Machine learning foundations

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2025

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. Linear algebra
2. Gradient of a function
3. Two simple machine learning models
   - Linear model
   - Nearest-neighbours model
4. Probability theory
5. Model capacity, underfitting and overfitting
6. Model selection
7. Bias and variance trade-off
8. Maximum likelihood estimation
9. Model evaluation
10. Supervised and unsupervised learning algorithms
11. Ensambling

Note on the slides

This set of slides is larger than the one used during the lectures. It includes some additional material that you can use as a guide when studying.

Linear algebra

Materials:

- Chapter I.2 from Goodfellow et al., *Deep Learning*
- Kolter et al., "Linear Algebra Review and Reference"

Scalars

- A scalar is a single number (integer, real, rational, ...).
- Denoted by italics a, n, x

Vectors

- A vector is a 1-D array of numbers (integer, real, rational, ...)

  $$\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{bmatrix}$$

- Example notation for type and size

  $\boldsymbol{x} \in \mathbb{R}^n$

Matrices

- A matrix is a 2-D array of numbers

$$\begin{bmatrix} a_{1,1} & a_{1,2} \\ a_{2,1} & a_{2,2} \end{bmatrix}$$

- Example notation for type and shape
  $\mathbf{A} \in \mathbb{R}^{m \times n}$

Tensors

- A tensor is an array of numbers that may have
  - a zero dimensions and be a scalar,
  - one dimension and be a vector,
  - two dimensions and be a matrix,
  - more dimensions ...

Side note: One of the most popular frameworks for implementing deep machine learning models is called TensorFlow (https://www.tensorflow.org/).

Transpose matrix

$$(\boldsymbol{A}^T)_{i,j} = \boldsymbol{A}_{j,i}$$

$$\boldsymbol{A} = \begin{bmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \\ A_{3,1} & A_{3,2} \end{bmatrix} \Rightarrow \begin{bmatrix} A_{1,1} & A_{2,1} & A_{3,1} \\ A_{1,2} & A_{2,2} & A_{3,2} \end{bmatrix}$$

The transpose matrix is a mirror image with regard to the main diagonal

$$(\boldsymbol{AB})^T = \boldsymbol{B}^T\boldsymbol{A}^T$$

Identity matrix

- Identity matrix $\boldsymbol{I}_3$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

- The identity matrices are neutral elements in matrix-matrix and matrix-vector multiplication, e.g.

$$\forall \boldsymbol{x} \in \mathbb{R}^n : \boldsymbol{I}_n \boldsymbol{x} = \boldsymbol{x} \boldsymbol{I}_n = \boldsymbol{x}$$

Matrix (dot) product

$$\boldsymbol{C} = \boldsymbol{AB}$$

The matrices must be compatible: an $m \times n$ matrix is multiplied with an $n \times r$ matrix and as a result an $m \times r$ matrix is obtained

$$C_{i,j} = \sum_{k} A_{i,k} B_{k,j}$$

$$\boldsymbol{A} \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \\ 10 & 11 & 12 \end{bmatrix} \times \boldsymbol{B} \begin{bmatrix} 1 & 2 & 3 & 4 & 5 \\ 6 & 7 & 8 & 9 & 10 \\ 11 & 12 & 13 & 14 & 15 \end{bmatrix} = \boldsymbol{C} \begin{bmatrix} 4 \times 5 \end{bmatrix}$$

$$C_{2,5} = A_{2,1} B_{1,5} + A_{2,2} B_{2,5} + A_{2,3} B_{3,5} = 4 \cdot 5 + 5 \cdot 10 + 6 \cdot 15 = 160$$

Matrix (dot) product

- In general matrix multiplication is not commutative, i.e., most of the time $\boldsymbol{AB} \neq \boldsymbol{BA}$.
- Depending on the dimensions sometimes $\boldsymbol{AB}$ or $\boldsymbol{BA}$ are not possible.
- As a special case the matrix can be a (column or row) vector; an $m \times n$ matrix is multiplied with a $n \times 1$ vector to obtain a $m \times 1$ vector.

Systems of linear equations

$$A_{1,1}x_1 + A_{1,2}x_2 + \ldots + A_{1,n}x_n = b_1$$

$$A_{2,1}x_1 + A_{2,2}x_2 + \ldots + A_{2,n}x_n = b_2$$

$$\ldots$$

$$A_{m,1}x_1 + A_{m,2}x_2 + \ldots + A_{m,n}x_n = b_m$$

- $A_{*,*}$ and b_* are the knowns, x_* are the unknowns.
- In matrix form: $\boldsymbol{Ax} = \boldsymbol{b}$

Systems of linear equations

- $\boldsymbol{Ax} = \boldsymbol{b}$ expands to

$$\boldsymbol{A}_{1,:}\boldsymbol{x}_1 = \boldsymbol{b}_1$$

$$\boldsymbol{A}_{2,:}\boldsymbol{x}_2 = \boldsymbol{b}_2$$

$$\dots$$

$$\boldsymbol{A}_{m,:}\boldsymbol{x}_m = \boldsymbol{b}_m$$

Solving systems of linear equations

- A linear system of equations can have
  - no solutions,
  - many solutions,
  - exactly one solution.
- Only one solution implies that multiplication by a matrix is an invertible operation.

Matrix inversion

- Matrix inverse is defined with

$$\boldsymbol{A}^{-1}\boldsymbol{A} = \boldsymbol{I}_n$$

- A system of linear equations can be solved using inverse matrix

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$$

$$\boldsymbol{A}^{-1}\boldsymbol{A}\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{b}$$

$$\boldsymbol{I}_n\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{b}$$

$$\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{b}$$

- This is useful mostly for abstract analysis.
- From a numerical point of view there are much more efficient methods.

Invertibility

A matrix cannot be inverted if

- the number of rows and columns is not the same, or
- some rows and columns are "redundant" ("linearly dependent", "low rank").

Moore-Penrose pseudoinverse

- Matrix inversion is not defined on matrices that are no square.
- The **Moore-Penrose pseudoinverse** is defined as

$$\boldsymbol{A}^{+} = \lim_{\alpha \searrow 0} (\boldsymbol{A}^{T}\boldsymbol{A} + \alpha \boldsymbol{I})^{-1}\boldsymbol{A}^{T}$$

Moore-Penrose pseudoinverse

Now we can consider

$$\boldsymbol{x} = \boldsymbol{A}^{+}\boldsymbol{y}$$

- If the equation has
  - exactly one solution: this is the same as inverse,
  - no solution: gives the solution with the smallest error, $\|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{y}\|_2$
  - many solutions: gives the solution with the smallest norm of $\boldsymbol{x}$.

Singular value decomposition

- Similar to eigenvalue decomposition
- More general: matrix need not be square

$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^T$$

- ***U*** and ***V*** are square matrices and are both orthogonal, ***D*** is diagonal.
- The diagonal elements of D are called **singular values** of matrix ***A***; the columns of ***U*** and ***V*** are **left-singular** and **right-singular vectors** of ***A***, respectively.

Computing the pseudoinverse

- Efficient implementations are based on the formula allowed by the singular decomposition

$$\boldsymbol{A}^{+} = \boldsymbol{V}\boldsymbol{D}^{+}\boldsymbol{U}^{T}$$

- $\boldsymbol{U}, \boldsymbol{D}, \boldsymbol{V}$ are from the singular value decomposition of $\boldsymbol{A}$.
- The pseudoinverse $\boldsymbol{D}^{+}$ of $\boldsymbol{D}$ is obtained by taking the reciprocal non-zero elements and after that taking the transpose of the resulting matrix.

Norms

- Norms are functions that measure how "large" a vector is.
- Similar to a distance between zero and the point represented by the vector
  - $f(\boldsymbol{x}) = 0 \Rightarrow \boldsymbol{x} = 0$
  - $f(\boldsymbol{x} + \boldsymbol{y}) \leq f(\boldsymbol{x}) + f(\boldsymbol{y})$ **(the triangle inequality)**
  - $\forall \alpha \in \mathbb{R} : f(\alpha \boldsymbol{x}) = \alpha f(\boldsymbol{x})$

Norms

- L^p- norm

$$\|\boldsymbol{x}\|_p = \left(\sum_i |x_i|^p \right)^{\frac{1}{p}}$$

  - Most popular L^2-norm (for $p = 2$)
  - L_1-norm (for $p = 1$): $\|\boldsymbol{x}\|_1 = \sum_i |x_i|$
  - Max norm (for infinite p): $\|\boldsymbol{x}\|_\infty = \max_i |x_i|$

Special vectors and matrices

- Unit vector $\left\|\boldsymbol{x}\right\|_n = 1$
- Symmetric matrix $\boldsymbol{A} = \boldsymbol{A}^T$
- Orthogonal matrix

$$\boldsymbol{A}\boldsymbol{A}^T = \boldsymbol{I} = \boldsymbol{A}^T\boldsymbol{A}$$

- It follows that for orthogonal matrices $\boldsymbol{A}^T = \boldsymbol{A}^{-1}$

Eigendecomposition

- Eigenvector and eigenvalue

$$\boldsymbol{A}\boldsymbol{x} = \lambda \boldsymbol{x}$$

- Eigendomdecomposition of a matrix

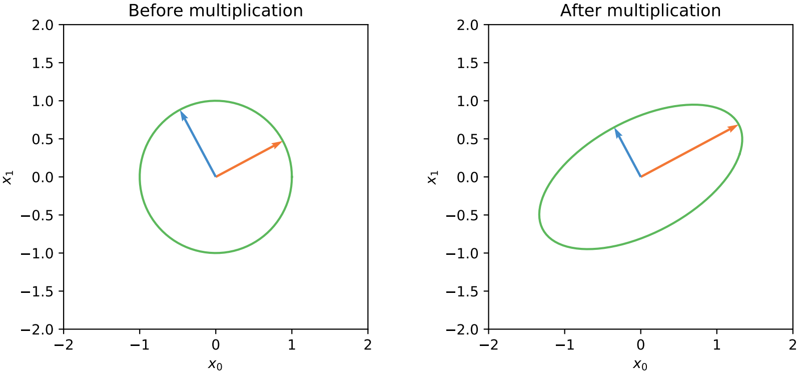
$$\boldsymbol{A} = \boldsymbol{V}\mathrm{diag}(\lambda)\boldsymbol{A}^{-1}$$

where $\mathrm{diag}(\lambda)$ is a diagonal matrix having the (scalar) eigenvalues λ as diagonal elements.

Eigendecomposition

- Every real symmetric matrix has a real orthogonal eigendecomposition
$$\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^T$$
where $\boldsymbol{Q}$ is an orthogonal matrix composed of eigenvectors of $\boldsymbol{A}$ and $\boldsymbol{\Lambda}$ is a diagonal matrix.
- The eigenvalue Λ_{ii} is associated with the eigenvector in column i of $\boldsymbol{Q}$, denoted as $\boldsymbol{Q}_{:,i}$.
- We can think of $\boldsymbol{A}$ as scaling space by factor λ_i in the direction of its corresponding eigenvector $v^{(i)}$ (represented by $\boldsymbol{Q}_{:,i}$).

Effect of eigenvalues



Eigendecomposition

- From the eigendecomposition we learn useful properties of the matrix.
- The eigendecomposition of a real symmetric matrix is used in optimization of quadratic expressions of the form $f(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x}$ under the constraint $\|\boldsymbol{x}\|_2 = 1$.
- For instance, if $\boldsymbol{x} = \boldsymbol{v}^{(i)}$, then $f(\boldsymbol{x}) = \lambda_i$, when $\boldsymbol{v}^{(i)}$ is an eigenvector of A and λ_i is its corresponding eigenvalue.
- The maximal (minimal) value of f within the constraint region is equal to the maximal (minimal) eigenvalue.

Trace

- A **trace** of a matrix is defined as

$$Tr(\boldsymbol{A}) = \sum_i \boldsymbol{A}_{i,i}$$

- Expressions in terms of the trace operators allow to exploit many useful identities, e.g.

$$Tr(\boldsymbol{ABC}) = Tr(\boldsymbol{BCA}) = Tr(\boldsymbol{CAB})$$

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
$$\hat{y} = \hat{w}_0 + \sum_{j=1}^{p} x_j \hat{w}_j$$
- $\hat{w}_i$ $(0 \leq i \leq p)$ 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

Some hyper(space) terminology:

- Points $\boldsymbol{x}, \hat{y}$ form a **hyperplane** in the $(p+1)$-dimensional input-output hyperspace.
- If $\boldsymbol{x}$ is extended with constant 1 then the hyperplane includes the origin and it forms a **subspace**.
- If 1 is not included then the hyperplane is an **affine** set and it cuts the y-axis at the point $(\mathbf{0}, \hat{w}_0)$, where the vector $\mathbf{0}$ has all x_i coordinates equal to 0.
- Reminder: from now on we assume that 1 is included in $\boldsymbol{x}$ and $\hat{w}_0$ in $\hat{\boldsymbol{w}}/$
- The function $f(\boldsymbol{x}) = \boldsymbol{w}^T\boldsymbol{x}$ defined on the p-dimensional (input) space is a **linear** function (we omit the hats over the ws since now we consider them as free variables).
- The gradient $\nabla f(\boldsymbol{x})$ is a vector pointing along the direction of maximal change.

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**

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

    assuming N input-output pairs.
- 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

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

Discussion point 1

Why we cannot simply solve for $\hat{\boldsymbol{w}}$ in the following way?

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

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

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

Linear model fit by least squares

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

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

.

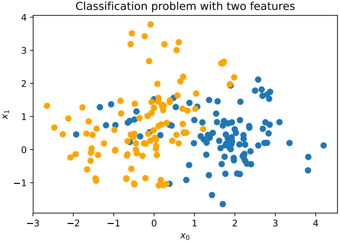
- This is called "making a prediction" for $\boldsymbol{x}_i$.
- The entire fitted surface (hyperplane) is fully characterized by the parameter vector $\hat{\boldsymbol{w}}$.
- After fitting the model, we can "discard" the training dataset.

Example: Linear model fit by least squares

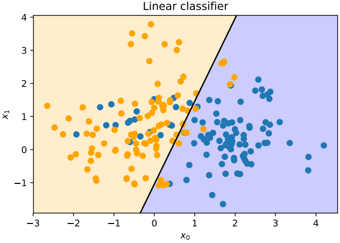
- Scatter plot (on next slide) of training data on a pair of inputs x_1 and x_2
- Output class variable g has two values BLUE and ORANGE.
- Linear regression model fitted with the response variable y coded as 0 for BLUE and 1 for ORANGE.
- Fitted values $\hat{y}$ converted to a fitted class variable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



Classification problem with two features



Linear classifier

Example: Linear model fit by least squares

- Two classes separated in the plane ($\mathbb{R}^2$) by the decision boundary $\{\boldsymbol{x} : \boldsymbol{w}^T\boldsymbol{x} = 0.5\}$
- $\{\boldsymbol{x} : \boldsymbol{w}^T\boldsymbol{x} < 0.5\}$ set of BLUE points
- $\{\boldsymbol{x} : \boldsymbol{w}^T\boldsymbol{x} \geq 0.5\}$ set of ORANGE points

Example: Linear model fit by least squares

- Wrong classifications on both sides of the boundary
- Are the errors caused by the model or are they unavoidable?
- Two possible scenarios
  - **Scenario 1**: data generated from bivariate Gaussian distribution
  - **Scenario 2**: data generated from 10 Gaussian distributions; the means of these distributions are also distributed as Gaussian
- In Scenario 1 the linear boundary is the best we can do since the overlap is inevitable.
- In Scenario 2 the linear boundary is unlikely to be optimal (in fact the boundary is non-linear and disjoint).

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

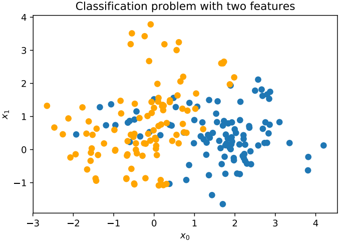
$$\hat{y}(\boldsymbol{x}) = \frac{1}{k} \sum_{\boldsymbol{x}_i \in N_k(\boldsymbol{x})} y_i$$

  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.

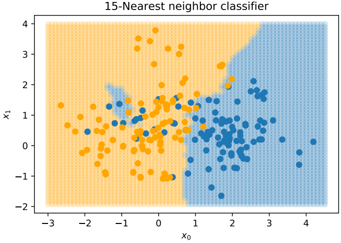
Back to the BLUE and ORANGE example

- 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

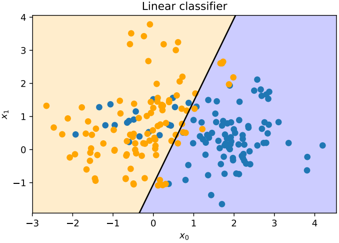


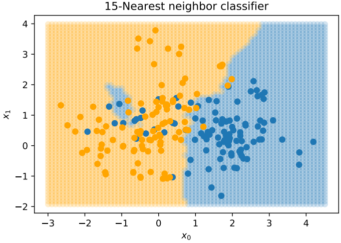
Classification problem with two features



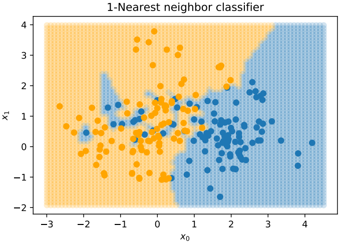
15-Nearest neighbor classifier

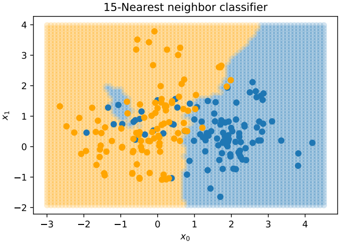
Linear classifier vs. 15-Nearest neighbour


Linear classifier


15-Nearest neighbor classifier

1-Nearest neighbour vs. 15-Nearest neighbour





Comparison of the techniques

- 15-NN seems to work better than the linear classifier since fewer points are missclassified.
- On the other hand, **none** of the points in the 1-NN case was misclassified!?
- Actually with the 1-NN method the error on **training data** is always 0.
- An independent test set needed to obtain a better comparison of the methods.

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).

Discussion point 2

Assume that you are building a machine learning model to be used as an *aid* by clinicians for decision making. The inputs to the model are a number of *biomarkers* describing the condition of the patient.

The clinician specifies that they are interested in a model that is *interpretable*, i.e. a model that will not only output a prediction but also give an indication about which biomarkers are important when making the prediction.

You can either use a linear model or a k-NN classifier. What is the better choice in your opinion?

Probability theory

Materials:

- Chapter I.3 from Goodfellow et al., *Deep Learning*

Probability theory

- Probability theory is a mathematical framework for dealing with uncertainty, i.e., modeling and analyzing uncertain events and statements
- In AI probability theory is used in two major ways:
  - To design AI systems, i.e., derive models and expressions and the corresponding algorithms.
  - To analyze the behaviour of the AI systems.

Probability theory

- A **random variable** is a variable that can take values randomly.
- We will denote random variables with plain (ordinary text) typeface and their values with standard math typeface for example, if the random variable is denoted as x its values can be x_1 and x_2.
- A vector-valued random variable is denoted with bold typeface, e.g. $\mathbf{x}$.
- On its own a random variable just denotes the set of its possible values; to get its full meaning in needs to be coupled with a distribution.

Probability theory

- There are two types of random variables: **discrete** and **continuous**.
- Consequently there are two ways to describe probability distributions: **probability mass functions** and **probability density functions**.

Probability mass function

- The domain of a probability mass function P is the set of all possible states of the random variable x.
- $\forall x \in \mathrm{x} : 0 \leq P((x) \leq 1$
    - An impossible event has probability 0 and no state can be less probable than that.
    - An event that is guaranteed to happen has probability 1 and no state can have a greater chance of occurring.
- $\sum_{x \in \mathrm{x}} P(x) = 1$
    - We say that x is **normalized**.
- Example: Uniform distribution: $P(\mathrm{x} = x_i) = \frac{1}{k}$.

Probability density function

- The domain of the probability density function p must be the set of all possible states of x.
- $\forall x \in \mathrm{x} : p(x) \geq 0$.
- $$\int p(x)dx = 1$$
- Example: uniform distribution $u(x; a, b) = \frac{1}{b-a}$, for $x \in [a, b]$

Conditional probability

- **Conditional probability** is the probability of some event provided that some other event has happened.
- Given two random variables x and y, the conditional probability that y has value y provided that we know that x has value x is given by

$$P(\mathrm{y} = y \mid \mathrm{x} = x) = \frac{P(\mathrm{x},\mathrm{y})}{P(\mathrm{x} = x)}$$

- Another way to see this formula is

$$P(\mathrm{x},\mathrm{y}) = P(\mathrm{x} = x)P(\mathrm{y} = y \mid \mathrm{x} = x)$$

i.e., the probability of x and y occurring together is equal to the probability of occurrence of x times the probability of y occurring provided x has occurred.

Expectation

- 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
- $$\mathbb{E}_{\mathrm{x}\sim P}[f(x)] = \sum_{x} P(x)f(x)$$
- $$\mathbb{E}_{\mathrm{x}\sim P}[f(x)] = \int p(x)f(x)dx$$
- Linarity of expectations:

$$\mathbb{E}_{\mathrm{x}}[\alpha f(x) + \beta g(x)] = \alpha\mathbb{E}_{\mathrm{x}}[f(x)] + \beta\mathbb{E}_{\mathrm{x}}[g(x)]$$

Variance and covariance

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

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

  Square root of the variance is called **standard deviation**.

- The **covariance** is a measure of linear relation as well as scale between

  $$\mathrm{Cov}(f(x), g(x)) = \mathbb{E}[f(x) - E[(f(x)])(g(x) - E[g(x)])]$$

Covariance matrix

- The **covariance matrix** of a random vector $\boldsymbol{x} \in \mathbb{R}^n$ is a $n \times n$ matrix with elements

$$\mathrm{Cov}(\boldsymbol{x})_{i,j} = \mathrm{Cov}(x_i, x_j)$$

- The diagonal elements of the matrix give the variance

$$\mathrm{Cov}(\mathrm{x}_i, \mathrm{x}_i) = \mathrm{Var}(\mathrm{x}_i)$$

Bernouli Distribution

- A distribution over a single binary random variable
- Controlled by a single parameter $\phi \in [0, 1]$ which corresponds to the probability of the random variable taking the value 1
- Properties:

$$
\begin{aligned}
P(\mathrm{x}) = 1) &= \phi \\
P(\mathrm{x} = 0) &= 1 - \phi \\
P(\mathrm{x} = x) &= \phi^{x}(1 - \phi)^{1-x} \\
\mathbb{E}_{\mathsf{x}}[\mathsf{x}] &= \phi \\
Var(\mathsf{x}) &= \phi(1 - \phi)
\end{aligned}
$$

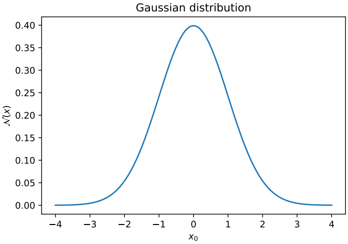
Gaussian distribution

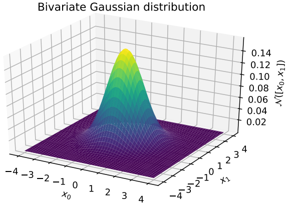
- The most commonly used distribution, also called **normal distribution**.
- Controlled by two parameters $\mu \in \mathbb{R}$ (the **mean**) and $\sigma \in (0, \infty)$, (the **standard deviation**)

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

$$\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sqrt{\frac{1}{(2\pi)^n \det(\Sigma)}} \exp\left(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{\mu})\right)$$

Gaussian distribution



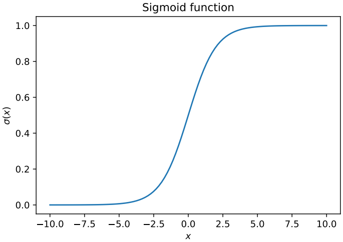


Logistic sigmoid

- A useful function that we are going to consider

$$\sigma(x) = \frac{1}{1 + \exp(-x)}$$

- The Logistic (sigmoid) function is commonly used to parametrize Bernoulli distributions.



Bayes' rule

- Suppose know $P(\mathrm{y} \mid \mathrm{x})$, but we actually need $P(\mathrm{x} \mid \mathrm{y})$. If we know $P(\mathrm{x})$ then we can compute

$$P(\mathrm{x} \mid \mathrm{y}) = \frac{P(\mathrm{y} \mid \mathrm{x})P(\mathrm{x})}{P(\mathrm{y})}$$

  Although it appears in the formula prior knowledge $P(\mathrm{y}$ is not needed since usually it can be computed as $\sum_{\mathrm{x}} P(\mathrm{y} \mid \mathrm{x})P(\mathrm{x})$

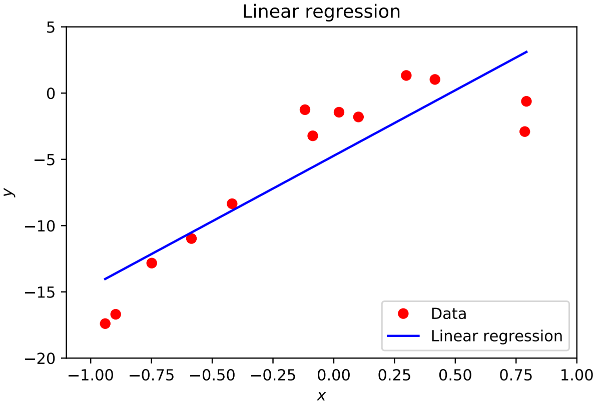
- It can be straightforwardly derived from the conditional probability formula.
- It could have be named also after Laplace who independently found it, generalized it, and introduced it in practice.

Model capacity, underfitting and overfitting

Materials:

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

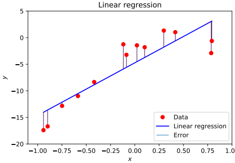
Linear regression

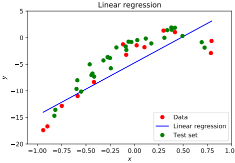


$$\hat{y} = \hat{w}_0 + \sum_{i=1}^{n} x_i \hat{w}_i$$
$$\hat{y} = \boldsymbol{x}^T \hat{\boldsymbol{w}}$$

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.
- During the training (learning) we aim at reducing the training error.
- If that is the end goal, we only have an optimization problem, not a machine learning one.





Generalization error

- **Generalization error**, also called **test error** is defined as the expected error on new, previously unseen data.
- Unlike in simple optimization, in machine learning our main goal is to minimize the **generalization error**.
- Usually the generalization error is estimated by measuring the performance on a **test data set** which must be independent from the training set.

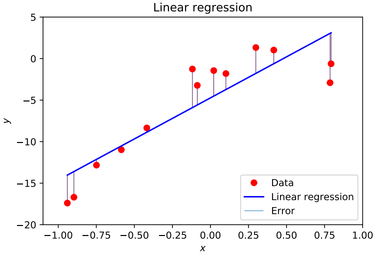
Example: Linear regression

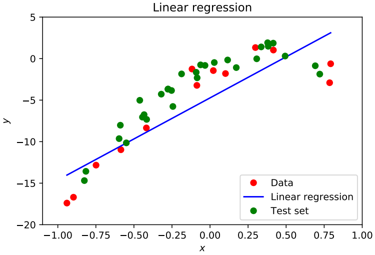
- Previously, we trained the model by minimizing the training error

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

- 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.

Discussion point 3

Can you name a scenario in medical image analysis practice where the i.i.d. assumptions are bound to be broken?

Underfitting and overfitting

- The factor that determines how well a machine algorithm will perform is its ability to
  1. Make the training error small.
  2. Make the difference between the training and test error small.
- These two factors correspond to the two central challenges in machine learning: **underfitting** and **overfitting**.
- Underfitting occurs when the model is not able to produce a sufficiently small training error.
- Overfitting occurs when the gap between the training and test errors is too large.

Model capacity

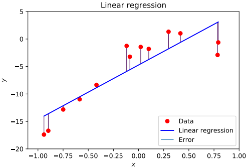
- A **capacity of the model** is its ability to fit a wide variety of functions.
- Low capacity models struggle to fit the training set (underfitting).
- Models with high capacity have danger to overfit the training data (e.g., by "memorizing" training samples).
- The capacity can be controlled by choosing 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.

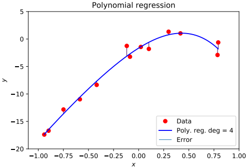
Polynomial regression

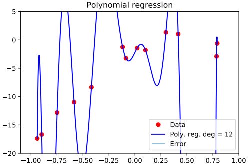
- The linear regression algorithm can be generalized to include all polynomial functions instead of just the linear ones.
- The linear regression model is then just a special case restricted to a polynomial of degree one: $\hat{y} = b + wx$.
- Moving to degree two to we obtain: $\hat{y} = b + w_1x + w_2x^2$.
  - 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.: $\hat{y} = b + w_1x + w_2 \sin(x) + w_3\sqrt{x}$.
- 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

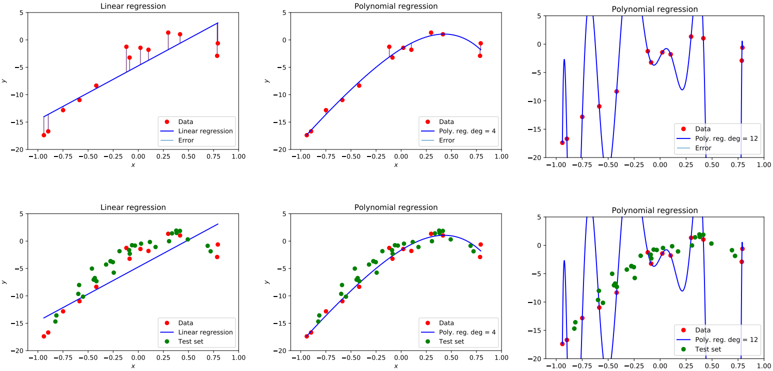






Polynomial regression

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



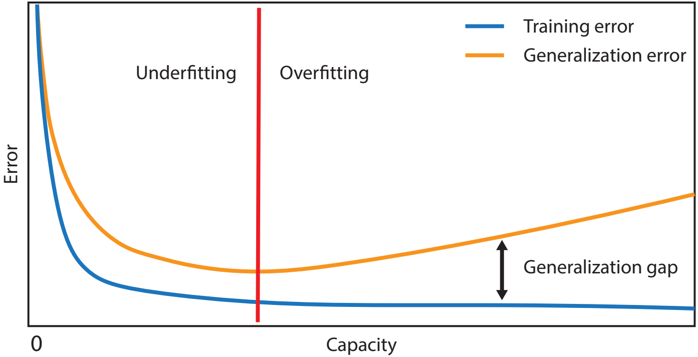
Overfitting and underfitting in polynomial estimation

- Models with low capacity are not up to the task.
- Models with high-capacity can solve a complex task, but when the capacity is too high for the concrete (training) task there is the danger of overfitting.
- In our example: the linear function is unable to capture the curvature so it undefits.
- The degree-12 predictor is capable of fitting the training data, but it also able to find infinitely many functions that pass through the same points, so it has high probability of overfitting.
- The degree-4 function is the right solution and it generalizes well on the new data.

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(see next slide).

Generalization and capacity



Training set size

- Training and generalization error vary as the size of the training data set varies.
- Expected generalization error never increases as the size of the training set increases.
- Any fixed parametric model will asymptotically approach an error value that exceeds the so called Bayes error.
- It is possible for the model to have optimal capacity and still have a large gap between training and generalization errors.
- In that case the gap usually can be reduced with increasing the number of training examples.

Training set size

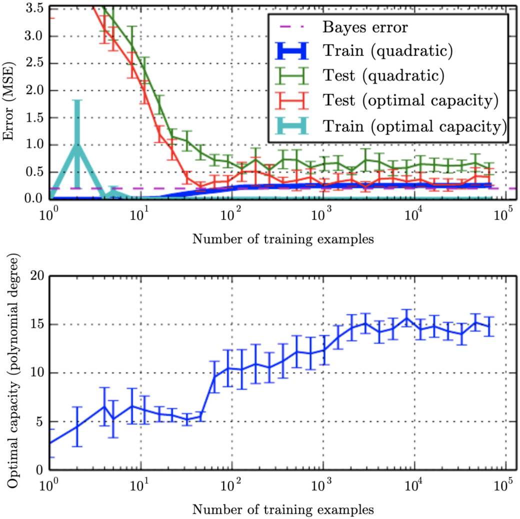


Figure from Goodfellow et al., *Deep Learning*

The No Free Lunch theorem

- **No Free Lunch Theorem** for machine learning (Wolpert, 1996):
  Averaged over all possible data-generating distributions every classification algorithm has the same error rate when tested on new unobserved data.
- In some sense, no machine algorithm is universally better than any other algorithm.
- An interesting, but mainly theoretical result.
- In practice we often have an information about the probability distributions we deal with and can tailor our algorithms to perform well with particular distributions.

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.

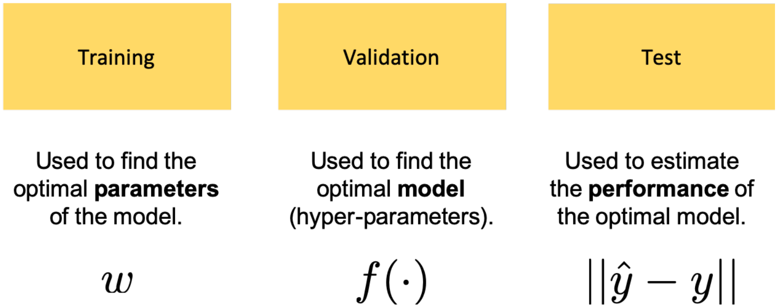
Choice of training, validation, and test sets

- 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.
- One subset is used to learn the parameters of the algorithm and the other is the validation set.
- The subset used to learn the parameters is still typically called a **training set**.

Choice of training, validation, and test sets

- Since the validation set is used to determine the hyperparameters it will typically underestimate the generalization error.
- However, it will usually better predict the generalization error than the training set.
- After the completion of the hyperparameters optimization we can estimate the generalization error using the test data.
- In practice the testing should be done also on different test data to avoid the test data becoming “stale”.

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	$f(\cdot)$	$\|\|\hat{y} - y\|\|$

Discussion point 4

How large should the training, validation and testing datasets be as a percentage (%) of the total available data?

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**.

Cross-validation

- The original data is partitioned into k (disjoint) subsets.
- The average error can be estimated by taking the average over k trials.
- In trial i, the i-th subset is used as test set and the rest as training set.
- Problem: no unbiased estimators of the variance of such average error exist, but there are approximations that are used in practice.

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.
- It can also be a whole function, e.g., the linear function or polynomial of some degree, like in the polynomial regression.

Point estimation

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

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

- 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.

Function estimation

- In **function estimation**, we assume that there is a (true) function that describes the (approximate) relationship between $\boldsymbol{x}$ and $\boldsymbol{y}$

$$\boldsymbol{y} = f(\boldsymbol{x}) + \epsilon$$

  where ϵ is the part of $\boldsymbol{y}$ which is not predictable from $\boldsymbol{x}$
- The goal is to find the **function estimate** (**model**) $\hat{f}$ which is a good approximation of f.
- The linear regression and polynomial regression can be seen both illustrate scenarios that can be interpreted as either estimating a parameter $\boldsymbol{w}$ or estimating a function $\hat{f}$.

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

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

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 $\mathrm{Var}(\hat{\theta})$ over the training set as a random variable.
- Alternatively we can compute the **standard error** (the square root of the variance) $\mathrm{SE}(\hat{\theta})$.
- 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.

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

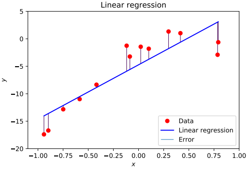
- The smaller MSE the better - so minimizing both the bias and variance is always preferable.

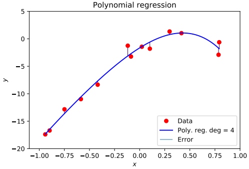
Bias and variance

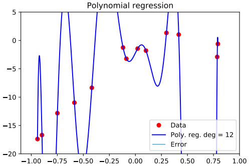
- Our original goal was to provide a mathematical support for the notions of capacity, underfitting, and overfitting.
- Indeed there is a close relationship between these three concepts and bias and variance.
- When generalization error is measured by MSE (and hence indirectly via bias and variance) 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

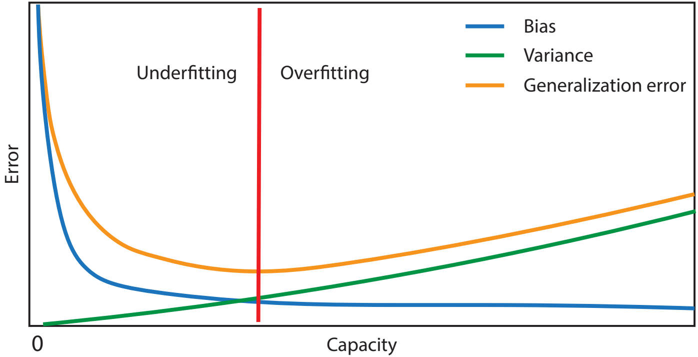
How will the estimated regression model change when one training data point is replaced with another one?







Bias and variance



Consistency

- So far we considered fixed size of the training data sets.
- We expect that as the number m of training examples grows the estimators will converge to the true value of the parameters.
- More formally this is captured in the notion of **consistency**

  $$\text{plim}_{m\to\infty}\hat{\theta}_m = \theta$$

  where plim denotes convergence in probability: for any $\epsilon > 0$, $P(\mid \hat{\theta}_m - \theta \mid > \epsilon) \to 0$ as $m \to \infty$.
- For consistent models the bias decreases as m increases, however a decreasing bias (when m increases) does not imply consistency.

Maximum likelihood estimation

Materials:

- Chapter I.5.5 from Goodfellow et al., *Deep Learning*

Maximum likelihood estimation

- We would like to have some principle from which we can derive good estimator functions for a large scale of models.
- The **maximum likelihood estimation** is the most common such principle.
- Given observation data and a corresponding (statistical) model our goal is to find the parameter vector which imply the highest probability to obtain the data.

Maximum likelihood estimation

- Consider a set of m examples $\mathbb{X} = \{\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \dots, \boldsymbol{x}^{(m)}\}$ drawn independently from the true but unknown distribution $p_{\text{data}}(\mathbf{x})$.
- Let $p_{\text{model}}(\mathbf{x}; \boldsymbol{\theta})$ be a parametric family of probability distributions, i.e., for each $\boldsymbol{\theta}$ we get a different distribution p_{model}.
- $p_{\text{model}}(\boldsymbol{x}; \boldsymbol{\theta})$ maps any configuration $\boldsymbol{x}$ to a real number estimating the (true) probability $p_{\text{data}}(\boldsymbol{x})$

Maximum likelihood estimation

- The maximum likelihood estimator for $\boldsymbol{\theta}$ is then defined as

$$\boldsymbol{\theta}_{\mathrm{ML}} = \mathrm{argmax}_{\boldsymbol{\theta}} p_{\mathrm{model}}(\mathbb{X}; \boldsymbol{\theta}) = \mathrm{argmax}_{\boldsymbol{\theta}} \prod_{i=1}^{m} p_{\mathrm{model}}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta})$$

  Note that also the empirical distribution $\hat{p}_{\mathrm{data}}$ is implicitly present in the formula through $\boldsymbol{x}^{(i)}$.

- A more convenient equivalent optimization problem is obtained by taking logarithm of the product

$$\boldsymbol{\theta}_{\mathrm{ML}} = \mathrm{argmax}_{\boldsymbol{\theta}} p_{\mathrm{model}}(\mathbb{X}; \boldsymbol{\theta}) = \sum_{i=1}^{m} \log p_{\mathrm{model}} \boldsymbol{x}^{(i)}; \boldsymbol{\theta})$$

Maximum likelihood estimation

- We can further rescale by dividing the expression by m

$$\boldsymbol{\theta}_{\mathrm{ML}} = \mathrm{argmax}_{\boldsymbol{\theta}} p_{\mathrm{model}}(\mathbb{X};\boldsymbol{\theta})$$

$$\boldsymbol{\theta}_{\mathrm{ML}} = \mathrm{argmax}_{\boldsymbol{\theta}} \mathbb{E}_{\mathbf{x}\sim\hat{p}_{\mathrm{data}}} \log p_{\mathrm{model}}(\boldsymbol{x};\boldsymbol{\theta})$$

- In this way the problem is expressed as an equivalent expectation problem (now the empirical distribution $\hat{p}_{\mathrm{data}}$ becomes explicit).

Maximum likelihood estimation

- Perhaps more straightforwardly, the maximum likelihood estimation can be seen as minimizing the dissimilarity between $\hat{p}_{\text{data}}$ and p_{model}.
- The degree of dissimilarity is given by the KL-divergence

$$D_{\text{KL}}(\hat{p}_{\text{data}} \| p_{\text{model}}) = \mathbb{E}_{\mathbf{x} \sim \hat{p}_{\text{data}}} [\log \hat{p}_{\text{data}}(\boldsymbol{x}) - \log p_{\text{model}}(\boldsymbol{x})]$$

- Only the term of the right is function of the model, so it is the only one which needs to be minimized

$$-\mathbb{E}_{\mathbf{x} \sim \hat{p}_{\text{data}}} [\log p_{\text{model}}(\boldsymbol{x})]$$

  which is equivalent with the maximization problem from the previous slide.
- It boils down to minimizing the **cross-entropy** between the two distributions.

Maximum likelihood estimation

- **The maximum likelihood estimation can be seen as an attempt to make the model distribution** p_{model} **to match the empirical distribution** $\hat{p}_{\text{data}}$.
- Ideally we would like to match the data generating distribution p_{data}, but we do not have access to it.

Conditional log likelihood and mean square error

- The maximal likelihood estimator can be generalized to estimate a conditional probability $P(\mathbf{y} \mid \mathbf{x}; \boldsymbol{\theta})$.
- Let all inputs be given by $\boldsymbol{X}$ and all observed outputs by $\boldsymbol{Y}$. Then the conditional maximum likelihood estimator is

$$\boldsymbol{\theta}_{\mathrm{ML}} = \arg\ \max_{\theta} P(\boldsymbol{Y} \mid \boldsymbol{X}; \boldsymbol{\theta})$$

- If the examples are assumed to be i.i.d., then this can be decomposed into

$$\boldsymbol{\theta}_{\mathrm{ML}} = \arg\ \max_{\theta} \sum_{i=1}^{m} \log P(\boldsymbol{y}^{(i)} \mid \boldsymbol{x}^{(i)}; \boldsymbol{\theta})$$

Example: linear regression as maximum likelihood

- The linear regression seen as an algorithm that learns to take an input $\boldsymbol{x}$ and produce output $\hat{y}$.
- This function from $\boldsymbol{x}$ to $\hat{y}$ is chosen to minimize the mean squared error.
- This criterion was introduced more or less arbitrarily.
- We revisit linear regression from the point of view of maximal likelihood.
- We think of the model as producing a conditional distribution $p(y \mid \boldsymbol{x})$ instead of a single prediction $\hat{y}$.

Example: linear regression as maximum likelihood

- With an infinitely large training set we might see several examples whit the same input $\boldsymbol{x}$ but different y.
- The learning algorithm needs to fit the distribution to all these y corresponding to the same $\boldsymbol{x}$.
- To derive the linear regression algorithm we assume $p(y \mid \boldsymbol{x}) = \mathcal{N}(y; \hat{y}(\boldsymbol{x}; \boldsymbol{w}), \sigma^2)$, where $\hat{y}(\boldsymbol{x}; \boldsymbol{w})$ gives the (prediction of the) mean of the normal distribution and σ is fixed to some chosen constant.
- The parameter vector θ corresponds in this case to $\boldsymbol{w}$.

Example: linear regression as maximum likelihood

- By substituting (the full Gaussian function version of) $p(y \mid \boldsymbol{x})$ in the conditional log-likelihood formula we obtain

$$\sum_{i=1}^{m} \log p(\boldsymbol{x}^{(i)} \mid y^{(i)}; \boldsymbol{\theta}) = -m \log \sigma - \frac{m}{2} \log(2\pi) - \sum_{i=1}^{m} \frac{\left\| \hat{y}^{(i)} - y^{(i)} \right\|^2}{2\sigma^2}$$

  where $\hat{y}^{(i)}$ is the linear regression on the i-th input $\boldsymbol{x}^{(i)}$.

- By comparing with the mean squared error

$$\mathrm{MSE}_{\mathrm{train}} = \frac{1}{m} \sum_{i=1}^{m} \left\| \hat{y}^{(i)} - y^{(i)} \right\|^2$$

  one can see that maximizing the log-likelihood with respect to $\boldsymbol{w}$ results with the same estimate of $\boldsymbol{x}$ as minimizing MSE. (The third term in the log-likelihood forumula, needs to be as small as possible.)

Properties of maximum likelihood

- It can be shown that the maximum likelihood estimator is the best asymptotically, i.e. as $m \to \infty$, in terms of its convergence rate.
- **Property of consistency**: as the number of training examples approaches infinity the maximum likelihood estimate of a parameter converges towards the true parameter value.
- The maximum likelihood estimator has the property of consistency provided:
    - The true distribution p_{data} is in the model family $p_{\text{model}}(\cdot; \boldsymbol{\theta})$
    - p_{data} corresponds to exactly one value of $\boldsymbol{\theta}$

Model evaluation

Materials:

- Fawcett, “An introduction to ROC analysis”

Model evaluation

- To quantitatively evaluate a machine learning algorithm we need to define a **performance measure**.
- Usually the performance measure is specific to the task carried out by the algorithm.
- For classification tasks a natural measure is the model **accuracy**.
- The **accuracy** is defined as the proportion of examples for which the model produces the correct output.
- An equivalent (complementary) measure is the **error rate** defined as the proportion of incorrect outputs.

Model evaluation

- The best way to evaluate a machine learning algorithm is by applying it to a **test set** data which has not been seen before.
- Ideally there should be **no overlap** between the **test set** and the **training set** used to obtain the model.

Binary classification

- We consider **binary classification** problems, i.e., problems using only two classes/
- Formally each input example $x^{(i)}$ needs to be mapped into one element of the set $\{\boldsymbol{p}, \boldsymbol{n}\}$ of **true** classes.
- A **classification model** (**classifier**) is a function from the input examples to the set $\{\boldsymbol{Y}, \boldsymbol{N}\}$ of **predicted classes** or **hypothesized classes**.
- $\boldsymbol{p}, \boldsymbol{n}$ correspond to $\boldsymbol{Y}, \boldsymbol{N}$, respectively.

Binary classification

- For a given classifier there are four possible outcomes.
- If the true class of $x^{(i)}$ is $\boldsymbol{p}$ and the predicted class is $\boldsymbol{Y}$ then we have a **true positive** (TP); if it was classified $\boldsymbol{N}$, then we have a **false negative** (FN).
- Symmetrically, a $x^{(i)}$ with true class $\boldsymbol{n}$ which is assigned a predicted class $\boldsymbol{N}$ is a **true negative** (TN); if the predicted class is $\boldsymbol{Y}$, then it is a false positive (FP).

Confusion matrix

These four combinations can be put together in a **confusion matrix**, also called **contingency table**.

		True class	
		p	***n***
Predicted class	***Y***	True positives (TP)	False positives (FP)
	N	False negatives (FN)	True negatives (TN)

Binary classifications metrics

- Using the four basic categories of prediction outcomes (TP, FP, TN, FN) we can derive various **measures** of performance of classification models.
- For instance the accuracy can be defined as

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

- Also quite frequently used measures are

$$Sensitivity = \frac{TP}{TP + FN} \quad Specificity = \frac{TN}{TN + FP} \quad Precision = \frac{TP}{TP + FP}$$

Binary classification metrics

- Sensitivity is also called **recall**, **true positive rate** or **hit rate**.
- In medical contexts the sensitivity can be interpreted as a measure of the extent to which diseased individuals are correctly diagnosed.
- In general: measures the proportion of the target group the method is able to detect, i.e. how sensitive is to this group.
- Specificity is also called **true negative rate** or **selectivity**.
- In medical contexts the specificity can be interpreted as a measure of the extent to which healthy individuals are correctly diagnosed.
- The precision tells us which proportion of the positive predictions is correct.

Discussion point 6

You have developed a method for some image analysis diagnostic task that has very high sensitivity (e.g. 0.99) but relatively low specificity (e.g. 0.25).
Can this be still a useful tool for clinicians and if so in what context?

Binary classification metrics

- Sometimes the above mentioned measures are not sufficient.
- For example, in a population in which the percentage of healthy individuals is much larger than the diseased individuals, it is easy to achieve high specificity by trivially classifying each patient as healthy.
- We can obtain more objective evaluation by combing metrics.
- The metrics F_1 is the harmonic mean (average) of the precision and recall (sensitivity)

$$\frac{2}{F_1} = \frac{1}{Precision} + \frac{1}{Recall} \text{ or } F_1 = 2 \cdot \frac{Precision \cdot Recall}{Precision + Recall}$$

Areas under the curve measures

- (Binary) classifications often depend on some parameter (e.g., threshold).
- Hence on way to combine two metrics is by assigning them to the axes of a coordinate system and varying this parameter to construct a graphical plot.
- We obtain a curve (actually, most of the time series of points) such that each point corresponds to a particular parameter value.
- The area under the curve is a measure of how good is the classification.

Receiver Operating Characteristic (ROC) curve

- The ROC curve plots the true positive rate (sensitivity) versus the false positive rate (1 - specificity).

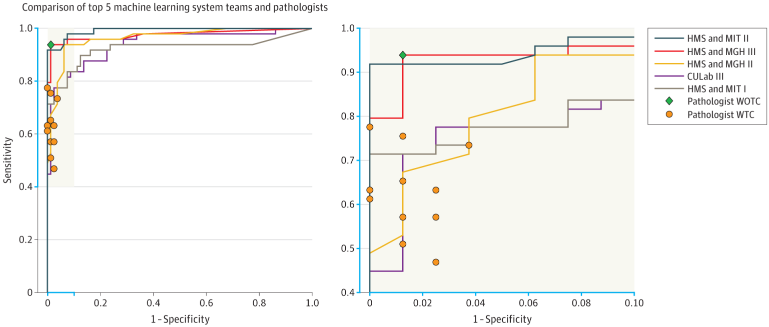


Figure from Bejnordi et al., “Diagnostic assessment of deep learning algorithms for detection of lymph node metastases in women with breast cancer”

Receiver Operating Characteristic (ROC) curve

- There are several characteristic points points in the ROC space:
  - (0,0) corresponds to the strategy of never making a positive classification.
  - (1,1) is the opposite: unconditionally issuing a positive classification.
  - (0,1) represents perfect classification.
  - Obviously we strive to achieve this ideal point as as a result have as much as possible area under the curve covered (ideally it should cover the whole square corresponding to the ROC space)
- A less common example of a measure combination into a graphical plot is the precision-recall plot (recall on the *x*-axis, precision on the *y*-axis).

Supervised and unsupervised learning algorithms

Materials:

- Chapters I.5.6 and I.5.7 from Goodfellow et al., *Deep Learning*

Supervised learning algorithms

- Learning algorithms that learn based on a given training examples $\boldsymbol{x}$ and their corresponding outputs $\boldsymbol{y}$.
  - Linear and logistic regressions
  - Support vector machines
  - k-nearest neighbours
  - Decision trees

Unsupervised learning algorithms

- Unsupervised algorithms experience only "features", but not supervision feedback.
- The distinction with the supervised algorithms is not always clear since there is no good test to distinguish if something is a feature or a target provided by the supervisor.
- Rule of thumb: in unsupervised algorithms no human annotation is needed for the training examples.
  - Principal component analysis
  - *k*-means clustering
  - t-Distributed Stochastic Neighbor Embedding
  - Generative adversarial networks

Ensambling

Materials:

- Chapter II.7.11 from Goodfellow et al., *Deep Learning*

Bagging and other ensemble methods

- **Bagging** (short for **b**ootstrap **agg**regat**ing**) is a technique for reducing of the generalization error by combining several models.
- Train models separately and let them vote on the right output.
- An example of a general strategy in machine learning called **model averaging**.
- Methods using this strategy are called *ensemble methods*.
- The rationale behind the combining of models is that usually different models will not make the same error.

Bagging

- Different ensemble methods compose the ensemble of models in different ways.
- One way would be to choose the models, training algorithms and objective functions as different as possible.
- In contrast, begging allows the same kind of model, algorithm and objective function to be reused several times.

Bagging

- Bagging constructs *k* different data sets.
- Each data set
  - has the same size as the original set and
  - is constructed by sampling with repetition from the original data set
- For each data set a different model is produced.
- Each model reflects the differences between the (training) data sets.

Bagging example

Training an “8 detector” with two resampled datasets: a “cartoon” example.

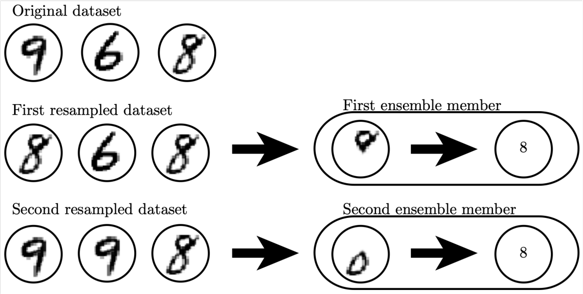


Figure from Goodfellow et al., *Deep Learning*

Model averaging for neural networks

- Neural networks profit from model averaging even when they are trained on the same data set.
- This is because with random initialization, minibatches (subsets of the training set), hyperparameters, non-determinism in the implementation a sufficient variety between the models can be achieved.

Model averaging in general

- In general, it is considered that model averaging always improves the generalization error.
- In theory, with sufficient computer memory and time one can always improve the results by combining several methods.
- Therefore, when testing/benchmarking (new) methods it is considered "fair" to use only a single model.
- Machine learning contests are usually won by using model averaging.
- **Boosting** is similar to ensembling, only the models (neural networks) are added **incrementally** to the ensemble.

In summary...

EXAMPLES
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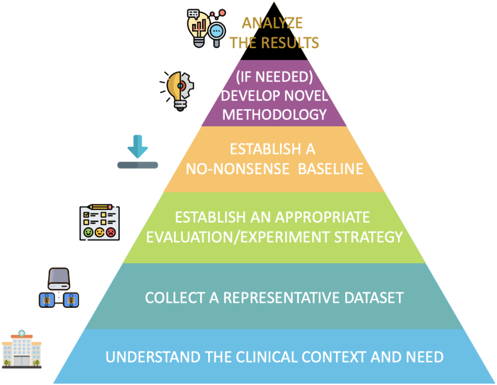
ANALYZE THE RESULTS
(IF NEEDED) DEVELOP NOVEL METHODOLOGY
ESTABLISH A NO-NONSENSE BASELINE
ESTABLISH AN APPROPRIATE EVALUATION/EXPERIMENT STRATEGY
COLLECT A REPRESENTATIVE DATASET
UNDERSTAND THE CLINICAL CONTEXT AND NEED

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

Acknowledgements

The slides for this lecture were prepared by Mitko Veta and Dragan Bošnacki.
Some of the slides are based on the accompanying lectures of Goodfellow et al., *Deep Learning*.

References

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