LDA proposes to model all conditional distributions $P(X = x_j|Y = C_k) = P_k(x)$ as Gaussian distributions $P_k(x) \sim \mathcal{N}(\mu_k, \Sigma)$.
Classes have **different means** μ_k but the **same covariance matrix** Σ.

Recall that: $\mathcal{N}(\mu_k, \Sigma) \propto \frac{1}{|\Sigma|^{1/2}} \exp(-\frac{1}{2}(x - \mu_k)^T \Sigma^{-1}(x - \mu_k))$

Linear discriminant analysis (LDA)

We can notice that:

$$
\begin{aligned}
f^*(x_j) &= \arg\max_{C_k} P_{C_k}(x_j)\pi_{C_k} = \arg\min_{C_k} -2\log[P_{C_k}(x_j)\pi_{C_k}] \\
&\propto \arg\min_{C_k} (x-\mu_k)^T\Sigma^{-1}(x-\mu_k) + \log(|\Sigma|) - 2\log(\pi_{C_k}) \\
&= \arg\min_{C_k} -2x^T\Sigma^{-1}\mu_k + \mu_k^T\Sigma^{-1}\mu_k - 2\log(\pi_{C_k}) \\
&= \arg\min_{C_k} \underbrace{\mu_k^T\Sigma^{-1}\mu_k - 2\log(\pi_{C_k})}_{a_k} + x^T \underbrace{-2\Sigma^{-1}\mu_k}_{b_k}
\end{aligned}
\tag{41}
$$

This is a linear discriminant function !

Linear discriminant analysis (LDA)

In order to estimate μ_k and Σ, we can maximize the log-likelihood of the training set (x_i, y_i):

$$l(\mu_1, ..., \mu_K) = -\sum_{k=1}^{K} \sum_{i:y_i=k} \frac{1}{2}(x_i - \mu_k)^T \Sigma^{-1}(x_i - \mu_k) - \frac{1}{2} n \log(|\Sigma|) \quad (42)$$

Let $n_k = \#\{i : y_i = k\}$ be the number of observations in class k. The log-likelihood is maximized by:

$$\mu_k^* = \frac{1}{n_k} \sum_{i:y_i=k} x_i \quad \Sigma^* = \frac{1}{n} \sum_{k=1}^{K} \sum_{i:y_i=k} (x_i - \mu_k^*)(x_i - \mu_k^*)^T \quad (43)$$

The a priori probabilities π_{C_k} are estimated as the proportion of samples of class k: $\pi_{C_k}^* = \#\{i : y_i = k\}/n$

Linear discriminant analysis (LDA)

Thus, the best classifier under the assumption that $P_k(x) \sim \mathcal{N}(\mu_k, \Sigma)$ is given by:

$$f^*(x_j) \arg\min_{C_k} -2x_j^T(\Sigma^*)^{-1}\mu_k^* + (\mu_k^*)^T(\Sigma^*)^{-1}\mu_k^* - 2\log(\pi_{C_k}^*) \tag{44}$$

for every sample x_j. We can also notice that if we have two classes (0 and 1) their *linear* (in x_j) decision boundary is given by their log-ratio:

$$\begin{aligned}\log\frac{P(Y=C_0|X=x_j)}{P(Y=C_1|X=x_j)} &= \log\frac{\pi_0}{\pi_1} - \frac{1}{2}(\mu_0+\mu_1)^T\Sigma^{-1}(\mu_0-\mu_1) + \\ &+ x_j^T\Sigma^{-1}(\mu_0-\mu_1) = a + x^Tb = 0\end{aligned} \tag{45}$$

Linear discriminant analysis (LDA)

Pros

- Easy to interpret
- Fast to compute
- Optimal if Gaussian, homoscedasticity and linear assumptions are met

Cons

- Covariance matrix inversion might be ill-posed if $N << p$ (need of regularization)
- Sensitive to outliers (observations far from the boundary have all the same influence)
- Predictive power can decrease if variables are correlated

Summary

QDA and Naive Bayes

QDA

- In LDA we assume that classes have the same covariance matrix Σ. In QDA, each class has its own covariance matrix Σ_k.
- More flexible but also more parameters to compute

Naive Bayes

- In Naive Bayes, we also assume that all features are independent (given a certain class) which means that each class has its own *diagonal* covariance matrix Σ_k.
- Faster and easier to compute than QDA
- Be careful: features should not be correlated !

In both cases, the discriminant functions are **quadratic** !

QDA and Naive Bayes

$$
\begin{aligned}
f^*(x_j) &= \arg\min_{C_k} (x-\mu_k)^T \Sigma_k^{-1} (x-\mu_k) + \log(|\Sigma_k|) - 2\log(\pi_{C_k}) \\
&= \arg\min_{C_k} x^T \Sigma_k^{-1} x - 2x^T \Sigma_k^{-1} \mu_k + \mu_k^T \Sigma_k^{-1} \mu_k - 2\log(\pi_{C_k}) \\
&= \arg\min_{C_k} x^T \underbrace{A_k}_{\Sigma_k^{-1}} x + x^T \underbrace{b_k}_{-2\Sigma^{-1}\mu_k} + \underbrace{c_k}_{\mu_k^T \Sigma^{-1} \mu_k - 2\log(\pi_{C_k})}
\end{aligned}
\tag{46}
$$

This is a quadratic discriminant function !

Summary

Logistic regression

- Can we use a linear regression model $y = x^T \beta$ to predict categorical variables (i.e. for classification in $\mathcal{Y} = \{C_1, \ldots, C_K\}$) ?

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- Instead of predicting directly y, we could predict the probability of y being equal to a certain class knowing x (i.e. $P(Y = C_k | X = x)$. Is linear regression suited for predicting conditional probabilities ?

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- Again no, predicted values are usually unbounded $\rightarrow$ we have to force the outcome to be in the unit interval $[0, 1]$
- Furthermore, we want that $\sum_k P(Y = C_k | X = x) = 1$

Logistic regression

- Logistic regression uses the logistic function $l(x) = \frac{e^x}{1+e^x} = \frac{1}{1+e^{-x}}$ to bound the output between $[0, 1]$. Since we have K possible classes, we model each conditional probability of the classes as:

$$P(Y = C_k|X = x; \theta) = \frac{\exp(x^T \beta_k)}{1 + \sum_{l=1}^{K-1} \exp(x^T \beta_l)} \qquad k = 1, ..., K-1$$
$$P(Y = C_K|X = x; \theta) = \frac{1}{1 + \sum_{l=1}^{K-1} \exp(x^T \beta_l)} \tag{47}$$

- where we have chosen the last class K as reference one in order to have a sum equal to 1. This choice is arbitrary in that the estimates are equivariant wrt this choice
- θ is the entire set of parameters $\{\beta_k\}_{k=1}^{K-1}$

Logistic regression

- **Binomial** or binary logistic regression: y can only have two values ($K = 2$). It can be seen as a series of iid Bernoulli trials.
- **Multinomial** logistic regression: y can have three or more values not ordered ($K > 2$)

  In the following, we will discuss in detail the two-class $\{0, 1\}$ case where we can write that $P(Y = 1|X = x; \beta) = p(x; \beta)$ and $P(Y = 0|X = x; \beta) = 1 - p(x; \beta)$. It follows that:

$$p(x; \beta) = \frac{\exp(x^T \beta)}{1 + \exp(x^T \beta)} \tag{48}$$

  We can also compute the log-odds, namely the log of the likelihood of the first class with respect to the second one (resemblance with LDA...):

$$\log \frac{p(x; \beta)}{1 - p(x; \beta)} = x^T \beta \tag{49}$$

Logistic regression

$$\log \frac{p(x;\beta)}{1-p(x;\beta)} = x^T\beta \tag{50}$$

- The **linear** decision boundary is thus $x^T\beta = 0$
- We should predict $Y = 1$ when $p(x;\beta) > (1-p(x;\beta))$, which means when $x^T\beta \geq 0$, and $Y = 0$ when $p(x;\beta) < (1-p(x;\beta))$, that is when $x^T\beta < 0$
- Remember that x includes the constant term 1 to accommodate the intercept β_0

Logistic regression

- Logistic regression predicts conditional probabilities (not only classes) $\rightarrow$ we can fit it using maximum likelihood
- Given N training observations (i.e. images), each described by a set of features x_i and a known binary class y_i, they can be seen as a sequence of iid Bernoulli trials.
- Remember that the Bernoulli distribution is $P(Y = y) = p^y(1-p)^{1-y}$ where $y = \{0, 1\}$ which means that $P(Y = y) = p$ if $y = 1$, $P(Y = y) = 1 - p$ if $y = 0$ and 0 otherwise.
- The (conditional) likelihood of all N observations is:

$$L(\beta) = \prod_{i=1}^{N} P(Y = y_i | X = x_i; \beta) = \prod_{i=1}^{N} p(x_i; \beta)^{y_i} (1 - p(x_i; \beta))^{1-y_i} \quad (51)$$

Logistic regression

- It is more convenient to work with the log-likelihood $l(\beta) = \ln(L(\beta))$:

$$
\begin{aligned}
l(\beta) &= \sum_{i=1}^{N} y_i \ln(p(x_i;\beta)) + (1-y_i)\ln(1-p(x_i;\beta)) \\
&= \sum_{i=1}^{N} y_i \ln(P(Y=1|X=x;\beta)) + (1-y_i)\ln(P(Y=0|X=x;\beta)) \\
&= \sum_{i=1}^{N} y_i \ln\left(\frac{P(Y=1|X=x;\beta)}{P(Y=0|X=x;\beta)}\right) + \ln(P(Y=0|X=x;\beta)) \\
&= \sum_{i=1}^{N} y_i x_i^T\beta - \ln(1+e^{(x_i^T\beta)}) = -\ln\left(e^{(-y_i x_i^T\beta)}(1+e^{(x_i^T\beta)})\right)
\end{aligned}
\tag{52}
$$

- No closed form solution $\rightarrow$ gradient and Hessian computation

Logistic regression

- We could use a gradient ascent $\beta^{new} = \beta^{old} + \frac{\partial l(\beta^{old})}{\partial \beta}$:

$$\begin{aligned}\frac{\partial l(\beta)}{\partial \beta} &= \sum_{i=1}^{N} x_i(y_i - \frac{\exp(x_i^T\beta)}{1+\exp(x_i^T\beta)}) = \sum_{i=1}^{N} x_i(y_i - p(x_i;\beta)) \\ &= \sum_{i=1}^{N} x_i(y_i - P(Y=1|X=x_i;\beta))\end{aligned} \tag{53}$$

- the term within the parenthesis is the prediction error, namely the difference between the observed y_i and its predicted probability of being equal to 1. This is then multiplied by x_i, which accounts for the magnitude of the model $x_i^T\beta$ in making this prediction

Logistic regression

- Otherwise we could use the Newton's method:
  $\beta^{new} = \beta^{old} - \left(\frac{\partial l^2(\beta^{old})}{\partial \beta \beta^T}\right)^{-1} \frac{\partial l(\beta^{old})}{\partial \beta}$

$$\frac{\partial l^2(\beta)}{\partial \beta \beta^T} = \sum_{i=1}^{N} x_i x_i^T p(x_i;\beta)(1 - p(x_i;\beta)) \tag{54}$$

- in matrix notation

$$\beta^{new} = \beta^{old} + (X^T W X)^{-1} X^T (\mathbf{y} - \mathbf{p}) \tag{55}$$

- where $\mathbf{y}$ denotes the vector of y_i, $\mathbf{p}$ is a vector containing the $p(x_i;\beta^{old})$, X is a matrix with the x_i and W is a diagonal matrix containing the $p(x_i;\beta^{old})(1 - p(x_i;\beta^{old}))$

Logistic regression

- Please note that if $y \in \{-1; +1\}$, the loss is different but the gradient is the same ! We can choose as loss:

$$
\begin{aligned}
L(\beta) &= \prod_{i=1}^{N} p(x_i;\beta)^{\frac{y_i+1}{2}} (1 - p(x_i;\beta))^{\frac{1-y_i}{2}} \\
l(\beta) &= \sum_{i=1}^{N} \frac{y_i+1}{2} \ln(p(x_i;\beta)) + \frac{1-y_i}{2} \ln(1 - p(x_i;\beta)) = \\
&= \sum_{i=1}^{N} - \left(\frac{1-y_i}{2}\right) x_i^T \beta - \ln(1 + \exp(-x_i^T \beta)) \\
\frac{\partial l(\beta)}{\partial \beta} &= \sum_{i=1}^{N} x_i \left(\frac{1+y_i}{2} - p(x_i;\beta)\right)
\end{aligned}
\tag{56}
$$

Logistic regression

- An interesting choice of loss when $y \in \{-1; +1\}$ is $L(\beta) = \prod_{i=1}^{N} \frac{1}{1+\exp(-y_i x_i^T \beta)}$ which means maximizing

$$\begin{cases} p(x_i; \beta) = \frac{1}{1+\exp(-x_i^T \beta)}, & \text{if} \quad y_i = 1 \\ 1 - p(x_i; \beta) = \frac{1}{1+\exp(x_i^T \beta)}, & \text{if} \quad y_i = -1 \end{cases} \tag{57}$$

- This comes from the fact that

$$1 - \frac{1}{1+\exp(-x_i^T \beta)} = \frac{\exp(-x_i^T \beta)}{1+\exp(-x_i^T \beta)} \frac{\exp(x_i^T \beta)}{\exp(x_i^T \beta)} = \frac{1}{1+\exp(x_i^T \beta)} \tag{58}$$

- The gradient is as before $\frac{\partial l(\beta)}{\partial \beta} = \frac{-\partial \ln(1+\exp(-y_i x_i^T \beta))}{\partial \beta} = \frac{y_i x_i \exp(-y_i x_i^T \beta)}{1+\exp(-y_i x_i^T \beta)}$:

$$\begin{cases} x_i \left(\frac{\exp(-x_i^T \beta)}{1+\exp(-x_i^T \beta)} \right) = x_i (1 - p(x_i; \beta)), & \text{if} \quad y_i = 1 \\ -x_i \left(\frac{\exp(x_i^T \beta)}{1+\exp(x_i^T \beta)} \right) = -x_i p(x_i; \beta), & \text{if} \quad y_i = -1 \end{cases} \tag{59}$$

Logistic regression

- Similarly to OLS, we could also add a regularization on the parameters β like $||\beta||_2^2$ (i.e. Ridge, avoid overfitting) or $||\beta||_2$ (i.e. LASSO, variable selection)
- Logistic regression is similar to LDA (decision boundary as log-ratio is a linear function in x) but it makes *less assumptions* since conditional distributions are not assumed to follow a Gaussian distribution $\rightarrow$ if data are not Gaussian logistic regression is more robust to outliers

Summary

K-nearest-neighbour

In the discrete case with a L_2 norm, we select as best f^* the one that minimizes:

$$f^*(x_j) = \arg\min_f E_{Y|X}[L(Y, f(x_j))|X = x_j] = E_{Y|X}[Y|X = x_j] \quad (60)$$

The k-nearest-neighbour method approximates this solution by looking within a neighbourhood of every point x_j. More precisely :

$$f_k^*(x_j) = \text{Ave}(y_i|x_i \in N_k(x_j)) = \frac{1}{k} \sum_{x_i \in N_k(x_j)} y_i \quad (61)$$

where Ave is the average, $N_k(x_j)$ is the neighbourhood of x_j defined by the k closest points x_i in the Training set $\mathcal{T}$. Closeness implies a metric (Euclidean, cosine, etc.) !

K-nearest-neighbour

If $\mathcal{T}$ is large, it seems that we could always approximate $f(x_j)$ with a k-nearest-neighbour method, since we should always be able to find a fairly large neighbourhood of observations close to any x_j and average them.

Even in high dimension ? **Curse of dimensionality** ! If with $d = 1$ we need $N = 100$ points to accurately sample the space, we would need $N = 100^{10}$ points to preserve the same sampling density with $d = 10$!

K-nearest-neighbour - Bias-variance tradeoff

As before, let (x_0, y_0) be a test sample, $y_0 = x_0^T \beta + \epsilon_0$ the true model and $f_k^*(x_0)$ the k-nearest-neighbour estimate. The expected prediction error, that is the mean squared error (MSE) when using a L2-norm, of k-nearest-neighbour estimate at (x_0, y_0) is equal to:

$$\begin{aligned} \text{MSE} &= \mathbf{E}[(y_0 - f_k^*(x_0))^2] \\ &= \underbrace{\sigma^2}_{\text{irreducible error}} + \text{Var}_{\mathcal{T}}(f_k^*(x_0)) + \text{Bias}^2(f_k^*(x_0)) \\ &= \sigma^2 + \frac{\sigma^2}{k} + [f(x_0) - \mathbf{E}_{\mathcal{T}}[f_k^*(x_0)]]^2 \end{aligned} \tag{62}$$

When k increases the variance decreases but the bias is likely to increase $\rightarrow$ k can be chosen using CV !

K-nearest-neighbour

Pros

- Decision boundaries are non-convex in general
- It can be used with any metric
- It is naturally multi-class

Cons

- Curse of dimensionality
- Computational time can be long (need to compute many distances)

References

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