Machine learning foundations

Mitko Veta

Eindhoven University of Technology
Department of Biomedical Engineering

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Learning goals

At the end of this lecture you will:

- Have an understanding of the goal of machine learning (ML) models.
- *Have a good understanding of basic mathematical concepts used in ML and be able to apply them in the design and implementation of ML methods.
- Have a good understanding of the basic principles of machine learning (ML) and be able to apply them in the analysis of ML methods.
- Be able to design good experimental setups for developing ML models.
- *Have a good understanding of the different evaluation measures for ML models.

* Covered in video lectures

Overview

Topics covered in this lecture:

1. Gradient of a function
2. Two simple machine learning models
   Linear model
   Nearest-neighbours model
3. Model capacity, underfitting and overfitting
4. Model selection
5. Bias and variance trade-off

Prelude: Gradient of a function

Materials:

- Chapters I.4 and I.5 from Goodfellow et al., *Deep Learning*
- Kolter et al., "Linear Algebra Review and Reference"

Gradient of a function

- Let $f : \mathbb{R}^{m \times n} \mapsto \mathbb{R}$ be a function that takes $m \times n$ matrix $\boldsymbol{A}$ as input and returns a real number (scalar).
- A **gradient** of f with respect to A is the matrix

$$\nabla_{\boldsymbol{A}} f(\boldsymbol{A}) = \begin{bmatrix} \frac{\partial f}{\partial A_{11}} & \frac{\partial f}{\partial A_{12}} & \cdots & \frac{\partial f}{\partial A_{1n}} \\ \frac{\partial f}{\partial A_{21}} & \frac{\partial f}{\partial A_{22}} & \cdots & \frac{\partial f}{\partial A_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f}{\partial A_{m1}} & \frac{\partial f}{\partial A_{m2}} & \cdots & \frac{\partial f}{\partial A_{mn}} \end{bmatrix}$$

- i.e. an $m \times n$ matrix with

$$(\nabla_{\boldsymbol{A}} f(\boldsymbol{A}))_{ij} = \frac{\partial f}{\partial A_{ij}}$$

- The size of the gradient of $\boldsymbol{A}$ is the same as the size of A.

Gradient

- In the special (but more common) case when A is a vector we obtain the gradient

$$\nabla_{\boldsymbol{x}} f(\boldsymbol{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_m} \end{bmatrix}$$

- In general to define a gradient we require that the function returns a **real** value.

Jacobian

- The Jacobian $\boldsymbol{J_f}$ is a generalization of the gradient for vector valued functions.
- Let $\boldsymbol{f} : \mathbb{R}^n \mapsto \mathbb{R}^m$ be a function that takes n-dimensional vector $\boldsymbol{x}$ as input and returns a m-dimensional vector as an output.
- The Jacobian $\boldsymbol{J_f}$ is defined as

$$\boldsymbol{J_f} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \frac{\partial f_m}{\partial x_2} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

- Note that for the special case of a scalar-valued function, the Jacobian is the transpose of the gradient.

Optimization

- Most machine learning methods involve some kind of optimization.
  - One exception is the k-Nearest neighbour classifier introduced later.
- Optimization means minimizing or maximizing some function $f(\boldsymbol{x})$, i.e. finding the values of $\boldsymbol{x}$ for which $f(\boldsymbol{x})$ has a minimum or a maximum.
- Notation: $\boldsymbol{x}^* = \operatorname{argmin} f(\boldsymbol{x})$

Gradient-based optimization

- The derivative tells us how to change x in order to make a small improvement of $f(x)$.
- Therefore, derivatives can be useful in optimization.

Two simple machine learning models

Materials:

- Chapter 2.3 from Friedman et al., *The Elements of Statistical Learning*

Some notations

- We denote an input variable with the symbol x (scalar) or $\boldsymbol{x}$ (vector).
- The i-th component of a vector input $\boldsymbol{x}$ is denoted as x_i.
- Quantitative (numerical) outputs are denoted with y.
- Qualitative outputs are denoted with g (from group) and take values from a set $\mathcal{G}$.
- Matrices are denoted with bold and uppercase letters $\boldsymbol{X}$ for instance, a set of N input p-vectors $\boldsymbol{x}_i$ $(1 \leq i \leq N)$ is "packed" in a $N \times p$ input matrix $\boldsymbol{X}$.
- Since by default vectors are assumed to be column vectors, the rows of $\boldsymbol{X}$ are the transposes $\boldsymbol{x}_i^T$.

The learning task

- Given a value of the input vector $\boldsymbol{x}$ make a good prediction of the output y, denoted as $\hat{y}$.
- Both y and $\hat{y}$ should take values from the same numerical set.
- Similarly, g and $\hat{g}$ should both take values from the same set $\mathcal{G}$.
- We suppose that we have available a set of measurements $(\boldsymbol{x}_i, y_i)$ or $(\boldsymbol{x}_i, g_i)$ $(1 \leq i \leq N)$ called **training data** (in matrix form: $(\boldsymbol{X}, \boldsymbol{y})$ and/or $(\boldsymbol{X}, \boldsymbol{g})$).
- Our task is to construct a prediction rule based on the training data.

The learning task

Example:

- **Variable values**: Let g (and therefore also $\hat{g}$) be two valued (categorical), e.g. $\mathcal{G} = \{$BLUE, ORANGE$\}$.
- **Encoding of gs with ys**: Then each class can be encoded binary, i.e., with $y \in \{0, 1\}$, e.g., BLUE and ORANGE, would correspond to 0 and 1, respectively.
- **Predicted output values**: $\hat{y}$ ranges over the interval $[-\infty, +\infty]$ (of which $\{0, 1\}$ is a subset).
- **Prediction rule**: $\hat{g}$ is assigned a (class label) BLUE if $\hat{y} < 0.5$ and ORANGE, otherwise.

Two simple approaches to prediction

- Linear model fit
    - strong assumptions about the structure of the decision boundary
- k-nearest neighbours
    - weak assumptions about the structure of the decision boundary

Linear model fit by least squares

- Despite relative simplicity one of the most important statistical tools
- Input vector $\boldsymbol{x}^T = (x_1, x_2, \ldots, x_p)$
- Output y predicted using the model
$$\hat{y} = \hat{w}_0 + \textstyle\sum_{j=1}^{p} x_j \hat{w}_j$$
- $\hat{w}_i$ $(0 \leq i \leq p)$ are the parameters of the linear model
- In vector form
$$\hat{y} = \hat{\boldsymbol{w}}^T \boldsymbol{x} = \boldsymbol{x}^T \hat{\boldsymbol{w}}$$
using the fact that the scalar (inner) product of two vectors is a commutative operation.

Linear model fit by least squares

- We assume that w_0 is in $\boldsymbol{w}$ and 1 is included in $\boldsymbol{x}$.
- $\hat{y}$ is a scalar, but in general can be a k-vector $\hat{\boldsymbol{y}}$, in which case $\boldsymbol{w}$ becomes a $p \times k$ matrix of coefficients.

Linear model fit by least squares

- There are many ways to fit a linear model to a training dataset.
- **Least squares** method
  - We need to find coefficients $\hat{w}_i$ which minimize the error estimated with the **residual sum of squares**

$$\mathrm{RSS}(\boldsymbol{w}) = \sum_{i=1}^{N} (y_i - \boldsymbol{x}_i^T \boldsymbol{w})^2$$

    assuming N input-output pairs.
- $\mathrm{RSS}(\boldsymbol{w})$ is a quadratic function.
- A minimum always exists though not necessarily a unique one.

Linear model fit by least squares

- We look for the solution $\hat{\boldsymbol{w}}$ using the matrix notation:
- $\boldsymbol{y} = [y_1, y_2, \ldots, y_N]^T$ is the vector formed from the N output vectors and $\boldsymbol{X}$ is an $N \times p$ matrix

$$\mathrm{RSS}(\boldsymbol{w}) = (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w})^T(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w})$$

- To find the minimum we differentiate with respect to $\boldsymbol{w}$ which gives

$$-2\boldsymbol{X}^T(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w})$$

For details about the derivation check equations 4 and 5 in this document.

Linear model fit by least squares

- To find the minimum our derivative must be $\mathbf{0}$, hence:

$$\boldsymbol{X}^T(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}) = \mathbf{0}$$

$$\boldsymbol{X}^T\boldsymbol{y} - \boldsymbol{X}^T\boldsymbol{X}\boldsymbol{w} = \mathbf{0}$$

$$\boldsymbol{X}^T\boldsymbol{y} = \boldsymbol{X}^T\boldsymbol{X}\boldsymbol{w}$$

- If $\boldsymbol{X}^T\boldsymbol{X}$ is non-singular there exists a unique solution given by

$$\hat{\boldsymbol{w}} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

Linear model fit by least squares

- For each input $\boldsymbol{x}_i$ there corresponds the fitted output

$$\hat{y}_i = \hat{y}_i(\boldsymbol{x}_i) = \hat{\boldsymbol{w}}^T \boldsymbol{x}_i$$

.

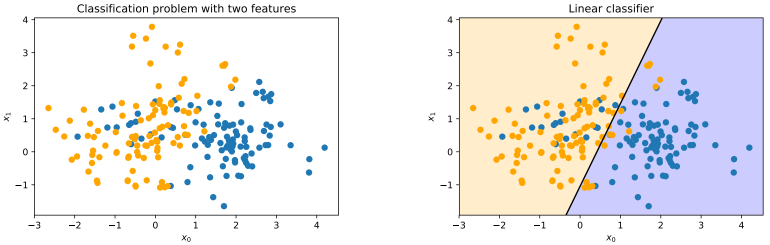
- This is called "making a prediction" for $\boldsymbol{x}_i$.
- The entire fitted surface (hyperplane) is fully characterized by the parameter vector $\hat{\boldsymbol{w}}$.
- After fitting the model, we can "discard" the training dataset.

Example: Linear model fit by least squares

- Scatter plot (on next slide) of training data on a pair of inputs x_1 and x_2
- Output class variable g has two values BLUE and ORANGE.
- Linear regression model fitted with the response variable y coded as 0 for BLUE and 1 for ORANGE.
- Fitted values $\hat{y}$ converted to a fitted class variable $\hat{g}$ as

$$\hat{g} = \begin{cases} \text{BLUE} & \text{if } \hat{y} \leq 0.5 \\ \text{ORANGE} & \text{if } \hat{y} > 0.5 \end{cases}$$

Example: Linear model fit by least squares



Nearest-neighbours model

- In nearest-neignbour methods $\hat{y}(\boldsymbol{x})$ is determined based on the inputs (points) in the training set $\mathcal{T}$ which are "closest" to the input $\boldsymbol{x}$.
- k-nearest neighbour fit is defined as

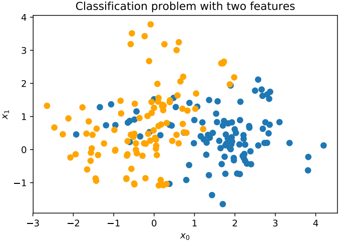
$$\hat{y}(\boldsymbol{x}) = \frac{1}{k} \sum_{\boldsymbol{x}_i \in N_k(\boldsymbol{x})} y_i$$

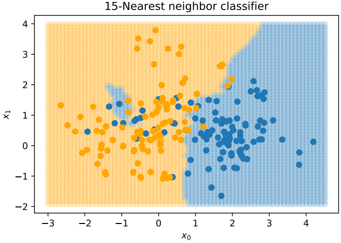
  where $N_k(\boldsymbol{x})$ is the neighbourhood of $\boldsymbol{x}$ consisting of the k "closest" points to $\boldsymbol{x}$.
- "Closeness" requires a definition of **metrics**.
- For the moment we assume Euclidian distance (each $\boldsymbol{x}$ is a point in the hyperspace).
- An average of the classes of the k closest points (but only for binary classification problem.

Back to the BLUE and ORANGE example

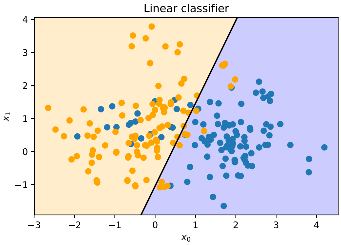
- We use the same training data as in the linear model example.
- New borderline between the classes generated with 15-nearest-neighbour model.
- Since ORANGE is encoded as 1 $\hat{y}$ is the proportion of ORANGE points in the 15-neighbourhood.
- Class ORANGE assigned to $\boldsymbol{x}$ if $\hat{y}(\boldsymbol{x}) > 0.5$ (majority is ORANGE).

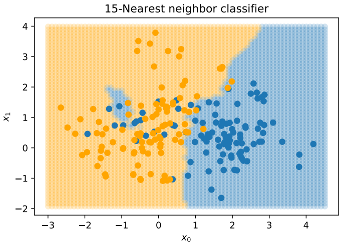
15-Nearest neighbour classifier



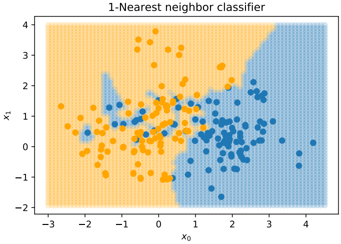


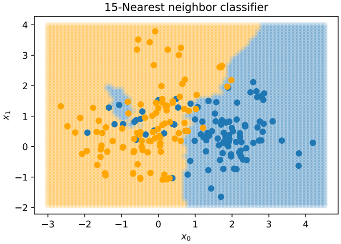
Linear classifier vs. 15-Nearest neighbour


Linear classifier


15-Nearest neighbor classifier

1-Nearest neighbour vs. 15-Nearest neighbour





Comparison of techniques

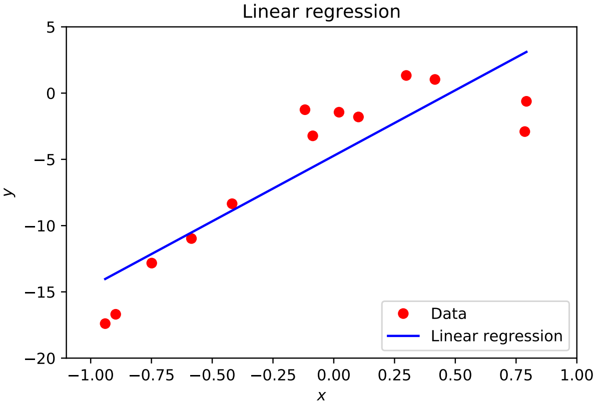
- At first sight it looks like k-NN has only one parameter, k versus p parameters (number of weights w_i) of the linear model.
- The **effective** number of parameters of k-NN is N/k which is in general bigger than p (N is the size of the training set).
- For instance, assume non-overlapping neighbourhoods
  - There will be N/k neighbourhoods.
  - To each neighbourhood there correspond one parameter (the mean of the elements of the neighbourhood).

Model capacity, underfitting and overfitting

Materials:

- Chapter I.5.2 from Goodfellow et al., *Deep Learning*

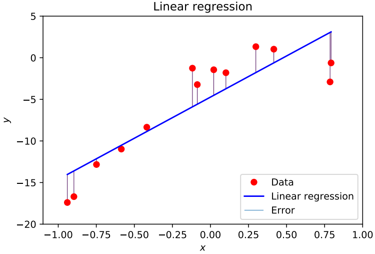
Linear regression

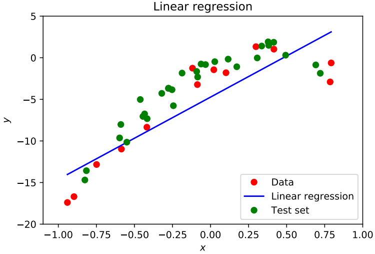


$$\hat{y} = \hat{w}_0 + \sum_{i=1}^{n} x_i \hat{w}_i$$
$$\hat{y} = \boldsymbol{x}^T \hat{\boldsymbol{w}}$$

Generalization

- The central challenge in machine learning is to design an algorithm which will perform well on new data (different from the training set data).
- This ability is called **generalization**.
- **Training error** is the error computed on the training set.





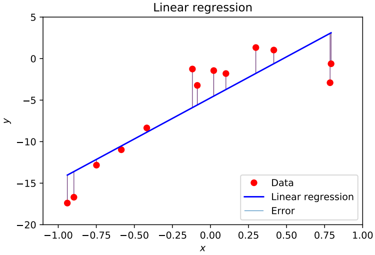
Example: Linear regression

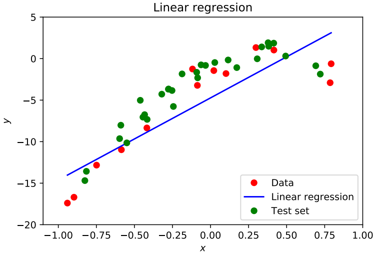
- Previously, we trained the model by minimizing the training error

$$\frac{1}{m^{(\text{train})}} \left\| \boldsymbol{X}^{(\text{train})} \hat{\boldsymbol{w}} - \boldsymbol{y}^{(\text{train})} \right\|_2^2$$

- We would like actually to minimize the test error

$$\frac{1}{m^{(\text{test})}} \left\| \boldsymbol{X}^{(\text{test})} \hat{\boldsymbol{w}} - \boldsymbol{y}^{(\text{test})} \right\|_2^2$$





Statistical learning theory

- **Statistical learning theory** provides methods to mathematically reason about the performance on the test set although we can observe only the training set.
- This is possible under some assumptions about the data sets
  - The training and test data are generated by drawing from a probability distribution over data sets. We refer to that as **data-generating process**.
  - **i.i.d. assumptions**
    - Examples in each data sets are **independent** from each other.
    - The training data set and the test data set are **identically distributed**, i.e., drawn from the same probability distribution.

Model capacity

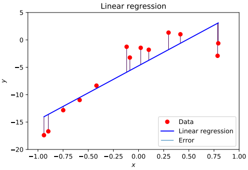
- A **capacity of the model** is its ability to fit a wide variety of functions.
- The capacity can be controlled by choosing its **hypothesis space**, i.e. the set of functions from which the learning algorithm is allowed to select the solution.
- Example: The linear regression algorithm has the set of all linear functions as its hypothesis space.

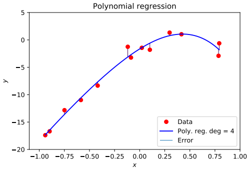
Polynomial regression

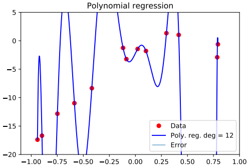
- The linear regression algorithm can be generalized to include all polynomial functions instead of just the linear ones.
- Moving to degree two to we obtain: $\hat{y} = b + w_1 x + w_2 x^2$.
  - This can be seen as adding a new feature x^2.
  - In fact, we can generalize this approach to create all sorts of hypothesis spaces, e.g.: $\hat{y} = b + w_1 x + w_2 \sin(x) + w_3 \sqrt{x}$.
- The **outuput** is still a **linear** function of the parameters, so in principle it can be trained in the same way as the linear regression.

Polynomial regression

A comparison of a linear, degree-4, and degree-12 polynomials as predictors

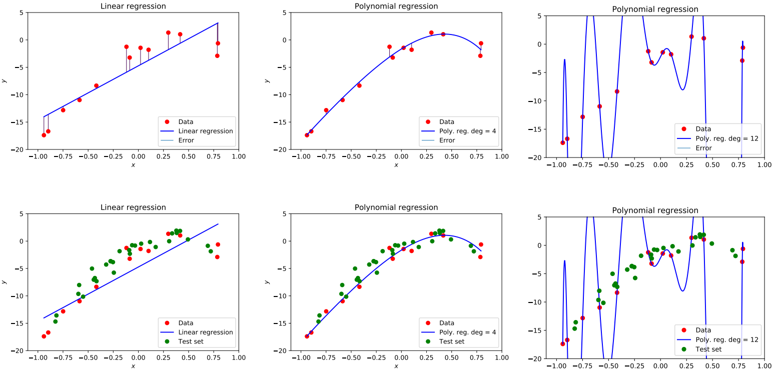






Polynomial regression

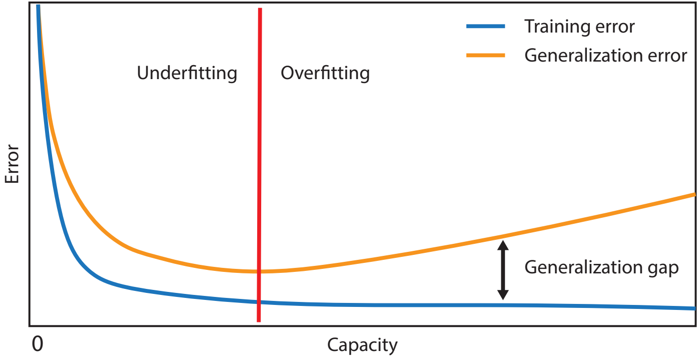
A comparison of a linear, degree-4, and degree-12 polynomials as predictors



Generalization and capacity

- Simpler functions generalize more easily, but we still need to choose a sufficiently complex hypothesis (function) to obtain small training error.
- Typically training error decreases with the increase of the model capacity until an (asymptotic) value is reached.
- The generalization error is U-shaped with the capacity range split in an underfitting and an overfitting zone.

Generalization and capacity



Regularization

- In addition to increasing and decreasing of the hypothesis space, i.e., the capacity, we can influence the learning algorithm by **giving preference to one solution over another in the hypothesis space**.
- In case both functions are eligible we can define a condition to express preference about one of the functions.
- The unpreferred solution is chosen only if it gives significantly better performance with the training data.
- *More on regularization in the next lecture.*

Model selection

Materials:

- Chapter I.5.3 from Goodfellow et al., *Deep Learning*

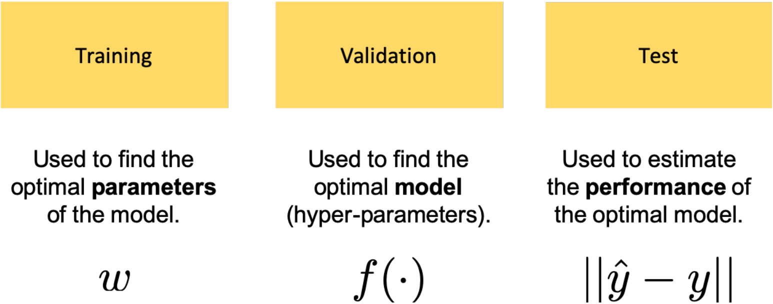
Hyperparameters and validation sets

- **Hyperparameters** are settings that can be used to control the behaviour of the algorithm.
- In general, the hyperparameters are not modified by the learning algorithm itself.
- **Example**: In **polynomial regression** the degree of the polynomial is a **capacity** hyperparameter.
- A setting can be chosen to be hyperparameter when it is **difficult to optimize** or - more often - when its derivation from the training set **can lead to overfitting**.
  - Example: in polynomial regression we can always fit the data better with a higher degree polynomial.

Choice of training, validation, and test sets

- The **validation set** is used during training to predict the behaviour (generalization error) of the algorithm on new data, i.e., on the test set and to chose the hyperparameters.
- Ideally these two sets are disjoint.
- The validation set is chosen from the training data.
- The training data is split in two disjoint subsets.

Choice of training, validation, and test sets



Training	Validation	Test
Used to find the optimal **parameters** of the model.	Used to find the optimal **model** (hyper-parameters).	Used to estimate the **performance** of the optimal model.
w	$f(\cdot)$	$\|\|\hat{y} - y\|\|$

Cross-validation

- Dividing the data set into disjoint training and test sets can result in a result in a too small validation and/or test set.
- In such cases all data is used to estimate the generalization error.
- We use procedures that repeat the training and testing on different randomly chosen subsets or splits of the original data set.
- The most common such procedure is the **k-fold cross-validation**.

Expectation (recap)

- The **expectation** or **expected** value of a function $f(x)$ with respect to a probability distribution $P(x)$ is the average value of f over all values x assuming they are drawn from P

$$\mathbb{E}_{x \sim P}[f(x)] = \sum_{x} P(x)f(x)$$

$$\mathbb{E}_{x \sim P}[f(x)] = \int p(x)f(x)dx$$

Variance (recap)

- The **variance** gives a measure of variation of the values of a random variable x

$$\mathrm{Var}(f(x)) = \mathbb{E}[(f(x) - E[f(x)])^2]$$

Bias and variance trade-off

Materials:

- Chapter I.5.4 from Goodfellow et al., *Deep Learning*

Point estimation

- For efficient design of learning algorithms it is useful to have formal characterizations of notions like generalization, overfitting and underfitting.
- To this end we introduce some definitions.
- **Point estimation** is the attempt to provide the single "best" prediction of some quantity of interest.
- The quantity of interest can be a single parameter, parameter vector of some model, e.g., the weights $\boldsymbol{w}$ in the linear regression model.

Point estimation

- Given a parameter $\boldsymbol{\theta}$ we denote its point estimate with $\hat{\boldsymbol{\theta}}$.
- As usual, let $\{\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(m)}\}$ be m independent and identically distributed (i.i.d.) data points.
- A **point estimator** or **statistic** is any function of the data

$$\hat{\boldsymbol{\theta}}_m = g(\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(m)})$$

- This definition is very general. For instance, that the value returned by g need not be close to the true value $\boldsymbol{\theta}$. Also g might return a value which is outside the values that $\boldsymbol{\theta}$ is allowed to have.

Point estimation

- Of course, a good estimator is still a function that returns values close to $\boldsymbol{\theta}$.
- Since the data is drawn from a random process, point estimate $\hat{\boldsymbol{\theta}}$ is considered to be a random variable and $\boldsymbol{\theta}$ is fixed, but unknown parameter.

Bias

- A bias of an estimator $\hat{\boldsymbol{\theta}}_m$ is defined as

$$\text{bias}(\hat{\boldsymbol{\theta}}_m) = \mathbb{E}(\hat{\boldsymbol{\theta}}_m) - \boldsymbol{\theta}$$

  where the expectation is over the data and $\boldsymbol{\theta}$ is the true underlying value.
- An estimator $\hat{\boldsymbol{\theta}}_m$ is **unbiased** if $\text{bias}(\hat{\boldsymbol{\theta}}_m) = 0$. Note that this implies $\mathbb{E}(\hat{\boldsymbol{\theta}}_m) = \boldsymbol{\theta}$.
- $\hat{\boldsymbol{\theta}}_m$ is **asymptotically unbiased** if $\lim_{m\to\infty} \text{bias}(\hat{\boldsymbol{\theta}}_m) = 0$ (implying $\lim_{m\to\infty} \mathbb{E}(\hat{\boldsymbol{\theta}}_m) = \boldsymbol{\theta}$).

Bias: example

- **Example**: Consider samples $\{x^{(1)}, \ldots, x^{(m)}\}$ i.i.d distributed according to the Gaussian distribution

$$p(x^{(i)}; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2}\frac{x^{(i)} - \mu}{\sigma^2}\right)$$

- The **sample mean** is a common estimator of the Gaussian mean parameter

$$\hat{\mu}_m = \frac{1}{m}\sum_{i=1}^{m} x(i)$$

Bias: example

We compute the bias as expectation by substituting the Gaussian distribution in the formula

$$\begin{aligned}
\text{bias}(\mu_m) &= \mathbb{E}[\mu_m] - \mu \\
&= \mathbb{E}\left[\tfrac{1}{m}\textstyle\sum_{i=1}^{m} x^{(i)}\right] - \mu \\
&= \left(\tfrac{1}{m}\textstyle\sum_{i=1}^{m} \mathbb{E}[x^{(i)}]\right) - \mu \\
&= \left(\tfrac{1}{m}\textstyle\sum_{i=1}^{m} \mu\right) - \mu \\
&= \mu - \mu = 0
\end{aligned}$$

The sample mean is an unbiased estimator of Gaussian mean parameter.

Bias: example

- **Example**: Estimators of the variance of a Gaussian distribution
- We compare two different estimators of the variance σ^2 parameter
- **Sample variance**

$$\hat{\sigma}^2 = \frac{1}{m} \sum_{1}^{m} \left(x^{(i)} - \hat{\mu}_m \right)^2$$

  where $\hat{\mu}$ is the sample mean.

- We are interested in computing

$$\text{bias}(\hat{\sigma}_m^2) = \mathbb{E}[\hat{\sigma}_m^2] - \sigma^2$$

Bias: example

- First we evaluate $\mathbb{E}[\hat{\sigma}_m^2]$:

$$\mathbb{E}[\hat{\sigma}_m^2] = \mathbb{E}\left[\frac{1}{m}\sum_{1}^{m}\left(x^{(i)} - \hat{\mu}_m\right)^2\right] = \frac{m-1}{m}\sigma^2$$

- Back to the bias

$$\text{bias}(\hat{\sigma}_m^2) = \mathbb{E}[\hat{\sigma}_m^2] - \sigma^2 = \frac{m-1}{m}\sigma^2 - \sigma^2 = -\frac{\sigma^2}{m}$$

- Therefore the sample variance is a **biased** estimator.

Bias: example

- The **unbiased variance estimator** is defined as

$$\tilde{\sigma}^2 = \frac{1}{m-1} \sum_{1}^{m} \left(x^{(i)} - \hat{\mu}_m\right)^2$$

- Indeed

$$\mathbb{E}[\tilde{\sigma}_m^2] = \mathbb{E}\left[\frac{1}{m-1} \sum_{1}^{m} \left(x^{(i)} - \hat{\mu}_m\right)^2\right] = \frac{m-1}{m-1}\sigma^2 = \sigma^2$$

and the bias is 0.

Variance and standard error

- Another important feature of an estimator is its variance.
- The **variance** of an estimator is simple its statistical variance $\text{Var}(\hat{\theta})$ over the training set as a random variable.
- Alternatively we can compute the **standard error** (the square root of the variance) $\text{SE}(\hat{\theta})$.
- The variance or the standard error provide a measure how much the estimate would vary as we resample the data independently from the underlying data generating process.
- We would prefer a relatively low variance of the estimator.

Variance and standard error

- The standard error of the mean estimator is given as

$$\mathrm{SE}(\hat{\mu}) = \sqrt{\mathrm{Var}\left[\frac{1}{m}\sum_{i=1}^{m} x^{(i)}\right]} = \frac{\sigma}{\sqrt{m}}$$

  where σ is the true variance of the distribution, i.e., the samples $x^{(i)}$.

- Neither the square root of the sample variance nor the square root of the unbiased estimator of the variance give an unbiased estimate of the standard deviation.
- Both approaches underestimate the true standard deviation.
- However, for large m the approximation works quite well.

Variance and standard error

- In machine learning the generalization error is estimated based on the sample mean of the error on the test set.
- The accuracy of the estimate depends on the number of the examples.
- From the statistical theory (central limit theorem) we know that the mean is distributed with normal distribution for which we can establish confidence intervals.
- For instance, the 95% confidence interval is given by

$$[\hat{\mu_m} - 1.96\mathrm{SE}(\hat{\mu}_m), \hat{\mu_m} + 1.96\mathrm{SE}(\hat{\mu}_m)]$$

- Then we can say that algorithm A is better than algorithm B of the confidence upper bound for the error of A is less than the corresponding lower bound of B.

Trading off bias and variance to minimize mean squared error

- Bias and variance measure two different sources of error in an estimator.
- Bias measures the expected deviation with the true value of the estimator.
- Variance provides a measure of the deviation from the expected value of the estimator depending on the particular data sampling.

Trading off bias and variance to minimize mean squared error

- Often we need to make a trade-off between these two.
- The most common way to do this is via cross-validation.
- An alternative is to compare the **mean squared error** (MSE) of the estimates.

$$\text{MSE} = \mathbb{E}[(\hat{\theta}_m - \theta)^2] = \text{bias}(\hat{\theta}_m)^2 + \text{Var}(\hat{\theta}_m)$$

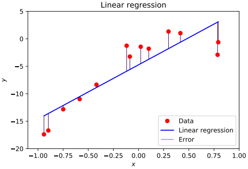
- The smaller MSE the better - so minimizing both the bias and variance is always preferable.

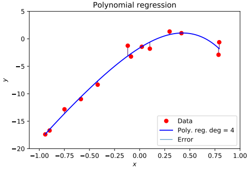
Bias and variance

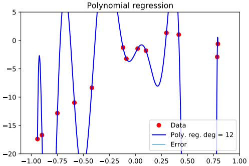
- Our original goal was to provide a mathematical support for the notions of capacity, underfitting, and overfitting.
- Indeed there is a close relationship between these three concepts and bias and variance.
- When generalization error is measured by MSE (and hence indirectly via bias and variance) increasing capacity tends to increase variance and decrease bias.
- Again the generalization as a function of capacity is given by an U-shaped curve.

Discussion

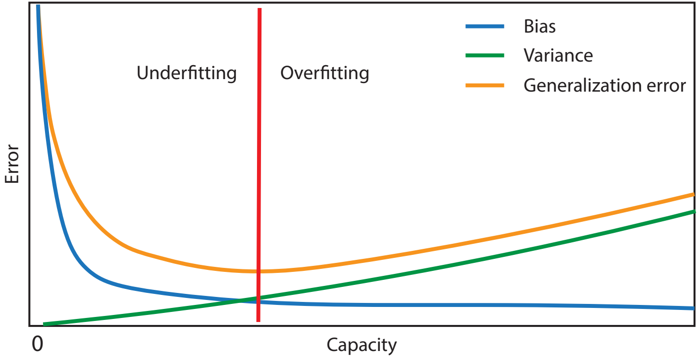
How will the estimated regression model change when one training data point is replaced with another one?



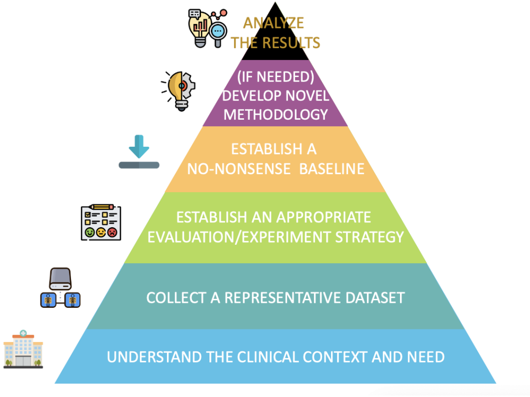




Bias and variance



In summary...



ANALYZE THE RESULTS

(IF NEEDED) DEVELOP NOVEL METHODOLOGY

ESTABLISH A NO-NONSENSE BASELINE

ESTABLISH AN APPROPRIATE EVALUATION/EXPERIMENT STRATEGY

COLLECT A REPRESENTATIVE DATASET

UNDERSTAND THE CLINICAL CONTEXT AND NEED

Important: introductory topics covered in video lecture

These topics are covered in the extended slide stack and video lecture (links in Cavas) and are exam material:

- Linear algebra
- Probability theory
- Maximum-likelihood estimation
- Supervised and unsupervised algorithms
- Ensambling

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The slides for this lecture were prepared by Mitko Veta and Dragan Bošnacki.
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References

- Friedman, J., T. Hastie, and R. Tibshirani. *The Elements of Statistical Learning*. Springer series in statistics New York, 2001.
- Goodfellow, I., Y. Bengio, and A. Courville. *Deep Learning*. MIT Press, 2016.
- Kolter, Z. and C. Do. "Linear Algebra Review and Reference". In: (2015).