



Notes on  
**Machine Learning Lecture**

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**DISCLAIMER**

These are my notes and associated further reading that regards my understanding of Machine Learning based on the Universiteit Gent 2022 winter lecture. Non-cited statements come from the lecture. I also make notes to myself. If the reader finds something useful, I encourage them to investigate further. Non-cited charts were created by me, and their nonprofit-related usage is allowed with a citation.

The following text is from me to me; to prepare myself for the examination and enhance my knowledge of related topics. The empty spaces are for me to write once I print these notes.

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Before you write:

1. What are the keywords?
2. What are the assumptions of the model or algorithm?
3. What are the main take away?
4. Flow Charts?
5. Advantages and Disadvantages
6. Are they linear or non-linear transformations / models

## 1 First Steps in Supervised Learning

### 1.1 What is Machine Learning?

Machine Learning is the field that generates algorithms that learn from data so they can predict or make decisions based on their learning. One aims to **build a model for data by optimizing the performance criterion using training data**. See Figure 1 for the different fields surrounding machine learning.

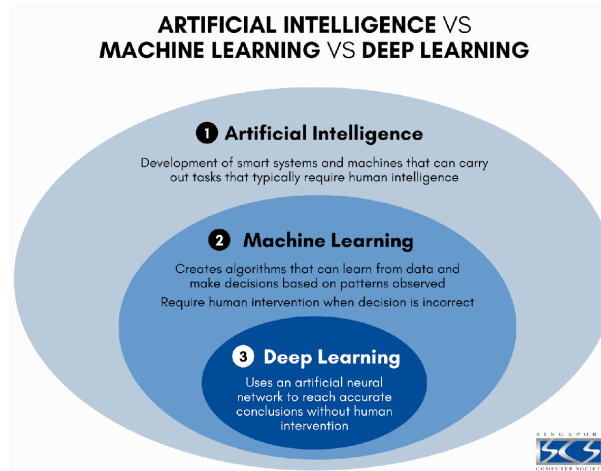


Figure 1: Surrounding fields in Machine Learning. Image from [1].

To understand machine learning algorithms, it is necessary to know about Probability Theory and Statistics. It is also desired to have efficient programming knowledge, so this is an interdisciplinary field.

Learning algorithms are implemented when no rules are available to establish the relationship between the input and the output. It is also possible that the algorithm is required to adapt to different environments.

### 1.2 Types of Machine Learning

There are three main different types of machine learning; these are depicted in Figure 2.

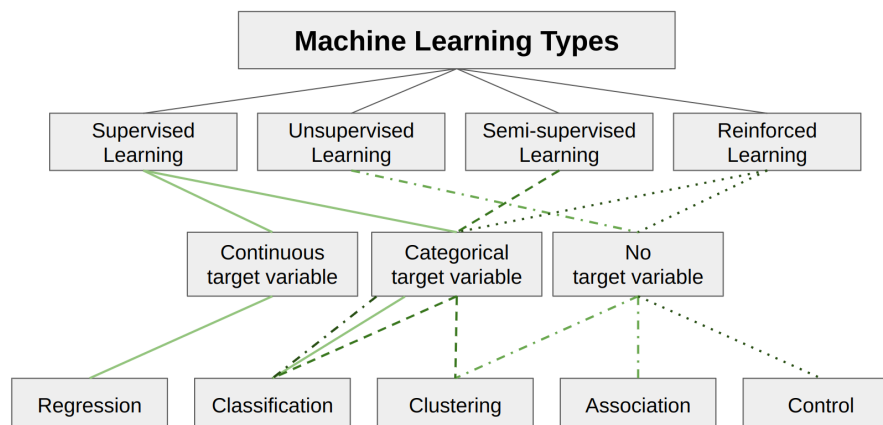


Figure 2: Different types of machine learning. Image inspired from [2].

- **Supervised:** here, the expert gives the algorithm the output data (as labels for classification) so that the input-output relationship can be modeled. The type of tasks covered here are:
  - Regression: when the output is numerical.
  - Classification: when the output is categorical.
- **Unsupervised:** the aim is to learn without an output; this approach allows us to model the structure of the data or the underlying profile of the data; they can become *discriminative* or *generative*<sup>1</sup>; for instance, Gaussian mixture models<sup>2</sup>, random forests, and neural networks are discriminative models. Generative models are often used as pre-processing in deep learning [4].

<sup>1</sup>The algorithm focuses on devising the decision boundary (without underlying assumptions on data) or on modeling the joint distribution of inputs and outputs, respectively.

<sup>2</sup>See more in [3].

- Clustering: hierarchic and nonhierarchic are their sub-branches; more might be investigated. Clustering can be both discriminative and generative.
- Association / Transformation of Features: the aim is to uncover latent variables or compress information. This can either improve or worsen the interpretability of the model, e.g. Principal Component Analysis (PCA); see Figure 3.

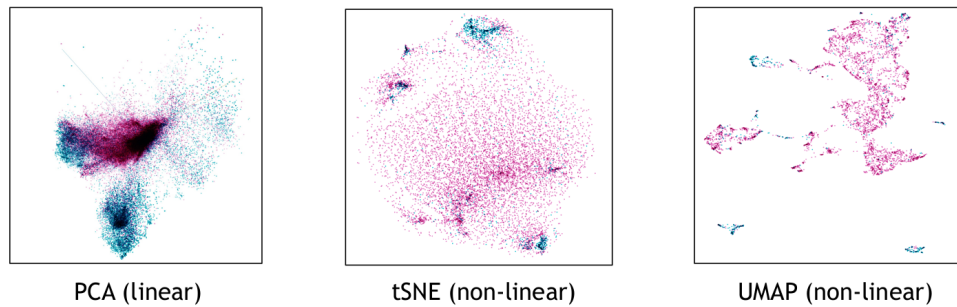


Figure 3: Different types of feature transformation, showing PCA (left), t-Distributed Stochastic Neighbor Embedding (center), and Uniform Manifold Approximation and Projection (right). Image inspired from lecture 1.

- **Semi-supervised Learning:** as the name suggests, this is a mixture of the previous two and is typically implemented when the cost of labeling is high [2].
- **Reinforced Learning:** this method uses gathered information from the interaction with the environment to maximize reward and reduce risks [2]; this can be implemented for real-time decisions.

### 1.3 Supervised Learning

The notation used in the lecture is the following<sup>3</sup>:

- Ground truth:  $\mathbf{y} = f(\mathbf{x}) + \varepsilon$
- Training data:  $\mathbf{X}, \mathbf{Y} : (\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)$
- Hypothesis:  $f(\mathbf{x}) \sim g(\mathbf{x}, \mathbf{X}, \boldsymbol{\theta}) + \varepsilon$ ; best model that can be learned from a certain model family.
- Loss function:  $\mathcal{L}(\boldsymbol{\theta} | \mathbf{X})$
- Learning:  $\hat{\boldsymbol{\theta}} = \operatorname{argmin}_{\boldsymbol{\theta}} (\mathbb{E}[\mathcal{L}(\boldsymbol{\theta} | \mathbf{X})])$ ; minimize expected loss on new data.

Notice that  $f(\mathbf{x})$  is unknown. In general, finding the optimal parameters that will minimize the expected loss function on new data is necessary. Optimal parameters depend on the assumption made on data. Finding non-parametric algorithms in supervised learning for regression and classification is also possible, e.g., K-nearest neighbors (KNN). See Figure 4 for a better comparison.

**! Algs:** KNN (regression and classification), decision trees (regression and classification), linear discriminate (regression and classification), and non-linear feature expansion (regression).

Consider mentioning the training/inference time and memory scale w.r.t. dataset size when describing an algorithm. These issues become relevant once the quality of the data has been addressed.

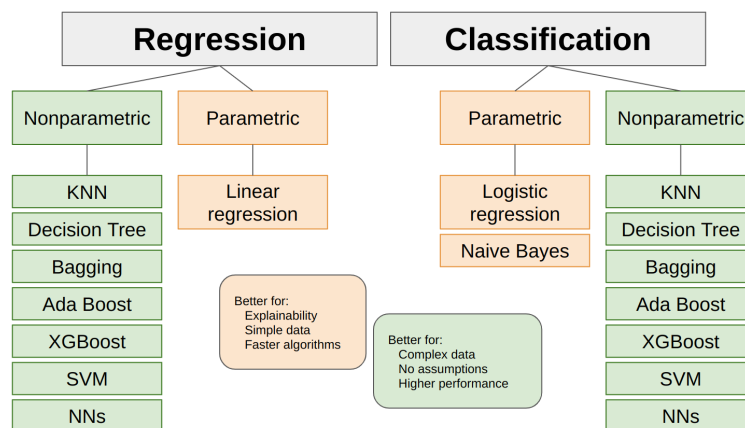


Figure 4: Types of algorithms in supervised learning and some examples. Image inspired from [6].

<sup>3</sup>However, the nomenclature is not always maintained; therefore, you might find the notation following in [5]. To avoid confusion, it is explained in the text what variables mean.

## 1.4 Evaluating Models and Conditions for Generalization

Machine learning aims to achieve **generalization**; the algorithm should perform well when new data is introduced. To understand how this is feasible, important concepts will be introduced.

- **Loss function**: this is among the most important metric in machine learning. This function allows the user to tell how good a model's prediction is, based on the *the loss*. This transforms the learning into an optimization problem by defining a loss function and optimizing it to its minimum. More on this shall be explored [7]. **!** Different loss functions, different predictions.
- **Empirical Risk Minimization (ERM)**: the understanding of ERM permits us to understand the limits of an algorithm, which also allows the development of practical skills in machine learning [8]. The concept of empirical risk arises from the fact that the user cannot access the *true error* since the algorithm only receives a sample of an unknown distribution from the data. However, estimating the *training error* – the error the algorithm incurs over the training sample [9] is possible. In short, ERM is the search for a predictor (or model) that minimizes the training error; this can be depicted in the following expression

$$\hat{\theta} = \underset{\theta}{\operatorname{argmin}} \left( \frac{1}{N} \sum_{j=1}^N \mathcal{L}(x_j | \theta, \mathbf{X}) \right). \quad (1)$$

Remember that the model represents your **hypothesis**. ERM: the search for the best model that minimizes training error.

- **Test Error**: because the ERM does not tell the user how well the algorithm is capable to predict on new data, what is typically done is to split the available data such that, once the algorithm has been trained (found  $\hat{\theta}$ ), the algorithm can be assessed on the performance on the *test data*. **!** WARNING: depending on how you split the data, how likely you are introducing *leakage* in your model.
- **redo IID Assumption**: Identically and Independent Assumption:
  - Indetically: training, validation, test, and new incoming data are drawn from the same underlying joint distribution. In other words, all datasets must have the same statistical properties: mean, standard deviation, and other characteristics [10].

Violating this assumption creates

- \* prediction bias; predictions are not characteristic of the real world due to lack of representative groups, e.g., training facial recognition on engineering students: population not very diverse, very few women, no children, no elderly people. This can also result from lack of balanced classes.

Feature and label bias can be considered a violation of the “identically distributed” part of the i.i.d. assumption.

- Independent: no subgroups of samples correlated in any type of data subset (training, validation, and test); in other words, any data point should not provide information on the occurrence or value of another data point [10]. Usually, The correlation is attributed to **latent variables**, a.k.a. unknown or unobserved variables.

Violating this assumption creates

- \* bias;

Violation of any assumption leads to poorer generalization, and they can be interconnected. **!!!** I think what is important in this discussion is identifying the source of a violation rather than the independent consequence because the violation of each might result in a similar consequence. FOCUS ON THE SOURCE RATHER THAN THE CONSEQUENCE.

—

For instance, the characteristic clusters in **STDB5** for the spherical and non-spherical tokamaks violate the identical assumption. This might not necessarily mean that spherical tokamaks must have their own scaling law (?). In reality, there is no continuum in aspect ratio to effectively assess whether they are *identical* machines. This implies too much money to discover.

## 1.5 Model Selection: hyperparameter analysis

When one changes the hyperparameters of an algorithm, it can be considered a different model than before; for instance, the number of features one uses is a hyperparameter. How can one tell which model is better compared to another? It is recommended to follow the diagram shown in Figure 5, left.

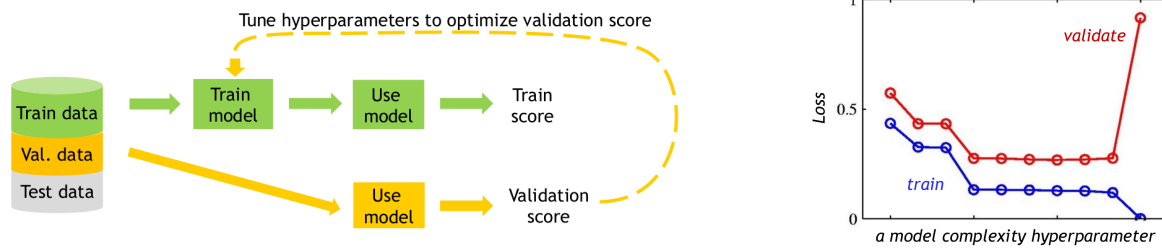


Figure 5: Left: data split for model assessment, all data subsets are assumed to follow IID assumption. Right: validation curve; if the IID assumption is not fulfilled, the curves will not look similar; this is why it is recommended to look at this plot at the beginning. Sometimes, the validation curve is plotted with accuracy or another metric, like  $F_1$ -score. Images from lecture 1.

When you tune the model's hyperparameters, you also change the model complexity; the validation curve is assessed from this analysis. The validation curve plots a model performance metric vs. the algorithm's complexity [11]. The typical behavior is that the validation error goes down as the complexity increases, but the error goes up again at some point; see Figure 5, right. **More on this will be explained when the bias-variance decomposition in a model is studied.** Once the ideal model has been found, the train and validation datasets are merged to obtain the overall train and test errors without further modification. This is depicted in Figure 6

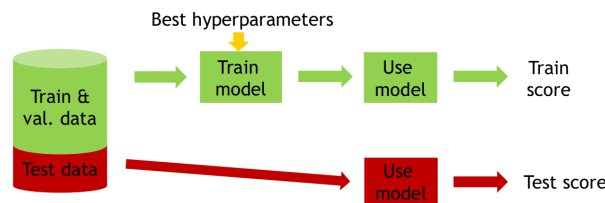


Figure 6: Data split for model assessment, final stage. Image from lecture 1.

If the validation and training data are too small, the model will likely have a poor choice of hyperparameters and might overfit. Again, beware of how you split the data, as you might introduce a source of leakage.

Another discussion brought on the analysis of model complexity is the choosing of features. In general, it is not ideal to have too many features due to what is known as *the curse of dimensionality*. The reasoning is that a higher number of features implies a more complex model, and the more complex the model, the more data it requires to perform well. For instance, consider the case of fitting data with a polynomial of degree  $d$  with  $F$  total number of features. The complexity of the said model is  $\mathcal{O}(F^d)$ ; from this, it is possible to observe that the selection of features becomes a serious matter for optimal performance, directly affecting its generalization capability.

Here are some forms of **regularization** for optimal model selection:

- Spend time searching for the optimal subset of features to avoid the "curse of dimensionality".
- If possible, reduce the number of hyperparameters (this is a matter in neural networks).
- Constrain parameter space: the idea is that you assess for a region in parameter space where you know solutions will lead to an optimal generalization, e.g.  $L_1$  and  $L_2$  regularization, more on this in the incoming chapter.
- When working with optimization algorithms, such as gradient descent, avoid over-tuning in training data (e.g. early stopping).

## 1.6 Summary

**Key words:** empirical risk minimization (ERM), validation curves, curse of dimensionality.



## 2 Supervised Parametric Linear Models and Introduction to SVM

Three central concepts must be understood when discussing parametric models: loss function, regularization, and optimization [5]. To understand these concepts, let us have a look at the equation that *models* the true input-output relationship

$$y = f(\mathbf{x}) + \varepsilon. \quad (2)$$

Depending on the assumptions, is the algorithm; for instance, if  $f(\mathbf{x}) = \boldsymbol{\theta}^T \mathbf{x}$  is linear, and the noise is Gaussian  $\varepsilon \sim \mathcal{N}(0, \sigma^2)$ , you retrieve ordinary least squares [5]. Derive the previous statement:

Of course,  $f(\mathbf{x})$  can be non-linear, and other assumptions can be imposed over the irreducible noise, depending on the problem; for instance, the assumption of  $\varepsilon \sim$  Laplace distribution, one obtains the *absolute error loss* [5]. However, if one keeps the assumption of Gaussian noise, one will obtain a Gaussian joint likelihood [5], which eases the interpretation and working of the model's predictions.

The main objective of the learning algorithm is to learn enough from the training data to properly predict or make decisions on unseen data; this is known as *generalization*. A model may also learn the noise from the training data rather than the underlying properties of it; this is known as *overfitting*. The loss function is implemented to prevent overfitting so that the model does not mimic the training data.

### 2.1 Loss Functions

Recall that, the learning of an algorithm means that one is dealing with an optimization algorithm [5] of the parameters  $\boldsymbol{\theta}$ . As previously mentioned, the optimization problem is formulated as follows

$$\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}}{\operatorname{argmin}} \left( \frac{1}{N} \sum_{i=1}^N \mathcal{L}(y_i, f_{\boldsymbol{\theta}}(\mathbf{x}_i)) \right), \quad (3)$$

here, one observes

- the **loss function**  $\mathcal{L}(y_i, f_{\boldsymbol{\theta}}(\mathbf{x}_i))$ , and
- the **cost function**  $J(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^N \mathcal{L}(y_i, f_{\boldsymbol{\theta}}(\mathbf{x}_i))$ .

It is possible that a solution to the optimization problem is not exactly and is not directly computable; this is particularly common in non-linear functions, e.g. no closed-form solution exists for logistic regression. Therefore, a solution might be found through numerical optimization [5]. However, the ultimate goal is not solving Eq. (3), but rather

$$\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}}{\operatorname{argmin}} (E_{\text{new}}(\boldsymbol{\theta})), \quad (4)$$

with  $E_{\text{new}}(\boldsymbol{\theta}) = \mathbb{E}_* [E(\hat{y}, y_*)]$ , being the expected error on predictions w.r.t. unseen data. Nevertheless, one does not have access to this information; for this reason that **the loss minimization is the representative for generalization** [5]. Therefore, it is of crucial importance that the machine learning practitioner understands that the training objective, Eq. (3), is just a proxy for the actual objective, Eq. (4). The authors in [5] stress on the following observations

- optimization accuracy  $\neq$  statistical accuracy,
- loss function  $\neq$  error function, and
- explicit vs implicit regularization (explain *asymptotic minimizer* and *strictly proper*<sup>4</sup> functions).

<sup>4</sup>Hint: the downside of Hinge loss; remedy: squared Hinge loss. Do not forget to see p.105 in [5].

It is important to understand that selecting the loss and error functions comes as part of the model's design. There is no right nor wrong selection, but rather, what represents best your data. For instance, one has

- linear regression: linear in the parameter model and  $\mathcal{L}$  being the squared error loss; and,
- support vector classification: linear in the parameter model and  $\mathcal{L}$  being the Hinge loss [5].

IMPORTANT: a loss function is said to be robust if the training data containing a considerable amount of outliers only has a minor impact on the learned model [5].

### 2.1.1 Regression

As already discussed, some loss functions come naturally from the assumptions made on the data, such as the *squared error loss*

$$\mathcal{L}(y, \hat{y}) = (\hat{y} - y)^2, \quad (5)$$

coming from a Gaussian noise in Eq. (2); and, the *absolute error loss*

$$\mathcal{L}(y, \hat{y}) = |\hat{y} - y|, \quad (6)$$

if the noise in Eq. (2) is  $\varepsilon \sim L(0, b_\varepsilon)$  Laplacian [5]. However, not all loss functions come from an instinctive derivation from data assumption; some are designed to achieve a superior generalization. For instance, the *Huber loss*

$$\mathcal{L}(y, \hat{y}) = \begin{cases} \frac{1}{2}(\hat{y} - y)^2 & \text{if } |\hat{y} - y| < 1 \\ |\hat{y} - y| - \frac{1}{2} & \text{else.} \end{cases} \quad (7)$$

This is a combination of the previous two; this is because the absolute error is more robust to outliers than the squared error [5]. Another variation to this idea is depicted with the  $\epsilon$ -insensitive loss

$$\mathcal{L}(y, \hat{y}) = \begin{cases} 0 & \text{if } |\hat{y} - y| < \epsilon \\ |\hat{y} - y| - \epsilon & \text{else,} \end{cases} \quad (8)$$

where  $\epsilon$  is left to be chosen for the design, notice that the  $\epsilon$ -insensitive loss leaves a tolerance width  $2\epsilon$  around the observed  $y$  and, outside the region, behaves like the absolute error loss [5]. This loss function proves particularly useful for support vector regression [5]. See Figure 7 to compare the robustness of the functions mentioned in this section.

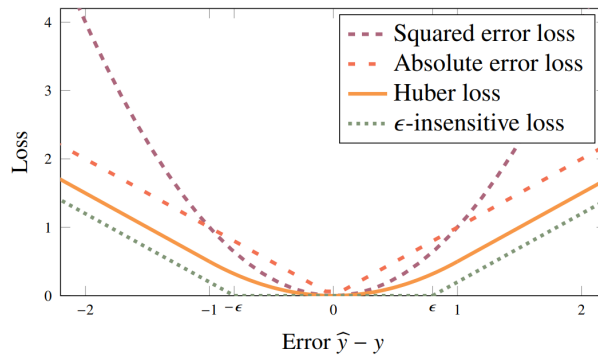


Figure 7: Different loss functions for regression given a specific error function. Image from [5].

### 2.1.2 Classification

An instinctive loss function for binary classification could have similar behaviour to the Heaviside function; there is one known as the *misclassification loss* written as

$$\mathcal{L}(y, \hat{y}) = \begin{cases} 0 & \text{if } \hat{y} = y \\ 1 & \text{else.} \end{cases} \quad (9)$$

Despite that one might have the goal of suppressing the misclassification rate the most, this is not the commonly chosen loss function for three main reasons (explain). The usage of the *cross-entropy loss*

$$\mathcal{L}(y, g(\mathbf{x})) = \begin{cases} \ln(g(\mathbf{x})) & \text{if } y = 1 \\ \ln(1 - g(\mathbf{x})) & \text{if } y = -1 \end{cases} \quad (10)$$

is more used. Here,  $g(\mathbf{x})$  is the probability that the observation  $\mathbf{x}$  belongs to a class; this allows a complete statistical description of the output-input conditional distribution [5]. To understand other families of loss functions, it is essential to comprehend the concept of **margins**. In general, it is defined that **the margin of a classifier for a data point  $(\mathbf{x}, y)$  is  $y \cdot f(\mathbf{x})$** ; so that if the margin has the same sign, the classification is considered correct, otherwise incorrect [5]. This construction helps when the classifier does not have a probabilistic interpretation. Still, rather it is just being represented with an underlying function  $f(\mathbf{x})$ ; it can be seen as a measure of certainty in a prediction [5] (!!! think: similarity between error in regression loss functions and margin in classification loss functions). From the construction of the margin, it is possible to assign a small loss to a positive (correct classification) margin and a considerable loss to a negative margin. Figure 8 shows diverse loss functions for classification with different robustness to outliers.

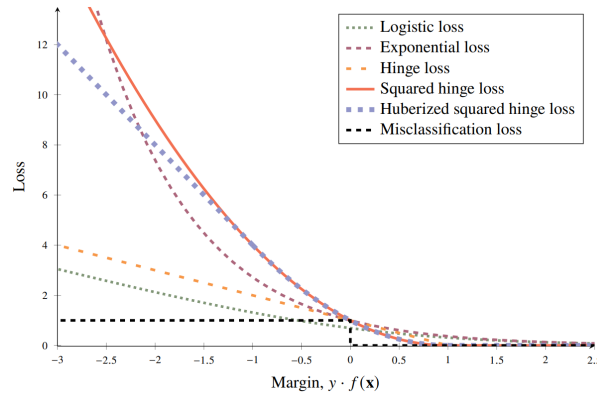


Figure 8: Different loss functions for classification given the margin. Image from [5].

Write the expressions for the different loss functions shown in the image with their respective properties and algorithms usage. Explain losses for multiclass classification.

## 2.2 Learning parameters for Specific Cases

Explain the solution and main characteristics when minimizing the loss functions for regression and classification using MSE (or SSE) and log-loss, respectively. Explain gradient descent and compare with coordinate descent.

### 2.2.1 DEMO: Gradient descent for linear regression notebook

Make your notes.

## 2.3 Overfitting and Explicit Regularization

As mentioned, generalization is when an algorithm performs well on unseen data. Overfitting happens when proper generalization is not achieved, and the algorithm only performs well on the training dataset; there are many causes of overfitting, one being a model being too complex (e.g. number of features being used).

The goal of regularization in parametric models is that: "if a model with small values of the parameter  $\hat{\theta}$  fits the data almost as well as a model with larger parameter values, the one with small parameter values should be preferred." [5]

Regularization is the act of preventing overfitting. For implicit regularization, one can modify the expression of the loss function; for instance, **Ridge regression** or  **$L^2$  regularization** is the addition of a function that penalizes high weights in polynomial regression (because high values of weights mean high complexity algorithm). The resultant expression is the following

$$\mathcal{L}(y, \hat{y}) = \frac{1}{2}(\hat{y} - y)^2 + \lambda \cdot \|\mathbf{w}\|_2^2. \quad (11)$$

With  $\lambda \geq 0$ , one always has a unique solution to regression – the best value is obtained through cross-validation.  $\lambda = 0$  gives OLS solution. Notice that the modified equation presents a trade-off between having the perfect fit and enforcing the regressor parameters to being close to zero; the greater  $\lambda$ , the closer to zero the  $\hat{\theta}$  values. Given the loss function with Ridge regression, one obtains [5]

$$\hat{\theta} = \left( \mathbf{X}^T \mathbf{X} + n\lambda \mathbf{I}_{p+1} \right)^{-1} \mathbf{X}^T \mathbf{y}, \quad (12)$$

with  $n$  denoting the number of observations in the dataset. Another type of regularization is known as **LASSO** or  **$L^1$  regularization**, and it is of the following form

$$\mathcal{L}(y, \hat{y}) = \frac{1}{2}(\hat{y} - y)^2 + \lambda \cdot \|\mathbf{w}\|_1, \quad (13)$$

where  $\|\mathbf{w}\|_1$  is the 1-norm  $\|\mathbf{w}\|_1 = |w_1| + |w_2| \dots + |w_p|$  [5]. It is worth noting that there is no closed-form solution to this loss function; numerical optimization algorithms must be used to solve the LASSO regression. The effect of this type of regularization is that it can *switch-off* some coefficients (by setting specific weights to zero) and provide sparse solutions; it is for this reason that, sometimes, this is a method of feature selection [5].

Following images from the book [5].

### General Explicit Regularisation

$L^1$  and  $L^2$  regularisation are two common examples of what we refer to as explicit regularisation since they are both formulated as modifications of the cost function. They suggest a general pattern on which explicit regularisation can be formulated:

$$\hat{\theta} = \arg \min_{\theta} \underbrace{J(\theta; \mathbf{X}, \mathbf{y})}_{(i)} + \underbrace{\lambda}_{(iii)} \underbrace{R(\theta)}_{(ii)}. \quad (5.26)$$

This expression contains three important elements:

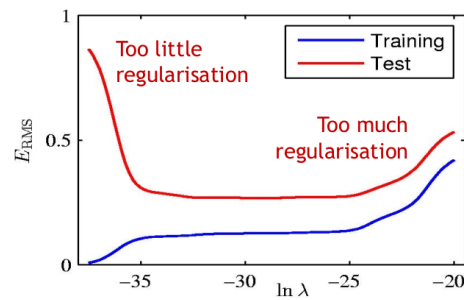
- (i) the cost function, which encourages a good fit to the training data;
- (ii) the regularisation term, which encourages small parameter values; and
- (iii) the regularisation parameter  $\lambda$ , which determines the trade-off between (i) and (ii).

<b>Method</b>	<b>What is optimisation used for?</b>			<b>What type of optimisation?</b>			
	<i>Training</i>	<i>Hyper-parameters</i>	<i>Nothing</i>	<i>Closed-form*</i>	<i>Grid search</i>	<i>Gradient-based</i>	<i>Stochastic gradient descent</i>
<i>k-NN</i>							
<i>Trees</i>							
<i>Linear regression</i>							
<i>Linear regression with <math>L^2</math>-regularisation</i>							
<i>Linear regression with <math>L^1</math>-regularisation</i>							
<i>Logistic regression</i>							
<i>Deep learning</i>							
<i>Random forests</i>							
<i>AdaBoost</i>							
<i>Gradient boosting</i>							
<i>Gaussian processes</i>							
*including coordinate descent							

Generalisation: perform well on unseen data!

Train model on training data

More complex model:  
training error decreases



Evaluate model on separate test data:  
at some point **test error goes up again**.

⇒ *Overfitting to the training data!*

⇒ *Select best degree based on unseen data!*

### 2.3.1 DEMO: Linear regression regularization notebook

Make your notes.

|

## 2.4 Classification: Linear Support Vector Machine

## 2.5 Classification: Soft Margin Support Vector Machine

## 2.6 Summary

**Keywords:** asymptotic minimizer, strictly proper, margins, optimization, open- and closed-form solutions.

# 3 Reasoning About Models and Data

## 3.1 Error Functions for Model Selection

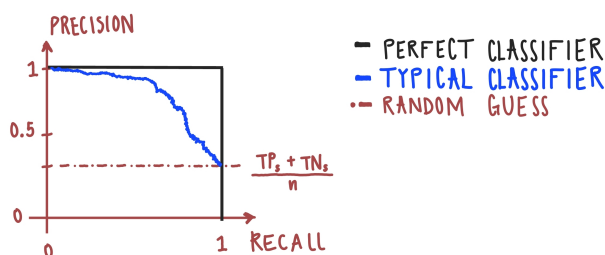
Describe the confusion matrix and why it is needed.

|

For the following, add comments based on slides.

Table 1: Some of the obtainable metrics from a confusion matrix [5], [12]. Remember that  $n$  is a dataset's total number of observations.

Metric	Formula	Description
Misclassification Rate	$\frac{FNs + FPs}{n}$	Fraction of predictions being incorrect
Accuracy	$\frac{TNs + TP_s}{n}$	Complement of misclassification rate
Precision	$\frac{TP_s}{TP_s + FPs}$	Fraction of predicted positives actually being positive
Recall	$\frac{TP_s}{TP_s + FNs}$	Fraction of actual positives correctly predicted
Fall-out	$\frac{FPs}{FPs + TNs}$	Probability of false alarm
Specificity	$\frac{TP_s}{FPs + TNs}$	Compliment of fall-out
False discovery rate	$\frac{FPs}{FPs + TP_s}$	Fraction of incorrect positive predictions
False negative rate	$\frac{FNs}{FNs + TP_s}$	Fraction of actual positive incorrectly classified
False omission rate	$\frac{FNs}{FNs + FPs}$	Fraction of incorrect negative relative to tall incorrect classifications
Prevalence	$\frac{FNs + TP_s}{n}$	Proportion of actual positive instances in the dataset
F <sub>1</sub> -score	$\frac{2 \cdot precision \cdot recall}{precision + recall}$	Harmonic mean of precision and recall
F <sub><math>\beta</math></sub> -score	$\frac{(1 + \beta^2) \cdot precision \cdot recall}{\beta^2 (precision + recall)}$	Used to account that recall is $\beta$ -times as important as precision



Explain RoC curve.

Explain hypothesis testing and its importance.

### 3.2 Bias and Variance

For this discussion, the **IID assumption is conserved**. This discussion centers on *What happens if you train a model multiple times on different IID data sets of the same size?* The answer is that one gets **different models**, with the difference being more notorious if the complexity of the model is high; however, the difference decreases if the amount of data increases in each case. This is depicted in Figure 9

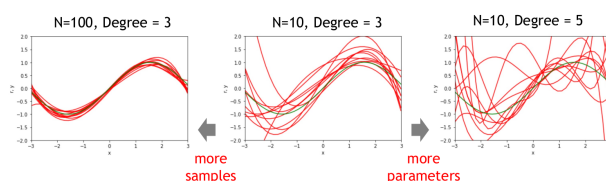


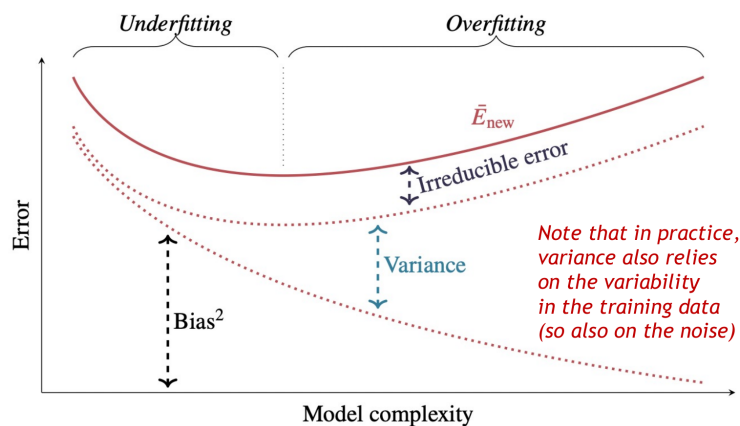
Figure 9: Image from lecture 3.

Explain what bias and variance are **in statistics**.

An **estimator** or a model  $g()$  is an instance of a model family being fed with a fixed number of observations in the dataset.

Derive an estimator's bias and variance decomposition (see the summary slide of bias and variance).

Explain the theoretical plot of generalization error [5]:



The trade-off between model complexity and dataset size opens the discussion on

- **MODEL BIAS:** this theoretical concept cannot be measured because the user cannot access the underlying data distribution. This characterizes being
  - **the expectation** across various models trained with different data subsets of the expected model error on unseen data, compared to the ground truth.
  - **the capability** of the chosen estimator to approximate the ground truth.

High bias implies that the model is too simple to extract suitable information from the features; this is also referred to as **underfitting**. The result of high bias can be a high observation of error; however, this could also be from a large amount of irreducible error (see plot above), meaning that features do not carry the necessary information for estimation.

- **MODEL VARIANCE:** this theoretical concept cannot be measured because the user cannot access the underlying data distribution. This characterizes being
  - **the variance** across various models trained with different data subsets of the expected model error on unseen data, compared to the ground truth.
  - **the sensitivity** of the chosen estimator to variability in training data.

When high variance is observed, this is because the model is **overfitting** the training data, so it is suggested to either obtain more data or make the model less complex.

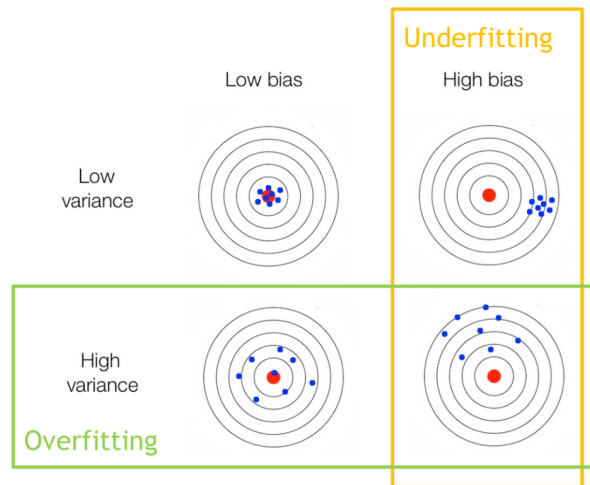


Figure 10: In the bull's eye plots, each blue dot represents the average error on unseen data of a model trained on a different dataset; the red mark represents the perfect model. Without better data, model generalization error trades-off between high variance and low bias and vice versa. Image from lecture 3.

Bias and variance trade-off if you keep the amount of data and the model type fixed but tune the model complexity.

A model can be complex enough to overfit the training data but still be unable to capture the ground truth due to a large irreducible error; hence, **it is possible to have both in a model**.

Figure 11 considers how the generalization error and variance change as the dataset size increases for a theoretical example with known ground truth and noise-free error.

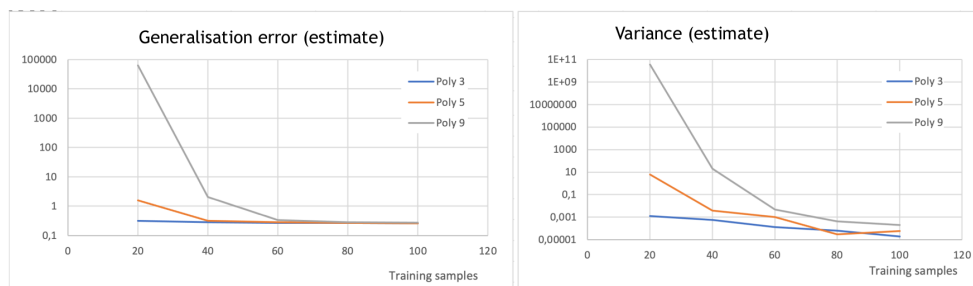


Figure 11: Variation on training dataset size and generalization error with variance with known ground truth and controlled noise; thus, this is an ideal case. Image from lecture 3.

From this, it is possible to observe that, for greater datasets, the generalization error decreases and converges to the irreducible error while the variance converges to zero. It is important to understand that **convergence is slower for more complex models or complex noise**.

#### LEARNING CURVES: when ground-truth is not available – sampling impact from training dataset

In practice, bias and variance cannot be estimated since one cannot access the underlying data distribution. For this, it is possible to obtain the learning curves that yield information on whether the model has high variance and/or bias by sampling the impact of training dataset size from the total training set. Figure 12 shows the learning curves for two situations.

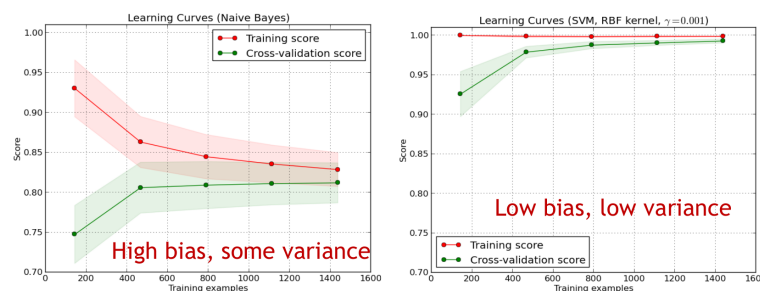


Figure 12: Learning curves with accuracy score; finding learning curves with the loss instead of the score is also possible. On the left-hand side (low  $N$ , both plots): insufficient data, severe overfitting, training performance close to perfect, validation performance very bad. On the right-hand side (high  $N$ , both plots): hopefully enough data and less overfitting. Limit to infinity: training and validation curves converge to the same value. Image from lecture 3.



Here are a couple of observations:

- If training and validation sets are identically distributed, **and** validation set is large enough: scores should converge to the same value.
- Extrapolation towards *converged value* estimates the best possible generalization error, i.e. model bias + irreducible error.
- More complex models should give lower errors: lower model bias, same irreducible; if not: irreducible error dominates (or other data problem).
- Variability of scores does NOT reflect variance.

### Learning vs (Cross)-Validation Curves

- Learning:
  - Plot shows the average training loss/score in the y-axis.
  - Number of samples per training in the x-axis.
- Cross-Validation:
  - Plot shows the average validation loss/score in the y-axis.
  - Serves as an estimate for loss on unseen data.
  - Hyperparameter variation in the x-axis (e.g., regularisation parameter  $\lambda$ , number of features, polynomial degree, training time (#batches) in gradient descent, number of neurons in a neural network, etc.)

### 3.3 Risks of Data Splitting and IID Assumption Fulfillment

There are some issues when one performs data splitting for model development; for instance, if the training set is too small, there is a risk of overfitting. If the validation set is too small, poor hyperparameter choice is possible. If the test set is too small, the test score might not represent its generalization capacity well. Nevertheless, these are not the only risks of data splitting; one must ensure that the IID assumption is fulfilled as best as possible.

As mentioned, **non-independent data can lead to leakage** of information from validation or test sets into training, resulting in optimistic scores but disappointing performance in the real world. Here are some of the causes:

- Validation and/or test data not sampled independently from train data (the split was not independent). Think of an example!
- Some model or preprocessing parameters are tuned on validation and/or test data. Example: normalizing data based on all data's average and standard deviation (instead of just training data).
- Not enough data to average on latent variables and give identically distributed sets to the three splits.

**Example:** suppose you have 440 data points from 8 different hospitals; for splitting this dataset, in practice, one has two options

- one randomly shuffles all data, then splits into 3 sets.
  - Positive aspect: three datasets come from the same distribution; hence, one IID was fulfilled w.r.t. local dataset.
  - Negative aspects: they are not identically w.r.t. the underlying distribution or ground truth; hence, there is a risk of overfitting on these eight hospitals. Furthermore, there is a risk of leakage: records from a single patient could end in training and test sets.
- one randomly selects hospitals to create the three datasets (e.g. 3 for the train, 2 for the validation, and 3 for the test) – this is a **grouped split**.
  - Positive aspect: there is no risk of leakage as **they are independent datasets** (one IID fulfilled w.r.t. underlying distribution).
  - Negative aspect: sets not identically distributed w.r.t. local dataset and underlying distribution.

Mention the other splitting forms and when they are used for specific cases.

### 3.4 Robust Validation Strategies

When dealing with too little data, it is possible to make use of cross-validation, which consists in averaging across results for multiple train-validate splits given a single dataset. The idea is that one trains the model multiple times (with different train/validation split each time) to then average the validation score across the training runs for model selection. Here are some of the benefits:

- more robust estimate of the error on unseen data,
- allows reducing the size of the validation set (more data for training),
- allows a more in-depth analysis of distribution issues, and
- shows variability across validation errors that combine different training sets (variance) and different validation sets.

Here are some of the types of cross-validation:

- **k-fold cross-validation:** split training data into k folds (typically 5 to 10) considering the IID assumption.

- Train k times, each time using different fold as validation fold
- Use average of k validation scores to estimate out-of-sample performance
- Use this estimate to select best hyperparameters (factors)

train	train	train	train	val
train	train	train	val	train
train	train	val	train	train
train	val	train	train	train
val	train	train	train	train

**After final parameter selection: use all train & validation data to train final model – final evaluation on the test set (stage 2 – refit option = True)!**

- **Grouped kCV:** assures independence (one of IID) by splitting per group. The number of folds is upper-bounded by the number of groups in the dataset.
- **Stratified kCV:** assures identically distributed (one of IID) by splitting with the assurance of the same amounts of classes in all splits. The number of folds upper-bounded by the number of samples in the smallest class.
- **Stratified-Grouped kCV:** assures both identically distributed and independence (two of IID) by assuring the previous two characteristics.
- Explain multiple random splits and bootstrapping.

The same loss function (for training) and error function (for hyperparameter tuning) should be used in all cases. Here are some characteristics according to the number of folds:

- **Fewer folds:** less averaging (more sensitive to the variability of the training set), BUT each fold is more representative because there is more data. This is okay if the given dataset is large. Also, this implies less training time.
- **More folds:** more robust for small datasets and optimally use data for training; however, it takes more time for training.
  - EXTREME CASE: leave-one-out: only one data point is left for validation, and everything else is used for training. **Use LOOCV for small datasets or when estimated model performance is critical!**

### 3.5 Analysis of Model Performance

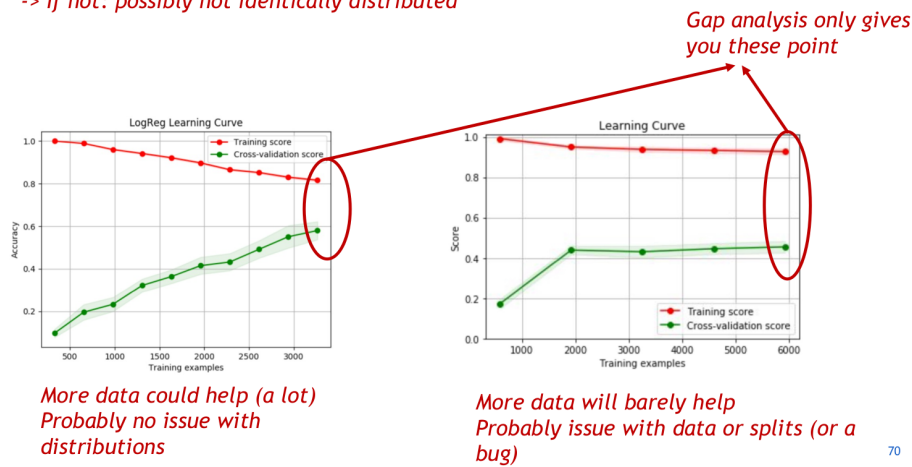
When reporting the model scores (train, validation, and test), it is natural to observe two types of gaps: train-validation and validation-test; how large these gaps are will tell the user the possible problems within the model and suggest possible actions to mitigate them. If

- **train-validation gap is too large:** this may be an overfitting issue; here, it is recommended to plot the validation curves and check whether the hyperparameter tuning was correctly done. It is also possible that there are too many features, and feature engineering might be required. Finally, one can also try a simpler model. **If overfitting**

**is not the issue**, it is possible that the corresponding datasets are not identically distributed; for this, plotting learning curves and fold analysis is recommended. If possible, try to increment the size of the validation dataset. The following image shows how to determine whether this is an overfitting or IID issue.

-> If more data would help: probably just overfitting

-> If not: possibly not identically distributed



70

Explain what exactly fold analysis means.

- **validation-test gap is too large:** leakage may be the main cause of this gap; for this, it is recommended to enhance the splitting of the datasets to ensure independence. If splitting is not the source of leakage, then it is possible that it comes from incorrect preprocessing: everything computed from data **MUST** be refitted for each fold. It is possible that overfitting in the validation set is the cause due to extreme hyperparameter tuning; for this, the tuning of fewer hyperparameters could help. If possible, adding more data to the validation set is recommended. A violation of the identically distributed can also be the cause; maybe test data was collected separately.
- In both scenarios, falling back on domain knowledge and thinking is recommended.

Gaps indicate unreliable estimation of the algorithm's performance on unseen data; if they remain, it is recommended to attempt a simpler model: higher bias and lower variance can avoid 'unpleasant surprises' in the real world. It is also possible to implement **error analysis**, which requires the implementation of diverse confusion matrices to gain a complete overview of what could be wrong. Mention and explain the three different confusion matrices.

Explain which other types of examinations could be implemented on the given dataset.

### 3.6 Augmentation

Explain augmentation: why is it needed? How does it differentiate from data cleaning? advantages and disadvantages. How does/can each affect your model? What happens if you do too much or too little of either?

### 3.7 Summary

Chapter 11: gaps, learning curves, error analysis, model debugging, and augmentation.

**Keywords:** estimator, model bias and model variance, learning curves, leakage, grouped split, validation strategy,

## 4 Clustering – K-Means and Clustering Mixture Models

### 4.1 Latent Variables

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### 4.2 K-Means Clustering

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### 4.3 Mixture Distributions: Mixture of Gaussians

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### 4.4 Expectation-Maximization (EM) Algorithm

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## 4.5 Summary

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## 5 The Data Pipeline (DP) and Ramp-Up Towards Non-Linear Models

### 5.1 DP Cleaning

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### 5.2 DP Feature Extraction / Expansion

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### 5.3 DP Transformations and Embeddings

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### 5.4 DP Dimensionality Reduction

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### 5.5 Introduction to Kernels

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## 5.6 Summary

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## 6 Directed and Undirected Graphical Models

### 6.1 Directed Graphical Models: Bayesian Networks

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### 6.2 Undirected Graphical Models: Markov Random Fields

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### 6.3 Inference in Graphical Models

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### 6.4 Summary

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## 7 Bayesian Estimation

### 7.1 Regression

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#### 7.1.1 Polynomial Fitting

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#### 7.1.2 General Least-Squares

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#### 7.1.3 Overfitting Problem

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#### 7.1.4 Ridge Regression

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### 7.2 Probability Concepts

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### 7.3 A Probabilistic View on Regression

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#### 7.3.1 Least-Squares Estimation as Maximum Likelihood

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#### 7.3.2 Maximum-A-Priori (MAP) Estimation

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#### 7.3.3 Bayesian Curve Fitting

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### 7.4 Summary

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## 8 Hidden Markov Models and Gaussian Processes

### 8.1 Introduction

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## 8.2 Models for Sequential Data

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## 8.3 Hidden Markov Models

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## 8.4 Extensions

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## 8.5 Introduction to Gaussian Processes

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## 8.6 Regression

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### 8.6.1 Covariance Function

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### 8.6.2 Prediction

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### 8.6.3 Implementation

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### 8.6.4 Hyperparameters

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### 8.6.5 Sequential Sampling

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## 8.7 Optimization

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## 8.8 Classification

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## 8.9 Summary

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## 9 Combining Multiple Learners – Ensembles

### 9.1 Introduction

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### 9.2 Bagging, Boosting, and AdaBoost

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### 9.3 Loss Function and Viola-Jones Face Detector

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### 9.4 Decision Trees: CART Framework

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### 9.5 Random Forests

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## 9.6 Summary

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## 10 Neural Networks and Feature Learning

### 10.1 Introduction

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### 10.2 Multi-Layer Perceptrons (MLP)

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#### 10.2.1 Back Propagation

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### 10.3 Convolutional Neural Networks (CNN)

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### 10.4 Overfitting and Regularisation

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## 10.5 Auto-encoders and Embeddings

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## 10.6 Deep Learning Extensions

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## 10.7 Recurrent Neural Networks

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## 10.8 Summary

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# 11 Ethical Aspects in Machine Learning

## 11.1 Examples of Powerful Algorithms and Ethical Concerns

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## 11.2 Overconfidence and Unreliability of Models

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## 11.3 Model Explainability

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## 11.4 FAIRNESS: Criteria, Mitigation & “Fairness by Awareness”

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## 11.5 Summary

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