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
- Two simple machine learning models Linear model Nearest-neighbours model
- 4. Probability theory

Linear algebra

Materials:

- Chapter I.2 from deeplearning
- linearalgebra

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

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

Matrix (dot) product

$$C = AB$$

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 $AB \neq BA$.
- Depending on the dimensions sometimes AB or 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 equations

ightharpoonup Ax = b expands to

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

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

$$\boldsymbol{A}_{m,:}\boldsymbol{x}_m = \boldsymbol{b}_m \tag{4}$$

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

$$Ax = b$$
 $A^{-1}Ax = A^{-1}b$
 $I_nx = A^{-1}b$
 $x = A^{-1}b$

- ▶ 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").

Norms

- ▶ Norms are functions that measure how "large" a vector is.
- Similar to a distance between zero and the point represented by the vector
 - $f(x) = 0 \Rightarrow x = 0$
 - $f(x + y) \le f(x) + f(y)$ (the triangle inequality)

Norms

 $ightharpoonup L^p$ - 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): $\|x\|_1 = \sum_i |x_i|$
- Max norm (for infinite p): $||x||_{\infty} = \max_i |x_i|$

Special vectors and matrices

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

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

lacktriangle It follows that for orthogonal matrices $oldsymbol{A}^T = oldsymbol{A}^{-1}$

Eigendecomposition

► Eigenvector and eigenvalue

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

► Eigendomdecomposition of a matrix

$${m A} = {m V} {\sf diag}(\lambda) {m A}^{-1}$$

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

Eigendecomposition

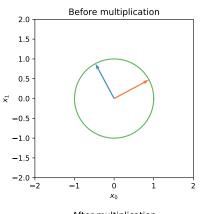
 Every real symmetric matrix has a real orthogonal eigendecomposition

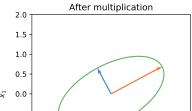
$$\mathbf{A} = \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^T$$

where $m{Q}$ is an orthogonal matrix composed of eigenvectors of $m{A}$ and $m{\Lambda}$ 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 \boldsymbol{A} as scaling space by factor λ_i in the direction of its corresponding eigenvector $\boldsymbol{v}^{(i)}$ (represented by $\boldsymbol{Q}_{:,i}$).

Effect of eigenvalues





Singular value decomposition

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

$$A = UDV^T$$

- ▶ 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.

Moore-Penrose pseudoinverse

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

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

Moore-Penrose pseudoinverse

Now we can consider

$$x = A^+ y$$

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

Computing the pseudoinverse

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

$$A^+ = VD^+U^T$$

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

Gradient-based optimization

Materials:

- Chapters I.4 and I.5 from deeplearning
- linearalgebra

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

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

 \triangleright 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 **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

$$abla_{m{x}}f(m{x}) = egin{bmatrix} rac{\partial f}{\partial x_1} \ rac{\partial f}{\partial x_2} \ rac{\partial f}{\partial x_m} \end{bmatrix}$$

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

Jacobian

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

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

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

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 **elements**

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 (x_i, y_i) or (x_i, g_i) $(1 \le i \le N)$ called **training data** (in matrix form: (X, y) and/or (X, 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 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 $\mathbf{x}^T = (x_1, x_2, \dots, x_p)$
- Output y predicted using the model

$$\hat{y} = \hat{w_0} + \sum_{j=1}^p x_j \hat{w_j}$$

- \hat{w}_i $(0 \le i \le p)$ 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 w and 1 is included in x.
- \hat{y} is a scalar, but in general can be a k-vector \hat{y} , in which case w becomes a $p \times k$ matrix of coefficients.

Linear model fit by least squares

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

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

assuming N input-output pairs.

- ▶ RSS(w) is a quadratic function.
- A minimum always exists though not necessarily a unique one.

Linear model fit by least squares

- ightharpoonup We look for the solution $\hat{\boldsymbol{w}}$ using the matrix notation:
- **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

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

► To find the minimum we differentiate with respect to **w** which gives

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

using the rule $(AB)^T = B^T A^T$ this is equivalent to

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

Linear model fit by least squares

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

$$X^{T}(y - Xw) = 0$$

 $X^{T}y - X^{T}Xw = 0$
 $X^{T}y = X^{T}Xw$

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

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

Question: Why not simply $\mathbf{y} - \mathbf{X}\mathbf{w} = \mathbf{0} \rightarrow \mathbf{y} = \mathbf{X}\mathbf{w} \rightarrow \hat{\mathbf{w}} = \mathbf{X}^{-1}\mathbf{y}$?

Linear model fit by least squares

 \triangleright For each input x_i there corresponds the fitted output

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

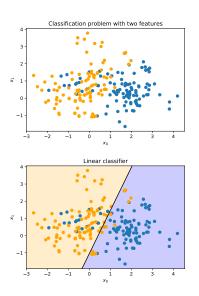
- ▶ This is called "making a prediction" for x_i .
- The entire fitted surface (hyperplane) is fully characterized by the parameter vector $\hat{\boldsymbol{w}}$.
- After fitting the model, we can "discard" the training dataset.

Example: Linear model fit by least squares

- Scatter plot 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

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

Example: Linear model fit by least squares



Example: Linear model fit by least squares

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

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

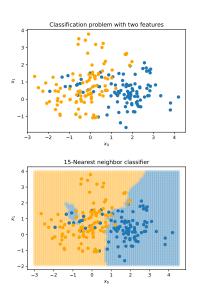
where $N_k(x)$ is the neighbourhood of x consisting of the k "closest" points to x.

- "Closeness" requires a definition of metrics.
- ► For the moment we assume Euclidian distance (each *x* is a point in the hyperspace).
- ▶ An average of the classes of the *k* closest points

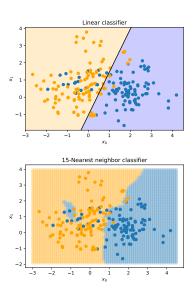
Back to the BLUE and ORANGE example

- 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 ŷ is the proportion of ORANGE points in the 15-neighbourhood
- ► Class ORANGE assigned to x if $\hat{y}(x) > 0.5$ (majority is ORANGE)

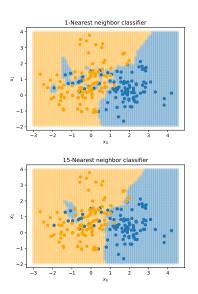
15-Nearest neighbour classifier



Linear classifier vs. 15-Nearest neighbour



1-Nearest neighbour vs. 15-Nearest neighbour



Comparison of 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).

Materials:

► Chapter I.3 from deeplearning

- Probability theory is a mathematical framework for dealing with uncertainty, i.e., modeling and analyzing uncertain events and statements
- In Al 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.

- ► A **random variable** is a variable that can take values randomly.
- 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.

- 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.
- $\forall x \in x : 0 \le P((x) \le 1)$
 - 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.
- - 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.
- $\forall x \in \mathsf{x} : p(x) \geq 0.$

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

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

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

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

Linarity of expectations:

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

Variance and covariance

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

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

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

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

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

Covariance matrix

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

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

▶ The diagonal elements of the matrix give the variance

$$Cov(x_i, x_i) = Var(x_i)$$

Bernouli Distribution

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

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

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

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

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

$$Var(x) = \phi(1 - \phi)$$

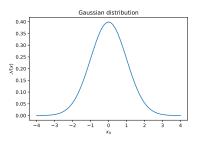
Gaussian distribution

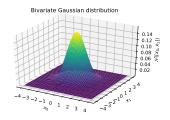
- The most commonly used distribution, also called normal distribution.
- ► Controlled by two parameters $\mu \in \mathbb{R}$ (the **mean**) and $\sigma \in (0, \infty)$, (the **standard deviation**)

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

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

Gaussian distribution



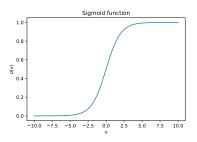


Logistic sigmoid

A useful function that we are going to consider

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

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



Bayes' rule

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

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

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

- 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.

Acknowledgements

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Some of the slides are based on the accompanying lectures of **deeplearning**.

References