Machine learning foundations I

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2021

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.

Overview

Topics covered in this lecture:

1. Linear algebra

2. Gradient-based optimization

3. Two simple machine learning models
   Linear model
   Nearest-neighbours model

4. Probability theory

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

$$
\begin{aligned}
A_{1,1}x_1 + A_{1,2}x_2 + \ldots + A_{1,n}x_n &= b_1 \\
A_{2,1}x_1 + A_{2,2}x_2 + \ldots + A_{2,n}x_n &= b_2 \\
&\ldots \\
A_{m,1}x_1 + A_{m,2}x_2 + \ldots + A_{m,n}x_n &= b_m
\end{aligned}
$$

- $A_{*,*}$ 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

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

- $\boldsymbol{U}$ and $\boldsymbol{V}$ are square matrices and are both orthogonal, $\boldsymbol{D}$ is diagonal.
- The diagonal elements of D are called **singular values** of matrix $\boldsymbol{A}$; the columns of $\boldsymbol{U}$ and $\boldsymbol{V}$ are **left-singular** and **right-singular vectors** of $\boldsymbol{A}$, 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 $\|\boldsymbol{x}\|_n = 1$
- 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

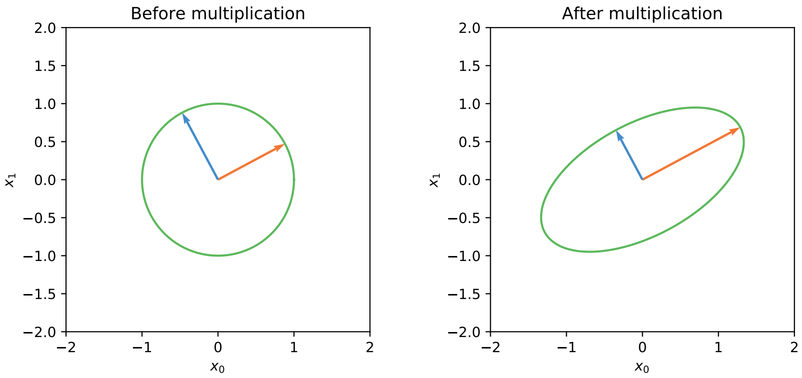
$$\boldsymbol{A} = \boldsymbol{V}\mathrm{diag}(\lambda)\boldsymbol{A}^{-1}$$

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.

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

Gradient-based optimization

Materials:

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

Gradient

- 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 case when A is a vector we obtain the (possibly more familiar) 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**

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

    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

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

Discussion point

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

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

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

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

Linear model fit by least squares

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

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

.

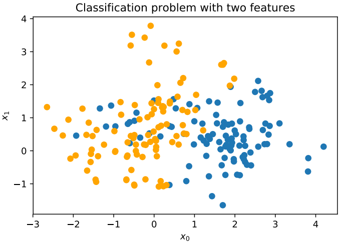
- This is called "making a prediction" for $\boldsymbol{x}_i$.
- The entire fitted surface (hyperplane) is fully characterized by the parameter vector $\hat{\boldsymbol{w}}$.
- After fitting the model, we can "discard" the training dataset.

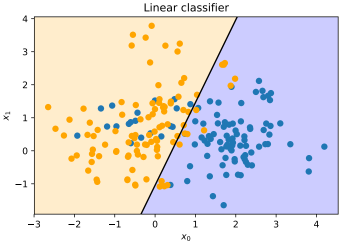
Example: Linear model fit by least squares

- 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





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).

Discussion point

What is the expression for the Euclidean distance between two vectors (points) **a** and **b** in vector form?

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

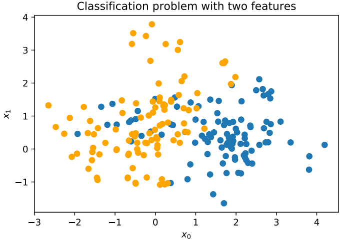
$$\hat{y}(\boldsymbol{x}) = \frac{1}{k} \sum_{\boldsymbol{x}_i \in N_k(\boldsymbol{x})} y_i$$

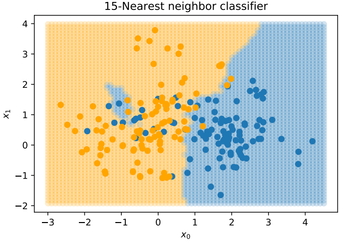
  where $N_k(\boldsymbol{x})$ is the neighbourhood of $\boldsymbol{x}$ consisting of the k "closest" points to $\boldsymbol{x}$.
- "Closeness" requires a definition of **metrics**.
- For the moment we assume Euclidian distance (each $\boldsymbol{x}$ is a point in the hyperspace).
- An average of the classes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

Back to the BLUE and ORANGE example

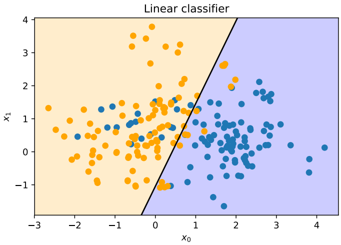
- We use the same training data as in the linear model example.
- New borderline between the classes generated with 15-nearest-neighbour model.
- Since ORANGE is encoded as 1 $\hat{y}$ is the proportion of ORANGE points in the 15-neighbourhood.
- Class ORANGE assigned to $\boldsymbol{x}$ if $\hat{y}(\boldsymbol{x})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

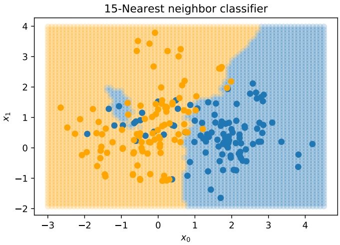
15-Nearest neighbour classifier



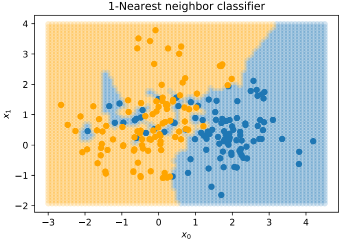


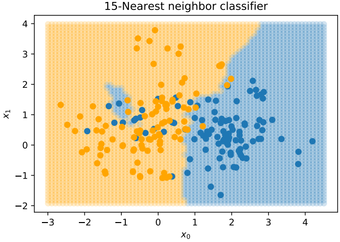
Linear classifier vs. 15-Nearest neighbour





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

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:

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

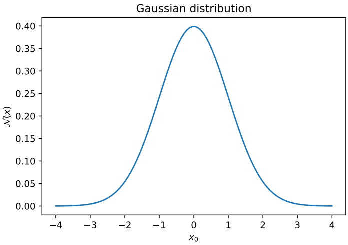
Gaussian distribution

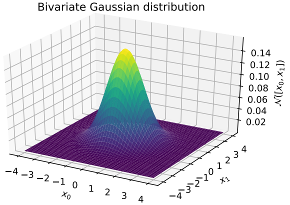
- The most commonly used distribution, also called **normal distribution**.
- Controlled by two parameters $\mu \in \mathbb{R}$ (the **mean**) and $\sigma \in (0, \infty)$, (the **standard deviation**)

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

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

Gaussian distribution



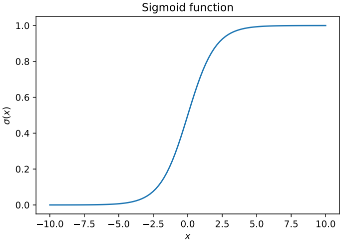


Logistic sigmoid

- 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.

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*.

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