

Machine learning foundations I

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Learning goals

At the end of this lecture you will:

- ▶ Have an understanding of the goal of machine learning (ML) models.
- ▶ Have a good understanding of basic mathematical concepts used in ML and be able to apply them in the design and implementation of ML methods.

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 (self-study)

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 1.2 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, ...)

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

- ▶ Example notation for type and size

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

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

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

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

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

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

Identity matrix

- ▶ Identity matrix 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.

$$\forall \mathbf{x} \in \mathbb{R}^n : I_n \mathbf{x} = \mathbf{x} I_n = \mathbf{x}$$

Matrix (dot) product

$$\mathbf{C} = \mathbf{AB}$$

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

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

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

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

Matrix (dot) product

- ▶ In general matrix multiplication is not commutative, i.e., most of the time $\mathbf{AB} \neq \mathbf{BA}$.
- ▶ Depending on the dimensions sometimes \mathbf{AB} or \mathbf{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

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

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

...

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

- ▶ $A_{*,*}$ and b_* are the knowns, x_* are the unknowns.
- ▶ In matrix form: **$A\mathbf{x} = \mathbf{b}$**

Systems of linear equations

► $\mathbf{Ax} = \mathbf{b}$ expands to

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

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

...

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

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

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

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

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

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

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

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

- ▶ 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 not square.
- ▶ The **Moore-Penrose pseudoinverse** is defined as

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

Moore-Penrose pseudoinverse

Now we can consider

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

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

Singular value decomposition

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

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

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

Computing the pseudoinverse

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

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

- ▶ \mathbf{U} , \mathbf{D} , \mathbf{V} are from the singular value decomposition of \mathbf{A} .
- ▶ The pseudoinverse \mathbf{D}^+ of \mathbf{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
 - ▶ $f(\mathbf{x}) = 0 \Rightarrow \mathbf{x} = 0$
 - ▶ $f(\mathbf{x} + \mathbf{y}) \leq f(\mathbf{x}) + f(\mathbf{y})$ (**the triangle inequality**)
 - ▶ $\forall \alpha \in \mathbb{R} : f(\alpha \mathbf{x}) = \alpha f(\mathbf{x})$

Norms

- ▶ L^p - norm

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

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

Special vectors and matrices

- ▶ Unit vector $\|\mathbf{x}\|_n = 1$
- ▶ Symmetric matrix $\mathbf{A} = \mathbf{A}^T$
- ▶ Orthogonal matrix

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

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

Eigendecomposition

- ▶ Eigenvector and eigenvalue

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

- ▶ Eigendecomposition of a matrix

$$\mathbf{A} = \mathbf{V}\text{diag}(\lambda)\mathbf{A}^{-1}$$

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

Eigendecomposition

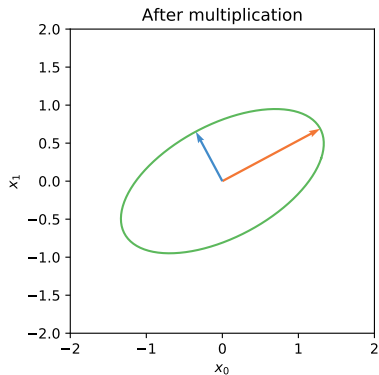
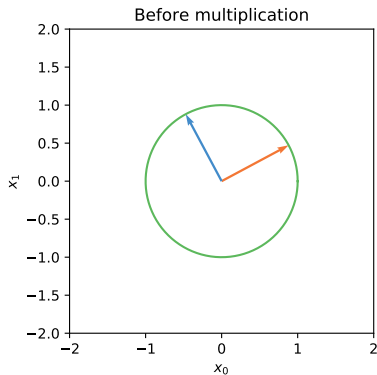
- ▶ Every real symmetric matrix has a real orthogonal eigendecomposition

$$\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T$$

where \mathbf{Q} is an orthogonal matrix composed of eigenvectors of \mathbf{A} and $\mathbf{\Lambda}$ is a diagonal matrix.

- ▶ The eigenvalue Λ_{ii} is associated with the eigenvector in column i of \mathbf{Q} , denoted as $\mathbf{Q}_{:,i}$.
- ▶ We can think of \mathbf{A} as scaling space by factor λ_i in the direction of its corresponding eigenvector $\mathbf{v}^{(i)}$ (represented by $\mathbf{Q}_{:,i}$).

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 $f(\mathbf{x}) = \mathbf{x}^T \mathbf{A} \mathbf{x}$ under the constraint $\|\mathbf{x}\|_2 = 1$.
- ▶ For instance, if $\mathbf{x} = \mathbf{v}^{(i)}$, then $f(\mathbf{x}) = \lambda_i$, when $\mathbf{v}^{(i)}$ 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.

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

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

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

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

Gradient-based optimization

Materials:

- ▶ Chapters 1.4 and 1.5 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 \mathbf{A} as input and returns a real number (scalar).
- ▶ A **gradient** of f with respect to A is the matrix

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

- ▶ i.e. an $m \times n$ matrix with

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

- ▶ The size of the gradient of \mathbf{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

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

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

Jacobian

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

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

- ▶ 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 $f(\mathbf{x})$, i.e. finding the values of \mathbf{x} for which $f(\mathbf{x})$ has a minimum or a maximum.
- ▶ Notation: $\mathbf{x}^* = \operatorname{argmin} f(\mathbf{x})$

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 \mathbf{x} (vector).
- ▶ The i -th component of a vector input \mathbf{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 \mathbf{X} for instance, a set of N input p -vectors \mathbf{x}_i ($1 \leq i \leq N$) is "packed" in a $N \times p$ input matrix \mathbf{X} .
- ▶ Since by default vectors are assumed to be column vectors, the rows of \mathbf{X} are the transposes \mathbf{x}_i^T .

The learning task

- ▶ Given a value of the input vector \mathbf{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 (\mathbf{x}_i, y_i) or (\mathbf{x}_i, g_i) ($1 \leq i \leq N$) called **training data** (in matrix form: (\mathbf{X}, \mathbf{y}) and/or (\mathbf{X}, \mathbf{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. $\mathcal{G} = \{\text{BLUE}, \text{ORANGE}\}$.
- ▶ **Encoding of g s with y s:** 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 $\mathbf{x}^T = (x_1, x_2, \dots, x_p)$
- ▶ 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

$$\hat{y} = \hat{\mathbf{w}}^T \mathbf{x} = \mathbf{x}^T \hat{\mathbf{w}}$$

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

Linear model fit by least squares

Some hyper(space) terminology:

- ▶ Points \mathbf{x}, \hat{y} form a **hyperplane** in the $(p + 1)$ -dimensional input-output hyperspace.
- ▶ If \mathbf{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 \mathbf{x} and \hat{w}_0 in $\hat{\mathbf{w}}$.
- ▶ The function $f(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$ defined on the p -dimensional (input) space is a **linear** function (we omit the hats over the \mathbf{w} s since now we consider them as free variables).
- ▶ The gradient $\nabla f(\mathbf{x})$ 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**

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

assuming N input-output pairs.

- ▶ $\text{RSS}(\mathbf{w})$ 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 $\hat{\mathbf{w}}$ using the matrix notation:
- ▶ $\mathbf{y} = [y_1, y_2, \dots, y_N]^T$ is the vector formed from the N output vectors and \mathbf{X} is an $N \times p$ matrix

$$\text{RSS}(\mathbf{w}) = (\mathbf{y} - \mathbf{X}\mathbf{w})^T(\mathbf{y} - \mathbf{X}\mathbf{w})$$

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

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

Linear model fit by least squares

- ▶ To find the minimum our derivative must be **0**, hence:

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

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

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

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

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

Discussion point

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

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

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

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

Linear model fit by least squares

- ▶ For each input \mathbf{x}_i there corresponds the fitted output

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

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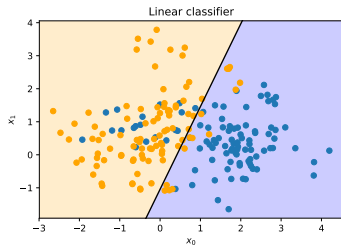
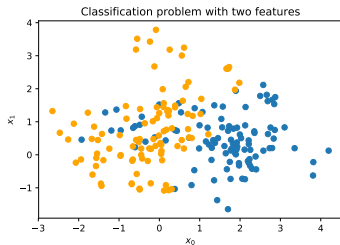
- ▶ This is called “making a prediction” for \mathbf{x}_i .
- ▶ The entire fitted surface (hyperplane) is fully characterized by the parameter vector $\hat{\mathbf{w}}$.
- ▶ After fitting the model, we can “discard” the training dataset.

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 $\{\mathbf{x} : \mathbf{w}^T \mathbf{x} = 0.5\}$
- ▶ $\{\mathbf{x} : \mathbf{w}^T \mathbf{x} < 0.5\}$ set of BLUE points
- ▶ $\{\mathbf{x} : \mathbf{w}^T \mathbf{x} \geq 0.5\}$ 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-neighbour methods $\hat{y}(\mathbf{x})$ is determined based on the inputs (points) in the training set \mathcal{T} which are "closest" to the input \mathbf{x} .
- ▶ k -nearest neighbour fit is defined as

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

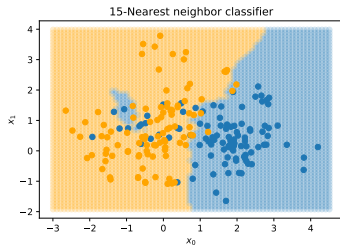
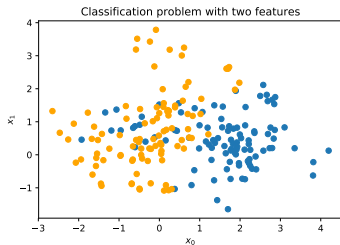
where $N_k(\mathbf{x})$ is the neighbourhood of \mathbf{x} consisting of the k "closest" points to \mathbf{x} .

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

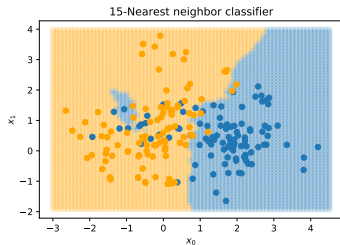
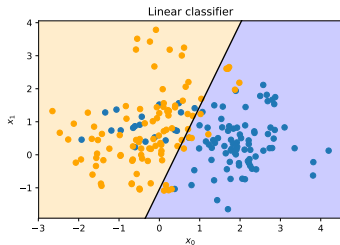
Back to the BLUE and ORANGE example

- ▶ 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 \mathbf{x} if $\hat{y}(\mathbf{x}) > 0.5$ (majority is ORANGE).

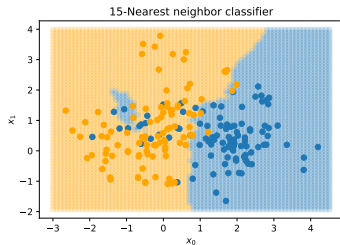
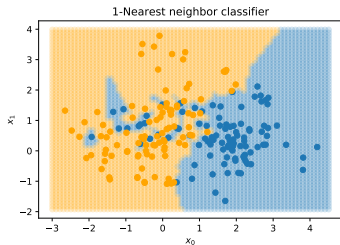
15-Nearest neighbour classifier



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 1.3 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 .
- ▶ $\forall x \in \mathcal{X} : 0 \leq P(x) \leq 1$
 - ▶ 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.
- ▶ $\sum_{x \in \mathcal{X}} P(x) = 1$
 - ▶ We say that x is **normalized**.
- ▶ Example: Uniform distribution: $P(x = x_i) = \frac{1}{k}$.

Probability density function

- ▶ The domain of the probability density function p must be the set of all possible states of x .
- ▶ $\forall x \in x : p(x) \geq 0$.



$$\int p(x) dx = 1$$

- ▶ 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

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

- ▶ Another way to see this formula is

$$P(x,y) = P(x = x)P(y = y \mid x = x)$$

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



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



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

- ▶ Linearity of expectations:

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

Variance and covariance

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

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

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

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

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

Covariance matrix

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

$$\text{Cov}(\mathbf{x})_{i,j} = \text{Cov}(x_i, x_j)$$

- ▶ The diagonal elements of the matrix give the variance

$$\text{Cov}(x_i, x_i) = \text{Var}(x_i)$$

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:

$$P(x = 1) = \phi$$

$$P(x = 0) = 1 - \phi$$

$$P(x = x) = \phi^x (1 - \phi)^{1-x}$$

$$\mathbb{E}_x[x] = \phi$$

$$\text{Var}(x) = \phi(1 - \phi)$$

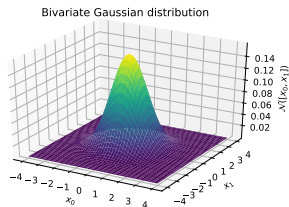
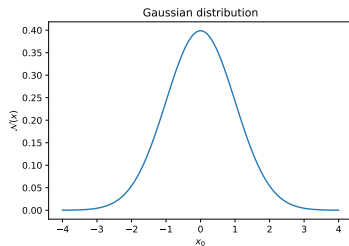
Gaussian distribution

- ▶ 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**)

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

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

Gaussian distribution

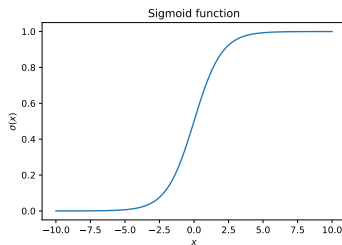


Logistic sigmoid

- ▶ 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 $P(y | x)$, but we actually need $P(x | y)$. If we know $P(x)$ then we can compute

$$P(x | y) = \frac{P(y | x)P(x)}{P(y)}$$

Although it appears in the formula prior knowledge $P(y)$ is not needed since usually it can be computed as $\sum_x P(y | x)P(x)$




- ▶ 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.

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