The A”allon koneoppimisen sanakirja

Alexander Jung[1], Konstantina Olioumtsevits[1], Ekkehard Schnoor[1], Tommi Flores Ryynänen[1], Juliette Gronier[2] ja Salvatore Rastelli[1]
Käännös Mikko Seesto[1], Janita Thusberg[1] ja Helli Manninen[1]
[1]Aalto-yliopisto [2]ENS Lyon

22. lokakuuta 2025

please cite as: A. Jung, K. Olioumtsevits, E. Schnoor, T. Ryynänen, J. Gronier ja S. Rastelli, *Aallon koneoppimisen sanakirja*. Käännös J. Thusberg, H. Manninen ja M. Seesto. Espoo, Suomi: Aalto-yliopisto, 2025.

Acknowledgment

This dictionary of machine learning evolved through the development and teaching of several courses, including CS-E3210 Machine Learning: Basic Principles, CS-C3240 Machine Learning, CS-E4800 Artificial Intelligence, CS-EJ3211 Machine Learning with Python, CS-EJ3311 Deep Learning with Python, CS-E4740 Federated Learning, and CS-E407507 Human-Centered Machine Learning. These courses were offered at Aalto University `https://www.aalto.fi/en`, to adult learners via The Finnish Institute of Technology (FITech) `https://fitech.io/en/`, and to international students through the European University Alliance Unite! `https://www.aalto.fi/en/unite`.

We are grateful to the students who provided valuable feedback that helped shape this dictionary. Special thanks to Mikko Seesto for his meticulous proofreading.

This work was supported by

- the Research Council of Finland (grant 331197, 363624, 349966);
- the European Union (grant 952410);
- the Jane and Aatos Erkko Foundation (grant A835);
- Business Finland, as part of the project Forward-Looking AI Governance in Banking and Insurance (FLAIG).

Sisällys

Lists of Symbols

Sets and Functions

$a \in \mathcal{A}$	The object a is an element of the set $\mathcal{A}$.
$a := b$	We use a as a shorthand for b.
$\lvert\mathcal{A}\rvert$	The cardinality (i.e., number of elements) of a finite set $\mathcal{A}$.
$\mathcal{A} \subseteq \mathcal{B}$	$\mathcal{A}$ is a subset of $\mathcal{B}$.
$\mathcal{A} \subset \mathcal{B}$	$\mathcal{A}$ is a strict subset of $\mathcal{B}$.
$\mathcal{A} \times \mathcal{B}$	The Cartesian product of the sets $\mathcal{A}$ and $\mathcal{B}$.
$\mathbb{N}$	The natural numbers 1, 2, ...
$\mathbb{R}$	The real numbers x [1].
$\mathbb{R}_+$	The nonnegative real numbers $x \geq 0$.
$\mathbb{R}_{++}$	The positive real numbers $x > 0$.
$\{0, 1\}$	The set consisting of the two real numbers 0 and 1.
$[0, 1]$	The closed interval of real numbers x with $0 \leq x \leq 1$.

$\arg\min_{\mathbf{w}} f(\mathbf{w})$	The set of minimizers for a real-valued function $f(\mathbf{w})$. See also: function.
$\mathbb{S}^{(n)}$	The set of unit-norm vectors in $\mathbb{R}^{n+1}$. See also: norm, vector.
$\exp(a)$	The exponential function evaluated at the real number $a \in \mathbb{R}$. See also: function.
$\log a$	The logarithm of the positive number $a \in \mathbb{R}_{++}$.
$f(\cdot): \mathcal{A} \to \mathcal{B} : a \mapsto f(a)$	A function (or map) from a set $\mathcal{A}$ to a set $\mathcal{B}$, which assigns to each input $a \in \mathcal{A}$ a well-defined output $f(a) \in \mathcal{B}$. The set $\mathcal{A}$ is the domain of the function f and the set $\mathcal{B}$ is the co-domain of f. Machine learning (ML) aims to learn a function h that maps featuret $\mathbf{x}$ of a data point to a prediction $h(\mathbf{x})$ for its label y. See also: function, map, ML, feature, data point, prediction, label.
$\text{epi}(f)$	The epigraph of a real-valued function $f : \mathbb{R}^d \to \mathbb{R}$. See also: epigraph, function.
$\frac{\partial f(w_1, \ldots, w_d)}{\partial w_j}$	The partial derivative (if it exists) of a real-valued function $f : \mathbb{R}^d \to \mathbb{R}$ with respect to w_j [2, Ch. 9]. See also: function.

$\nabla f(\mathbf{w})$

The gradient of a differentiable real-valued function $f : \mathbb{R}^d \to \mathbb{R}$ is the vector $\nabla f(\mathbf{w}) = \big(\partial f/\partial w_1, \ldots, \partial f/\partial w_d\big)^T \in \mathbb{R}^d$ [2, Ch. 9].

See also: gradient, differentiable, function, vector.

Matrices and Vectors

$\mathbf{x} = \left(x_1, \ldots, x_d\right)^T$	A vector of length d, with its jth entry being x_j. See also: vector.
$\mathbb{R}^d$	The set of vectors $\mathbf{x} = \left(x_1, \ldots, x_d\right)^T$ consisting of d real-valued entries $x_1, \ldots, x_d \in \mathbb{R}$. See also: vector.
$\mathbf{I}_{l\times d}$	A generalized identity matrix with l rows and d columns. The entries of $\mathbf{I}_{l\times d} \in \mathbb{R}^{l\times d}$ are equal to 1 along the main diagonal and otherwise equal to 0. See also: matrix.
$\mathbf{I}_d, \mathbf{I}$	A square identity matrix of size $d \times d$. If the size is clear from context, we drop the subscript. See also: matrix.
$\|\mathbf{x}\|_2$	The Euclidean (or ℓ_2) norm of the vector $\mathbf{x} = \left(x_1, \ldots, x_d\right)^T \in \mathbb{R}^d$ defined as $\|\mathbf{x}\|_2 := \sqrt{\sum_{j=1}^d x_j^2}$. See also: norm, vector.
$\|\mathbf{x}\|$	Some norm of the vector $\mathbf{x} \in \mathbb{R}^d$ [3]. Unless otherwise specified, we mean the Euclidean norm $\|\mathbf{x}\|_2$. See also: norm, vector.
$\mathbf{x}^T$	The transpose of a matrix that has the vector $\mathbf{x} \in \mathbb{R}^d$ as its single column. See also: matrix, vector.

$\mathbf{X}^T$	The transpose of a matrix $\mathbf{X} \in \mathbb{R}^{m \times d}$. A square real-valued matrix $\mathbf{X} \in \mathbb{R}^{m \times m}$ is called symmetric if $\mathbf{X} = \mathbf{X}^T$. See also: matrix.
$\mathbf{X}^{-1}$	The inverse matrix of a matrix $\mathbf{X} \in \mathbb{R}^{d \times d}$. See also: inverse matrix, matrix.
$\mathbf{0} = \big(0, \ldots, 0\big)^T$	The vector in $\mathbb{R}^d$ with each entry equal to zero. See also: vector.
$\mathbf{1} = \big(1, \ldots, 1\big)^T$	The vector in $\mathbb{R}^d$ with each entry equal to one. See also: vector.
$\big(\mathbf{v}^T, \mathbf{w}^T\big)^T$	The vector of length $d + d'$ obtained by concatenating the entries of vector $\mathbf{v} \in \mathbb{R}^d$ with the entries of $\mathbf{w} \in \mathbb{R}^{d'}$. See also: vector.
$\text{span}\{\mathbf{B}\}$	The span of a matrix $\mathbf{B} \in \mathbb{R}^{a \times b}$, which is the subspace of all linear combinations of the columns of $\mathbf{B}$, such that $\text{span}\{\mathbf{B}\} = \big\{\mathbf{B}\mathbf{a} : \mathbf{a} \in \mathbb{R}^b\big\} \subseteq \mathbb{R}^a$. See also: matrix.
$\text{null}(\mathbf{A})$	The nullspace of a matrix $\mathbf{A} \in \mathbb{R}^{a \times b}$, which is the subspace of vectors $\mathbf{a} \in \mathbb{R}^b$ such that $\mathbf{A}\mathbf{a} = \mathbf{0}$. See also: nullspace, matrix, vector.

$\det(\mathbf{C})$	The determinant of the matrix $\mathbf{C}$. See also: determinant, matrix.
$\mathbf{A} \otimes \mathbf{B}$	The Kronecker product of $\mathbf{A}$ and $\mathbf{B}$ [4]. See also: Kronecker product.

Probability Theory

$\mathbf{x} \sim p(\mathbf{z})$	The random variable (RV) $\mathbf{x}$ is distributed according to the probability distribution $p(\mathbf{z})$ [5], [6]. See also: RV, probability distribution.
$\mathbb{E}_p\{f(\mathbf{z})\}$	The expectation of an RV $f(\mathbf{z})$ that is obtained by applying a deterministic function f to an RV $\mathbf{z}$ whose probability distribution is $\mathbb{P}(\mathbf{z})$. If the probability distribution is clear from context, we just write $\mathbb{E}\{f(\mathbf{z})\}$. See also: expectation, RV, function, probability distribution.
$\mathrm{cov}\,(x, y)$	The covariance between two real-valued RVs defined over a common probability space. See also: covariance, RV, probability distribution.
$\mathbb{P}(\mathbf{x}, y)$	A (joint) probability distribution of an RV whose realizationt are data points with features $\mathbf{x}$ and label y. See also: probability distribution, RV, realization, data point, feature, label.
$\mathbb{P}(\mathbf{x}\|y)$	A conditional probability distribution of an RV $\mathbf{x}$ given the value of another RV y [7, Sec. 3.5]. See also: probability distribution, RV.
$\mathbb{P}(\mathcal{A})$	The probability of the measurable event $\mathcal{A}$. See also: probability, measurable, event.

$\mathbb{P}(\mathbf{x}; \mathbf{w})$	A parameterized probability distribution of an RV $\mathbf{x}$. The probability distribution depends on a parameter vector $\mathbf{w}$. For example, $\mathbb{P}(\mathbf{x}; \mathbf{w})$ could be a multivariate normal distribution with the parameter vector $\mathbf{w}$ given by the entries of the mean vector $\mathbb{E}\{\mathbf{x}\}$ and the kovarianssimatriisi $\mathbb{E}\Big\{ \big(\mathbf{x} - \mathbb{E}\{\mathbf{x}\}\big) \big(\mathbf{x} - \mathbb{E}\{\mathbf{x}\}\big)^{T} \Big\}$. See also: probability distribution, parameter, probabilistic model.
$\mathcal{N}(\mu, \sigma^2)$	The probability distribution of a Gaussian random variable (Gaussian RV) $x \in \mathbb{R}$ with mean (or expectation) $\mu = \mathbb{E}\{x\}$ and variance $\sigma^2 = \mathbb{E}\big\{(x - \mu)^2\big\}$. See also: probability distribution, Gaussian RV.
$\mathcal{N}(\boldsymbol{\mu}, \mathbf{C})$	The multivariate normal distribution of a vector-valued Gaussian RV $\mathbf{x} \in \mathbb{R}^d$ with mean (or expectation) $\boldsymbol{\mu} = \mathbb{E}\{\mathbf{x}\}$ and kovarianssimatriisi $\mathbf{C} = \mathbb{E}\big\{ \big(\mathbf{x} - \boldsymbol{\mu}\big) \big(\mathbf{x} - \boldsymbol{\mu}\big)^{T} \big\}$. See also: multivariate normal distribution, Gaussian RV.
Ω	A sample space of all possible outcomes of a random experiment. See also: event.
$\mathcal{F}$	A collection of measurable subsets of a sample space Ω. See also: sample space, event.
$\mathcal{P}$	A probability space that consists of a sample space Ω, a σ-algebra $\mathcal{F}$ of measurable subsets of Ω, and a probability distribution $\mathbb{P}(\cdot)$. See also: sample space, measurable, probability distribution.

Machine Learning

r	An index $r = 1, 2, \ldots$ that enumerates data points. See also: data point.
m	The number of data points in (i.e., the size of) a tietoaineisto. See also: data point, tietoaineisto.
$\mathcal{D}$	A tietoaineisto $\mathcal{D} = \{\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(m)}\}$ is a list of individual data points $\mathbf{z}^{(r)}$, for $r = 1, \ldots, m$. See also: tietoaineisto, data point.
d	The number of features that characterize a data point. See also: feature, data point.
x_j	The jth feature of a data point. The first feature is denoted by x_1, the second feature x_2, and so on. See also: data point, feature.
$\mathbf{x}$	The feature vector $\mathbf{x} = \big(x_1, \ldots, x_d\big)^T$ of a data point. The vector's entries are the individual features of a data point. See also: feature vector, data point, vector, feature.
$\mathcal{X}$	The feature space $\mathcal{X}$ is the set of all possible values that the features $\mathbf{x}$ of a data point can take on. See also: feature space, feature, data point.

$\mathbf{z}$	Instead of the symbol $\mathbf{x}$, we sometimes use $\mathbf{z}$ as another symbol to denote a vector whose entries are the individual features of a data point. We need two different symbols to distinguish between raw and learned features [8, Ch. 9]. See also: vector, feature, data point.
$\mathbf{x}^{(r)}$	The feature vector of the rth data point within a tietoaineisto. See also: feature vector, data point, tietoaineisto.
$x_j^{(r)}$	The jth feature of the rth data point within a tietoaineisto. See also: feature, data point, tietoaineisto.
$\mathcal{B}$	A mini-batch (or subset) of randomly chosen data points. See also: batch, data point.
B	The size of (i.e., the number of data points in) a mini-batch. See also: data point, batch.
y	The label (or quantity of interest) of a data point. See also: label, data point.
$y^{(r)}$	The label of the rth data point. See also: label, data point.
$\left(\mathbf{x}^{(r)}, y^{(r)}\right)$	The features and label of the rth data point. See also: feature, label, data point.

$\mathcal{Y}$	The label space $\mathcal{Y}$ of an ML method consists of all potential label values that a data point can carry. The nominal label space might be larger than the set of different label values arising in a given tietoaineisto (e.g., a training set). ML problems (or methods) using a numeric label space, such as $\mathcal{Y} = \mathbb{R}$ or $\mathcal{Y} = \mathbb{R}^3$, are referred to as regression problems (or methods). ML problems (or methods) that use a discrete label space, such as $\mathcal{Y} = \{0, 1\}$ or $\mathcal{Y} = \{cat, dog, mouse\}$, are referred to as luokittelu problems (or methods). See also: label space, ML, label, data point, tietoaineisto, training set, regression, luokittelu.
η	Learning rate (or step size) used by gradient-based methods. See also: learning rate, step size, gradient-based methods.
$h(\cdot)$	A hypothesis map that maps the features of a data point to a prediction $\hat{y} = h(\mathbf{x})$ for its label y. See also: hypothesis, map, feature, data point, prediction, label.
$\mathcal{Y}^{\mathcal{X}}$	Given two sets $\mathcal{X}$ and $\mathcal{Y}$, we denote by $\mathcal{Y}^{\mathcal{X}}$ the set of all possible hypothesis maps $h : \mathcal{X} \to \mathcal{Y}$. See also: hypothesis, map.
$\mathcal{H}$	A hypothesis space or model used by an ML method. The hypothesis space consists of different hypothesis maps $h : \mathcal{X} \to \mathcal{Y}$, between which the ML method must choose. See also: hypothesis space, model, ML, hypothesis, map.

$d_{\text{eff}}(\mathcal{H})$	The effective dimension of a hypothesis space $\mathcal{H}$. See also: effective dimension, hypothesis space.
B^2	The squared harha of a learned hypothesis $\hat{h}$, or its parameters. Note that $\hat{h}$ becomes an RV if it is learned from data points being RVs themselves. See also: harha, hypothesis, parameter, RV, data point.
V	The variance of a learned hypothesis $\hat{h}$, or its parameters. Note that $\hat{h}$ becomes an RV if it is learned from data points being RVs themselves. See also: variance, hypothesis, parameter, RV, data point.
$L((\mathbf{x}, y), h)$	The loss incurred by predicting the label y of a data point using the prediction $\hat{y} = h(\mathbf{x})$. The prediction $\hat{y}$ is obtained by evaluating the hypothesis $h \in \mathcal{H}$ for the feature vector $\mathbf{x}$ of the data point. See also: loss, label, data point, prediction, hypothesis, feature vector.
E_v	The validation error of a hypothesis h, which is its average loss incurred over a validation set. See also: validation error, hypothesis, loss, validation set.
$\widehat{L}\big(h\|\mathcal{D}\big)$	The empirical risk, or average loss, incurred by the hypothesis h on a tietoaineisto $\mathcal{D}$. See also: empirical risk, loss, hypothesis, tietoaineisto.

E_t	The training error of a hypothesis h, which is its average loss incurred over a training set. See also: training error, hypothesis, loss, training set.
t	A discrete-time index $t = 0, 1, \ldots$ used to enumerate sequential events (or time instants). See also: event.
t	An index that enumerates learning tasks within a multitask learning problem. See also: learning task, multitask learning.
α	A regularization parameter that controls the amount of regularization. See also: regularization, parameter.
$\lambda_j(\mathbf{Q})$	The jth eigenvalue (sorted in either ascending or descending order) of a positive semi-definite (psd) matrix $\mathbf{Q}$. We also use the shorthand λ_j if the corresponding matrix is clear from context. See also: eigenvalue, psd, matrix.
$\sigma(\cdot)$	The activation function used by an artificial neuron within an artificial neural network (ANN). See also: activation function, ANN.
$\mathcal{R}_{\hat{y}}$	A decision region within a feature space. See also: decision region, feature space.

$\mathbf{w}$	A parameter vector $\mathbf{w} = \big(w_1, \ldots, w_d\big)^T$ of a model, e.g., the weights of a linear model or an ANN. See also: parameter, vector, model, weights, linear model, ANN.
$h^{(\mathbf{w})}(\cdot)$	A hypothesis map that involves tunable model parameters $w_1, \ldots, w_d$ stacked into the vector $\mathbf{w} = \big(w_1, \ldots, w_d\big)^T$. See also: hypothesis, map, model parameters, vector.
$\phi(\cdot)$	A feature map $\phi : \mathcal{X} \to \mathcal{X}' : \mathbf{x} \mapsto \phi\big(\mathbf{x}\big)$ that transforms the feature vector $\mathbf{x}$ of a data point into a new feature vector $\mathbf{x}' = \phi\big(\mathbf{x}\big) \in \mathcal{X}'$. See also: feature map.
$K\big(\cdot, \cdot\big)$	Given some feature space $\mathcal{X}$, a kernel is a map $K : \mathcal{X} \times \mathcal{X} \to \mathbb{C}$ that is psd. See also: feature space, kernel, map, psd.
$\mathrm{VCdim}\,(\mathcal{H})$	The Vapnik–Chervonenkis dimension (VC dimension) of the hypothesis space $\mathcal{H}$. See also: VC dimension, hypothesis space.

Federated Learning

$\mathcal{G} = (\mathcal{V}, \mathcal{E})$	An undirected graph whose nodes $i \in \mathcal{V}$ represent devicet within a federated learning network (FL network). The undirected weighted edges $\mathcal{E}$ represent connectivity between devices and statistical similarities between their tietoaineistot and learning tasks. See also: graph, device, FL network, tietoaineisto, learning task.
$i \in \mathcal{V}$	A node that represents some device within an FL network. The device can access a local dataset and train a local model. See also: device, FL network, local dataset, local model.
$\mathcal{G}^{(\mathcal{C})}$	The induced subgraph of $\mathcal{G}$ using the nodes in $\mathcal{C} \subseteq \mathcal{V}$.
$\mathbf{L}^{(\mathcal{G})}$	The Laplacian matrix of a graph $\mathcal{G}$. See also: Laplacian matrix, graph.
$\mathbf{L}^{(\mathcal{C})}$	The Laplacian matrix of the induced graph $\mathcal{G}^{(\mathcal{C})}$. See also: Laplacian matrix, graph.
$\mathcal{N}^{(i)}$	The neighborhood of the node i in a graph $\mathcal{G}$. See also: neighborhood, graph.
$d^{(i)}$	The weighted node degree $d^{(i)} := \sum_{i' \in \mathcal{N}^{(i)}} A_{i,i'}$ of node i. See also: node degree.
$d^{(\mathcal{G})}_{\max}$	The maximum weighted node degree of a graph $\mathcal{G}$. See also: maximum, node degree, graph.

$\mathcal{D}^{(i)}$	The local dataset $\mathcal{D}^{(i)}$ carried by node $i \in \mathcal{V}$ of an FL network. See also: local dataset, FL network.
m_i	The number of data points (i.e., sample size) contained in the local dataset $\mathcal{D}^{(i)}$ at node $i \in \mathcal{V}$. See also: data point, sample size, local dataset.
$\mathbf{x}^{(i,r)}$	The features of the rth data point in the local dataset $\mathcal{D}^{(i)}$. See also: feature, data point, local dataset.
$y^{(i,r)}$	The label of the rth data point in the local dataset $\mathcal{D}^{(i)}$. See also: label, data point, local dataset.
$\mathbf{w}^{(i)}$	The local model parameters of device i within an FL network. See also: model parameters, device, FL network.
$L_i\left(\mathbf{w}\right)$	The local loss function used by device i to measure the usefulness of some choice $\mathbf{w}$ for the local model parameters. See also: loss function, device, model parameters.
$L^{(\mathrm{d})}\left(\mathbf{x}, h\big(\mathbf{x}\big), h'\big(\mathbf{x}\big)\right)$	The loss incurred by a hypothesis h' on a data point with features $\mathbf{x}$ and label $h\big(\mathbf{x}\big)$ that is obtained from another hypothesis. See also: loss, hypothesis, data point, feature, label.

$\text{stack}\left\{\mathbf{w}^{(i)}\right\}_{i=1}^{n}$

The vector $\left(\left(\mathbf{w}^{(1)}\right)^T, \ldots, \left(\mathbf{w}^{(n)}\right)^T\right)^T \in \mathbb{R}^{dn}$ that is obtained by vertically stacking the local model parameters $\mathbf{w}^{(i)} \in \mathbb{R}^d$, for $i = 1, \ldots, n$.

See also: vector, model parameters.

Tools

characteristic function The characteristic function of a real-valued RV x is the function [6, Sec. 26]

$$\phi_x(t) := \mathbb{E}\exp(jtx) \text{ with } j = \sqrt{-1}.$$

The characteristic function uniquely determines the probability distribution of x.

See also: RV, probability distribution.

continuous A function $f : \mathbb{R}^d \to \mathbb{R}$ is continuous at a point $\mathbf{x}' \in \mathbb{R}^d$ if for every $\epsilon > 0$ there is a $\delta > 0$ such that for all $\mathbf{x} \in \mathbb{R}^d$ with $\|\mathbf{x} - \mathbf{x}'\|_2 < \delta$, it holds that $|f(\mathbf{x}) - f(\mathbf{x}')| < \epsilon$ [2]. In other words, we can make $f(\mathbf{x})$ arbitrarily close to $f(\mathbf{x}')$ by choosing $\mathbf{x}$ sufficiently close to $\mathbf{x}'$. If f is continuous at every point $\mathbf{x}' \in \mathbb{R}^d$, then f is said to be continuous on $\mathbb{R}^d$. The notion of a continuous function can be naturally extended to functions between general metric spaces [2].

See also: Euclidean space, metric.

convergence TBD.

convex optimization TBD.

determinant The determinant $\det(\mathbf{A})$ of a square matrix $\mathbf{A} = \left(\mathbf{a}^{(1)}, \ldots, \mathbf{a}^{(d)}\right) \in \mathbb{R}^{d \times d}$ is a function of its columns $\mathbf{a}^{(1)}, \ldots, \mathbf{a}^{(d)} \in \mathbb{R}^d$, i.e., it satisfies the following properties [**?**]:

- Normalized:

$$\det(\mathbf{I}) = 1$$

- Multilinear:

$$\det\left(\mathbf{a}^{(1)}, \ldots, \alpha\mathbf{u} + \beta\mathbf{v}, \ldots, \mathbf{a}^{(d)}\right) = \alpha \det\left(\mathbf{a}^{(1)}, \ldots, \mathbf{u}, \ldots, \mathbf{a}^{(d)}\right) + \beta \det\left(\mathbf{a}^{(1)}, \ldots, \mathbf{v}, \ldots, \mathbf{a}^{(d)}\right)$$

- Antisymmetric:

$$\det\left(\ldots, \mathbf{a}^{(j)}, \ldots, \mathbf{a}^{(j')}, \ldots\right) = -\det\left(\ldots, \mathbf{a}^{(j')}, \ldots, \mathbf{a}^{(j)}, \ldots\right).$$

We can interpret a matrix $\mathbf{A}$ as a linear transformation on $\mathbb{R}^d$. The determinant $\det(\mathbf{A})$ characterizes how volumes in $\mathbb{R}^d$ (and their orientation) are altered by this transformation (see Fig. 1) [3], [**?**]. In particular, $\det(\mathbf{A}) > 0$ preserves orientation, $\det(\mathbf{A}) < 0$ reverses orientation, and $\det(\mathbf{A}) = 0$ collapses volume entirely, indicating that $\mathbf{A}$ is non-invertible. The determinant also satisfies $\det(\mathbf{AB}) = \det(\mathbf{A}) \cdot \det(\mathbf{B})$, and if $\mathbf{A}$ is diagonalizable with eigenvalues $\lambda_1, \ldots, \lambda_d$, then $\det(\mathbf{A}) = \prod_{j=1}^{d} \lambda_j$ [**?**]. For the special cases $d = 2$ (i.e., two-dimensional or 2-D) and $d = 3$ (i.e., three-dimensional or 3-D), the determinant can be interpreted as an oriented area or volume spanned by the column vectors of $\mathbf{A}$.

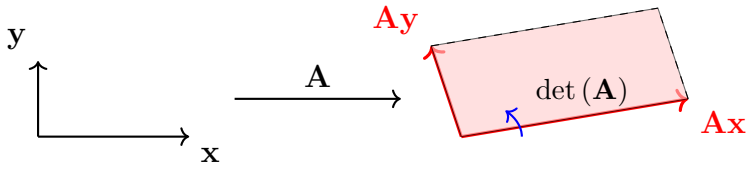


Fig. 1. We can interpret a square matrix $\mathbf{A}$ as a linear transformation of $\mathbb{R}^d$ into itself. The determinant $\det(\mathbf{A})$ characterizes how this transformation alters an oriented volume.

See also: eigenvalue, inverse matrix.

function A function between two sets $\mathcal{U}$ and $\mathcal{V}$ assigns each element $u \in \mathcal{U}$ exactly one element $f(u) \in \mathcal{V}$ [2]. We write this as

$$f : \mathcal{U} \to \mathcal{V} : u \mapsto f(u)$$

where $\mathcal{U}$ is the domain and $\mathcal{V}$ the co-domain of f. That is, a function f defines a unique output $f(u) \in \mathcal{V}$ for every input $u \in \mathcal{U}$ (see Fig. 2).

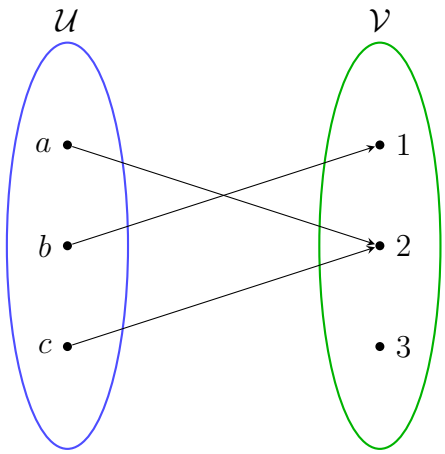


Fig. 2. A function $f\colon \{a, b, c\} \to \{1, 2, 3\}$ mapping each element of the domain to exactly one element of the co-domain.

Hessian Consider a function $f : \mathbb{R}^d \to \mathbb{R}$ for which the second-order partial derivatives exist at $\mathbf{x}'$. Then, the Hessian $\nabla^2 f(\mathbf{x}')$ of f at $\mathbf{x}$ is defined as the matrix of second-order partial derivatives of f at $\mathbf{x}'$,

$$\nabla^2 f(\mathbf{x}') = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_d} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_d \partial x_1} & \frac{\partial^2 f}{\partial x_d \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_d^2} \end{bmatrix}.$$

If the second-order partial derivatives are continuous in a neighborhood around $\mathbf{x}'$, then the Hessian is a symmetric matrix, i.e., $\frac{\partial^2 f}{\partial x_j \partial x_{j'}} = \frac{\partial^2 f}{\partial x_{j'} \partial x_j}$ for all j, j' [2]. If additionally f is convex, then the Hessian is a psd matrix [**?**].

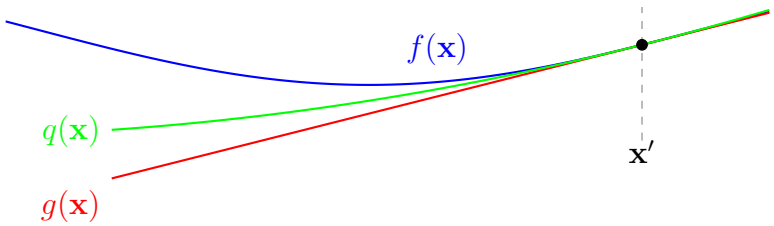


Fig. 3. A function $f(\mathbf{x})$ that is sufficiently smooth at a point $\mathbf{x}'$ can be locally approximated by a quadratic function $q(\mathbf{x})$ which allows for a more accurate approximation compared to a linear function $g(\mathbf{x})$.

The Hessian $\nabla^2 f(\mathbf{x}')$ can be used to compute a quadratic function

$$q(\mathbf{x}) = (1/2)(\mathbf{x} - \mathbf{x}')^T \underbrace{\nabla^2 f(\mathbf{x}')}_{\text{Hessian}}(\mathbf{x} - \mathbf{x}') + (\mathbf{x} - \mathbf{x}')^T \underbrace{\nabla f(\mathbf{x}')}_{\text{gradient}} + f(\mathbf{x}')$$

that approximates f locally around $\mathbf{x}'$.

See also: differentiable, matrix, function, quadratic function.

map We use the term map as a synonym for function.

See also: function.

matrix A matrix of size $m \times d$ is a 2-D array of numbers, which is denoted by

$$\mathbf{A} = \begin{bmatrix} A_{1,1} & A_{1,2} & \dots & A_{1,d} \\ A_{2,1} & A_{2,2} & \dots & A_{2,d} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m,1} & A_{m,2} & \dots & A_{m,d} \end{bmatrix} \in \mathbb{R}^{m \times d}.$$

Here, $A_{r,j}$ denotes the matrix entry in the rth row and the jth column. Matrices are useful representations of various mathematical objects [**?**], including the following:

- Systems of linear equations: We can use a matrix to represent a system of linear equations

$$\begin{pmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \quad \text{compactly as} \quad \mathbf{A}\mathbf{w} = \mathbf{y}.$$

  One important example of systems of linear equations is the optimality condition for the model parameters within linear regression.

- Linear mapt: Consider a d-dimensional vector space $\mathcal{U}$ and a m-dimensional vector space $\mathcal{V}$. If we fix a basis $\mathbf{u}^{(1)}, \ldots, \mathbf{u}^{(d)}$ for $\mathcal{U}$ and a basis $\mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(m)}$ for $\mathcal{V}$, each matrix $\mathbf{A} \in \mathbb{R}^{m \times d}$ naturally defines a linear map $\alpha : \mathcal{U} \to \mathcal{V}$ (see Fig. 4) such that

$$\mathbf{u}^{(j)} \mapsto \sum_{r=1}^{m} A_{r,j} \mathbf{v}^{(r)}.$$

- Tietoaineistot: We can use a matrix to represent a tietoaineisto. Each row corresponds to a single data point, and each column corresponds to a specific feature or label of a data point.

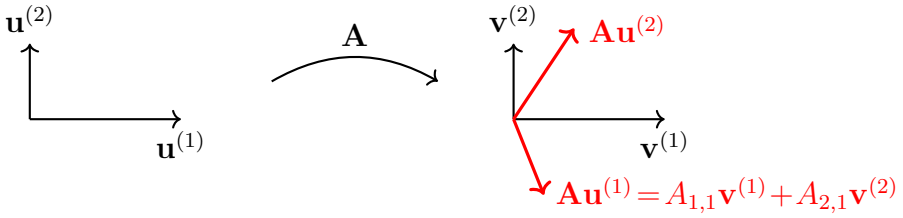


Fig. 4. A matrix $\mathbf{A}$ defines a linear map between two vector spacet.

See also: linear map, tietoaineisto, linear model.

Newton's method Newton's method is an iterative optimization method for finding local minima or maxima of a differentiable objective function $f(\mathbf{w})$. Like gradient-based methods, Newton's method also computes a new estimate $\widehat{\mathbf{w}}_{k+1}$ by optimizing a local approximation of $f(\mathbf{w})$ around the current estimate $\widehat{\mathbf{w}}_k$. In contrast to gradient-based methods, which use the gradient to build a local linear approximation, Newton's method uses the Hessian matrix to build a local quadratic approximation. In particular, starting from an initial estimate $\widehat{\mathbf{w}}_0$, Newton's method iteratively updates the estimate according to

$$\widehat{\mathbf{w}}_{k+1} = \widehat{\mathbf{w}}_k - \left(\nabla^2 f\left(\widehat{\mathbf{w}}_k\right)\right)^{-1} \nabla f\left(\widehat{\mathbf{w}}_k\right), \text{ for } k = 0, 1, \ldots.$$

Here, $\nabla f\left(\widehat{\mathbf{w}}_k\right)$ is the gradient, and $\nabla^2 f(\mathbf{w}^{(k)})$ is the Hessian of the objective function f. Since using a quadratic function as local approximation is more accurate than using a linear function (which is a special case of a quadratic function), Newton's method tends to converge faster than gradient-based methods (see Fig. 5). However, this faster convergence comes at the increased computational complexity of the iterations. Indeed, each iteration of Newton's method requires the inversion of the Hessian.

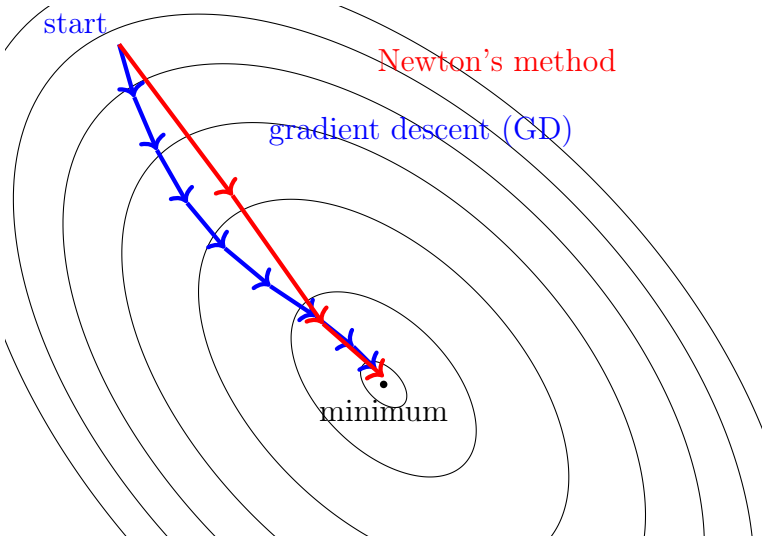


Fig. 5. Comparison of GD (blue) and Newton's method (red) paths toward the minimum of a loss function.

See also: optimization method, gradient, Hessian, GD.

optimization problem An optimization problem is a mathematical structure consisting of an objective function $f : \mathcal{U} \to \mathcal{V}$ defined over an optimization variable $\mathbf{w} \in \mathcal{U}$, together with a feasible set $\mathcal{W} \subseteq \mathcal{U}$. The co-domain $\mathcal{V}$ is assumed to be ordered, meaning that for any two elements $\mathbf{a}, \mathbf{b} \in \mathcal{V}$, we can determine whether $\mathbf{a} < \mathbf{b}$, $\mathbf{a} = \mathbf{b}$, or $\mathbf{a} > \mathbf{b}$. The goal of optimization is to find those values $\mathbf{w} \in \mathcal{W}$ for which the objective $f(\mathbf{w})$ is extremal—i.e., minimal or maximal [?], [?], [?].
See also: objective function.

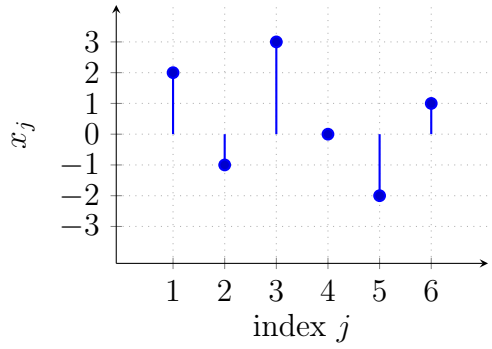
stochastic process A stochastic process is a collection of RVs defined on a common probability space and indexed by some set $\mathcal{I}$ [?], [?], [?]. The

index set $\mathcal{I}$ typically represents time or space, allowing us to represent random phenomena that evolve across time or spatial dimensions—for example, sensor noise or financial time series. Stochastic processes are not limited to temporal or spatial settings. For instance, random grapht such as the Erdős–Rényi (ER) graph or the stochastic block model (SBM) can also be viewed as stochastic processes. Here, the index set $\mathcal{I}$ consists of node pairs that index RVs whose values encode the presence or weight of an edge between two nodes. Moreover, stochastic processes naturally arise in the analysis of stochastic algorithmt, such as stochastic gradient descent (SGD), which construct a sequence of RVs.
See also: RV, SBM, SGD, uncertainty, probabilistic model.

vector A vector is an element of a vector space. In the context of ML, a particularly important example of a vector space is the Euclidean space $\mathbb{R}^d$, where $d \in \mathbb{N}$ is the (finite) dimension of the space. A vector $\mathbf{x} \in \mathbb{R}^d$ can be represented as a list or one-dimensional (1-D) array of real numbers, i.e., $x_1, \ldots, x_d$ with $x_j \in \mathbb{R}$ for $j = 1, \ldots, d$. The value x_j is the jth entry of the vector $\mathbf{x}$. It can also be useful to view a vector $\mathbf{x} \in \mathbb{R}^d$ as a function that maps each index $j \in \{1, \ldots, d\}$ to a value $x_j \in \mathbb{R}$, i.e., $\mathbf{x} : j \mapsto x_j$. This perspective is particularly useful for the study of kernel methodt. See Fig. 6 for the two views of a vector.

2, –1, 3, 0, –2, 1

(a)



(b)

Fig. 6. Two equivalent views of a vector $\mathbf{x} = \big(2, -1, 3, 0, -2, 1\big)^T \in \mathbb{R}^6$. (a) As a numeric array. (b) As a map $j \mapsto x_j$.

See also: vector space, Euclidean space, linear map.

vector space A vector space $\mathcal{V}$ (also called linear space) is a collection of elements, called vectors, along with the following two operations (see also Fig. 7): 1) addition (denoted by $\mathbf{v} + \mathbf{w}$) of two vectors $\mathbf{v}, \mathbf{w}$; and 2) multiplication (denoted by $c \cdot \mathbf{v}$) of a vector $\mathbf{v}$ with a scalar c that belongs to some number field (with a typical choice for this field being $\mathbb{R}$). The defining property of a vector space is that it is closed under two specific operations. First, if $\mathbf{v}, \mathbf{w} \in \mathcal{V}$, then $\mathbf{v} + \mathbf{w} \in \mathcal{V}$. Second, if $\mathbf{v} \in \mathcal{V}$ and $c \in \mathbb{R}$, then $c\mathbf{v} \in \mathcal{V}$.

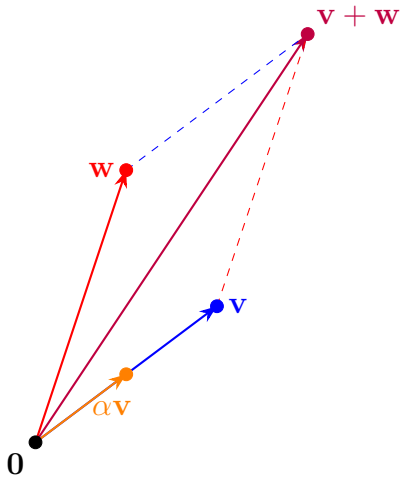


Fig. 7. A vector space $\mathcal{V}$ is a collection of vectors such that scaling and adding them always yields another vector in $\mathcal{V}$.

A common example of a vector space is the Euclidean space $\mathbb{R}^n$, which is widely used in ML to represent tietoaineistot. We can also use $\mathbb{R}^n$ to represent, either exactly or approximately, the hypothesis space used by an ML method. Another example of a vector space, which is naturally associated with every probability space $\mathcal{P} = \big(\Omega, \mathcal{R}, \mathbb{P}(\cdot)\big)$, is the collection of all real-valued RVs $x : \Omega \to \mathbb{R}$ [1], [**?**].

See also: vector, Euclidean space, linear model, linear map.

Machine Learning Concepts

absolute error loss Consider a data point with features $\mathbf{x} \in \mathcal{X}$ and numeric label $y \in \mathbb{R}$. As its name suggests, the absolute error loss incurred by a hypothesis $h : \mathcal{X} \to \mathbb{R}$ is defined as

$$L\left((\mathbf{x}, y), h\right) = |y - h(\mathbf{x})|.$$

Fig. 8 depicts the absolute error loss for a fixed data point with feature vector $\mathbf{x}$ and label y. It also indicates the loss values incurred by two different hypotheses h' and h''. Similar to the squared error loss, the absolute error loss is also a convex function of the prediction $\hat{y} = h(\mathbf{x})$. However, in contrast to the squared error loss, the absolute error loss is non-smooth, as it is not differentiable at the optimal prediction $\hat{y} = y$. This property makes empirical risk minimization (ERM)-based methods using the absolute error loss computationally more demanding [**?**], [**?**]. To build intuition, it is useful to consider the two hypotheses depicted in Fig. 8. Just by inspecting the slope of L around $h'(\mathbf{x})$ and $h''(\mathbf{x})$, it is impossible to determine whether we are very close to the optimum (at h') or still far away (at h''). As a result, any optimization method that is based on local approximations of the loss function (such as subgradient descent) must use a decreasing learning rate to avoid overshooting when approaching the optimum. This required decrease in learning rate tends to slow down the convergence of the optimization method. Besides the increased computational complexity, using absolute error loss in ERM can be beneficial in the presence of outliert in the training set. In contrast to the squared error loss, the slope of the absolute error loss

does not increase with increasing prediction error $y - h(\mathbf{x})$. As a result, the effect of introducing an outlier with large prediction error on the solution $\hat{h}$ of ERM with absolute error loss is much smaller compared with the effect on the solution of ERM with squared error loss.

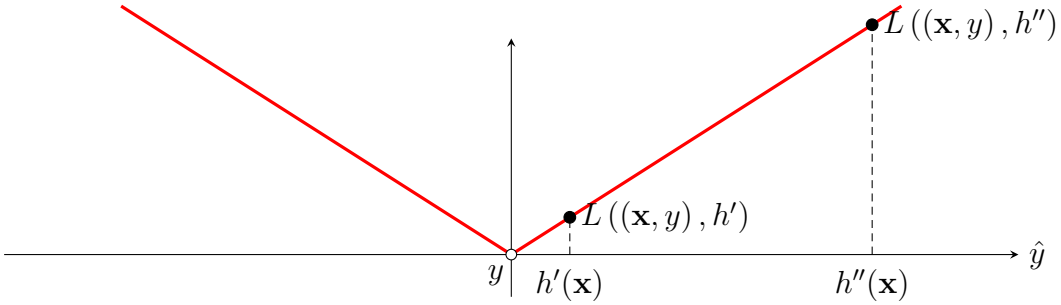


Fig. 8. For a data point with numeric label $y \in \mathbb{R}$, the absolute error $|y - h(\mathbf{x})|$ can be used as a loss function to guide the learning of a hypothesis h.

See also: data point, feature, label, loss, ERM, subgradient descent.

activation The output of an artificial neuron within an ANN is referred to as its activation. In particular, the activation is obtained by applying a (typically nonlinear) activation function to a weighted sum of its inputs.
See also: ANN, deep net.

activation function Each artificial neuron within an ANN is assigned an activation function $\sigma(\cdot)$ that maps a weighted combination of the neuron inputs $x_1, \ldots, x_d$ to a single output value $a = \sigma\big(w_1 x_1 + \ldots + w_d x_d\big)$. Note that each neuron is parameterized by the weights $w_1, \ldots, w_d$.
See also: ANN, activation, function, weights.

algebraic connectivity The algebraic connectivity of an undirected graph is the second-smallest eigenvalue λ_2 of its Laplacian matrix. A graph is connected if and only if $\lambda_2 > 0$.

See also: graph, eigenvalue, Laplacian matrix.

algoritmi An algorithm is a precise, step-by-step specification for producing an output from a given input within a finite number of computational steps [**?**]. For example, an algorithm to train a linear model explicitly describes how to transform a given training set into model parameters through a sequence of gradient steps. To study algorithms rigorously, we can represent (or approximate) them by different mathematical structures [**?**]. One approach is to represent an algorithm as a collection of possible executions. Each individual execution is then a sequence of the form

$$\text{input}, s_1, s_2, \ldots, s_T, \text{output}.$$

This sequence starts from an input and progresses via intermediate steps until an output is delivered. Crucially, an algorithm encompasses more than just a mapping from input to output; it also includes intermediate computational steps $s_1, \ldots, s_T$.

See also: linear model, training set, model parameters, gradient step, model, stochastic.

application programming interface (API) An API is a formal mechanism that allows software components to interact in a structured and modular way [**?**]. In the context of ML, APIs are commonly used to provide access to a trained ML model. Users—whether humans or mac-

hines—can submit the feature vector of a data point and receive a corresponding prediction. Suppose a trained ML model is defined as $\widehat{h}(x) := 2x + 1$. Through an API, a user can input $x = 3$ and receive the output $\widehat{h}(3) = 7$ without knowledge of the detailed structure of the ML model or its training. In practice, the model is typically deployed on a server connected to the Internet. Clients send requests containing feature values to the server, which responds with the computed prediction $\widehat{h}(\mathbf{x})$. APIs promote modularity in ML system design, i.e., one team can develop and train the model, while another team handles integration and user interaction. Publishing a trained model via an API also offers practical advantages. For instance, the server can centralize computational resources that are required to compute predictions. Furthermore, the internal structure of the model remains hidden—which is useful for protecting intellectual property or trade secrets. However, APIs are not without risk. Techniques such as model inversion can potentially reconstruct a model from its predictions using carefully selected feature vectors.

See also: ML, model, feature vector, data point, prediction, feature, model inversion.

tekoäly AI refers to systems that behave rationally in the sense of maximizing a long-term reward. The ML-based approach to AI is to train a model to predict optimal actions. These predictions are computed from observations about the state of the environment. The choice of loss function sets AI applications apart from more basic ML applications. AI systems rarely have access to a labeled training set that allows the

average loss to be measured for any possible choice of model parameters. Instead, AI systems use observed reward signals to estimate the loss incurred by the current choice of model parameters.

See also: ML, reinforcement learning (RL).

neuroverkko An ANN is a graphical (signal-flow) representation of a function that maps features of a data point at its input to a prediction for the corresponding label at its output. The fundamental unit of an ANN is the artificial neuron, which applies an activation function to its weighted inputs. The outputs of these neurons serve as inputs for other neurons, forming interconnected layers.

See also: function, feature, data point, prediction, label, activation function, layer.

attack An attack on an ML system refers to an intentional action—either active or passive—that compromises the system's integrity, availability, or confidentiality. Active attacks involve perturbing components such as tietoaineistot (via data poisoning) or communication links between devices within an ML application. Passive attacks, such as privacy attacks, aim to infer sensitive attributet without modifying the system. Depending on their goal, we distinguish among denial-of-service attackt, backdoor attacks, and privacy attacks.

See also: data poisoning, privacy attack, sensitive attribute, denial-of-service attack, backdoor.

attention Some ML applications involve data points composed of smaller units, known as tokens. For example, a sentence consists of words,

an image of pixel patches, and a network of nodes. In practice, the tokens within a single data point are typically not independent of one another, but rather, each token pays attention to specific other tokens. Probabilistic models provide a principled framework for representing and analyzing such dependencies [**?**]. Attention mechanisms use a more direct approach without explicit reference to a probabilistic model. The idea is to represent the relationship between two tokens i and i' using a parameterized function $f^{(\mathbf{w})}(i, i')$, where the parameters $\mathbf{w}$ are learned via a variant of ERM. Practical attention mechanisms differ in their precise choice of attention model $f^{(\mathbf{w})}(i, i')$ as well as in the precise ERM variant used to learn the parameters $\mathbf{w}$. One widely used family of attention mechanisms defines the parameters $\mathbf{w}$ in terms of two vectors associated with each token i, i.e., a query vector $\mathbf{q}^{(i)}$ and a key vector $\mathbf{k}^{(i')}$. For a given token i with query $\mathbf{q}^{(i)}$, and another token i' with key $\mathbf{k}^{(i')}$, the quantity $\left(\mathbf{q}^{(i)}\right)^{\top}\mathbf{k}^{(i')}$ quantifies the extent to which token i attends to (or depends on) token i' (see Fig. 9).

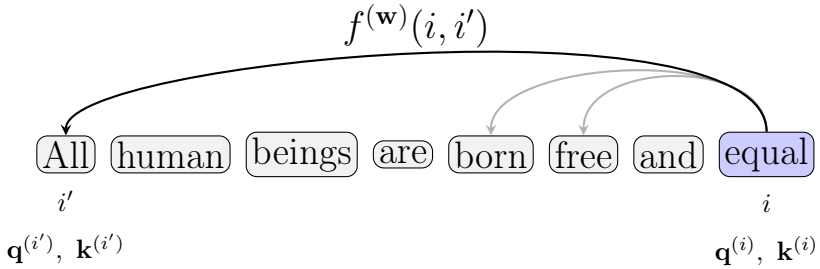


Fig. 9. Attention mechanisms learn a parameterized function $f^{(\mathbf{w})}(i, i')$ to measure how much token i attends to token i'. One widely used construction of $f^{(\mathbf{w})}(i, i')$ uses query and key vectors, denoted by $\mathbf{q}^{(i)}$ and $\mathbf{k}^{(i)}$, assigned to each token i [**?**].

See also: function.

autoenkoodaaja An autoencoder is an ML method that simultaneously learns an encoder map $h(\cdot) \in \mathcal{H}$ and a decoder map $h^*(\cdot) \in \mathcal{H}^*$. It is an instance of ERM using a loss computed from the reconstruction error $\mathbf{x} - h^*\big(h\big(\mathbf{x}\big)\big)$.

See also: feature learning, dimensionality reduction.

backdoor A backdoor attack refers to the intentional manipulation of the training process underlying an ML method. This manipulation can be implemented by perturbing the training set (i.e., through data poisoning) or via the optimization algorithm used by an ERM-based method. The goal of a backdoor attack is to nudge the learned hypothesis $\hat{h}$ toward specific predictions for a certain range of feature values. This range of feature values serves as a key (or trigger) to unlock a backdoor

in the sense of delivering anomalous predictions. The key $\mathbf{x}$ and the corresponding anomalous prediction $\hat{h}(\mathbf{x})$ are only known to the attacker. See also: ML, training set, data poisoning, algorithm, ERM, hypothesis, prediction, feature.

backpropagation Backpropagation is an algorithm for computing the gradient $\nabla_{\mathbf{w}} f(\mathbf{w})$ of an objective function $f(\mathbf{w})$ that depends on the model parameters $\mathbf{w}$ of an ANN. One example of such an objective function is the average loss incurred by the ANN on a batch of data points. This algorithm is a direct application of the chain rule from calculus to efficiently compute partial derivatives of the loss function with respect to the model parameters. Backpropagation consists of two consecutive phases, also illustrated in Fig. 10. The first phase includes the forward pass, where a batch of data points is fed into the ANN. The ANN processes the input through its layers using its current weights, ultimately producing a prediction at its output. The prediction of the batch is compared to the true label using a loss function, which quantifies the prediction error. The second phase includes the backward pass (i.e., backpropagation), where the error is backpropagated through the ANN layers. The obtained partial derivatives with respect to the ANN parameters $w_1, \ldots, w_d$ constitute the gradient $\nabla f(\mathbf{w})$, which can be used, in turn, to implement a gradient step.

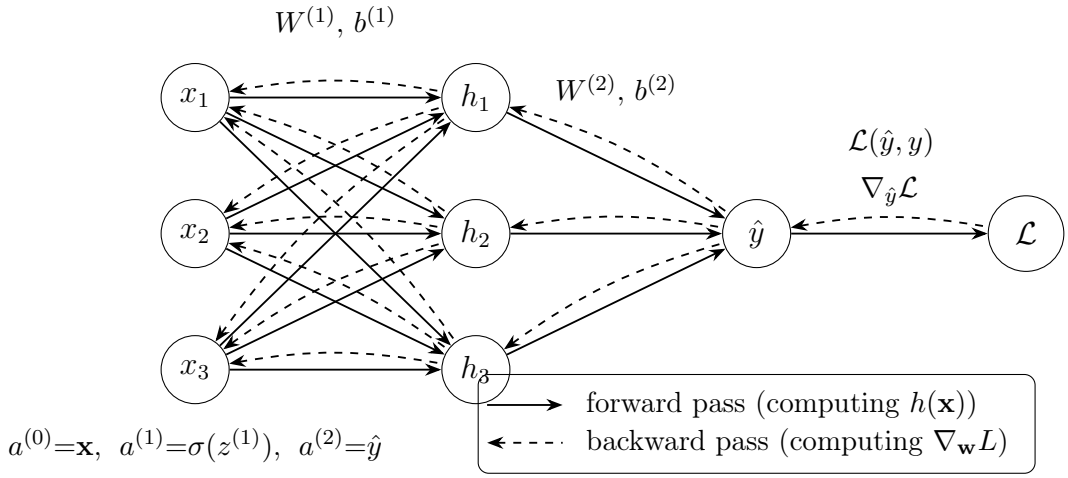


Fig. 10. Solid arrows show the forward pass (i.e., data flow and loss calculation), while dashed arrows show the gradient correction flow during the backward pass for updating the parameters $W^{(x)}$, $b^{(x)}$.

See also: ANN, loss function, GD, optimization method.

bagging (or bootstrap aggregation) Bagging (or bootstrap aggregation) is a technique to improve (the robustness of) a given ERM-based ML method. The idea is to use the uusio-otanta to generate perturbed copies of a given tietoaineisto and to learn a separate hypothesis for each copy. We then predict the label of a data point by combining or aggregating the individual predictions of each separate hypothesis. For hypothesis maps delivering numeric label values, this aggregation could be implemented by computing the average of individual predictions. Bagging is an example of an ensemble method, with base learners using the same model but different training sets.

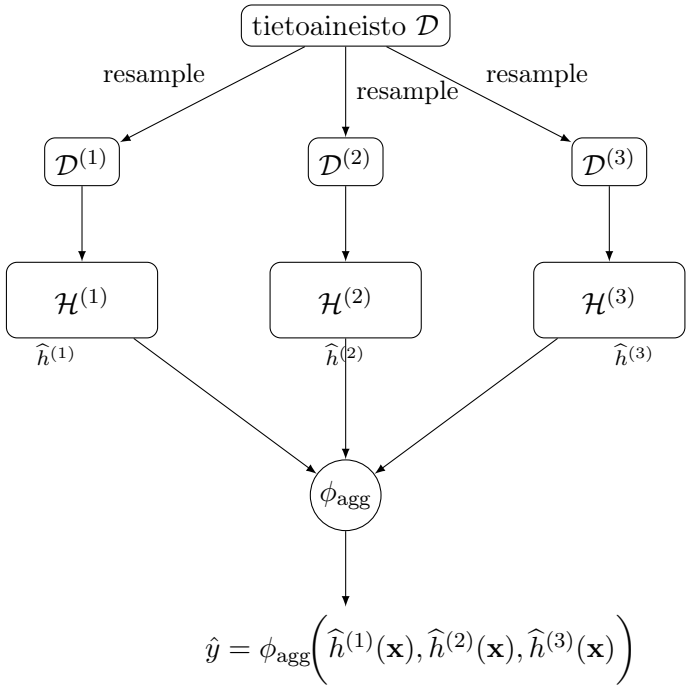


Fig. 11. A simple example of bagging. Three base learners use different variations $\mathcal{D}^{(1)}, \ldots, \mathcal{D}^{(3)}$ of the original tietoaineisto $\mathcal{D}$ to learn the hypotheses $\widehat{h}^{(1)}, \ldots, \widehat{h}^{(3)}$. The prediction $\hat{y}$ for a data point with feature vector $\mathbf{x}$ is obtained by applying an aggregation rule ϕ_{agg} to the individual predictions $\widehat{h}^{(1)}(\mathbf{x})$, $\widehat{h}^{(2)}(\mathbf{x})$, $\widehat{h}^{(3)}(\mathbf{x})$.

See also: robustness, uusio-otanta, ensemble.

vertailutaso Consider some ML method that produces a learned hypothesis (or trained model) $\hat{h} \in \mathcal{H}$. We evaluate the quality of a trained model by computing the average loss on a test set. But how can we assess whether the resulting test set performance is sufficiently good? How can we determine if the trained model performs close to optimal such that

there is little point in investing more resources (for data collection or computation) to improve it? To this end, it is useful to have a reference (or baseline) level against which we can compare the performance of the trained model.

Such a reference value might be obtained from human performance, e.g., the misclassification rate of dermatologists who diagnose cancer from visual inspection of skin [**?**]. Another source for a baseline is an existing, but for some reason unsuitable, ML method. For example, the existing ML method might be computationally too expensive for the intended ML application. Nevertheless, its test set error can still serve as a baseline. Another, somewhat more principled, approach to constructing a baseline is via a probabilistic model. In many cases, given a probabilistic model $p(\mathbf{x}, y)$, we can precisely determine the minimum achievable risk among any hypotheses (not even required to belong to the hypothesis space $\mathcal{H}$) [**?**].

This minimum achievable risk (referred to as the Bayes risk) is the risk of the Bayes estimator for the label y of a data point, given its features $\mathbf{x}$. Note that, for a given choice of loss function, the Bayes estimator (if it exists) is completely determined by the probability distribution $p(\mathbf{x}, y)$ [**?**, Ch. 4]. However, computing the Bayes estimator and Bayes risk presents two main challenges. First, the probability distribution $p(\mathbf{x}, y)$ is unknown and must be estimated from observed data. Second, even if $p(\mathbf{x}, y)$ were known, computing the Bayes risk exactly may be computationally infeasible [**?**]. A widely used probabilistic model is the multivariate normal distribution $(\mathbf{x}, y) \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ for data points

characterized by numeric features and labels. Here, for the squared error loss, the Bayes estimator is given by the posterior mean $\mu_{y|\mathbf{x}}$ of the label y, given the features $\mathbf{x}$ [**?**], [**?**]. The corresponding Bayes risk is given by the posterior variance $\sigma^2_{y|\mathbf{x}}$ (see Fig. 12).

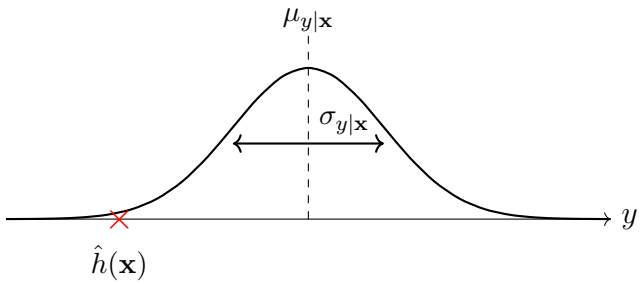


Fig. 12. If the features and the label of a data point are drawn from a multivariate normal distribution, we can achieve the minimum risk (under squared error loss) by using the Bayes estimator $\mu_{y|\mathbf{x}}$ to predict the label y of a data point with features $\mathbf{x}$. The corresponding minimum risk is given by the posterior variance $\sigma^2_{y|\mathbf{x}}$. We can use this quantity as a baseline for the average loss of a trained model $\hat{h}$.

See also: Bayes risk, Bayes estimator.

batch In the context of SGD, a batch refers to a randomly chosen subset of the overall training set. We use the data points in this subset to estimate the gradient of training error and, in turn, to update the model parameters.

See also: SGD, training set, data point, gradient, training error, model parameters.

batch learning In batch learning (also known as offline learning), the ML model is trained on the entire tietoaineisto in a single training iteration, instead of updating it incrementally as data arrive. All available data are inputted into a learning algorithm, resulting in a model that can make predictions. Since these tietoaineistot tend to be large, training is computationally expensive and time-consuming, so it is typically performed offline. After learning, the model will be static and will not adapt to new data automatically. Updating the model with new information requires retraining the model entirely. Once the model has been trained, it is launched into production where it cannot be updated. Training a model can take many hours, so many models in production settings are updated cyclically on a periodic schedule when the data distribution is stable. For example, a retail analytics team could retrain their demand forecast model every Sunday using the previous week's sales data to predict next week's demand. If a system needs to be constantly updated to rapidly changing data, such as in stock price prediction, a more adaptable solution such as online learning is necessary.

See also: batch, model, tietoaineisto, online learning.

Bayes estimator Consider a probabilistic model with a joint probability distribution $p(\mathbf{x}, y)$ over the features $\mathbf{x}$ and the label y of a data point. For a given loss function $L(\cdot, \cdot)$, we refer to a hypothesis h as a Bayes estimator if its risk $\mathbb{E}\{L((\mathbf{x}, y), h)\}$ is the minimum achievable risk [**?**]. Note that whether a hypothesis qualifies as a Bayes estimator depends on the underlying probability distribution and the choice for the loss

function $L(\cdot, \cdot)$.

See also: probabilistic model, hypothesis, risk.

Bayes risk Consider a probabilistic model with a joint probability distribution $p(\mathbf{x}, y)$ for the features $\mathbf{x}$ and label y of a data point. The Bayes risk is the minimum possible risk that can be achieved by any hypothesis $h : \mathcal{X} \rightarrow \mathcal{Y}$. Any hypothesis that achieves the Bayes risk is referred to as a Bayes estimator [?].

See also: probabilistic model, risk, Bayes estimator.

harha Consider an ML method using a parameterized hypothesis space $\mathcal{H}$. It learns the model parameters $\mathbf{w} \in \mathbb{R}^d$ using the tietoaineisto

$$\mathcal{D} = \left\{ \left(\mathbf{x}^{(r)}, y^{(r)}\right) \right\}_{r=1}^{m}.$$

To analyze the properties of the ML method, we typically interpret the data points as realizations of independent and identically distributed (i.i.d.) RVs,

$$y^{(r)} = h^{(\overline{\mathbf{w}})}\left(\mathbf{x}^{(r)}\right) + \boldsymbol{\varepsilon}^{(r)}, r = 1, \ldots, m.$$

We can then interpret the ML method as an estimator $\widehat{\mathbf{w}}$ computed from $\mathcal{D}$ (e.g., by solving ERM). The (squared) bias incurred by the estimate $\widehat{\mathbf{w}}$ is then defined as $B^2 := \left\| \mathbb{E}\{\widehat{\mathbf{w}}\} - \overline{\mathbf{w}} \right\|_2^2$.

See also: i.i.d., RV, probabilistic model, estimation error.

boosting Boosting is an iterative optimization method to learn an accurate hypothesis map (or strong learner) by sequentially combining less accurate hypothesis maps (referred to as weak learners) [?, Ch. 10]. For example, weak learners are shallow decision treet that are combined to

obtain a deep decision tree. Boosting can be understood as a generalization of gradient-based methods for ERM using parametric models and smooth loss functiont [**?**]. Just as GD iteratively updates model parameters to reduce the empirical risk, boosting iteratively combines (e.g., by summation) hypothesis maps to reduce the empirical risk (see Fig. 13). A widely used instance of the generic boosting idea is referred to as gradient boosting, which uses gradients of the loss function for combining the weak learners [**?**].

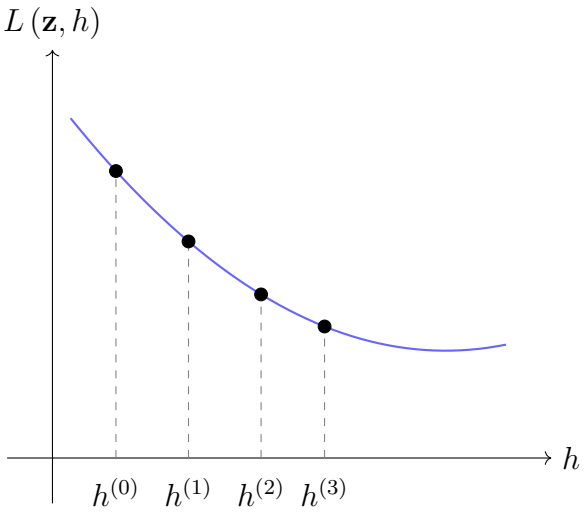


Fig. 13. Boosting methods construct a sequence of hypothesis maps $h^{(0)}$, $h^{(1)}$, ... that are increasingly strong learners (i.e., incurring a smaller loss).

See also: optimization method, hypothesis, map, decision tree, generalization, gradient-based methods, ERM, model, smooth, loss function, GD, model parameters, empirical risk, gradient, loss, gradient step.

uusio-otanta For the analysis of ML methods, it is often useful to interpret a given set of data points $\mathcal{D} = \{\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(m)}\}$ as realizations of i.i.d. RVs drawn from a common probability distribution $p(\mathbf{z})$. In practice, the probability distribution $p(\mathbf{z})$ is unknown and must be estimated from $\mathcal{D}$. The bootstrap approach uses the histogram of $\mathcal{D}$ as an estimator for $p(\mathbf{z})$.

See also: i.i.d., RV, probability distribution, histogram.

central limit theorem (CLT) Consider a sequence of i.i.d. RVs $x^{(r)}$, for $r = 1, 2, \ldots$, each with mean zero and finite variance $\sigma^2 > 0$. The CLT states that the normalized sum

$$s^{(m)} := \frac{1}{\sqrt{m}} \sum_{r=1}^{m} x^{(r)}$$

converges in distribution to a Gaussian RV with mean zero and variance σ^2 as $m \to \infty$ [**?**, Proposition 2.17]. One elegant way to derive the CLT is via the characteristic function of the normalized sum $s^{(m)}$. Let $\phi(t) = \mathbb{E}\{\exp(jtx)\}$ (with the imaginary unit $j = \sqrt{-1}$) be the common characteristic function of each sum and $x^{(r)}$, and let $\phi^{(m)}(t)$ denote the characteristic function of $s^{(m)}$. Define an operator $\mathcal{T}$ acting on characteristic functions such that

$$\phi^{(m)}(t) = \mathcal{T}(\phi^{(m-1)})(t) := \phi\left(\frac{t}{\sqrt{m}}\right) \cdot \phi^{(m-1)}\left(\frac{\sqrt{m-1}}{\sqrt{m}} t\right).$$

This fixed-point iteration captures the effect of recursively adding an i.i.d. RV $\mathbf{x}^{(m)}$ and rescaling. Iteratively applying $\mathcal{T}$ leads to convergence of $\phi^{(m)}(t)$ toward the fixed point

$$\phi^*(t) = \exp\left(-t^2\sigma^2/2\right)$$

which is the characteristic function of a Gaussian RV with mean zero and variance σ^2. Generalizations of the CLT allow for dependent or nonidentically distributed RVs [**?**, Sec. 2.8].

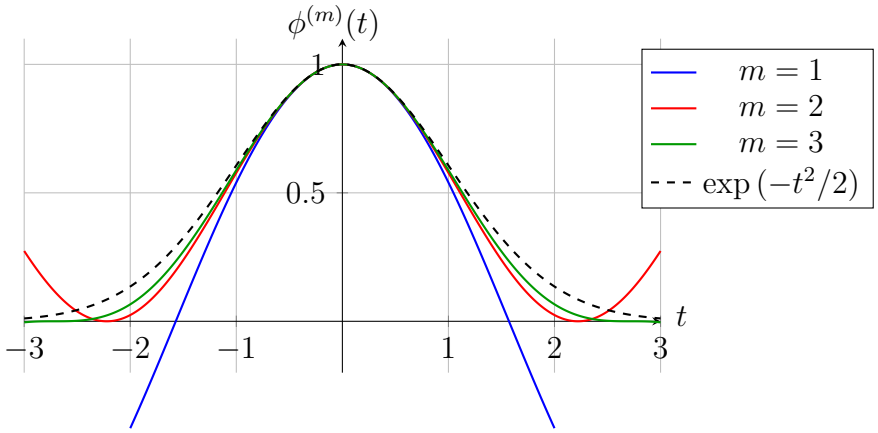


Fig. 14. Characteristic functions of normalized sums of i.i.d. RVs $x^{(r)} \in \{-1, 1\}$ for $r = 1, \ldots, m$ compared to the Gaussian limit.

See also: RV, Gaussian RV.

luokittelu Classification is the task of determining a discrete-valued label y for a given data point, based solely on its features $\mathbf{x}$. The label y belongs to a finite set, such as $y \in \{-1, 1\}$ or $y \in \{1, \ldots, 19\}$, and represents the category to which the corresponding data point belongs. See also: label, data point, feature.

luokitin A classifier is a hypothesis (i.e., a map) $h(\mathbf{x})$ used to predict a label taking on values from a finite label space. We might use the function value $h(\mathbf{x})$ itself as a prediction $\hat{y}$ for the label. However, it is customary to use a map $h(\cdot)$ that delivers a numeric quantity. The prediction is

then obtained by a simple thresholding step. For example, in a binary luokittelu problem with a label space $\mathcal{Y} \in \{-1, 1\}$, we might use a real-valued hypothesis map $h(\mathbf{x}) \in \mathbb{R}$ as a classifier. A prediction $\hat{y}$ can then be obtained via thresholding,

$$\hat{y} = 1 \text{ for } h(\mathbf{x}) \geq 0 \text{ and } \hat{y} = -1 \text{ otherwise.} \tag{1}$$

We can characterize a classifier by its decision regions $\mathcal{R}_a$, for every possible label value $a \in \mathcal{Y}$.

See also: hypothesis, luokittelu, decision region.

rypäs A cluster is a subset of data points that are more similar to each other than to the data points outside the cluster. The quantitative measure of similarity between data points is a design choice. If data points are characterized by Euclidean feature vectors $\mathbf{x} \in \mathbb{R}^d$, we can define the similarity between two data points via the Euclidean distance between their feature vectors. An example of such clusters is shown in Fig. 15.

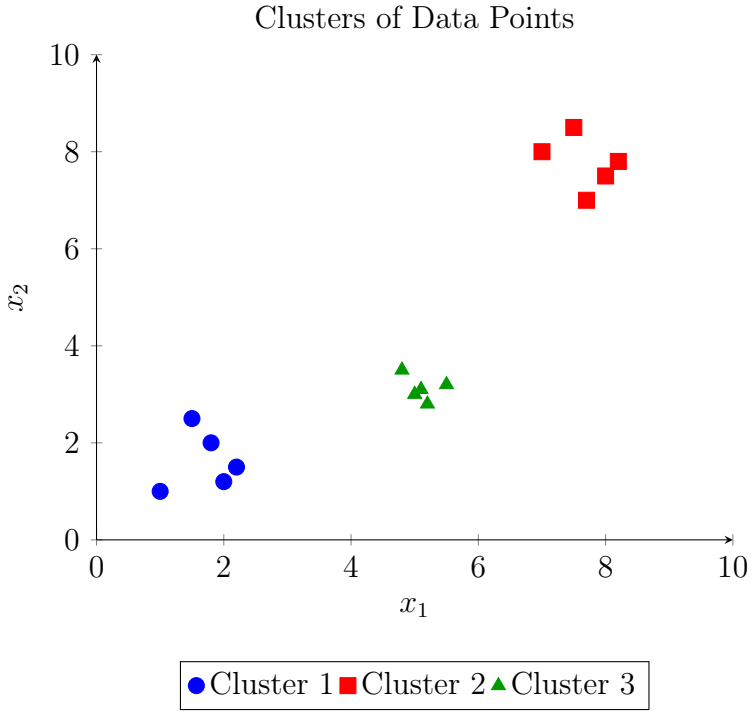


Fig. 15. Illustration of three clusters in a 2-D feature space. Each cluster groups data points that are more similar to each other than to those in other clusters, based on the Euclidean distance.

See also: data point, feature vector, feature space.

cluster centroid Klusterointi methods decompose a given tietoaineisto into few rypäst. Different klusterointi methods use different representations for these ryppäät. If data points are characterized by numerical feature vectors $\mathbf{x} \in \mathbb{R}^d$, we can use some vector $\boldsymbol{\mu} \in \mathbb{R}^d$, referred to as rypäs centroid, to represent a rypäs. For example, if a rypäs consists of a set of data points, we use the average of their feature vectors as a rypäs centroid. However, there are also other choices for how to construct a

rypäs centroid.

See also: klusterointi, feature vector, k-means.

clustered federated learning (CFL) CFL trains local models for the devices in a federated learning (FL) application by using a clustering assumption, i.e., the devices of an FL network form ryppäät. Two devices in the same rypäs generate local datasets with similar statistical properties. CFL pools the local datasets of devices in the same rypäs to obtain a training set for a rypäs-specific model. Generalized total variation minimization (GTVMin) clusters devices implicitly by enforcing approximate similarity of model parameters across well-connected nodes of the FL network.

See also: FL, clustering assumption, FL network, rypäs, graph clustering.

klusterointi Clustering methods decompose a given set of data points into a few subsets, which are referred to as ryppäät. Each rypäs consists of data points that are more similar to each other than to data points outside the rypäs. Different clustering methods use different measures for the similarity between data points and different forms of rypäs representations. The clustering method k-means uses the average feature vector of a rypäs (i.e., the rypäs mean) as its representative. A popular soft clustering method based on Gaussian mixture model (GMM) represents a rypäs by a multivariate normal distribution.

See also: rypäs, k-means, soft clustering, GMM.

clustering assumption The klusterointi assumption postulates that data points in a tietoaineisto form a (small) number of groups or ryppäät.

Data points in the same rypäs are more similar to each other than those outside the rypäs [?]. We obtain different klusterointi methods by using different notions of similarity between data points.

See also: klusterointi, data point, tietoaineisto, rypäs.

computational aspects By computational aspects of an ML method, we mainly refer to the computational resources required for its implementation. For example, if an ML method uses iterative optimization techniques to solve ERM, then its computational aspects include: 1) how many arithmetic operations are needed to implement a single iteration (i.e., a gradient step); and 2) how many iterations are needed to obtain useful model parameters. One important example of an iterative optimization technique is GD.

See also: ML, ERM, gradient step, model parameters, GD.

concentration inequality An upper bound on the probability that an RV deviates more than a prescribed amount from its expectation [?].

See also: probability, RV, expectation.

concept activation vector (CAV) Consider a deep net, consisting of several hidden layers, trained to predict the label of a data point from its feature vector. One way to explain the behavior of the trained deep net is by using the activations of a hidden layer as a new feature vector $\mathbf{z}$. We then probe the geometry of the resulting new feature space by applying the deep net to data points that represent a specific concept $\mathcal{C}$. By applying the deep net also to data points that do not belong to this concept, we can train a binary linear classifier $g(\mathbf{z})$ that distinguishes

between concept and non-concept data points based on the activations of the hidden layer. The resulting decision boundary is a hyperplane whose normal vector is the CAV for the concept $\mathcal{C}$.

See also: deep net, linear model, trustworthy artificial intelligence (trustworthy AI), interpretability, transparency.

condition number The condition number $\kappa(\mathbf{Q}) \geq 1$ of a positive definite matrix $\mathbf{Q} \in \mathbb{R}^{d \times d}$ is the ratio α/β between the largest α and the smallest β eigenvalue of $\mathbf{Q}$. The condition number is useful for the analysis of ML methods. The computational complexity of gradient-based methods for linear regression crucially depends on the condition number of the matrix $\mathbf{Q} = \mathbf{X}\mathbf{X}^T$, with the feature matrix $\mathbf{X}$ of the training set. Thus, from a computational perspective, we prefer features of data points such that $\mathbf{Q}$ has a condition number close to 1.

See also: matrix, eigenvalue, ML, gradient-based methods, linear regression, feature matrix, training set, feature, data point.

sekaannusmatriisi Consider data points characterized by features $\mathbf{x}$ and corresponding labels y. The labels take on values in a finite label space $\mathcal{Y} = \{1, \ldots, k\}$. For a given hypothesis h, the confusion matrix is a $k \times k$ matrix where each row corresponds to a different value of the true label $y \in \mathcal{Y}$ and each column to a different value of the prediction $h(\mathbf{x}) \in \mathcal{Y}$. The (c, c')th entry of the confusion matrix represents the fraction of data points with a true label $y = c$ that are predicted as $h(\mathbf{x}) = c'$. The main diagonal of the confusion matrix contains the fractions of correctly classified data points (i.e., those for which $y = h(\mathbf{x})$). The off-diagonal

entries contain the fractions of data points that are misclassified by h. See also: label, label space, hypothesis, matrix, luokittelu.

connected graph An undirected graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is connected if every non-empty subset $\mathcal{V}' \subset \mathcal{V}$ has at least one edge connecting it to $\mathcal{V} \setminus \mathcal{V}'$. See also: graph.

contraction operator An operator $\mathcal{F} : \mathbb{R}^d \to \mathbb{R}^d$ is a contraction if, for some $\kappa \in [0, 1)$,

$$\|\mathcal{F}\mathbf{w} - \mathcal{F}\mathbf{w}'\|_2 \leq \kappa \|\mathbf{w} - \mathbf{w}'\|_2 \text{ holds for any } \mathbf{w}, \mathbf{w}' \in \mathbb{R}^d.$$

convex A subset $\mathcal{C} \subseteq \mathbb{R}^d$ of the Euclidean space $\mathbb{R}^d$ is referred to as convex if it contains the line segment between any two points $\mathbf{x}, \mathbf{y} \in \mathcal{C}$ in that set. A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if its epigraph $\left\{ \left(\mathbf{w}^T, t \right)^T \in \mathbb{R}^{d+1} : t \geq f(\mathbf{w}) \right\}$ is a convex set [**?**]. We illustrate one example of a convex set and a convex function in Fig. 16.

(a) (b)

Fig. 16. (a) A convex set $\mathcal{C} \subseteq \mathbb{R}^d$. (b) A convex function $f : \mathbb{R}^d \to \mathbb{R}$.

See also: Euclidean space, function, epigraph.

convex clustering Consider a tietoaineisto $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)} \in \mathbb{R}^d$. Convex klusterointi learns vectors $\mathbf{w}^{(1)}, \ldots, \mathbf{w}^{(m)}$ by minimizing

$$\sum_{r=1}^{m} \left\|\mathbf{x}^{(r)} - \mathbf{w}^{(r)}\right\|_2^2 + \alpha \sum_{i,i' \in \mathcal{V}} \left\|\mathbf{w}^{(i)} - \mathbf{w}^{(i')}\right\|_p .$$

Here, $\|\mathbf{u}\|_p := \left(\sum_{j=1}^{d} |u_j|^p\right)^{1/p}$ denotes the p-norm (for $p \geq 1$). It turns out that many of the optimal vectors $\widehat{\mathbf{w}}^{(1)}, \ldots, \widehat{\mathbf{w}}^{(m)}$ coincide. A rypäs then consists of those data points $r \in \{1, \ldots, m\}$ with identical $\widehat{\mathbf{w}}^{(r)}$ [**?**], [**?**].

See also: tietoaineisto, convex, klusterointi, vector, norm, rypäs, data point.

Courant–Fischer–Weyl min–max characterization Consider a psd matrix $\mathbf{Q} \in \mathbb{R}^{d \times d}$ with eigenvalue decomposition (EVD) (or spectral decomposition), i.e.,

$$\mathbf{Q} = \sum_{j=1}^{d} \lambda_j \mathbf{u}^{(j)} \left(\mathbf{u}^{(j)}\right)^T .$$

Here, we use the ordered (in ascending order) eigenvalues

$$\lambda_1 \leq \ldots \leq \lambda_n .$$

The Courant–Fischer–Weyl min–max characterization [3, Th. 8.1.2] represents the eigenvalues of $\mathbf{Q}$ as the solutions to certain optimization problems.

See also: psd, matrix, EVD, eigenvalue, optimization problem.

covariance The covariance between two real-valued RVs x and y, defined on a common probability space, measures their linear dependence. It is

defined as

$$\mathrm{cov}\,(x, y) = \mathbb{E}\big\{\big(x - \mathbb{E}\{x\}\big)\big(y - \mathbb{E}\{y\}\big)\big\}.$$

A positive covariance indicates that x and y tend to increase together, while a negative covariance suggests that one tends to increase as the other decreases. If $\mathrm{cov}\,(x, y) = 0$, the RVs are said to be uncorrelated, though not necessarily statistically independent. See Fig. 17 for visual illustrations.

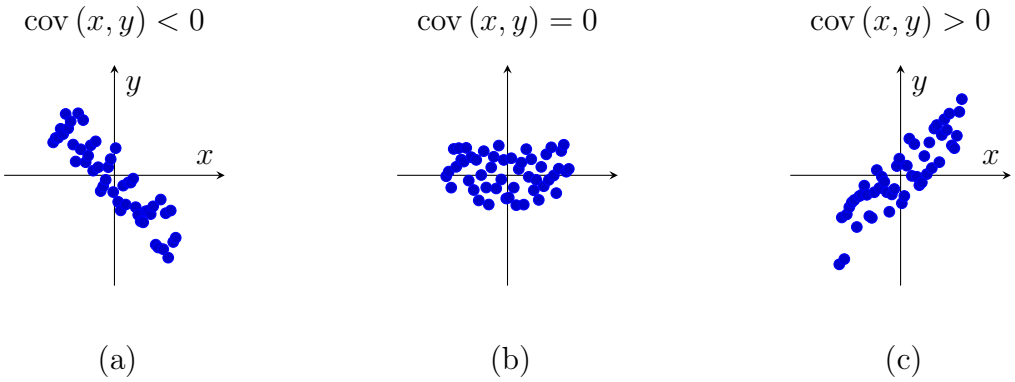


Fig. 17. Scatterplott illustrating realizations from three different probabilistic models for two RVs with different covariance values. (a) Negative. (b) Zero. (c) Positive.

See also: probabilistic model, expectation.

kovarianssimatriisi The covariance matrix of an RV $\mathbf{x} \in \mathbb{R}^d$ is defined as $\mathbb{E}\Big\{\big(\mathbf{x} - \mathbb{E}\{\mathbf{x}\}\big)\big(\mathbf{x} - \mathbb{E}\{\mathbf{x}\}\big)^T\Big\}$.
See also: covariance, matrix, RV.

data In the context of ML, the term data is often used synonymously with tietoaineisto [?, ?]. The ISO/IEC 2382:2015 standard defines data as a

re-interpretable representation of information in a formalized manner suitable for communication, interpretation, or processing [**?**].
See also: tietoaineisto, data point, sample.

data augmentation Data augmentation methods add synthetic data points to an existing set of data points. These synthetic data points are obtained by perturbations (e.g., adding noise to physical measurements) or transformations (e.g., rotations of images) of the original data points. These perturbations and transformations are such that the resulting synthetic data points should still have the same label. As a case in point, a rotated cat image is still a cat image even if their feature vectors (obtained by stacking pixel color intensities) are very different (see Fig. 18). Data augmentation can be an efficient form of regularization.

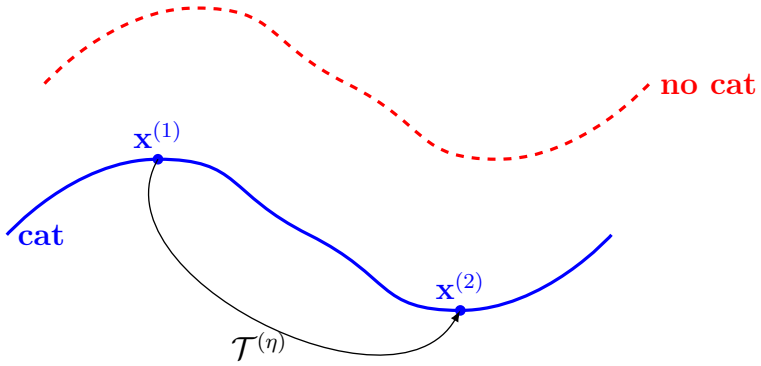


Fig. 18. Data augmentation exploits intrinsic symmetries of data points in some feature space $\mathcal{X}$. We can represent a symmetry by an operator $\mathcal{T}^{(\eta)} : \mathcal{X} \to \mathcal{X}$, parameterized by some number $\eta \in \mathbb{R}$. For example, $\mathcal{T}^{(\eta)}$ might represent the effect of rotating a cat image by η degrees. A data point with feature vector $\mathbf{x}^{(2)} = \mathcal{T}^{(\eta)}\big(\mathbf{x}^{(1)}\big)$ must have the same label $y^{(2)} = y^{(1)}$ as a data point with feature vector $\mathbf{x}^{(1)}$.

See also: data, data point, label, feature vector, regularization, feature space.

data minimization principle European data protection regulation includes a data minimization principle. This principle requires a data controller to limit the collection of personal information to what is directly relevant and necessary to accomplish a specified purpose. The data should be retained only for as long as necessary to fulfill that purpose [**?**, Article 5(1)(c)], [**?**].

See also: data.

datan normalisointi Data normalization refers to transformations applied

to the feature vectors of data points to improve the ML method's statistical aspects or computational aspects. For example, in linear regression with gradient-based methods using a fixed learning rate, convergence depends on controlling the norm of feature vectors in the training set. A common approach is to normalize feature vectors such that their norm does not exceed one [8, Ch. 5].

See also: data, feature vector, data point, ML, statistical aspects, computational aspects, linear regression, gradient-based methods, learning rate, convergence, norm, training set.

data point A data point is any object that conveys information [**?**]. Examples include students, radio signals, trees, images, RVs, real numbers, or proteins. We describe data points of the same type by two categories of properties. The first category includes features that are measurable or computable properties of a data point. These attributes can be automatically extracted or computed using sensors, computers, or other data collection systems. For a data point that represents a patient, one feature could be the body weight. The second category includes labels that are higher level facts (or quantities of interest)—that is, facts which typically require human expertise or domain knowledge to determine, rather than being directly measurable—associated with the data point. Determining the labels of a data point usually requires human expertise or domain knowledge. For a data point that represents a patient, a cancer diagnosis provided by a physician would serve as the label. Fig. 19 depicts an image as an example of a data point along with its features and labels. Importantly, what constitutes a feature or a label is not

inherent to the data point itself—it is a design choice that depends on the specific ML application.

A single data point.

Features:

- $x_1, \ldots, x_d$: Color intensities of all image pixels.
- x_{d+1}: Time-stamp of the image capture.
- x_{d+2}: Spatial location of the image capture.

Labels:

- y_1: Number of cows depicted.
- y_2: Number of wolves depicted.
- y_3: Condition of the pasture (e.g., healthy, overgrazed).

Fig. 19. Illustration of a data point consisting of an image. We can use different properties of the image as features and higher level facts about the image as labels.

The distinction between features and labels is not always clear-cut. A property that is considered a label in one setting (e.g., a cancer diagnosis) may be treated as a feature in another setting—particularly if reliable automation (e.g., via image analysis) allows it to be computed without human intervention. ML broadly aims to predict the label of a data point based on its features.

See also: data, feature, label, tietoaineisto.

data poisoning Data poisoning refers to the intentional manipulation (or fabrication) of data points to steer the training of an ML model [**?**], [**?**]. Data poisoning attacks take various forms, including backdoor and denial-of-service attacks. A backdoor attack implants triggers into training data, so that the trained model behaves normally on typical feature vectors but misclassifies a feature vector with a trigger pattern. A denial-of-service attack degrades the trained model's overall performance by injecting mislabeled or adversarial examples to prevent effective learning. Data poisoning is particularly concerning in decentralized or distributed ML settings (such as FL), where training data cannot be centrally verified.

See also: attack, backdoor, denial-of-service attack, trustworthy AI.

tietoaineisto A dataset is a set of distinct data points. In contrast to a sample, which is defined as a sequence of data points and may contain repetitions, a dataset is an unordered collection without duplicates. ML methods use datasets to train and validate models. The notion of a dataset is broad: data points may represent concrete physical entities

(such as humans or animals) or abstract objects (such as numbers). For illustration, Fig. 20 depicts a dataset whose data points are cows.

Fig. 20. A cow herd somewhere in the Alps.

Quite often, an ML engineer does not have direct access to the underlying dataset. For instance, accessing the dataset in Fig. 20 would require visiting the cow herd. In practice, we work with a more convenient representation (or approximation) of the dataset. Various mathematical models have been developed for this purpose [**?**], [**?**], [**?**], [**?**]. One of the most widely used is the relational model, which organizes data as a table (or relation) [**?**], [**?**]. A table consists of rows and columns: each row corresponds to a single data point, while each column represents a specific attribute of a data point. ML methods typically interpret these attributes as features or as a label of a data point. As an illustration, Table I shows a relational representation of the dataset from Fig. 20. In the relational model, the order of rows is immaterial, and each attribute (column) is associated with a domain that specifies the set of admissible values. In ML applications, these attribute domains correspond to the feature space and the label space.

TABLE I

A Relation (or Table) That Represents the Dataset in Fig. 20

Name	**Weight**	**Age**	**Height**	**Stomach temperature**
Zenzi	100	4	100	25
Berta	140	3	130	23
Resi	120	4	120	31

While the relational model is useful for the study of many ML applications, it may be insufficient regarding the requirements for trustworthy AI. Modern approaches like datasheets for datasets provide more comprehensive documentation, including details about the data collection process, intended use, and other contextual information [**?**].

See also: data point, data, feature, sample, feature space, label space.

decision boundary Consider a hypothesis map h that reads in a feature vector $\mathbf{x} \in \mathbb{R}^d$ and delivers a value from a finite set $\mathcal{Y}$. The decision boundary of h is the set of vectors $\mathbf{x} \in \mathbb{R}^d$ that lie between different decision regions. More precisely, a vector $\mathbf{x}$ belongs to the decision boundary if and only if each neighborhood $\{\mathbf{x}' : \|\mathbf{x} - \mathbf{x}'\| \leq \varepsilon\}$, for any $\varepsilon > 0$, contains at least two vectors with different function values.

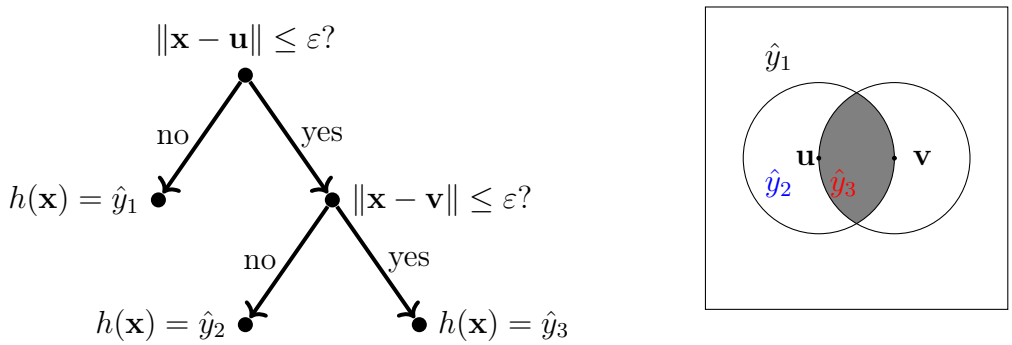
See also: hypothesis, map, feature vector, vector, decision region, neighborhood, function.

decision region Consider a hypothesis map h that delivers values from a finite set $\mathcal{Y}$. For each label value (i.e., category) $a \in \mathcal{Y}$, the hypothesis h determines a subset of feature values $\mathbf{x} \in \mathcal{X}$ that result in the same

output $h(\mathbf{x}) = a$. We refer to this subset as a decision region of the hypothesis h.

See also: hypothesis, map, label, feature.

decision tree A decision tree is a flowchart-like representation of a hypothesis map h. More formally, a decision tree is a directed graph containing a root node that reads in the feature vector $\mathbf{x}$ of a data point. The root node then forwards the data point to one of its child nodes based on some elementary test on the features $\mathbf{x}$. If the receiving child node is not a leaf node, i.e., it has child nodes itself, it represents another test. Based on the test result, the data point is forwarded to one of its descendants. This testing and forwarding of the data point is continued until the data point ends up in a leaf node without any children. See Fig. 21 for visual illustrations.



(a) (b)

Fig. 21. (a) A decision tree is a flowchart-like representation of a piecewise constant hypothesis $h : \mathcal{X} \to \mathbb{R}$. Each piece is a decision region $\mathcal{R}_{\hat{y}} := \{\mathbf{x} \in \mathcal{X} : h(\mathbf{x}) = \hat{y}\}$. The depicted decision tree can be applied to numeric feature vectors, i.e., $\mathcal{X} \subseteq \mathbb{R}^d$. It is parameterized by the threshold $\varepsilon > 0$ and the vectors $\mathbf{u}, \mathbf{v} \in \mathbb{R}^d$. (b) A decision tree partitions the feature space $\mathcal{X}$ into decision regions. Each decision region $\mathcal{R}_{\hat{y}} \subseteq \mathcal{X}$ corresponds to a specific leaf node in the decision tree.

See also: decision region.

deep net A deep net is an ANN with a (relatively) large number of hidden layers. Deep learning is an umbrella term for ML methods that use a deep net as their model [**?**].

See also: ANN, layer, ML, model.

degree of belonging Degree of belonging is a number that indicates the extent to which a data point belongs to a rypäs [8, Ch. 8]. The degree of belonging can be interpreted as a soft rypäs assignment. Soft clustering

methods can encode the degree of belonging with a real number in the interval $[0, 1]$. Hard clustering is obtained as the extreme case when the degree of belonging only takes on values 0 or 1.

See also: data point, rypäs, soft clustering, hard clustering.

denial-of-service attack A denial-of-service attack aims (e.g., via data poisoning) to steer the training of a model such that it performs poorly for typical data points.

See also: attack, data poisoning, model, data point.

density-based spatial clustering of applications with noise (DBSCAN) DBSCAN refers to a klusterointi algorithm for data points that are characterized by numeric feature vectors. Like k-means and soft clustering via GMM, DBSCAN also uses the Euclidean distances between feature vectors to determine the ryppäät. However, in contrast to k-means and GMM, DBSCAN uses a different notion of similarity between data points. DBSCAN considers two data points as similar if they are connected via a sequence (i.e., path) of nearby intermediate data points. Thus, DBSCAN might consider two data points as similar (and therefore belonging to the same cluster) even if their feature vectors have a large Euclidean distance.

See also: klusterointi, k-means, GMM, rypäs, graph.

device A physical system that can store and process data. In the context of ML, the term typically refers to a computer capable of reading data points from different sources and using them to train an ML model [**?**].

See also: data, ML, data point, model.

differentiable A real-valued function $f : \mathbb{R}^d \to \mathbb{R}$ is differentiable if it can be approximated locally at any point by a linear function. The local linear approximation at the point $\mathbf{x}$ is determined by the gradient $\nabla f(\mathbf{x})$ [2].
See also: function, gradient.

differential entropy For a real-valued RV $\mathbf{x} \in \mathbb{R}^d$ with a probability density function (pdf) $p(x)$, the differential entropy is defined as [**?**]

$$h(\mathbf{x}) := -\int p(\mathbf{x}) \log p(\mathbf{x})\, d\mathbf{x}.$$

Differential entropy can be negative and lacks some properties of entropy for discrete-valued RVs, such as invariance under a change of variables [**?**]. Among all RVs with a given mean $\boldsymbol{\mu}$ and kovarianssimatriisi $\boldsymbol{\Sigma}$, $h(\mathbf{x})$ is maximized by $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.
See also: uncertainty, probabilistic model.

differential privacy (DP) Consider some ML method $\mathcal{A}$ that reads in a tietoaineisto (e.g., the training set used for ERM) and delivers some output $\mathcal{A}(\mathcal{D})$. The output could be either the learned model parameters or the predictions for specific data points. DP is a precise measure of privacy leakage incurred by revealing the output. Roughly speaking, an ML method is differentially private if the probability distribution of the output $\mathcal{A}(\mathcal{D})$ remains largely unchanged if the sensitive attribute of one data point in the training set is changed. Note that DP builds on a probabilistic model for an ML method, i.e., we interpret its output $\mathcal{A}(\mathcal{D})$ as the realization of an RV. The randomness in the output can be ensured by intentionally adding the realization of an auxiliary RV (i.e., adding noise) to the output of the ML method.

See also: privacy leakage, sensitive attribute, privacy attack, privacy funnel.

dimensionality reduction Dimensionality reduction refers to methods that learn a transformation $h : \mathbb{R}^d \to \mathbb{R}^{d'}$ of a (typically large) set of raw features $x_1, \ldots, x_d$ into a smaller set of informative features $z_1, \ldots, z_{d'}$. Using a smaller set of features is beneficial in several ways:

- Statistical benefit: It typically reduces the risk of overfitting, as reducing the number of features often reduces the effective dimension of a model.
- Computational benefit: Using fewer features means less computation for the training of ML models. As a case in point, linear regression methods need to invert a matrix whose size is determined by the number of features.
- Visualization: Dimensionality reduction is also instrumental for data visualization. For example, we can learn a transformation that delivers two features z_1, z_2, which we can use, in turn, as the coordinates of a scatterplot. Fig. 22 depicts the scatterplot of handwritten digits that are placed using transformed features. Here, the data points are naturally represented by a large number of greyscale values (one value for each pixel).

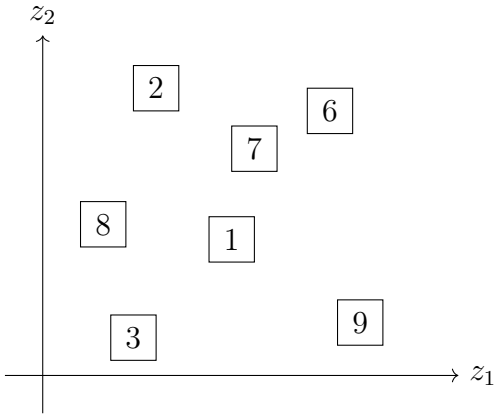


Fig. 22. Example of dimensionality reduction: High-dimensional image data (e.g., high-resolution images of handwritten digits) embedded into 2-D using learned features (z_1, z_2) and visualized in a scatterplot.

See also: overfitting, effective dimension, model, scatterplot.

discrepancy Consider an FL application with networked data represented by an FL network. FL methods use a discrepancy measure to compare hypothesis maps from local models at nodes i, i', connected by an edge in the FL network.

See also: FL, FL network, local model.

distributed algorithm A distributed algorithm is an algorithm designed for a special type of computer, i.e., a collection of interconnected computing devices (or nodes). These devices communicate and coordinate their local computations by exchanging messages over a network [**?**], [**?**]. Unlike a classical algorithm, which is implemented on a single device, a distributed algorithm is executed concurrently on multiple devices with computational capabilities. Similar to a classical algorithm, a distributed

algorithm can be modeled as a set of potential executions. However, each execution in the distributed setting involves both local computations and message-passing events. A generic execution might look as follows:

$$\begin{aligned}&\text{Node 1: input}_1,\ s_1^{(1)},\ s_2^{(1)},\ \ldots,\ s_{T_1}^{(1)},\ \text{output}_1;\\&\text{Node 2: input}_2,\ s_1^{(2)},\ s_2^{(2)},\ \ldots,\ s_{T_2}^{(2)},\ \text{output}_2;\\&\quad\vdots\\&\text{Node N: input}_N,\ s_1^{(N)},\ s_2^{(N)},\ \ldots,\ s_{T_N}^{(N)},\ \text{output}_N.\end{aligned}$$

Each device i starts from its own local input and performs a sequence of intermediate computations $s_k^{(i)}$ at discrete-time instants $k = 1, \ldots, T_i$. These computations may depend on both the previous local computations at the device and the messages received from other devices. One important application of distributed algoritmit is in FL where a network of devices collaboratively trains a personal model for each device.

See also: algorithm, device, event, FL, model.

dual norm Every norm $\|\cdot\|$ defined on a Euclidean space $\mathbb{R}^d$ has an associated dual norm, which is denoted by $\|\cdot\|_*$ and defined as $\|\mathbf{y}\|_* := \sup_{\|\mathbf{x}\|\leq 1} \mathbf{y}^T\mathbf{x}$. The dual norm measures the largest possible inner product between $\mathbf{y}$ and any vector in the unit ball of the original norm. For further details, see [**?**, Sec. A.1.6].

See also: norm, Euclidean space, vector.

edge weight Each edge $\{i, i'\}$ of an FL network is assigned a nonnegative edge weight $A_{i,i'} \geq 0$. A zero edge weight $A_{i,i'} = 0$ indicates the absence of an edge between nodes $i, i' \in \mathcal{V}$.

See also: FL network.

effective dimension The effective dimension $d_{\text{eff}}(\mathcal{H})$ of an infinite hypothesis space $\mathcal{H}$ is a measure of its size. Loosely speaking, the effective dimension is equal to the effective number of independent tunable model parameters. These parameters might be the coefficients used in a linear map or the weights and harha terms of an ANN.

See also: hypothesis space, model parameters, ANN.

eigenvalue We refer to a number $\lambda \in \mathbb{R}$ as an eigenvalue of a square matrix $\mathbf{A} \in \mathbb{R}^{d \times d}$ if there exists a nonzero vector $\mathbf{x} \in \mathbb{R}^d \setminus \{\mathbf{0}\}$ such that $\mathbf{A}\mathbf{x} = \lambda \mathbf{x}$.

See also: matrix, vector.

eigenvalue decomposition (EVD) The EVD for a square matrix $\mathbf{A} \in \mathbb{R}^{d \times d}$ is a factorization of the form

$$\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1}.$$

The columns of the matrix $\mathbf{V} = \big(\mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(d)}\big)$ are the eigenvectort of the matrix $\mathbf{V}$. The diagonal matrix $\mathbf{\Lambda} = \text{diag}\big\{\lambda_1, \ldots, \lambda_d\big\}$ contains the eigenvalues λ_j corresponding to the eigenvectors $\mathbf{v}^{(j)}$. Note that the above decomposition exists only if the matrix $\mathbf{A}$ is diagonalizable.

See also: matrix, eigenvector, eigenvalue.

eigenvector An eigenvector of a matrix $\mathbf{A} \in \mathbb{R}^{d \times d}$ is a nonzero vector $\mathbf{x} \in \mathbb{R}^d \setminus \{\mathbf{0}\}$ such that $\mathbf{A}\mathbf{x} = \lambda \mathbf{x}$ with some eigenvalue λ.

See also: matrix, vector, eigenvalue.

empirical risk The empirical risk $\widehat{L}\big(h|\mathcal{D}\big)$ of a hypothesis on a tietoaineisto $\mathcal{D}$ is the average loss incurred by h when applied to the data points in

$\mathcal{D}$.

See also: risk, hypothesis, tietoaineisto, loss, data point.

empirical risk minimization (ERM) ERM is the optimization problem of selecting a hypothesis $\hat{h} \in \mathcal{H}$ that minimizes the average loss (or empirical risk) on a training set $\mathcal{D}$. The hypothesis is chosen from a hypothesis space (or model) $\mathcal{H}$. The tietoaineisto $\mathcal{D}$ is referred to as training set. A plethora of ERM-based ML methods is obtained for different design choices for the tietoaineisto, model, and loss [8, Ch. 3]. Fig. 23 illustrates ERM for a linear model and data points that are characterized by a single feature x and a label y. The hypothesis h is a linear map that predicts the label of a data point as a linear function of its feature x, i.e., $h(x) = w_1 x + w_0$, where w_1 and w_0 are the model parameters of the hypothesis h. The ERM problem is to find the model parameters w_1 and w_0 that minimize the average loss (or empirical risk) incurred by the hypothesis h on the training set $\mathcal{D}$.

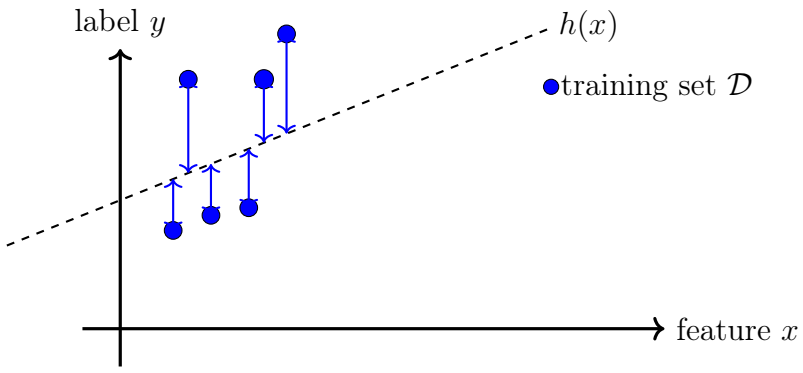


Fig. 23. ERM learns a hypothesis $h \in \mathcal{H}$, out of a model $\mathcal{H}$, by minimizing the average loss (or empirical risk) $1/m \sum_{r=1}^{m} L\left(\left(\mathbf{x}^{(r)}, y^{(r)}\right), h\right)$ incurred on a training set $\mathcal{D}$.

See also: optimization method, empirical risk, training set, loss, optimization problem.

ensemble An ensemble method combines multiple ML methods, referred to as base learners, to improve overall performance. The base learners can be obtained from ERM, using different choices for the loss, model, and training set. Ensemble methods exploit the diversity among these base learners to reduce errors. Loosely speaking, different base learners capture different aspects of the features of a data point. By aggregating the predictions of base learners, ensemble methods can often achieve better performance than any single base learner. Different ensemble methods use different constructions for the base learners and how to aggregate their predictions. For example, bagging (or bootstrap aggregation) methods use random sampling to construct different training

sets for the base learners. A well-known example of a bagging method is a random forest. On the other hand, boosting methods train base learners sequentially, where each new base learner focuses on correcting the errors of the previous ones. A third family of ensemble methods is stacking, where base learners are trained on the same training set but with potentially different models.

See also: bagging.

entropy Entropy quantifies the uncertainty or unpredictability associated with an RV [**?**]. For a discrete RV x taking on values in a finite set $\mathcal{S} = \{x_1, \ldots, x_n\}$ with a probability mass function $p_i := \mathbb{P}(x = x_i)$, the entropy is defined as

$$H(x) := -\sum_{i=1}^{n} p_i \log p_i.$$

Entropy is maximized when all outcomes are equally likely, and minimized (i.e., zero) when the outcome is deterministic. A generalization of the concept of entropy for continuous RVs is differential entropy.

See also: uncertainty, probabilistic model.

epigraph The epigraph of a real-valued function $f : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is the set of points lying on or above its graph (see Fig. 24), i.e.,

$$\operatorname{epi}(f) = \{(\mathbf{x}, t) \in \mathbb{R}^n \times \mathbb{R} \,|\, f(\mathbf{x}) \leq t\}.$$

A function is convex if and only if its epigraph is a convex set [**?**], [**?**].

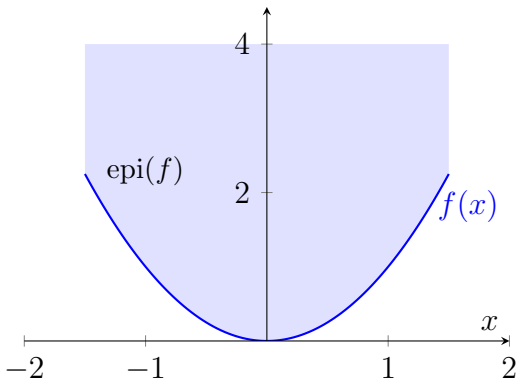


Fig. 24. Epigraph of the function $f(x) = x^2$ (i.e., the shaded area).

See also: function, convex.

epoch An epoch represents one complete pass of the entire training set through some learning algorithm. It refers to the point at which a model has processed every data point in the training set once. Training a model usually requires multiple epochs, since each iteration allows the model to refine the parameters and improve predictions. The number of epochs is something predefined by the user, and thus a hyperparameter, which plays a crucial role in determining how the model will generalize to unseen data. Too few epochs will result in underfitting, while too many epochs can result in overfitting.

See also: training set, algorithm, model, data point, parameter, prediction, underfitting, overfitting.

Erdős–Rényi graph (ER graph) An ER graph is a probabilistic model for grapht defined over a given node set $i = 1, \ldots, n$. One way to define the ER graph is via the collection of i.i.d. binary RVs $b^{(\{i,i'\})} \in \{0, 1\}$, for each

pair of different nodes i, i'. A specific realization of an ER graph contains an edge $\{i, i'\}$ if and only if $b^{(\{i,i'\})} = 1$. The ER graph is parameterized by the number n of nodes and the probability $\mathbb{P}(b^{(\{i,i'\})} = 1)$.

See also: graph, probabilistic model, i.i.d., RV, realization, probability.

estimation error Consider data points, each with feature vector $\mathbf{x}$ and label y. In some applications, we can model the relation between the feature vector and the label of a data point as $y = \bar{h}(\mathbf{x}) + \varepsilon$. Here, we use some true underlying hypothesis $\bar{h}$ and a noise term ε, which summarizes any modeling or labeling errors. The estimation error incurred by an ML method that learns a hypothesis $\widehat{h}$, e.g., using ERM, is defined as $\widehat{h}(\mathbf{x}) - \bar{h}(\mathbf{x})$, for some feature vector. For a parametric hypothesis space, which consists of hypothesis maps determined by model parameters $\mathbf{w}$, we can define the estimation error as $\Delta\mathbf{w} = \widehat{\mathbf{w}} - \overline{\mathbf{w}}$ [**?**], [**?**].

See also: data point, feature vector, label, hypothesis, ML, ERM, hypothesis space, map, model parameters.

Euclidean space The Euclidean space $\mathbb{R}^d$ of dimension $d \in \mathbb{N}$ consists of vectors $\mathbf{x} = \big(x_1, \ldots, x_d\big)$, with d real-valued entries $x_1, \ldots, x_d \in \mathbb{R}$. Such a Euclidean space is equipped with a geometric structure defined by the inner product $\mathbf{x}^T\mathbf{x}' = \sum_{j=1}^{d} x_j x'_j$ between any two vectors $\mathbf{x}, \mathbf{x}' \in \mathbb{R}^d$ [2].

See also: vector.

event Consider an RV $\mathbf{x}$, defined on some probability space $\mathcal{P}$, which takes values in a measurable space $\mathcal{X}$. An event $\mathcal{A} \subseteq \mathcal{X}$ is a subset of $\mathcal{X}$ such that the probability $\mathbb{P}(\mathbf{x} \in \mathcal{A})$ is well defined. In other words, the

preimage $\mathbf{x}^{-1}(\mathcal{A})$ of an event belongs to the σ-algebra of $\mathcal{P}$.

See also: RV, data point, independent and identically distributed assumption (i.i.d. assumption), probabilistic model.

expectation Consider a numeric feature vector $\mathbf{x} \in \mathbb{R}^d$ that we interpret as the realization of an RV with a probability distribution $p(\mathbf{x})$. The expectation of $\mathbf{x}$ is defined as the integral $\mathbb{E}\{\mathbf{x}\} := \int \mathbf{x} p(\mathbf{x})$. Note that the expectation is only defined if this integral exists, i.e., if the RV is integrable [2], [6], [**?**]. Fig. 25 illustrates the expectation of a scalar discrete RV x that takes on values from a finite set only.

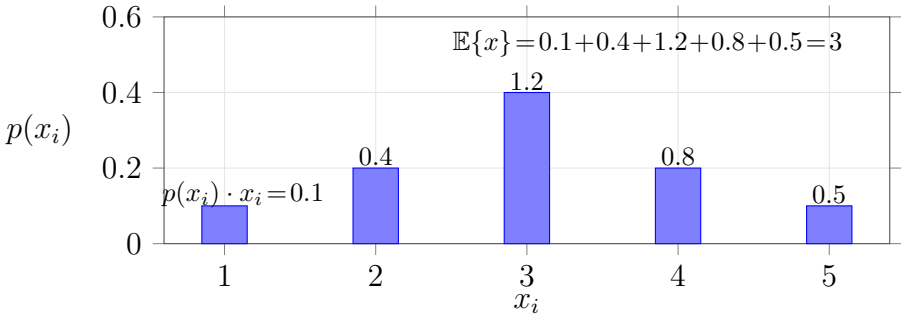


Fig. 25. The expectation of a discrete RV x is obtained by summing its possible values x_i, weighted by the corresponding probability $p(x_i) = \mathbb{P}(x = x_i)$.

See also: feature vector, realization, RV, probability distribution, probability.

expectation–maximization (EM) Consider a probabilistic model $\mathbb{P}(\mathbf{z}; \mathbf{w})$ for the data points $\mathcal{D}$ generated in some ML application. The maximum likelihood estimator for the model parameters $\mathbf{w}$ is obtained by maximizing $\mathbb{P}(\mathcal{D}; \mathbf{w})$. However, the resulting optimization problem might be

computationally challenging. EM approximates the maximum likelihood estimator by introducing a latent RV $\mathbf{z}$ such that maximizing $\mathbb{P}(\mathcal{D}, \mathbf{z}; \mathbf{w})$ would be easier [?], [?], [?]. Since we do not observe $\mathbf{z}$, we need to estimate it from the observed tietoaineisto $\mathcal{D}$ using a conditional expectation. The resulting estimate $\widehat{\mathbf{z}}$ is then used to compute a new estimate $\widehat{\mathbf{w}}$ by solving $\max_{\mathbf{w}} \mathbb{P}(\mathcal{D}, \widehat{\mathbf{z}}; \mathbf{w})$. The crux is that the conditional expectation $\widehat{\mathbf{z}}$ depends on the model parameters $\widehat{\mathbf{w}}$, which we have updated based on $\widehat{\mathbf{z}}$. Thus, we have to recalculate $\widehat{\mathbf{z}}$, which, in turn, results in a new choice $\widehat{\mathbf{w}}$ for the model parameters. In practice, we repeat the computation of the conditional expectation (i.e., the E-step) and the update of the model parameters (i.e., the M-step) until some stopping criterion is met.
See also: probabilistic model, maximum likelihood, optimization problem.

expert ML aims to learn a hypothesis h that accurately predicts the label of a data point based on its features. We measure the prediction error using some loss function. Ideally, we want to find a hypothesis that incurs minimal loss on any data point. We can make this informal goal precise via the i.i.d. assumption and by using the Bayes risk as the vertailutaso for the (average) loss of a hypothesis. An alternative approach to obtaining a vertailutaso is to use the hypothesis h' learned by an existing ML method. We refer to this hypothesis h' as an expert [?]. Regret minimization methods learn a hypothesis that incurs a loss comparable to the best expert [?], [?].
See also: loss function, vertailutaso, regret.

explainability We define the (subjective) explainability of an ML method

as the level of simulatability [?] of the predictions delivered by an ML system to a human user. Quantitative measures for the (subjective) explainability of a trained model can be constructed by comparing its predictions with the predictions provided by a user on a test set [?], [?]. Alternatively, we can use probabilistic models for data and measure the explainability of a trained ML model via the conditional (or differential) entropy of its predictions, given the user's predictions [?], [?].

See also: trustworthy AI, regularization.

explainable empirical risk minimization (EERM) EERM is an instance of structural risk minimization (SRM) that adds a regularization term to the average loss in the objective function of ERM. The regularization term is chosen to favor hypothesis maps that are intrinsically explainable for a specific user. This user is characterized by their predictions provided for the data points in a training set [?].

See also: SRM, regularization, ERM, training set.

explainable machine learning (XML) XML methods aim to complement each prediction with an explanation of how the prediction has been obtained. The construction of an explicit explanation might not be necessary if the ML method uses a sufficiently simple (or interpretable) model [?].

See also: prediction, explanation, ML, model.

explanation One approach to enhance the transparency of an ML method for its human user is to provide an explanation alongside the predictions delivered by the method. Explanations can take different forms. For

instance, they may consist of human-readable text or quantitative indicators, such as feature importance scores for the individual features of a given data point [**?**]. Alternatively, explanations can be visual—for example, intensity maps that highlight image regions that drive the prediction [**?**]. Fig. 26 illustrates two types of explanations. The first is a local linear approximation $g(\mathbf{x})$ of a nonlinear trained model $\hat{h}(\mathbf{x})$ around a specific feature vector $\mathbf{x}'$, as used in the method LIME. The second form of explanation depicted in the figure is a sparse set of predictions $\hat{h}(\mathbf{x}^{(1)}), \hat{h}(\mathbf{x}^{(2)}), \hat{h}(\mathbf{x}^{(3)})$ at selected feature vectors, offering concrete reference points for the user.

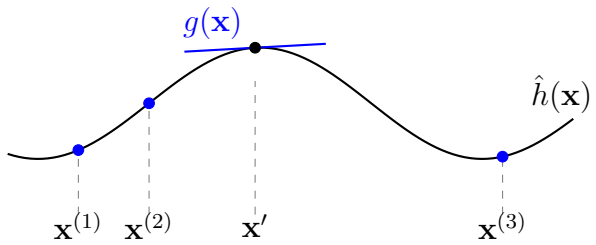


Fig. 26. A trained model $\hat{h}(\mathbf{x})$ can be explained locally at some point $\mathbf{x}'$ by a linear approximation $g(\mathbf{x})$. For a differentiable $\hat{h}(\mathbf{x})$, this approximation is determined by the gradient $\nabla\hat{h}(\mathbf{x}')$. Another form of explanation could be the function values $\hat{h}\big(\mathbf{x}^{(r)}\big)$ for $r = 1, 2, 3$.

See also: ML, prediction, feature, data point, luokittelu.

feature A feature of a data point is one of its properties that can be measured or computed easily without the need for human supervision. For example, if a data point is a digital image (e.g., stored as a `.jpeg` file), then we

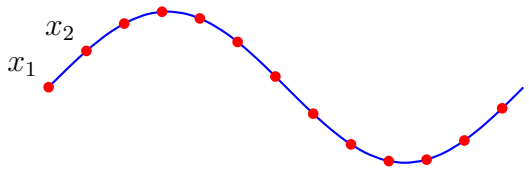


Fig. 27. An audio signal (blue waveform) and its discretized signal samples (red dots) which can be used as its features $x_1, \ldots, x_d$.

could use the red–green–blue (RGB) intensities of its pixels as features. Another example is shown in Fig. 27, where the the signal samples of a finite-duration audio signal are used as its features. Domain-specific synonyms for the term feature are "covariate," "explanatory variable," "independent variable," "input (variable)," "predictor (variable)," or "regressor" [?], [?], [?].

See also: data point.

feature learning Consider an ML application with data points characterized by raw features $\mathbf{x} \in \mathcal{X}$. Feature learning refers to the task of learning a map

$$\mathbf{\Phi} : \mathcal{X} \rightarrow \mathcal{X}' : \mathbf{x} \mapsto \mathbf{x}'$$

that reads in the features $\mathbf{x} \in \mathcal{X}$ of a data point and delivers new features $\mathbf{x}' \in \mathcal{X}'$ from a new feature space $\mathcal{X}'$. Different feature learning methods are obtained for different design choices of $\mathcal{X}, \mathcal{X}'$, for a hypothesis space $\mathcal{H}$ of potential maps $\mathbf{\Phi}$, and for a quantitative measure of the usefulness of a specific $\mathbf{\Phi} \in \mathcal{H}$. For example, principal component analysis (PCA) uses $\mathcal{X} := \mathbb{R}^d$, $\mathcal{X}' := \mathbb{R}^{d'}$ with $d' < d$, and a hypothesis space

$$\mathcal{H} := \left\{ \mathbf{\Phi} : \mathbb{R}^d \rightarrow \mathbb{R}^{d'} : \mathbf{x}' := \mathbf{F}\mathbf{x} \text{ with some } \mathbf{F} \in \mathbb{R}^{d' \times d} \right\}.$$

PCA measures the usefulness of a specific map $\mathbf{\Phi}(\mathbf{x}) = \mathbf{F}\mathbf{x}$ by the minimum linear reconstruction error incurred on a tietoaineisto such that

$$\min_{\mathbf{G}\in\mathbb{R}^{d\times d'}} \sum_{r=1}^{m} \left\| \mathbf{G}\mathbf{F}\mathbf{x}^{(r)} - \mathbf{x}^{(r)} \right\|_2^2 .$$

See also: feature, feature space, hypothesis space, PCA.

feature map A feature map refers to a function

$$\mathbf{\Phi} : \mathcal{X} \to \mathcal{X}', \quad \mathbf{x} \mapsto \mathbf{x}'$$

that transforms a feature vector $\mathbf{x} \in \mathcal{X}$ of a data point into a new feature vector $\mathbf{x}' \in \mathcal{X}'$, where $\mathcal{X}'$ is typically different from $\mathcal{X}$. The transformed representation $\mathbf{x}'$ is often more useful than the original $\mathbf{x}$. For instance, the geometry of data points may become more linear in $\mathcal{X}'$, allowing the application of a linear model to $\mathbf{x}'$. This idea is central to the design of kernel methods [**?**]. Other benefits of using a feature map include reducing overfitting and improving interpretability [**?**]. A common use case is data visualization, where a feature map with two output dimensions allows the representation of data points in a 2-D scatterplot. Some ML methods employ trainable feature maps, whose parameters are learned from data. An example is the use of hidden layers in a deep net, which act as successive feature maps [**?**]. A principled way to train a feature map is through ERM, using a loss function that measures reconstruction quality, e.g., $L = \|\mathbf{x} - r(\mathbf{x}')\|^2$, where $r(\cdot)$ is a trainable map that attempts to reconstruct $\mathbf{x}$ from the transformed

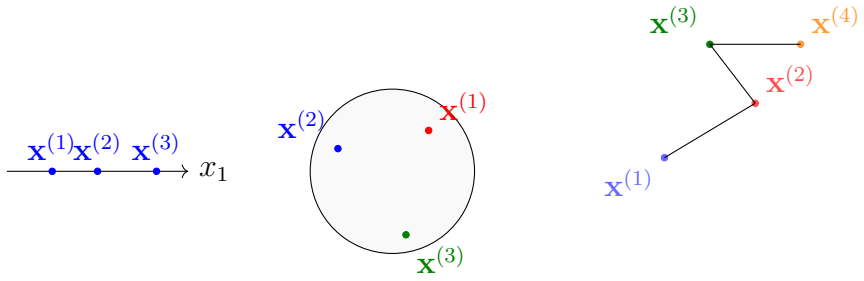
feature vector $\mathbf{x}'$.

See also: feature, map, kernel method, feature learning, PCA.

feature matrix Consider a tietoaineisto $\mathcal{D}$ with m data points with feature vectors $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)} \in \mathbb{R}^d$. It is convenient to collect the individual feature vectors into a feature matrix $\mathbf{X} := \big(\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)}\big)^T$ of size $m \times d$.

See also: tietoaineisto, data point, feature vector, feature, matrix.

feature space The feature space of a given ML application or method is constituted by all potential values that the feature vector of a data point can take on. For data points described by a fixed number d of numerical features, a common choice for the feature space is the Euclidean space $\mathbb{R}^d$. However, the mere presence of d numeric features does not imply that $\mathbb{R}^d$ is the most appropriate representation of the feature space. Indeed, the numerical features might be assigned to data points in a largely arbitrary or random manner, resulting in data points that are randomly scattered throughout $\mathbb{R}^d$ without any meaningful geometric structure. Feature learning methods try to learn a transformation of the original (potentially non-numeric) features to ensure a more meaningful arrangement of data points in $\mathbb{R}^d$. Three examples of feature spaces are shown in Fig. 28.



$\mathcal{X}^{(1)}$ $\mathcal{X}^{(2)}$ $\mathcal{X}^{(3)}$

(a) (b) (c)

Fig. 28. Three different feature spaces. (a) A linear space $\mathcal{X}^{(1)} = \mathbb{R}$. (b) A bounded convex set $\mathcal{X}^{(2)} \subseteq \mathbb{R}^2$. (c) A discrete space $\mathcal{X}^{(3)}$ whose elements are nodes of an undirected graph.

See also: feature vector, Euclidean space.

feature vector Feature vector refers to a vector $\mathbf{x} = \big(x_1, \ldots, x_d\big)^T$ whose entries are individual features $x_1, \ldots, x_d$. Many ML methods use feature vectors that belong to some finite-dimensional Euclidean space $\mathbb{R}^d$. For some ML methods, however, it can be more convenient to work with feature vectors that belong to an infinite-dimensional vector space (e.g., see kernel method).

See also: feature, vector, ML, Euclidean space, vector space.

federated averaging (FedAvg) FedAvg refers to a family of iterative FL algoritmit. It uses a server-client setting and alternates between clientwise local models retraining, followed by the aggregation of updated model parameters at the server [**?**]. The local update at client $i = 1, \ldots, n$

at time k starts from the current model parameters $\mathbf{w}^{(k)}$ provided by the server and typically amounts to executing few iterations of SGD. After completing the local updates, they are aggregated by the server (e.g., by averaging them). Fig. 29 illustrates the execution of a single iteration of FedAvg.

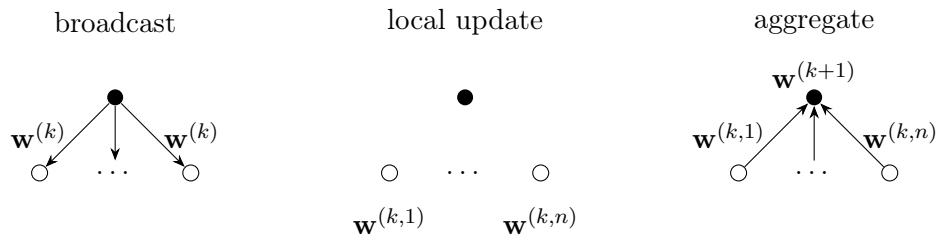


Fig. 29. Illustration of a single iteration of FedAvg, which consists of broadcasting model parameters by the server, performing local updates at clients, and aggregating the updates by the server.

See also: FL, algorithm, local model, SGD.

federated gradient descent (FedGD) An FL distributed algorithm that can be implemented as message passing across an FL network.

See also: FL, distributed algorithm, FL network, gradient step, gradient-based methods.

federated learning (FL) FL is an umbrella term for ML methods that train models in a collaborative fashion using decentralized data and computation.

See also: ML, model, data.

federated learning network (FL network) An FL network consists of an undirected weighted graph $\mathcal{G}$. The nodes of $\mathcal{G}$ represent devices that can access a local dataset and train a local model. The edges of $\mathcal{G}$ represent communication links between devices as well as statistical similarities between their local datasets. A principled approach to train the local models is GTVMin. The solutions of GTVMin are local model parameters that optimally balance the loss incurred on local datasets with their discrepancy across the edges of $\mathcal{G}$.

See also: FL, graph, device, GTVMin.

federated proximal (FedProx) FedProx refers to an iterative FL algorithm that alternates between separately training local models and combining the updated local model parameters. In contrast to FedAvg, which uses SGD to train local models, FedProx uses a proximal operator for the training [**?**].

See also: FL, algorithm, local model, model parameters, FedAvg, SGD, proximal operator.

federated relaxed (FedRelax) An FL distributed algorithm.

See also: FL, distributed algorithm.

federated stochastic gradient descent (FedSGD) An FL distributed algorithm that can be implemented as message passing across an FL network.

See also: FL, distributed algorithm, FL network, gradient step, gradient-based methods, SGD.

Finnish Meteorological Institute (FMI) The FMI is a government agency

responsible for gathering and reporting weather data in Finland.

See also: data.

fixed-point iteration A fixed-point iteration is an iterative method for solving a given optimization problem. It constructs a sequence $\mathbf{w}^{(0)}$, $\mathbf{w}^{(1)}$, ... by repeatedly applying an operator $\mathcal{F}$, i.e.,

$$\mathbf{w}^{(k+1)} = \mathcal{F}\mathbf{w}^{(k)}, \text{ for } k = 0, 1, \ldots. \tag{2}$$

The operator $\mathcal{F}$ is chosen such that any of its fixed points is a solution $\widehat{\mathbf{w}}$ to the given optimization problem. For example, given a differentiable and convex function $f(\mathbf{w})$, the fixed points of the operator $\mathcal{F} : \mathbf{w} \mapsto \mathbf{w} - \nabla f(\mathbf{w})$ coincide with the minimizers of $f(\mathbf{w})$. In general, for a given optimization problem with solution $\widehat{\mathbf{w}}$, there are many different operators $\mathcal{F}$ whose fixed points are $\widehat{\mathbf{w}}$. Clearly, we should use an operator $\mathcal{F}$ in (2) that reduces the distance to a solution such that

$$\underbrace{\left\|\mathbf{w}^{(k+1)} - \widehat{\mathbf{w}}\right\|_2}_{\overset{(2)}{=}\left\|\mathcal{F}\mathbf{w}^{(k)} - \mathcal{F}\widehat{\mathbf{w}}\right\|_2} \leq \left\|\mathbf{w}^{(k)} - \widehat{\mathbf{w}}\right\|_2 .$$

Thus, we require $\mathcal{F}$ to be at least non-expansive, i.e., the iteration (2) should not result in worse model parameters that have a larger distance to a solution $\widehat{\mathbf{w}}$. Furthermore, each iteration (2) should also make some progress, i.e., reduce the distance to a solution $\widehat{\mathbf{w}}$. This requirement can be made precise using the notion of a contraction operator [?], [?]. The operator $\mathcal{F}$ is a contraction operator if, for some $\kappa \in [0, 1)$,

$$\left\|\mathcal{F}\mathbf{w} - \mathcal{F}\mathbf{w}'\right\|_2 \leq \kappa \left\|\mathbf{w} - \mathbf{w}'\right\|_2 \text{ holds for any } \mathbf{w}, \mathbf{w}'.$$

For a contraction operator $\mathcal{F}$, the fixed-point iteration (2) generates a sequence $\mathbf{w}^{(k)}$ that converges quite rapidly. In particular [2, Th. 9.23],

$$\left\|\mathbf{w}^{(k)} - \widehat{\mathbf{w}}\right\|_2 \leq \kappa^k \left\|\mathbf{w}^{(0)} - \widehat{\mathbf{w}}\right\|_2 .$$

Here, $\left\|\mathbf{w}^{(0)} - \widehat{\mathbf{w}}\right\|_2$ is the distance between the initialization $\mathbf{w}^{(0)}$ and the solution $\widehat{\mathbf{w}}$. It turns out that a fixed-point iteration (2) with a firmly non-expansive operator $\mathcal{F}$ is guaranteed to converge to a fixed-point of $\mathcal{F}$ [**?**, Corollary 5.16]. Fig. 30 depicts examples of a firmly non-expansive operator, a non-expansive operator, and a contraction operator. All of these operators are defined on the 1-D space $\mathbb{R}$. Another example of a firmly non-expansive operator is the proximal operator of a convex function [**?**], [**?**].

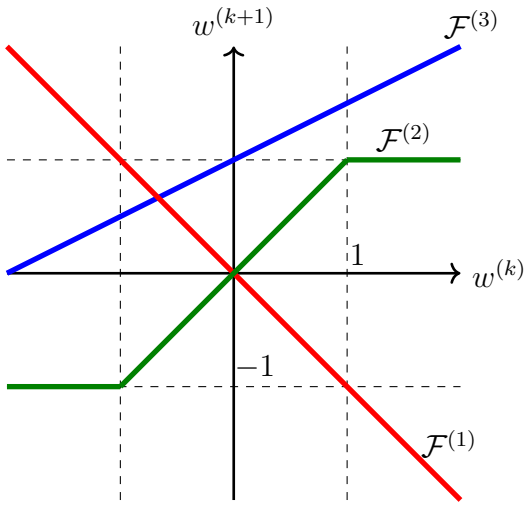


Fig. 30. Example of a non-expansive operator $\mathcal{F}^{(1)}$, a firmly non-expansive operator $\mathcal{F}^{(2)}$, and a contraction operator $\mathcal{F}^{(3)}$.

See also: optimization problem, differentiable, convex, function, model

parameters, contraction operator, proximal operator.

flow-based clustering Flow-based klusterointi groups the nodes of an undirected graph by applying k-means klusterointi to nodewise feature vectors. These feature vectors are built from network flows between carefully selected sources and destination nodes [**?**].

See also: klusterointi, graph, k-means, feature vector.

Gaussian mixture model (GMM) A GMM is a particular type of probabilistic model for a numeric vector $\mathbf{x}$ (e.g., the features of a data point). Within a GMM, the vector $\mathbf{x}$ is drawn from a randomly selected multivariate normal distribution $p^{(c)} = \mathcal{N}\left(\boldsymbol{\mu}^{(c)}, \mathbf{C}^{(c)}\right)$ with $c = I$. The index $I \in \{1, \ldots, k\}$ is an RV with probabilities $\mathbb{P}(I = c) = p_c$. Note that a GMM is parameterized by the probability p_c, the mean vector $\boldsymbol{\mu}^{(c)}$, and the kovarianssimatriisi $\mathbf{C}^{(c)}$ for each $c = 1, \ldots, k$. GMMs are widely used for klusterointi, density estimation, and as a generative model.

See also: probabilistic model, multivariate normal distribution, klusterointi.

Gaussian process (GP) A GP is a collection of RVs $\{f(\mathbf{x})\}_{\mathbf{x} \in \mathcal{X}}$ indexed by input values $\mathbf{x}$ from some input space $\mathcal{X}$ such that, for any finite subset $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)} \in \mathcal{X}$, the corresponding RVs $f(\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)})$ have a joint multivariate normal distribution

$$f\left(\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)}\right) \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{K}).$$

For a fixed input space $\mathcal{X}$, a GP is fully specified (or parameterized)

by: 1) a mean function $\mu(\mathbf{x}) = \mathbb{E}\{f(\mathbf{x})\}$; and 2) a covariance function $K\big(\mathbf{x}, \mathbf{x}'\big) = \mathbb{E}\{\big(f(\mathbf{x}) - \mu(\mathbf{x})\big)\big(f(\mathbf{x}') - \mu(\mathbf{x}')\big)\}$.

Example: We can interpret the temperature distribution across Finland (at a specific point in time) as the realization of a GP $f(\mathbf{x})$, where each input $\mathbf{x} = (\text{lat}, \text{lon})$ denotes a geographic location. Temperature observations from Finnish Meteorological Institute (FMI) weather stations provide values $f(\mathbf{x})$ at specific locations (see Fig. 31). A GP allows us to predict the temperature nearby FMI weather stations and to quantify the uncertainty of these predictions.

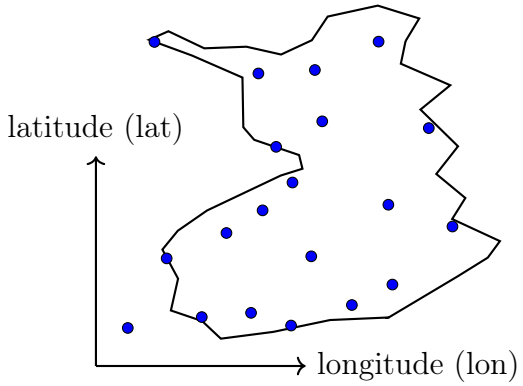


Fig. 31. For a given point in time, we can interpret the current temperature distribution over Finland as a realization of a GP indexed by geographic coordinates and sampled at FMI weather stations. The weather stations are indicated by blue dots.

See also: multivariate normal distribution, uncertainty, Gaussian RV.

Gaussian random variable (Gaussian RV) A standard Gaussian RV is

a real-valued RV x with pdf [7], [?], [?]

$$p(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-x^2/2\right).$$

Given a standard Gaussian RV x, we can construct a general Gaussian RV x' with mean μ and variance σ^2 via $x' := \sigma x + \mu$. The probability distribution of a Gaussian RV is referred to as normal distribution, denoted by $\mathcal{N}(\mu, \sigma^2)$.

A Gaussian random vector $\mathbf{x} \in \mathbb{R}^d$ with kovarianssimatriisi $\mathbf{C}$ and mean $\boldsymbol{\mu}$ can be constructed as [?], [?], [?]

$$\mathbf{x} := \mathbf{A}\mathbf{z} + \boldsymbol{\mu}$$

where $\mathbf{z} := \left(z_1, \ldots, z_d\right)^T$ is a vector of i.i.d. standard Gaussian RVs, and $\mathbf{A} \in \mathbb{R}^{d \times d}$ is any matrix satisfying $\mathbf{A}\mathbf{A}^T = \mathbf{C}$. The probability distribution of a Gaussian random vector is referred to as the multivariate normal distribution, denoted by $\mathcal{N}(\boldsymbol{\mu}, \mathbf{C})$.

We can interpret a Gaussian random vector $\mathbf{x} = \left(x_1, \ldots, x_d\right)$ as a stochastic process indexed by the set $\mathcal{I} = \{1, \ldots, d\}$. A GPt is a stochastic process over an arbitray index set $\mathcal{I}$ such that any restriction to a finite subset $\mathcal{I}' \subseteq \mathcal{I}$ yields a Gaussian random vector [?].

Gaussian RVs are widely used probabilistic models in the statistical analysis of ML methods. Their significance arises partly from the central limit theorem (CLT), which is a mathematically precise formulation of the following rule of thumb: The average of many independent RVs (not necessarily Gaussian themselves) tends toward a Gaussian RV [?].

The multivariate normal distribution is also distinct in that it represents maximum uncertainty. Among all vector-valued RVs with a given

kovarianssimatriisi $\mathbf{C}$, the RV $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{C})$ maximizes differential entropy [**?**, Th. 8.6.5]. This makes GPt a natural choice for capturing uncertainty (or lack of knowledge) in the absence of additional structural information.

See also: multivariate normal distribution, GP, probabilistic model, CLT, differential entropy.

general data protection regulation (GDPR) The GDPR was enacted by the European Union (EU), effective from 25 May 2018 [**?**]. It safeguards the privacy and data rights of individuals in the EU. The GDPR has significant implications for how data are collected, stored, and used in ML applications. Key provisions include the following:

- Data minimization principle: ML systems should only use the necessary amount of personal data for their purpose.
- Transparency and explainability: ML systems should enable their users to understand how the systems make decisions that impact the users.
- Data subject rights: Users should get an opportunity to access, rectify, and delete their personal data, as well as to object to automated decision-making and profiling.
- Accountability: Organizations must ensure robust data security and demonstrate compliance through documentation and regular audits.

See also: data, ML, data minimization principle, transparency, explainability.

generalization Generalization refers to the ability of a model trained on a training set to make accurate predictions on new unseen data points. This is a central goal of ML and AI, i.e., to learn patterns that extend beyond the training set. Most ML systems use ERM to learn a hypothesis $\hat{h} \in \mathcal{H}$ by minimizing the average loss over a training set of data points $\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(m)}$, which is denoted by $\mathcal{D}^{(\text{train})}$. However, success on the training set does not guarantee success on unseen data—this discrepancy is the challenge of generalization.

To study generalization mathematically, we need to formalize the notion of "unseen" data. A widely used approach is to assume a probabilistic model for data generation, such as the i.i.d. assumption. Here, we interpret data points as independent RVs with an identical probability distribution $p(\mathbf{z})$. This probability distribution, which is assumed fixed but unknown, allows us to define the risk of a trained model $\hat{h}$ as the expected loss

$$\bar{L}\big(\hat{h}\big) = \mathbb{E}_{\mathbf{z}\sim p(\mathbf{z})}\big\{L(\hat{h}, \mathbf{z})\big\}.$$

The difference between risk $\bar{L}\big(\hat{h}\big)$ and empirical risk $\widehat{L}\big(\hat{h}|\mathcal{D}^{(\text{train})}\big)$ is known as the generalization gap. Tools from probability theory, such as concentration inequalities and uniform convergence, allow us to bound this gap under certain conditions [**?**].

Generalization without probability: Probability theory is one way to study how well a model generalizes beyond the training set, but it is not the only way. Another option is to use simple deterministic changes to the data points in the training set. The basic idea is that a good model $\hat{h}$ should be robust, i.e., its prediction $\hat{h}(\mathbf{x})$ should not change much if

we slightly change the features $\mathbf{x}$ of a data point $\mathbf{z}$. For example, an object detector trained on smartphone photos should still detect the object if a few random pixels are masked [**?**]. Similarly, it should deliver the same result if we rotate the object in the image [**?**]. See Fig. 32 for a visual illustration.

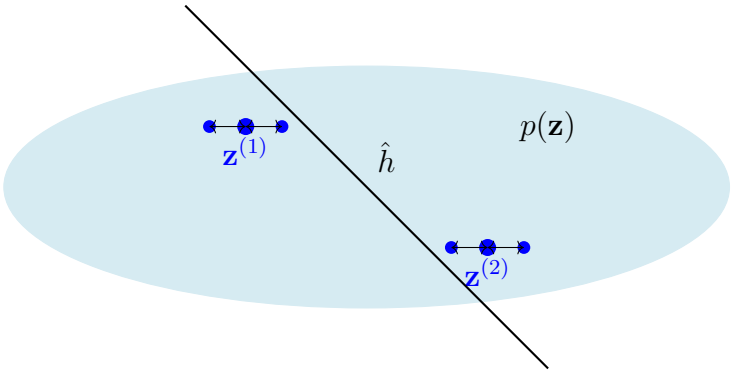


Fig. 32. Two data points $\mathbf{z}^{(1)}, \mathbf{z}^{(2)}$ that are used as a training set to learn a hypothesis $\hat{h}$ via ERM. We can evaluate $\hat{h}$ outside $\mathcal{D}^{(\text{train})}$ either by an i.i.d. assumption with some underlying probability distribution $p(\mathbf{z})$ or by perturbing the data points.

See also: ERM, i.i.d. assumption, overfitting, validation.

generalization gap Generalization gap is the difference between the performance of a trained model on the training set $\mathcal{D}^{(\text{train})}$ and its performance on data points outside $\mathcal{D}^{(\text{train})}$. We can make this notion precise by using a probabilistic model that allows us to compute the risk of a trained model as the expected loss. However, the probability distribution underlying this expectation is typically unknown and needs to be somehow estimated. Validation techniques use different constructions of a va-

lidation set, which is different from the training set, to estimate the generalization gap.

See also: generalization, validation, ERM, loss function.

generalized total variation (GTV) GTV is a measure of the variation of trained local models $h^{(i)}$ (or their model parameters $\mathbf{w}^{(i)}$) assigned to the nodes $i = 1, \ldots, n$ of an undirected weighted graph $\mathcal{G}$ with edges $\mathcal{E}$. Given a measure $d^{(h,h')}$ for the discrepancy between hypothesis maps h, h', the GTV is

$$\sum_{\{i,i'\} \in \mathcal{E}} A_{i,i'} d^{(h^{(i)}, h^{(i')})}.$$

Here, $A_{i,i'} > 0$ denotes the weight of the undirected edge $\{i, i'\} \in \mathcal{E}$.

See also: local model, model parameters, graph, discrepancy, hypothesis, map.

generalized total variation minimization (GTVMin) GTVMin is an instance of regularized empirical risk minimization (RERM) using the GTV of local model parameters as a regularizer [**?**].

See also: RERM, GTV, regularizer.

geometric median (GM) The GM of a set of input vectors $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)}$ in $\mathbb{R}^d$ is a point $\mathbf{z} \in \mathbb{R}^d$ that minimizes the sum of distances to the vectors [**?**] such that

$$\mathbf{z} \in \operatorname*{arg\,min}_{\mathbf{y} \in \mathbb{R}^d} \sum_{r=1}^{m} \left\| \mathbf{y} - \mathbf{x}^{(r)} \right\|_2 . \tag{3}$$

Fig. 33 illustrates a fundamental property of the GM: If $\mathbf{z}$ does not coincide with any of the input vectors, then the unit vectors pointing

from $\mathbf{z}$ to each $\mathbf{x}^{(r)}$ must sum to zero—this is the zero-subgradient (optimality) condition for (3). It turns out that the solution to (3) cannot be arbitrarily pulled away from trustworthy input vectors as long as they are the majority [?, Th. 2.2].

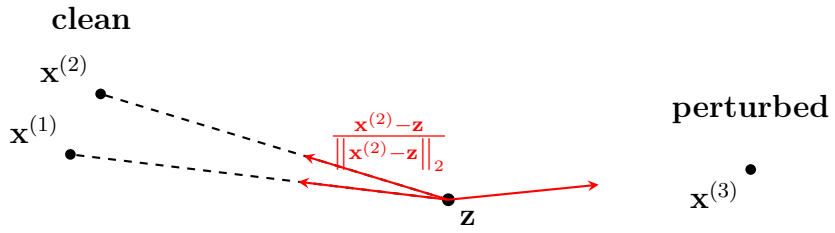


Fig. 33. Consider a solution $\mathbf{z}$ of (3) that does not coincide with any of the input vectors. The optimality condition for (3) requires that the unit vectors from $\mathbf{z}$ to the input vectors sum to zero.

See also: vector, subgradient.

gradient For a real-valued function $f : \mathbb{R}^d \to \mathbb{R} : \mathbf{w} \mapsto f(\mathbf{w})$, if a vector $\mathbf{g}$ exists such that $\lim_{\mathbf{w}\to\mathbf{w}'} f(\mathbf{w}) - \big(f(\mathbf{w}') + \mathbf{g}^T(\mathbf{w}-\mathbf{w}')\big)/\|\mathbf{w}-\mathbf{w}'\| = 0$, it is referred to as the gradient of f at $\mathbf{w}'$. If it exists, the gradient is unique and denoted by $\nabla f(\mathbf{w}')$ or $\nabla f(\mathbf{w})\big|_{\mathbf{w}'}$ [2].

See also: function, vector.

gradient descent (GD) GD is an iterative method for finding the minimum of a differentiable function $f : \mathbb{R}^d \to \mathbb{R}$. GD generates a sequence of estimates $\mathbf{w}^{(0)}$, $\mathbf{w}^{(1)}$, $\mathbf{w}^{(2)}$, ... that (ideally) converge to a minimum of f. At each iteration k, GD refines the current estimate $\mathbf{w}^{(k)}$ by taking a step in the direction of the steepest descent of a local linear approximation.

This direction is given by the negative gradient $\nabla f(\mathbf{w}^{(k)})$ of the function f at the current estimate $\mathbf{w}^{(k)}$. The resulting update rule is given by

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta \nabla f(\mathbf{w}^{(k)}) \tag{4}$$

where $\eta > 0$ is a suitably small step size. For a suitably choosen step size η, the update typically reduces the function value, i.e., $f(\mathbf{w}^{(k+1)}) < f(\mathbf{w}^{(k)})$. Fig. 34 illustrates a single GD step.

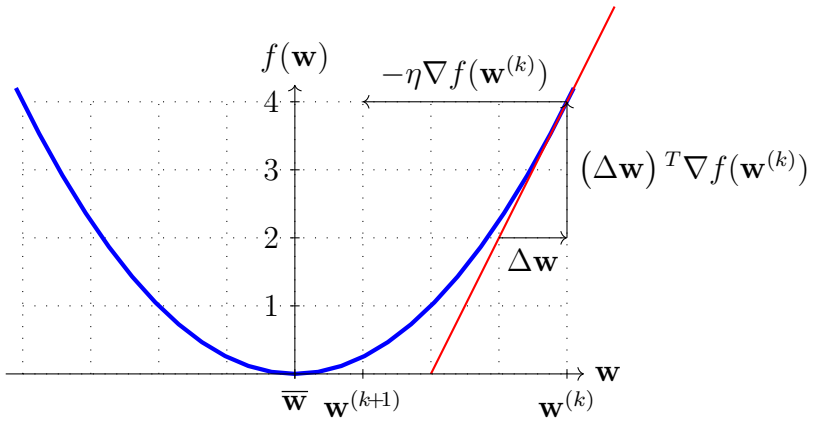


Fig. 34. A single gradient step (4) toward the minimizer $\overline{\mathbf{w}}$ of $f(\mathbf{w})$.

See also: minimum, differentiable, gradient, step size, gradient step.

gradient step Given a differentiable real-valued function $f(\cdot) : \mathbb{R}^d \to \mathbb{R}$ and a vector $\mathbf{w} \in \mathbb{R}^d$, the gradient step updates $\mathbf{w}$ by adding the scaled negative gradient $\nabla f(\mathbf{w})$ to obtain the new vector (see Fig. 35)

$$\widehat{\mathbf{w}} := \mathbf{w} - \eta \nabla f(\mathbf{w}). \tag{5}$$

Mathematically, the gradient step is an operator $\mathcal{T}^{(f,\eta)}$ that is parametrized by the function f and the step size η.

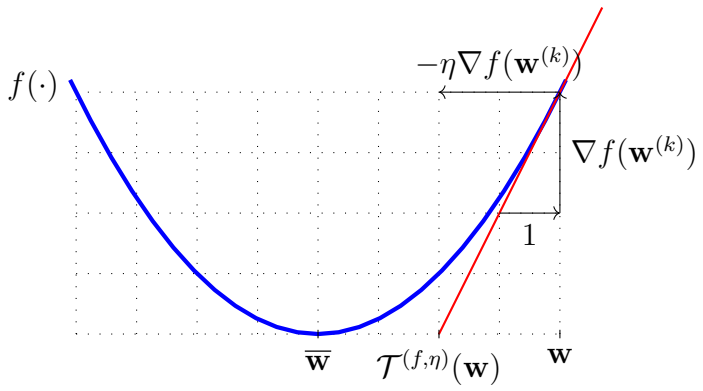


Fig. 35. The basic gradient step (5) maps a given vector $\mathbf{w}$ to the updated vector $\mathbf{w}'$. It defines an operator $\mathcal{T}^{(f,\eta)}(\cdot) : \mathbb{R}^d \to \mathbb{R}^d : \mathbf{w} \mapsto \widehat{\mathbf{w}}$.

Note that the gradient step (5) optimizes locally—in a neighborhood whose size is determined by the step size η—a linear approximation to the function $f(\cdot)$. A natural generalization of (5) is to locally optimize the function itself—instead of its linear approximation—such that

$$\widehat{\mathbf{w}} = \operatorname*{arg\,min}_{\mathbf{w}' \in \mathbb{R}^d} f(\mathbf{w}') + \frac{1}{\eta} \|\mathbf{w} - \mathbf{w}'\|_2^2 . \tag{6}$$

We intentionally use the same symbol η for the parameter in (6) as we used for the step size in (5). The larger the η we choose in (6), the more progress the update will make toward reducing the function value $f(\widehat{\mathbf{w}})$. Note that, much like the gradient step (5), the update (6) also defines an operator that is parameterized by the function $f(\cdot)$ and the learning rate η. For a convex function $f(\cdot)$, this operator is known as the proximal operator of $f(\cdot)$ [**?**].

See also: differentiable, function, vector, gradient, step size, neighbor-

hood, generalization, parameter, learning rate, convex, proximal operator.

gradient-based methods Gradient-based methods are iterative techniques for finding the minimum (or maximum) of a differentiable objective function of the model parameters. These methods construct a sequence of approximations to an optimal choice for model parameters that results in a minimum (or maximum) value of the objective function. As their name indicates, gradient-based methods use the gradients of the objective function evaluated during previous iterations to construct new, (hopefully) improved model parameters. One important example of a gradient-based method is GD.

See also: gradient, minimum, maximum, differentiable, objective function, model parameters, GD.

graph A graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is a pair that consists of a node set $\mathcal{V}$ and an edge set $\mathcal{E}$. In its most general form, a graph is specified by a map that assigns each edge $e \in \mathcal{E}$ a pair of nodes [**?**]. One important family of graphs is simple undirected graphs. A simple undirected graph is obtained by identifying each edge $e \in \mathcal{E}$ with two different nodes $\{i, i'\}$. Weighted graphs also specify numeric weights A_e for each edge $e \in \mathcal{E}$.

See also: map, weights.

graph clustering Graph klusterointi aims to cluster data points that are represented as the nodes of a graph $\mathcal{G}$. The edges of $\mathcal{G}$ represent pairwise similarities between data points. We can sometimes quantify the extent of these similarities by an edge weight [**?**], [**?**].

See also: graph, klusterointi, data point, edge weight.

hard clustering Hard klusterointi refers to the task of partitioning a given set of data points into (a few) nonoverlapping ryppäät. The most widely used hard klusterointi method is k-means.

See also: klusterointi, data point, rypäs, k-means.

high-dimensional regime The high-dimensional regime of ERM is characterized by the effective dimension of the model being larger than the sample size, i.e., the number of (labeled) data points in the training set. For example, linear regression methods operate in the high-dimensional regime whenever the number d of features used to characterize data points exceeds the number of data points in the training set. Another example of ML methods that operate in the high-dimensional regime is large neuroverkot, which have far more tunable weights (and bias terms) than the total number of data points in the training set. High-dimensional statistics is a recent main thread of probability theory that studies the behavior of ML methods in the high-dimensional regime [**?**], [**?**].

See also: ERM, effective dimension, overfitting, regularization.

Hilbert space A Hilbert space is a complete inner product space [**?**]. That is, it is a vector space equipped with an inner product between pairs of vectors, and it satisfies the additional requirement of completeness, i.e., every Cauchy sequence of vectors converges to a limit within the space. A canonical example of a Hilbert space is the Euclidean space $\mathbb{R}^d$, for some dimension d, consisting of vectors $\mathbf{u} = \big(u_1, \ldots, u_d\big)^T$ and

the standard inner product $\mathbf{u}^T\mathbf{v}$.

See also: vector space, vector, Euclidean space.

hinge loss Consider a data point characterized by a feature vector $\mathbf{x} \in \mathbb{R}^d$ and a binary label $y \in \{-1, 1\}$. The hinge loss incurred by a real-valued hypothesis map $h(\mathbf{x})$ is defined as

$$L\left((\mathbf{x}, y), h\right) := \max\{0, 1 - yh(\mathbf{x})\}. \tag{7}$$

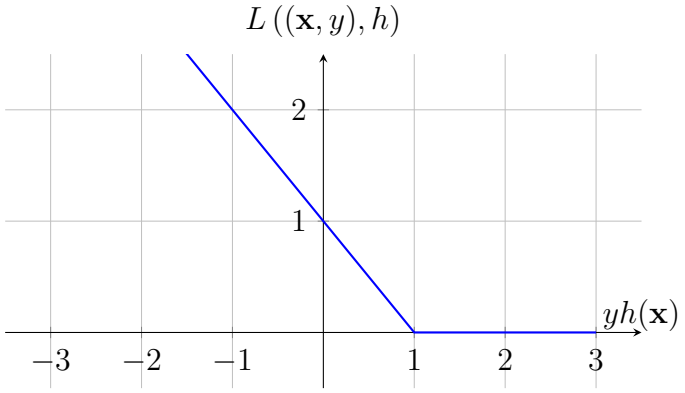


Fig. 36. The hinge loss incurred by the prediction $h(\mathbf{x}) \in \mathbb{R}$ for a data point with label $y \in \{-1, 1\}$. A regularized variant of the hinge loss is used by the support vector machine (SVM) [**?**].

See also: SVM, luokittelu, luokitin.

histogram Consider a tietoaineisto $\mathcal{D}$ that consists of m data points $\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(m)}$, each of them belonging to some cell $[-U, U] \times \ldots \times [-U, U] \subseteq \mathbb{R}^d$ with side length U. We partition this cell evenly into smaller elementary cells with side length Δ. The histogram of $\mathcal{D}$ assigns each elementary cell

to the corresponding fraction of data points in $\mathcal{D}$ that fall into this elementary cell. A visual example of such a histogram is provided in Fig. 37.

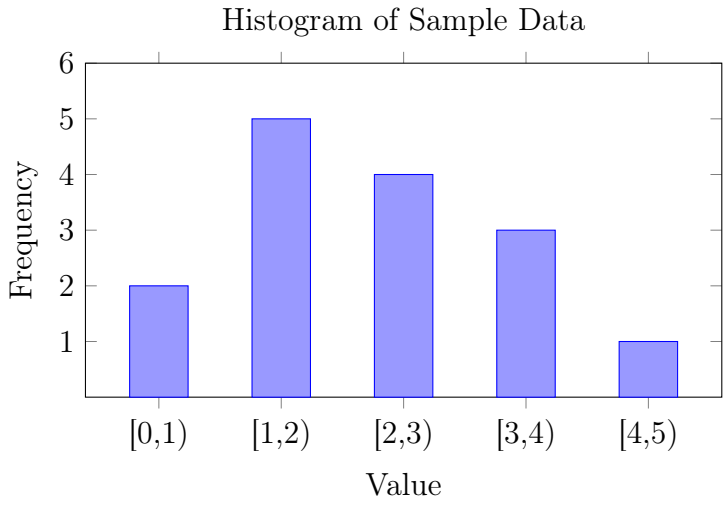


Fig. 37. A histogram representing the frequency of data points falling within discrete value ranges (i.e., bins). Each bar height shows the count of samples in the corresponding interval.

See also: tietoaineisto, data point, sample.

horizontal federated learning (HFL) HFL uses local datasets constituted by different data points but uses the same features to characterize them [**?**]. For example, weather forecasting uses a network of spatially distributed weather (observation) stations. Each weather station measures the same quantities, such as daily temperature, air pressure, and precipitation. However, different weather stations measure the characteristics or features of different spatiotemporal regions. Each spatiotemporal

region represents an individual data point, each characterized by the same features (e.g., daily temperature or air pressure).

See also: semi-supervised learning (SSL), FL, vertical federated learning (VFL).

Huber loss The Huber loss unifies the squared error loss and the absolute error loss.

See also: loss, squared error loss, absolute error loss.

Huber regression Huber regression refers to ERM-based methods that use the Huber loss as a measure of the prediction error. Two important special cases of Huber regression are least absolute deviation regression and linear regression. Tuning the threshold parameter of the Huber loss allows the user to trade the robustness of the absolute error loss against the computational benefits of the smooth squared error loss.

See also: least absolute deviation regression, linear regression, absolute error loss, squared error loss.

hypothesis A hypothesis refers to a map (or function) $h : \mathcal{X} \to \mathcal{Y}$ from the feature space $\mathcal{X}$ to the label space $\mathcal{Y}$. Given a data point with features $\mathbf{x}$, we use a hypothesis map h to estimate (or approximate) the label y using the prediction $\hat{y} = h(\mathbf{x})$. ML is all about learning (or finding) a hypothesis map h such that $y \approx h(\mathbf{x})$ for any data point (with features $\mathbf{x}$ and label y). Practical ML methods, limited by finite computational resources, must restrict learning to a subset of all possible hypothesis maps. This subset is called the hypothesis space or simply the model underlying the method.

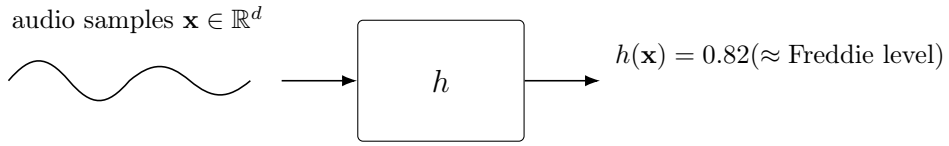


Fig. 38. A hypothesis $h : \mathcal{X} \to \mathcal{Y}$ maps the features $\mathbf{x} \in \mathcal{X}$ of a data point to a prediction $h(\mathbf{x}) \in \mathcal{Y}$ of the label. For example, the ML application `https://freddiemeter.withyoutube.com/` uses the samples of an audio recording as features predict how closely a person's singing resembles that of Freddie Mercury.

See also: map, function, prediction, model.

hypothesis space A hypothesis space is a mathematical model that characterizes the learning capacity of an ML method. The goal of such a method is to learn a hypothesis map that maps features of a data point to a prediction of its label. Given a finite amount of computational resources, a practical ML method typically explores only a restricted set of all possible maps from the feature space to the label space. Such a restricted set is referred to as a hypothesis space $\mathcal{H}$ underlying the ML method (see Fig. 39). For the analysis of a given ML method, the choice of a hypothesis space $\mathcal{H}$ is not unique, i.e., any superset containing all maps the method can learn is also a valid hypothesis space.

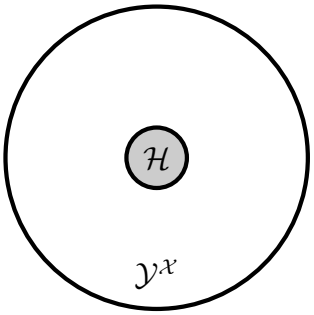


Fig. 39. The hypothesis space $\mathcal{H}$ of an ML method is a (typically very small) subset of the (typically very large) set $\mathcal{Y}^{\mathcal{X}}$ of all possible maps from the feature space $\mathcal{X}$ into the label space $\mathcal{Y}$.

On the other hand, from an ML engineering perspective, the hypothesis space $\mathcal{H}$ is a design choice for ERM-based methods. This design choice can be guided by the available computational resources and statistical aspects. For instance, if efficient matrix operations are feasible and a roughly linear relation exists between features and labels, a linear model can be a useful choice for $\mathcal{H}$.

See also: hypothesis, model, map, linear model.

independent and identically distributed (i.i.d.) A collection of RVs $\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(m)}$ is referred to as i.i.d. if each $\mathbf{z}^{(r)}$ follows the same probability distribution, and the RVs are mutually independent. That is, for any collection of events $\mathcal{A}_1, \ldots, \mathcal{A}_m$, we have

$$\mathbb{P}(\mathbf{z}^{(1)} \in \mathcal{A}_1, \ldots, \mathbf{z}^{(m)} \in \mathcal{A}_m) = \prod_{r=1}^{m} \mathbb{P}(\mathbf{z}^{(r)} \in \mathcal{A}_r).$$

See also: RV, probability distribution, event, data point, i.i.d. assumption.

independent and identically distributed assumption (i.i.d. assumption) The i.i.d. assumption interprets data points of a tietoaineisto as the realizations of i.i.d. RVs.

See also: i.i.d., data point, tietoaineisto, realization, RV.

interpretability An ML method is interpretable for a human user if they can comprehend the decision process of the method. One approach to develop a precise definition of interpretability is via the concept of simulatability, i.e., the ability of a human to mentally simulate the model behavior [**?**], [**?**], [**?**], [**?**], [**?**]. The idea is as follows: If a human user understands an ML method, then they should be able to anticipate its predictions on a test set. We illustrate such a test set in Fig. 40, which also depicts two learned hypotheses $\hat{h}$ and $\hat{h}'$. The ML method producing the hypothesis $\hat{h}$ is interpretable to a human user familiar with the concept of a linear map. Since $\hat{h}$ corresponds to a linear map, the user can anticipate the predictions of $\hat{h}$ on the test set. In contrast, the ML method delivering $\hat{h}'$ is not interpretable, because its behavior is no longer aligned with the user's expectations.

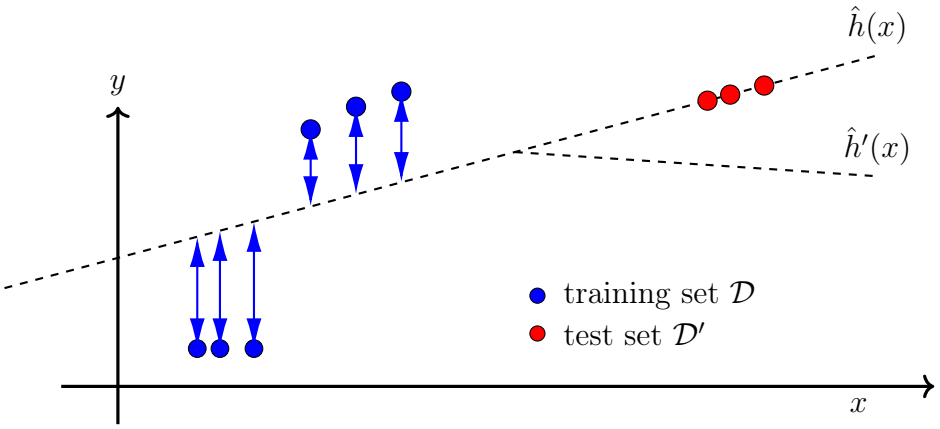


Fig. 40. We can assess the interpretability of trained ML models $\hat{h}$ and $\hat{h}'$ by comparing their predictions to pseudo-labels generated by a human user for $\mathcal{D}'$.

The notion of interpretability is closely related to the notion of explainability, as both aim to make ML methods more understandable for humans. In the context of Fig. 40, interpretability of an ML method $\hat{h}$ requires that the human user can anticipate its predictions on an arbitrary test set. This contrasts with explainability, where the user is supported by external explanations—such as saliency maps or reference examples from the training set—to understand the predictions of $\hat{h}$ on a specific test set $\mathcal{D}'$.

See also: explainability, trustworthy AI, regularization, LIME.

inverse matrix An inverse matrix $\mathbf{A}^{-1}$ is defined for a square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ that is of full rank, meaning its columns are linearly independent.

In this case, $\mathbf{A}$ is said to be invertible, and its inverse satisfies

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

A square matrix is invertible if and only if its determinant is nonzero. Inverse matrices are fundamental in solving systems of linear equations and in the closed-form solution of linear regression [?], [?]. The concept of an inverse matrix can be extended to matrices that are not square or not full rank. One may define a "left inverse" $\mathbf{B}$ satisfying $\mathbf{B}\mathbf{A} = \mathbf{I}$ or a "right inverse" $\mathbf{C}$ satisfying $\mathbf{A}\mathbf{C} = \mathbf{I}$. For general rectangular or singular matrices, the Moore–Penrose pseudoinverse $\mathbf{A}^{+}$ provides a unified concept of a generalized inverse matrix [3].

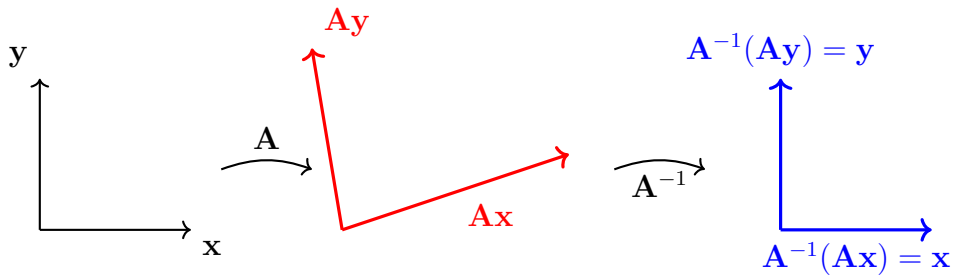


Fig. 41. A matrix $\mathbf{A}$ represents a linear transformation of $\mathbb{R}^2$. The inverse matrix $\mathbf{A}^{-1}$ represents the inverse transformation.

See also: matrix, determinant, linear regression, pseudoinverse.

Jacobi method The Jacobi method is an algorithm for solving systems of linear equations (i.e., a linear system) of the form $\mathbf{A}\mathbf{x} = \mathbf{b}$. Here, $\mathbf{A} \in \mathbb{R}^{d \times d}$ is a square matrix with nonzero main diagonal entries. The

method constructs a sequence $\mathbf{x}^{(0)}$, $\mathbf{x}^{(1)}$, ... by updating each entry of $\mathbf{x}^{(k)}$ according to

$$x_i^{(k+1)} = \frac{1}{a_{ii}} \left(b_i - \sum_{j \neq i} a_{ij} x_j^{(k)} \right).$$

Note that all entries $x_1^{(k)}$, ..., $x_d^{(k)}$ are updated simultaneously. The above iteration converges to a solution, i.e., $\lim_{k \to \infty} \mathbf{x}^{(k)} = \mathbf{x}$, under certain conditions on the matrix $\mathbf{A}$, e.g., being strictly diagonally dominant or symmetric positive definite [3], [?], [?]. Jacobi-type methods are appealing for large linear systems due to their parallelizable structure [?]. We can interpret the Jacobi method as a fixed-point iteration. Indeed, using the decomposition $\mathbf{A} = \mathbf{D} + \mathbf{R}$, with $\mathbf{D}$ being the diagonal of $\mathbf{A}$, allows us to rewrite the linear equation $\mathbf{A}\mathbf{x} = \mathbf{b}$ as a fixed-point equation

$$\mathbf{x} = \underbrace{\mathbf{D}^{-1}(\mathbf{b} - \mathbf{R}\mathbf{x})}_{\mathcal{F}\mathbf{x}}$$

which leads to the iteration $\mathbf{x}^{(k+1)} = \mathbf{D}^{-1}(\mathbf{b} - \mathbf{R}\mathbf{x}^{(k)})$.
As an example, for the linear equation $\mathbf{A}\mathbf{x} = \mathbf{b}$, where

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

the Jacobi method updates each component of $\mathbf{x}$ as follows:

$$\begin{aligned} x_1^{(k+1)} &= \frac{1}{a_{11}} \left(b_1 - a_{12} x_2^{(k)} - a_{13} x_3^{(k)} \right); \\ x_2^{(k+1)} &= \frac{1}{a_{22}} \left(b_2 - a_{21} x_1^{(k)} - a_{23} x_3^{(k)} \right); \\ x_3^{(k+1)} &= \frac{1}{a_{33}} \left(b_3 - a_{31} x_1^{(k)} - a_{32} x_2^{(k)} \right). \end{aligned}$$

See also: algorithm, matrix, fixed-point iteration, optimization method.

k-fold cross-validation (k-fold CV) k-fold CV is a method for learning and validating a hypothesis using a given tietoaineisto. This method divides the tietoaineisto evenly into k subsets or folds and then executes k repetitions of model training (e.g., via ERM) and validation. Each repetition uses a different fold as the validation set and the remaining $k-1$ folds as a training set. The final output is the average of the validation errors obtained from the k repetitions.

See also: ERM, validation, validation set, training set, validation error.

k-means The k-means principle is an optimization-based approach to the klusterointi of data points that are characterized by a numeric feature vector [8, Ch. 8]. As a hard clustering approach, k-means partitions a tietoaineisto into k disjoint subsets (or ryppäät), which are indexed by $c = 1, \ldots, k$. Each rypäs $\mathcal{C}$ is characterized by the average feature vector of data points that belong to it. This average (or mean) feature vector is referred to as the cluster centroid $\boldsymbol{\mu}^{(c)}$. A visual illustration is provided in Fig. 42.

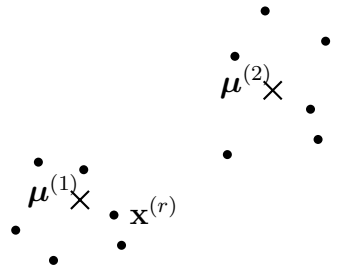


Fig. 42. A scatterplot of data points, indexed by $r = 1, \ldots, m$ and characterized by feature vectors $\mathbf{x}^{(r)} \in \mathbb{R}^2$. The scatterplot also includes two cluster centroids $\boldsymbol{\mu}^{(1)}, \boldsymbol{\mu}^{(2)} \in \mathbb{R}^2$.

In general, the k-means problem is a challenging optimization problem [**?**]. However, there is a simple iterative method for finding approximately optimal cluster centroids. This method, referred to as Lloyd's method, alternates between: 1) updating the rypäs assignments based on the nearest current cluster centroid; and 2) recalculating the cluster centroids given the updated rypäs assignments [**?**].

See also: hard clustering, rypäs.

kernel Consider a set of data points, each represented by a feature vector $\mathbf{x} \in \mathcal{X}$, where $\mathcal{X}$ denotes the feature space. A (real-valued) kernel is a function $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ that assigns to every pair of feature vectors $\mathbf{x}, \mathbf{x}' \in \mathcal{X}$ a real number $K\big(\mathbf{x}, \mathbf{x}'\big)$. This value is typically interpreted as a similarity measure between $\mathbf{x}$ and $\mathbf{x}'$. The defining property of a kernel is that it is symmetric, i.e., $K\big(\mathbf{x}, \mathbf{x}'\big) = K\big(\mathbf{x}', \mathbf{x}\big)$, and that for

any finite set of feature vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathcal{X}$, the matrix

$$\mathbf{K} = \begin{pmatrix} K(\mathbf{x}_1, \mathbf{x}_1) & K(\mathbf{x}_1, \mathbf{x}_2) & \ldots & K(\mathbf{x}_1, \mathbf{x}_n) \\ K(\mathbf{x}_2, \mathbf{x}_1) & K(\mathbf{x}_2, \mathbf{x}_2) & \ldots & K(\mathbf{x}_2, \mathbf{x}_n) \\ \vdots & \vdots & \ddots & \vdots \\ K(\mathbf{x}_n, \mathbf{x}_1) & K(\mathbf{x}_n, \mathbf{x}_2) & \ldots & K(\mathbf{x}_n, \mathbf{x}_n) \end{pmatrix} \in \mathbb{R}^{n \times n}$$

is psd. A kernel naturally defines a transformation of a feature vector $\mathbf{x}$ into a function $\mathbf{z} = K(\mathbf{x}, \cdot)$. The function $\mathbf{z}$ maps an input $\mathbf{x}' \in \mathcal{X}$ to the value $K(\mathbf{x}, \mathbf{x}')$. We can view the function $\mathbf{z}$ as a new feature vector that belongs to a feature space $\mathcal{X}'$ that is typically different from $\mathcal{X}$. This new feature space $\mathcal{X}'$ has a particular mathematical structure, i.e., it is a reproducing kernel Hilbert space (RKHS) [?], [?]. Since $\mathbf{z}$ belongs to a RKHS, which is a vector space, we can interpret it as a generalized feature vector. Note that a finite-length feature vector $\mathbf{x} = (x_1, \ldots, x_d)^T \in \mathbb{R}^d$ can be viewed as a function $\mathbf{x} : \{1, \ldots, d\} \rightarrow \mathbb{R}$ that assigns a real value to each index $j \in \{1, \ldots, d\}$.

See also: feature vector, feature space, Hilbert space, kernel method.

kernel method A kernel method is an ML method that uses a kernel K to map the original (i.e., raw) feature vector $\mathbf{x}$ of a data point to a new (transformed) feature vector $\mathbf{z} = K(\mathbf{x}, \cdot)$ [?], [?]. The motivation for transforming the feature vectors is that, by using a suitable kernel, the data points have a more "pleasant" geometry in the transformed feature space. For example, in a binary luokittelu problem, using transformed feature vectors $\mathbf{z}$ might allow us to use linear models, even if the data points are not linearly separable in the original feature space (see Fig. 43).

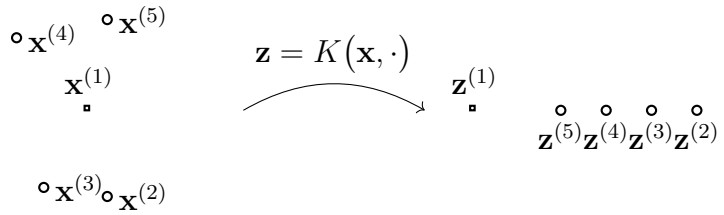


Fig. 43. Five data points characterized by feature vectors $\mathbf{x}^{(r)}$ and labels $y^{(r)} \in \{\circ, \square\}$, for $r = 1, \ldots, 5$. With these feature vectors, there is no way to separate the two classes by a straight line (representing the decision boundary of a linear classifier). In contrast, the transformed feature vectors $\mathbf{z}^{(r)} = K(\mathbf{x}^{(r)}, \cdot)$ allow us to separate the data points using a linear classifier.

See also: kernel, feature vector, feature space, linear classifier.

Kronecker product The Kronecker product of two matrices $\mathbf{A} \in \mathbb{R}^{m \times n}$ and $\mathbf{B} \in \mathbb{R}^{p \times q}$ is a block matrix denoted by $\mathbf{A} \otimes \mathbf{B}$ and defined as [3], [**?**]

$$\mathbf{A} \otimes \mathbf{B} = \begin{bmatrix} a_{11}\mathbf{B} & \cdots & a_{1n}\mathbf{B} \\ \vdots & \ddots & \vdots \\ a_{m1}\mathbf{B} & \cdots & a_{mn}\mathbf{B} \end{bmatrix} \in \mathbb{R}^{mp \times nq}.$$

The Kronecker product is a special case of the tensor product for matrices and is widely used in multivariate statistics, linear algebra, and structured ML models. It satisfies the identity $(\mathbf{A} \otimes \mathbf{B})(\mathbf{x} \otimes \mathbf{y}) = (\mathbf{A}\mathbf{x}) \otimes (\mathbf{B}\mathbf{y})$ for vectors $\mathbf{x}$ and $\mathbf{y}$ of compatible dimensions.

See also: matrix, ML, model, vector.

Kullback–Leibler divergence (KL divergence) The KL divergence is a quantitative measure of how different one probability distribution is

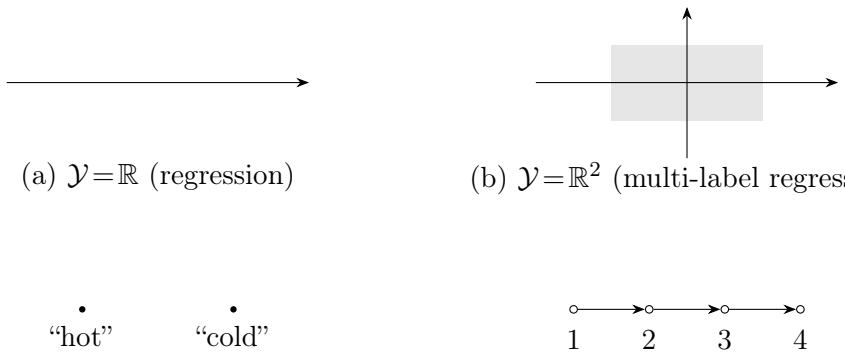
from another [?].

See also: probability distribution.

label A higher-level fact or quantity of interest associated with a data point. For example, if the data point is an image, the label could indicate whether the image contains a cat or not. Synonyms for label, commonly used in specific domains, include "response variable," "output variable," and "target" [?], [?], [?].

See also: data point, label space.

label space In a ML application, each data point is described by a set of features together with an associated label. The set of all admissible label values is called the label space, denoted by $\mathcal{Y}$. Importantly, $\mathcal{Y}$ may include values that no observed data point has as its label value. To a large extent, the choice of $\mathcal{Y}$ is up to the ML engineer and depends on the problem formulation. Fig. 44 shows some examples of label spacet that are commonly used in ML applications.



(a) $\mathcal{Y}=\mathbb{R}$ (regression)

(b) $\mathcal{Y}=\mathbb{R}^2$ (multi-label regression)

(c) $|\mathcal{Y}| = 2$ Binary luokittelu

(d) $\mathcal{Y}=\{1,2,3,4\}$ (ordinal regression)

Fig. 44. Examples of label spacet and corresponding flavours of ML.

The choice of label space $\mathcal{Y}$ determines the flavour of ML methods appropriate for the application at hand. Regression methods use the $\mathcal{Y} = \mathbb{R}$ while binary luokittelu methods use a label space $\mathcal{Y}$ that consists of two different elements, i.e., $|\mathcal{Y}| = 2$. Ordinal regression methods use a finite, ordered set of label values, e.g., $\mathcal{Y} = \{1, 2, 3, 4\}$ with the natural ordering $1 < 2 < 3 < 4$.

See also: data point,label, regression, luokittelu.

labeled data point A data point whose label is known or has been determined by some means that might require human labor.

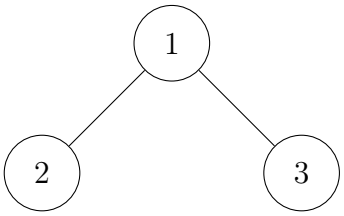
See also: data point, label.

Laplacian matrix The structure of a graph $\mathcal{G}$, with nodes $i = 1, \ldots, n$, can be analyzed using the properties of special matrices that are associated with $\mathcal{G}$. One such matrix is the graph Laplacian matrix $\mathbf{L}^{(\mathcal{G})} \in \mathbb{R}^{n \times n}$, which is defined for an undirected and weighted graph [**?**], [**?**]. It is

defined elementwise as (see Fig. 45)

$$L^{(\mathcal{G})}_{i,i'} := \begin{cases} -A_{i,i'}, & \text{for } i \neq i', \{i,i'\} \in \mathcal{E}; \\ \sum\limits_{i'' \neq i} A_{i,i''}, & \text{for } i = i'; \\ 0, & \text{else.} \end{cases}$$

Here, $A_{i,i'}$ denotes the edge weight of an edge $\{i,i'\} \in \mathcal{E}$.



(a)

$$\mathbf{L}^{(\mathcal{G})} = \begin{pmatrix} 2 & -1 & -1 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix}$$

(b)

Fig. 45. (a) Some undirected graph $\mathcal{G}$ with three nodes $i = 1, 2, 3$. (b) The Laplacian matrix $\mathbf{L}^{(\mathcal{G})} \in \mathbb{R}^{3 \times 3}$ of $\mathcal{G}$.

See also: graph, matrix, edge weight.

large language model (LLM) LLM is an umbrella term for ML methods that process and generate humanlike text. These methods typically use deep nets with billions (or even trillions) of parameters. A widely used choice for the network architecture is referred to as Transformers [**?**]. The training of LLMs is often based on the task of predicting a few words that are intentionally removed from a large text corpus. Thus, we can construct labeled data pointt simply by selecting some words from a given text as labels and the remaining words as features of data

points. This construction requires very little human supervision and allows for generating sufficiently large training sets for LLMs.

See also: deep net, labeled data point.

law of large numbers The law of large numbers refers to the convergence of the average of an increasing (large) number of i.i.d. RVs to the mean of their common probability distribution. Different instances of the law of large numbers are obtained by using different notions of convergence [**?**].

See also: convergence, i.i.d., RV, mean, probability distribution.

layer A deep net is an ANN that consists of consecutive layers, indexed by $\ell = 1, 2, \ldots, L$. The ℓ-th layer consists of artificial neurons $a_1^{(\ell)}, \ldots, a_{d^{(\ell)}}^{(\ell)}$ with the layer width $d^{(\ell)}$. Each of these artificial neurons evaluates an activation function for a weighted sum of the outputs (or activations) of the previous layer $\ell - 1$. The input to layer $\ell = 1$ is formed from weighted sums of the features of the data point for which the deep net computes a prediction. The outputs of the neurons in layer ℓ are then, in turn, used to form the inputs for the neurons in the next layer. The final (output) layer consists of a single neuron whose output is used as the prediction delivered by the deep net.

See also: deep net, ANN.

learning rate Consider an iterative ML method for finding or learning a useful hypothesis $h \in \mathcal{H}$. Such an iterative method repeats similar computational (update) steps that adjust or modify the current hypothesis to obtain an improved hypothesis. One well-known example of such an iterative learning method is GD and its variants, SGD and projected

gradient descent (projected GD). A key parameter of an iterative method is the learning rate. The learning rate controls the extent to which the current hypothesis can be modified during a single iteration. A well-known example of such a parameter is the step size used in GD [8, Ch. 5].

See also: ML, hypothesis, GD, SGD, projected GD, parameter, step size.

learning task Consider a tietoaineisto $\mathcal{D}$ consisting of multiple data points $\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(m)}$. For example, $\mathcal{D}$ can be a collection of images in an image database. A learning task is defined by specifying those properties (or attributes) of a data point that are used as its features and labels. Given a choice of model $\mathcal{H}$ and loss function, a learning task leads to an instance of ERM and can thus be represented by the associated objective function $\widehat{L}\big(h|\mathcal{D}\big)$ for $h \in \mathcal{H}$. Importantly, multiple distinct learning tasks can be constructed from the same tietoaineisto by selecting different sets of features and labels (see Fig. 46).

An image showing cows grazing in the Austrian countryside.

Task 1 (regression):
Features are the RGB values of all image pixels, and the label is the number of cows depicted.

Task 2 (luokittelu):
Features include the average green intensity of the image, and the label indicates whether cows should be moved to another location (i.e., yes/no).

Fig. 46. Two learning tasks constructed from a single image tietoaineisto. These tasks differ in feature selection and choice of label (i.e., the objective), but are both derived from the same tietoaineisto.

Different learning tasks arising from the same underlying tietoaineisto are often coupled. For example, when a probabilistic model is used to generate data points, statistical dependencies among different labels induce dependencies among the corresponding learning tasks. In general,

solving learning tasks jointly, e.g., using multitask learning methods, tends to be more effective than solving them independently (thereby ignoring dependencies among learning tasks) [?], [?], [?].

See also: tietoaineisto, model, loss function, objective function, multitask learning, label space.

least absolute deviation regression Least absolute deviation regression is an instance of ERM using the absolute error loss. It is a special case of Huber regression.

See also: ERM, absolute error loss, Huber regression.

least absolute shrinkage and selection operator (Lasso) The Lasso is an instance of SRM. It learns the weights $\mathbf{w}$ of a linear map $h(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$ from a training set. Lasso is obtained from linear regression by adding the scaled ℓ_1-norm $\alpha \|\mathbf{w}\|_1$ to the average squared error loss incurred on the training set.

See also: SRM, weights, linear map, training set, linear regression, norm, squared error loss.

linear classifier Consider data points characterized by numeric features $\mathbf{x} \in \mathbb{R}^d$ and a label $y \in \mathcal{Y}$ from some finite label space $\mathcal{Y}$. A linear luokitin is characterized by having decision regions that are separated by hyperplanes in $\mathbb{R}^d$ [8, Ch. 2].

See also: data point, feature, label, label space, luokitin, decision region.

linear map A linear map $f : \mathbb{R}^n \to \mathbb{R}^m$ is a function that satisfies additivity, i.e., $f(\mathbf{x} + \mathbf{y}) = f(\mathbf{x}) + f(\mathbf{y})$, and homogeneity, i.e., $f(c\mathbf{x}) = cf(\mathbf{x})$, for all vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ and scalars $c \in \mathbb{R}$. In particular, $f(\mathbf{0}) = \mathbf{0}$. Any

linear map can be represented as a matrix multiplication $f(\mathbf{x}) = \mathbf{A}\mathbf{x}$ for some matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$. The collection of real-valued linear maps for a given dimension n constitute a linear model, which is used in many ML methods.

See also: map, function, vector, matrix, linear model, ML.

linear model Consider an ML application involving data points, each represented by a numeric feature vector $\mathbf{x} \in \mathbb{R}^d$. A linear model defines a hypothesis space consisting of all real-valued linear maps from $\mathbb{R}^d$ to $\mathbb{R}$ such that

$$\mathcal{H}^{(d)} := \left\{ h : \mathbb{R}^d \to \mathbb{R} \mid h(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} \text{ for some } \mathbf{w} \in \mathbb{R}^d \right\}.$$

Each value of d defines a different hypothesis space, corresponding to the number of features used to compute the prediction $h(\mathbf{x})$. The choice of d is often guided not only by computational aspects (e.g., fewer features reduce computation) and statistical aspects (e.g., more features typically reduce harha and risk), but also by interpretability. A linear model using a small number of well-chosen features is generally considered more interpretable [**?**], [**?**]. The linear model is attractive because it can typically be trained using scalable convex optimization methods [**?**], [**?**]. Moreover, linear models often permit rigorous statistical analysis, including fundamental limits on the minimum achievable risk [**?**]. They are also useful for analyzing more complex nonlinear models such as neuroverkot. For instance, a deep net can be viewed as the composition of a feature map—implemented by the input and hidden layers—and a linear model in the output layer. Similarly, a decision tree can be

interpreted as applying a one-hot-encoded feature map based on decision regions, followed by a linear model that assigns a prediction to each region. More generally, any trained model $\hat{h} \in \mathcal{H}$ that is differentiable at some $\mathbf{x}'$ can be locally approximated by a linear map $g(\mathbf{x})$. Fig. 47 illustrates such a local linear approximation, defined by the gradient $\nabla \hat{h}(\mathbf{x}')$. Note that the gradient is only defined where $\hat{h}$ is differentiable. To ensure robustness in the context of trustworthy AI, one may prefer models whose associated map $\hat{h}$ is Lipschitz continuous. A classic result in mathematical analysis—Rademacher's Theorem—states that if $\hat{h}$ is Lipschitz continuous with some constant L over an open set $\Omega \subseteq \mathbb{R}^d$, then $\hat{h}$ is differentiable almost everywhere in Ω [**?**, Th. 3.1].

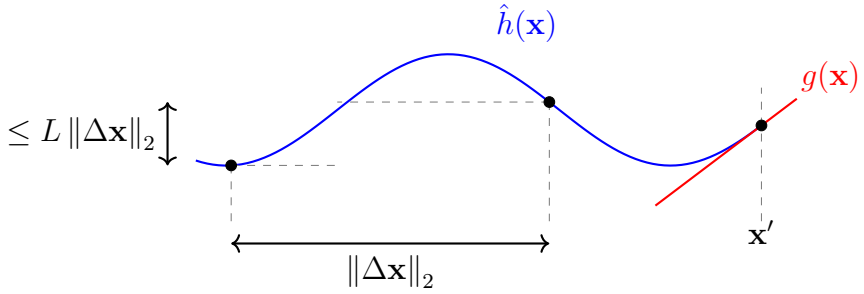


Fig. 47. A trained model $\hat{h}(\mathbf{x})$ that is differentiable at a point $\mathbf{x}'$ can be locally approximated by a linear map $g \in \mathcal{H}^{(d)}$. This local approximation is determined by the gradient $\nabla \hat{h}(\mathbf{x}')$.

See also: model, hypothesis space, linear map, interpretability, LIME.

linear regression Linear regression aims to learn a linear hypothesis map to predict a numeric label based on the numeric features of a data point. The quality of a linear hypothesis map is measured using the average

squared error loss incurred on a set of labeled data points, which we refer to as the training set.

See also: regression, hypothesis, map, label, feature, data point, squared error loss, labeled data point, training set.

local dataset The concept of a local tietoaineisto is in between the concept of a data point and a tietoaineisto. A local tietoaineisto consists of several individual data points characterized by features and labels. In contrast to a single tietoaineisto used in basic ML methods, a local tietoaineisto is also related to other local tietoaineistot via different notions of similarity. These similarities might arise from probabilistic models or communication infrastructure and are encoded in the edges of an FL network.

See also: tietoaineisto, data point, feature, label, ML, probabilistic model, FL network.

local interpretable model-agnostic explanations (LIME) Consider a trained model (or learned hypothesis) $\widehat{h} \in \mathcal{H}$, which maps the feature vector of a data point to the prediction $\widehat{y} = \widehat{h}$. LIME is a technique for explaining the behavior of $\widehat{h}$, locally around a data point with feature vector $\mathbf{x}^{(0)}$ [**?**]. The explanation is given in the form of a local approximation $g \in \mathcal{H}'$ of $\widehat{h}$ (see Fig. 48). This approximation can be obtained by an instance of ERM with a carefully designed training set. In particular, the training set consists of data points with feature vectors centered around $\mathbf{x}^{(0)}$ and the (pseudo-)label $\widehat{h}(\mathbf{x})$. Note that we can use a different model $\mathcal{H}'$ for the approximation from the original model $\mathcal{H}$.

For example, we can use a decision tree to locally approximate a deep net. Another widely used choice for $\mathcal{H}'$ is the linear model.

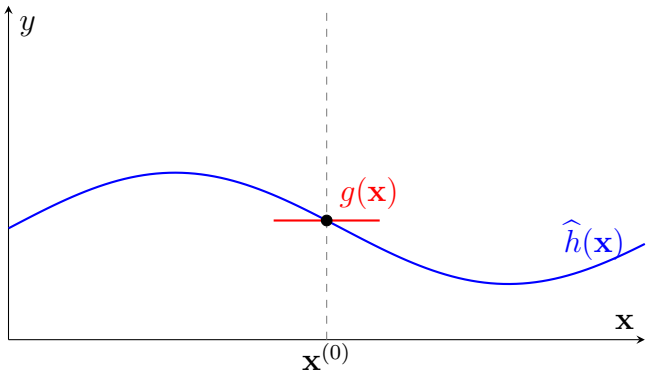


Fig. 48. To explain a trained model $\widehat{h} \in \mathcal{H}$, around a given feature vector $\mathbf{x}^{(0)}$, we can use a local approximation $g \in \mathcal{H}'$.

See also: model, explanation, ERM, training set, label, decision tree, deep net, linear model.

local model Consider a collection of devices that are represented as nodes $\mathcal{V}$ of an FL network. A local model $\mathcal{H}^{(i)}$ is a hypothesis space assigned to a node $i \in \mathcal{V}$. Different nodes can have different hypothesis spaces, i.e., in general, $\mathcal{H}^{(i)} \neq \mathcal{H}^{(i')}$ for different nodes $i, i' \in \mathcal{V}$.

See also: device, FL network, model, hypothesis space.

logistic loss Consider a data point characterized by the features $\mathbf{x}$ and a binary label $y \in \{-1, 1\}$. We use a real-valued hypothesis h to predict the label y from the features $\mathbf{x}$. The logistic loss incurred by this

prediction is defined as

$$L\left((\mathbf{x}, y), h\right) := \log\left(1 + \exp\left(-yh(\mathbf{x})\right)\right). \tag{8}$$

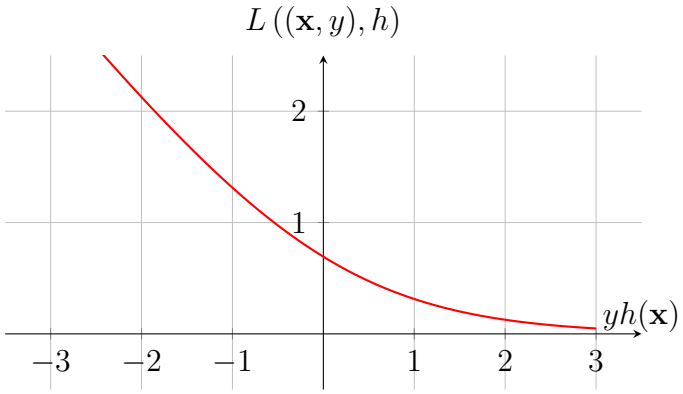


Fig. 49. The logistic loss incurred by the prediction $h(\mathbf{x}) \in \mathbb{R}$ for a data point with label $y \in \{-1, 1\}$.

Note that the expression (8) for the logistic loss applies only for the label space $\mathcal{Y} = \{-1, 1\}$ and when using the thresholding rule (1).

See also: data point, feature, label, hypothesis, loss, prediction, label space.

logistic regression Logistic regression learns a linear hypothesis map (or luokitin) $h(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$ to predict a binary label y based on the numeric feature vector $\mathbf{x}$ of a data point. The quality of a linear hypothesis map is measured by the average logistic loss on some labeled data points (i.e., the training set).

See also: regression, hypothesis, map, luokitin, label, feature vector, data point, logistic loss, labeled data point, training set.

loss ML methods use a loss function $L\left(\mathbf{z}, h\right)$ to measure the error incurred by applying a specific hypothesis to a specific data point. With a slight abuse of notation, we use the term loss for both the loss function L itself and the specific value $L\left(\mathbf{z}, h\right)$, for a data point $\mathbf{z}$ and hypothesis h.

See also: loss function, empirical risk.

loss function A loss function is a map

$$L : \mathcal{X} \times \mathcal{Y} \times \mathcal{H} \to \mathbb{R}_+ : \big(\big(\mathbf{x}, y\big), h\big) \mapsto L\left((\mathbf{x}, y), h\right).$$

It assigns a nonnegative real number (i.e., the loss) $L\left((\mathbf{x}, y), h\right)$ to a pair that consists of a data point, with features $\mathbf{x}$ and label y, and a hypothesis $h \in \mathcal{H}$. The value $L\left((\mathbf{x}, y), h\right)$ quantifies the discrepancy between the true label y and the prediction $h(\mathbf{x})$. Lower (closer to zero) values $L\left((\mathbf{x}, y), h\right)$ indicate a smaller discrepancy between prediction $h(\mathbf{x})$ and label y. Fig. 50 depicts a loss function for a given data point, with features $\mathbf{x}$ and label y, as a function of the hypothesis $h \in \mathcal{H}$.

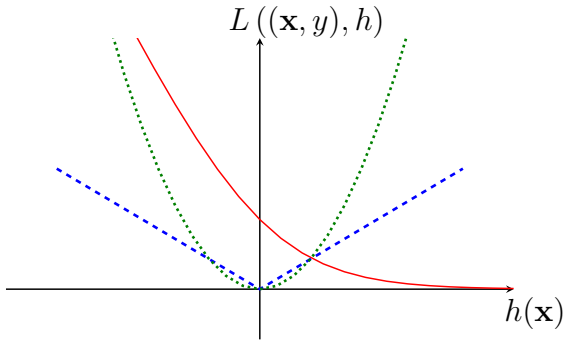


Fig. 50. Some loss function $L\left((\mathbf{x}, y), h\right)$ for a fixed data point, with feature vector $\mathbf{x}$ and label y, and a varying hypothesis h. ML methods try to find (or learn) a hypothesis that incurs minimal loss.

See also: loss, label, feature vector, ERM.

machine learning (ML) ML aims to predict a label from the features of a data point. ML methods achieve this by learning a hypothesis from a hypothesis space (or model) through the minimization of a loss function [8], [**?**]. One precise formulation of this principle is ERM. Different ML methods are obtained from different design choices for data points (i.e., their features and label), the model, and the loss function [8, Ch. 3].

See also: model, data, loss.

Markov decision process (MDP) An MDP is a mathematical structure that can be used to study RL applications. An MDP formalizes how reward signals depend on the predictions (and corresponding actions) made by an RL method. Formally, an MDP is a specific type of stochastic process defined by

- a state space $\mathcal{S}$;
- an action space $\mathcal{A}$ (where each action $a \in \mathcal{A}$ corresponds to a specific prediction made by the RL method);
- a transition function $\mathbb{P}(s' \mid s, a)$ specifying the probability distribution over the next state $s' \in \mathcal{S}$, given the current state $s \in \mathcal{S}$ and action $a \in \mathcal{A}$;
- a reward function $r(s, a) \in \mathbb{R}$ that assigns a numerical reward to each state-action pair.

The defining property of an MDP is the Markov property. That is, the next state s' and reward only depend on the current state s and action a, not on the entire history of interactions.

See also: RL, reward, prediction, stochastic process, function, probability distribution.

maximum The maximum of a set $\mathcal{A} \subseteq \mathbb{R}$ of real numbers is the greatest element in that set, if such an element exists. A set $\mathcal{A}$ has a maximum if it is bounded above and attains its supremum (or least upper bound) [2, Sec. 1.4].

See also: supremum.

maximum likelihood Consider data points $\mathcal{D} = \left\{\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(m)}\right\}$ that are interpreted as the realizations of i.i.d. RVs with a common probability distribution $\mathbb{P}(\mathbf{z}; \mathbf{w})$, which depends on the model parameters $\mathbf{w} \in \mathcal{W} \subseteq \mathbb{R}^n$. Maximum likelihood methods learn model parameters $\mathbf{w}$ by maximizing the probability (density) $\mathbb{P}(\mathcal{D}; \mathbf{w}) = \prod_{r=1}^{m} \mathbb{P}(\mathbf{z}^{(r)}; \mathbf{w})$ of the observed tietoaineisto. Thus, the maximum likelihood estimator is a solution to the optimization problem $\max_{\mathbf{w} \in \mathcal{W}} \mathbb{P}(\mathcal{D}; \mathbf{w})$.

See also: probability distribution, optimization problem, probabilistic model.

mean The mean of an RV $\mathbf{x}$, which takes on values in a Euclidean space $\mathbb{R}^d$, is its expectation $\mathbb{E}\{\mathbf{x}\}$. It is defined as the Lebesgue integral of $\mathbf{x}$ with respect to the underlying probability distribution P (e.g., see [2] or [6]), i.e.,

$$\mathbb{E}\{\mathbf{x}\} = \int_{\mathbb{R}^d} \mathbf{x} \, \mathrm{d}P(\mathbf{x}).$$

It is useful to think of the mean as the solution of the following risk minimization problem [7]:

$$\mathbb{E}\{\mathbf{x}\} = \arg\min_{\mathbf{c}\in\mathbb{R}^d} \mathbb{E}\big\{ \|\mathbf{x}-\mathbf{c}\|_2^2 \big\}.$$

We also use the term to refer to the average of a finite sequence $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)} \in \mathbb{R}^d$. However, these two definitions are essentially the same. Indeed, we can use the sequence $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)} \in \mathbb{R}^d$ to construct a discrete RV $\widetilde{\mathbf{x}} = \mathbf{x}^{(I)}$, with the index I being chosen uniformly at random from the set $\{1, \ldots, m\}$. The mean of $\widetilde{\mathbf{x}}$ is precisely the average $(1/m)\sum_{r=1}^{m} \mathbf{x}^{(r)}$.

See also: RV, expectation, probability distribution.

mean squared estimation error (MSEE) Consider an ML method that learns model parameters $\widehat{\mathbf{w}}$ based on some tietoaineisto $\mathcal{D}$. If we interpret the data points in $\mathcal{D}$ as i.i.d. realizations of an RV $\mathbf{z}$, we define the estimation error $\Delta\mathbf{w} := \widehat{w} - \overline{\mathbf{w}}$. Here, $\overline{\mathbf{w}}$ denotes the true model parameters of the probability distribution of $\mathbf{z}$. The MSEE is defined as the expectation $\mathbb{E}\big\{\big\|\Delta\mathbf{w}\big\|^2\big\}$ of the squared Euclidean norm of the estimation error [?], [?].

See also: RV, estimation error, probabilistic model, squared error loss.

measurable Consider a random experiment, such as recording the air temperature at an FMI weather station. The corresponding sample space Ω consists of all possible outcomes ω (e.g., all possible temperature values in degree Celsius). In many ML applications, we are not interested in the exact outcome ω, but only whether it belongs to a subset $\mathcal{A} \subseteq \Omega$ (e.g., "is the temperature below zero degrees?"). We call such a subset

$\mathcal{A}$ measurable if it is possible to decide, for any outcome ω, whether $\omega \in \mathcal{A}$ or not (see Fig. 51).

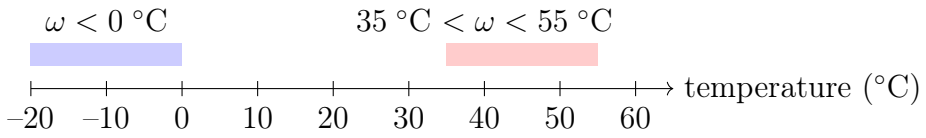


Fig. 51. A sample space constituted by all possible temperature values ω that may be experienced at an FMI station. Two measurable subsets of temperature values, denoted by $\mathcal{A}^{(1)}$ and $\mathcal{A}^{(2)}$, are highlighted. For any actual temperature value ω, it is possible to determine whether $\omega \in \mathcal{A}^{(1)}$ and whether $\omega \in \mathcal{A}^{(2)}$.

In principle, measurable sets could be chosen freely (e.g., depending on the resolution of the measuring equipment). However, it is often useful to impose certain completeness requirements on the collection of measurable sets. For example, the sample space itself should be measurable, and the union of two measurable sets should also be measurable. These completeness requirements can be formalized via the concept of σ-algebra (or σ-field) [1], [6], [**?**]. A measurable space is a pair $\left(\mathcal{X}, \mathcal{F}\right)$ that consists of an arbitrary set $\mathcal{X}$ and a collection $\mathcal{F}$ of measurable subsets of $\mathcal{X}$ that form a σ-algebra.

See also: sample space, probability.

median A median $\mathrm{med}\,(x)$ of a real-valued RV x is any number $m \in \mathbb{R}$ such

that $\mathbb{P}(x \leq m) \geq 1/2$ and $\mathbb{P}(x \geq m) \geq 1/2$ (see Fig. 52) [?].

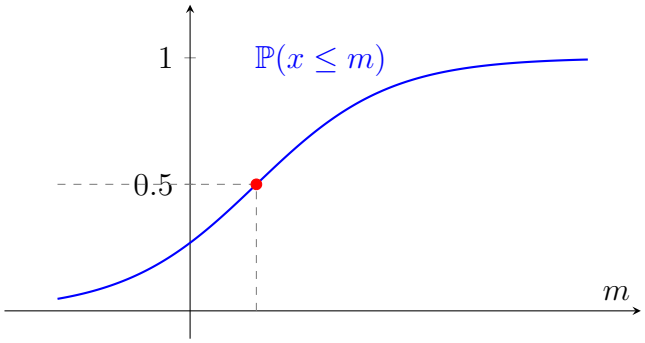


Fig. 52. A representation of a median.

We can define the median med $(\mathcal{D})$ of a tietoaineisto $\mathcal{D} = \{x^{(1)}, \ldots, x^{(m)} \in \mathbb{R}\}$ via a specific RV $\tilde{x}$ that is naturally associated with $\mathcal{D}$. In particular, this RV is constructed by $\tilde{x} = x^{(I)}$, with the index I being chosen uniformly at random from the set $\{1, \ldots, m\}$, i.e., $\mathbb{P}(I = r) = 1/m$ for all $r = 1, \ldots, m$. If the RV x is integrable, a median of x is the solution of the following optimization problem:

$$\min_{x' \in \mathbb{R}} \mathbb{E}|x - x'|.$$

Like the mean, the median of a tietoaineisto $\mathcal{D}$ can also be used to estimate parameters of an underlying probabilistic model. Compared with the mean, the median is more robust to outliert. For example, a median of a tietoaineisto $\mathcal{D}$ with more than one data point does not change even if we arbitrarily increase the largest element of $\mathcal{D}$ (see Fig. 53). In contrast, the mean will increase arbitrarily.

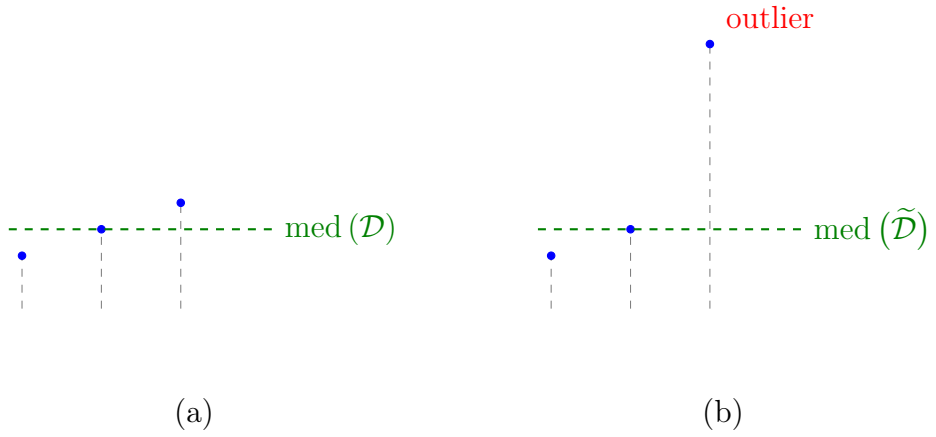


Fig. 53. The median is robust against outlier contamination. (a) Original tietoaineisto $\mathcal{D}$. (b) Noisy tietoaineisto $\widetilde{\mathcal{D}}$ including an outlier.

See also: mean, outlier, robustness.

metric In its most general form, a metric is a quantitative measure used to compare or evaluate objects. In mathematics, a metric measures the distance between two points and must follow specific rules, i.e., the distance is always nonnegative, zero only if the points are the same, symmetric, and it satisfies the triangle inequality [2]. In ML, a metric is a quantitative measure of how well a model performs. Examples include tarkkuus, precision, and the average 0/1 loss on a test set [**?**], [**?**]. A loss function is used to train models, while a metric is used to compare trained models.

See also: ML, model, tarkkuus, 0/1 loss, test set, loss function, loss, model selection.

minimum Given a set of real numbers, the minimum is the smallest of

those numbers. Note that for some sets, such as the set of negative real numbers, the minimum does not exist.

missing data Consider a tietoaineisto constituted by data points collected via some physical device. Due to imperfections and failures, some of the feature or label values of data points might be corrupted or simply missing. Data imputation aims to estimate these missing values [**?**]. We can interpret data imputation as an ML problem where the label of a data point is the value of the corrupted feature.
See also: feature, label.

model The study and design of ML methods is often based on a mathematical model [**?**]. Maybe the most widely used example of a mathematical model for ML is a hypothesis space. A hypothesis space consists of hypothesis maps that are used by an ML method to predict labels from the features of data points. Another important type of mathematical model is a probabilistic model, which consists of probability distributions that describe how data points are generated. Unless stated otherwise, we use the term model to refer specifically to the hypothesis space underlying an ML method. We illustrate one example of a hypothesis space and a probabilistic model in Fig. 54.

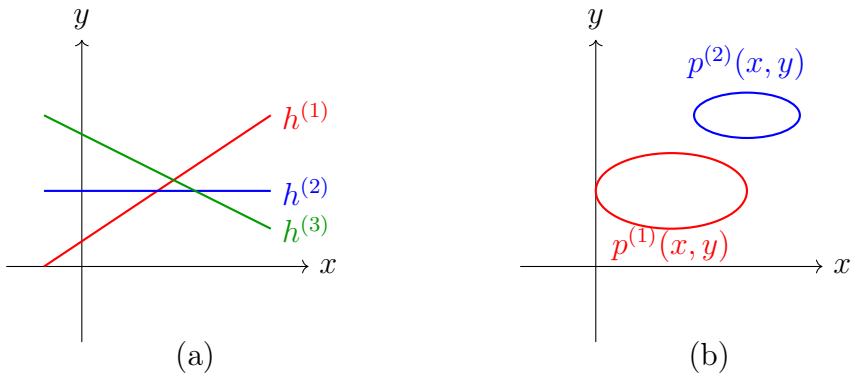


Fig. 54. Two types of mathematical models used in ML. (a) A hypothesis space consisting of three linear maps. (b) A probabilistic model consisting of probability distribution over the plane spanned by the feature and label values of a data point.

See also: hypothesis space, probabilistic model, probability distribution.

model inversion A model inversion is a form of privacy attack on an ML system. An adversary seeks to infer sensitive attributes of individual data points by exploiting partial access to a trained model $\hat{h} \in \mathcal{H}$. This access typically consists of querying the model for predictions $\hat{h}(\mathbf{x})$ using carefully chosen inputs. Basic model inversion techniques have been demonstrated in the context of facial image luokittelu, where images are reconstructed using the (gradient of) model outputs combined with auxiliary information such as a person's name [**?**] (see Fig. 55).

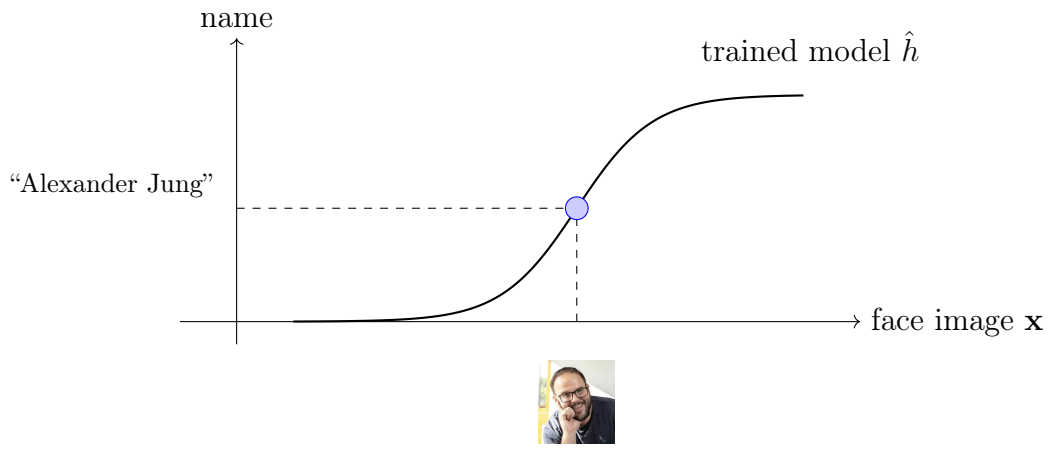


Fig. 55. Model inversion techniques implemented in the context of facial image classification.

See also: model, privacy attack, ML, sensitive attribute, data point, prediction, luokittelu, gradient, trustworthy AI, privacy protection.

model parameters Model parameters are quantities that are used to select a specific hypothesis map from a model. We can think of a list of model parameters as a unique identifier for a hypothesis map, similar to how a social security number identifies a person in Finland.

See also: model, parameter, hypothesis, map.

model selection In ML, model selection refers to the process of choosing between different candidate models. In its most basic form, model selection amounts to: 1) training each candidate model; 2) computing the validation error for each trained model; and 3) choosing the model with the smallest validation error [8, Ch. 6].

See also: ML, model, validation error.

multi-label classification Multi-label luokittelu problems and methods use data points that are characterized by several labels. As an example, consider a data point representing a picture with two labels. One label indicates the presence of a human in this picture and another label indicates the presence of a car.

See also: label, luokittelu, data point.

multiarmed bandit (MAB) An MAB problem is a precise mathematical formulation of a sequential decision-making task under uncertainty. At each discrete time step k, a learner selects one of several possible actions—called arms—from a finite set $\mathcal{A}$. Pulling arm a at time k yields a reward $r^{(a,k)}$ that is drawn from an unknown probability distribution $\mathbb{P}(r^{(a,k)})$. We obtain different classes of MAB problems by placing different restrictions on this probability distribution. In the simplest setting, the probability distribution $\mathbb{P}(r^{(a,k)})$ does not depend on t. Given an MAB problem, the goal is to construct ML methods that maximize the cumulative reward over time by strategically balancing exploration (i.e., gathering information about uncertain arms) and exploitation (i.e., selecting arms known to perform well). MAB problems form an important special case of RL problems [**?**], [**?**].

See also: reward, regret.

multitask learning Multitask learning aims to leverage relations between different learning tasks. Consider two learning tasks obtained from the same tietoaineisto of webcam snapshots. The first task is to predict the

presence of a human, while the second task is to predict the presence of a car. It may be useful to use the same deep net structure for both tasks and only allow the weights of the final output layer to be different.
See also: learning task, tietoaineisto, deep net, weights, layer.

multivariate normal distribution The multivariate normal distribution, which is denoted by $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, is a fundamental probabilistic model for numerical feature vectors of fixed dimension d. It defines a family of probability distributions over vector-valued RVs $\mathbf{x} \in \mathbb{R}^d$ [7], [**?**], [**?**]. Each distribution in this family is fully specified by its mean vector $\boldsymbol{\mu} \in \mathbb{R}^d$ and kovarianssimatriisi $\boldsymbol{\Sigma} \in \mathbb{R}^{d \times d}$. When the kovarianssimatriisi $\boldsymbol{\Sigma}$ is invertible, the corresponding probability distribution is characterized by the following pdf:

$$p(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^d \det(\boldsymbol{\Sigma})}} \exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right].$$

Note that this pdf is only defined when $\boldsymbol{\Sigma}$ is invertible. More generally, any RV $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ admits the following representation:

$$\mathbf{x} = \mathbf{A}\mathbf{z} + \boldsymbol{\mu}$$

where $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ is a standard normal vector and $\mathbf{A} \in \mathbb{R}^{d \times d}$ satisfies $\mathbf{A}\mathbf{A}^\top = \boldsymbol{\Sigma}$. This representation remains valid even when $\boldsymbol{\Sigma}$ is singular, in which case $\mathbf{A}$ is not full rank [**?**, Ch. 23]. The family of multivariate normal distributions is exceptional among probabilistic models for numerical quantities, at least for the following reasons. First, the family is closed under affine transformations, i.e.,

$$\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \text{ implies } \mathbf{B}\mathbf{x}+\mathbf{c} \sim \mathcal{N}\big(\mathbf{B}\boldsymbol{\mu} + \mathbf{c}, \mathbf{B}\boldsymbol{\Sigma}\mathbf{B}^T\big).$$

Second, the probability distribution $\mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$ maximizes the differential entropy among all distributions with the same kovarianssimatriisi $\mathbf{\Sigma}$ [?].
See also: probabilistic model, probability distribution, standard normal vector, differential entropy, Gaussian RV.

mutual information (MI) The MI $I(\mathbf{x}; y)$ between two RVs $\mathbf{x}$, y defined on the same probability space is given by [?]

$$I(\mathbf{x}; y) := \mathbb{E}\left\{\log \frac{p(\mathbf{x}, y)}{p(\mathbf{x})p(y)}\right\}.$$

It is a measure of how well we can estimate y based solely on $\mathbf{x}$. A large value of $I(\mathbf{x}; y)$ indicates that y can be well predicted solely from $\mathbf{x}$. This prediction could be obtained by a hypothesis learned by an ERM-based ML method.
See also: RV, probability space, prediction, hypothesis, ERM, ML.

nearest neighbor (NN) NN methods learn a hypothesis $h : \mathcal{X} \to \mathcal{Y}$ whose function value $h(\mathbf{x})$ is solely determined by the NNs within a given tietoaineisto. Different methods use different metrics for determining the NNs. If data points are characterized by numeric feature vectors, we can use their Euclidean distances as the metric.
See also: hypothesis, function, tietoaineisto, metric, data point, feature vector, neighbors.

neighborhood Consider some metric space $\mathcal{X}$ with metric $d : \mathcal{X} \times \mathcal{X} \to \mathbb{R}_+$. The neighborhood of a point $\mathbf{x} \in \mathcal{X}$ is the set of other points having a sufficiently small distance to $\mathbf{x}$. For example, the ϵ-neighborhood of $\mathbf{x}$ is

defined as

$$\{\mathbf{x}' \in \mathcal{X} : d(\mathbf{x}, \mathbf{x}') \leq \epsilon\}.$$

If $\mathcal{X}$ is an undirected graph, which is a special case of a metric space, the neighborhood of a node $i \in \mathcal{V}$ is the set of its neighbors.

See also: neighbors, metric.

neighbors The neighbors of a node $i \in \mathcal{V}$ within an FL network are those nodes $i' \in \mathcal{V} \setminus \{i\}$ that are connected (via an edge) to node i.

See also: FL network.

networked data Networked data consist of local datasets that are related by some notion of pairwise similarity. We can represent networked data using a graph whose nodes carry local datasets and whose edges encode pairwise similarities. An example of networked data can be found in FL applications where local datasets are generated by spatially distributed devices.

See also: data, local dataset, graph, FL, device.

networked exponential families (nExpFam) A collection of exponential families, each of them assigned to a node of an FL network. The model parameters are coupled via the network structure by requiring them to have a small GTV [**?**].

See also: FL network, model parameters, GTV.

networked federated learning (NFL) NFL refers to methods that learn personalized models in a distributed fashion. These methods learn from local datasets that are related by an intrinsic network structure.

See also: model, local dataset, FL.

networked model A networked model over an FL network $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ assigns a local model (i.e., a hypothesis space) to each node $i \in \mathcal{V}$ of the FL network $\mathcal{G}$.

See also: model, FL network, local model, hypothesis space.

node degree The degree $d^{(i)}$ of a node $i \in \mathcal{V}$ in an undirected graph is the number of its neighbors, i.e., $d^{(i)} := \left|\mathcal{N}^{(i)}\right|$.

See also: graph, neighbors.

non-smooth We refer to a function as non-smooth if it is not smooth [**?**].

See also: function, smooth.

norm A norm is a function that maps each (vector) element of a vector space to a nonnegative real number. This function must be homogeneous and definite, and it must satisfy the triangle inequality [**?**].

See also: function, vector, vector space.

nullspace The nullspace of a matrix $\mathbf{A} \in \mathbb{R}^{d' \times d}$, denoted by null($\mathbf{A}$), is the set of all vectors $\mathbf{n} \in \mathbb{R}^{d}$ such that

$$\mathbf{A}\mathbf{n} = \mathbf{0}.$$

Consider a feature learning method that uses the matrix $\mathbf{A}$ to transform a feature vector $\mathbf{x} \in \mathbb{R}^{d}$ of a data point into a new feature vector $\mathbf{z} = \mathbf{A}\mathbf{x} \in \mathbb{R}^{d'}$. The nullspace null($\mathbf{A}$) characterizes all directions in the original feature space $\mathbb{R}^{d}$ along which the transformation $\mathbf{A}\mathbf{x}$ remains unchanged. In other words, adding any vector from the nullspace to a feature vector $\mathbf{x}$ does not affect the transformed representation $\mathbf{z}$. This property can be exploited to enforce invariances in the predictions

(computed from $\mathbf{Ax}$). Fig. 56 illustrates one such invariance. It shows rotated versions of two handwritten digits, which approximately lie along 1-D curves in the original feature space. These curves are aligned with a direction vector $\mathbf{n} \in \mathbb{R}^d$. To ensure that the trained model is invariant to such rotations, we can choose the transformation matrix $\mathbf{A}$ such that $\mathbf{n} \in \text{null}(\mathbf{A})$. This ensures that $\mathbf{Ax}$, and hence the resulting prediction, is approximately insensitive to rotations of the input image.

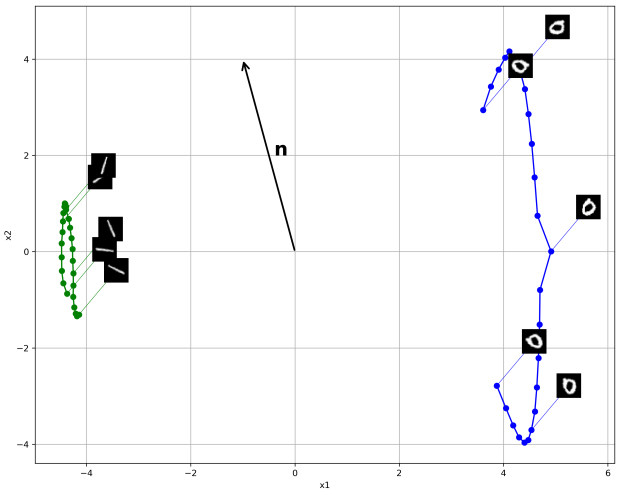


Fig. 56. Rotated handwritings of two different digits. The rotations are approximately aligned along straight lines parallel to the vector $\mathbf{n}$. For a binary luokitin distinguishing between these digits, a natural choice is a linear feature map $\mathbf{x} \mapsto \mathbf{Ax}$ with a matrix $\mathbf{A}$ whose nullspace contains $\mathbf{n}$, i.e., $\mathbf{n} \in \text{null}(\mathbf{A})$.

See also: matrix, feature map, feature learning.

Python demo: click me

objective function An objective function is a map that assigns a numeric objective value $f(\mathbf{w})$ to each choice $\mathbf{w}$ of some variable that we want to optimize (see Fig. 57). In the context of ML, the optimization variable could be the model parameters of a hypothesis $h^{(\mathbf{w})}$. Common objective functions include the risk (i.e., expected loss) or the empirical risk (i.e., average loss over a training set). ML methods apply optimization techniques, such as gradient-based methods, to find the choice $\mathbf{w}$ with the optimal value (e.g., the minimum or the maximum) of the objective function.

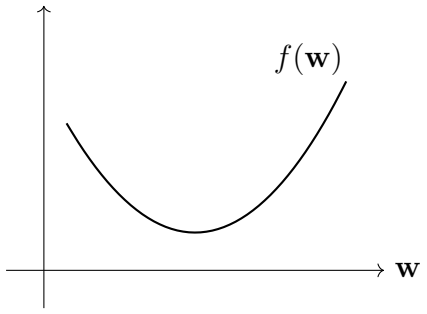


Fig. 57. An objective function maps each possible value $\mathbf{w}$ of an optimization variable, such as the model parameters of an ML model, to a value $f(\mathbf{w})$ that measures the usefulness of $\mathbf{w}$.

See also: loss, empirical risk, ERM, optimization problem.

online algorithm An online algorithm processes input data incrementally, receiving data points sequentially and making decisions or producing outputs (or decisions) immediately without having access to the entire

input in advance [?], [?]. Unlike an offline algorithm, which has the entire input available from the start, an online algorithm must handle uncertainty about future inputs and cannot revise past decisions. Similar to an offline algorithm, we represent an online algorithm formally as a collection of possible executions. However, the execution sequence for an online algorithm has a distinct structure as follows:

$$\text{in}_1,\ s_1,\ \text{out}_1,\ \text{in}_2,\ s_2,\ \text{out}_2,\ \ldots,\ \text{in}_T,\ s_T,\ \text{out}_T.$$

Each execution begins from an initial state (i.e., in_1) and proceeds through alternating computational steps, outputs (or decisions), and inputs. Specifically, at step k, the algorithm performs a computational step s_k, generates an output out_k, and then subsequently receives the next input (data point) in_{k+1}. A notable example of an online algorithm in ML is online gradient descent (online GD), which incrementally updates model parameters as new data points arrive.

See also: algorithm, data, data point, uncertainty, ML, online GD, model parameters, online learning.

online gradient descent (online GD) Consider an ML method that learns model parameters $\mathbf{w}$ from some parameter space $\mathcal{W} \subseteq \mathbb{R}^d$. The learning process uses data points $\mathbf{z}^{(t)}$ that arrive at consecutive time instants $t = 1, 2, \ldots$. Let us interpret the data points $\mathbf{z}^{(t)}$ as i.i.d. copies of an RV $\mathbf{z}$. The risk $\mathbb{E}\{L(\mathbf{z}, \mathbf{w})\}$ of a hypothesis $h^{(\mathbf{w})}$ can then (under mild conditions) be obtained as the limit $\lim_{T\to\infty}(1/T)\sum_{t=1}{}^{T} L\left(\mathbf{z}^{(t)}, \mathbf{w}\right)$. We might use this limit as the objective function for learning the model parameters $\mathbf{w}$. Unfortunately, this limit can only be evaluated if we wait

infinitely long in order to collect all data points. Some ML applications require methods that learn online, i.e., as soon as a new data point $\mathbf{z}^{(t)}$ arrives at time t, we update the current model parameters $\mathbf{w}^{(t)}$. Note that the new data point $\mathbf{z}^{(t)}$ contributes the component $L\left(\mathbf{z}^{(t)}, \mathbf{w}\right)$ to the risk. As its name suggests, online GD updates $\mathbf{w}^{(t)}$ via a (projected) gradient step such that

$$\mathbf{w}^{(t+1)} := P_{\mathcal{W}}\big(\mathbf{w}^{(t)} - \eta_t \nabla_{\mathbf{w}} L\left(\mathbf{z}^{(t)}, \mathbf{w}\right)\big). \tag{9}$$

Note that (9) is a gradient step for the current component $L\left(\mathbf{z}^{(t)}, \cdot\right)$ of the risk. The update (9) ignores all previous components $L\left(\mathbf{z}^{(t')}, \cdot\right)$, for $t' < t$. It might therefore happen that, compared with $\mathbf{w}^{(t)}$, the updated model parameters $\mathbf{w}^{(t+1)}$ increase the retrospective average loss $\sum_{t'=1}^{t-1} L\left(\mathbf{z}^{(t')}, \cdot\right)$. However, for a suitably chosen learning rate η_t, online GD can be shown to be optimal in practically relevant settings. By optimal, we mean that the model parameters $\mathbf{w}^{(T+1)}$ delivered by online GD after observing T data points $\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(T)}$ are at least as good as those delivered by any other learning method [**?**], [**?**].

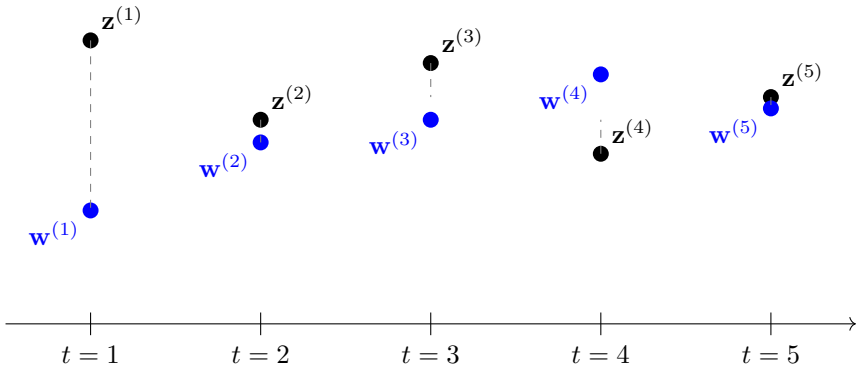


Fig. 58. An instance of online GD that updates the model parameters $\mathbf{w}^{(t)}$ using the data point $\mathbf{z}^{(t)} = x^{(t)}$ arriving at time t. This instance uses the squared error loss $L\left(\mathbf{z}^{(t)}, w\right) = (x^{(t)} - w)^2$.

See also: objective function, GD, gradient step, online learning.

online learning Some ML methods are designed to process data in a sequential manner, updating their model parameters one at a time, as new data points become available. A typical example is time-series data, such as daily minimum and maximum temperatures recorded by an FMI weather station. These values form a chronological sequence of observations. During each time step t, online learning methods update (or refine) the current hypothesis $h^{(t)}$ (or model parameters $\mathbf{w}^{(t)}$) based on the newly observed data point $\mathbf{z}^{(t)}$.

See also: online GD, online algorithm.

optimism in the face of uncertainty ML methods learn model parameters $\mathbf{w}$ according to some performance criterion $\bar{f}(\mathbf{w})$. However, they usually cannot access $\bar{f}(\mathbf{w})$ directly but rely on an estimate (or approxi-

mation) $f(\mathbf{w})$ of $\bar{f}(\mathbf{w})$. As a case in point, ERM-based methods use the average loss on a given tietoaineisto (i.e., the training set) as an estimate for the risk of a hypothesis. Using a probabilistic model, one can construct a confidence interval $\left[l^{(\mathbf{w})}, u^{(\mathbf{w})}\right]$ for each choice $\mathbf{w}$ for the model parameters. One simple construction is $l^{(\mathbf{w})} := f(\mathbf{w}) - \sigma/2$, $u^{(\mathbf{w})} := f(\mathbf{w}) + \sigma/2$, with σ being a measure of the (expected) deviation of $f(\mathbf{w})$ from $\bar{f}(\mathbf{w})$. We can also use other constructions for this interval as long as they ensure that $\bar{f}(\mathbf{w}) \in \left[l^{(\mathbf{w})}, u^{(\mathbf{w})}\right]$ with a sufficiently high probability. An optimist chooses the model parameters according to the most favorable—yet still plausible—value $\tilde{f}(\mathbf{w}) := l^{(\mathbf{w})}$ of the performance criterion (see Fig. 59). Two examples of ML methods that use such an optimistic construction of an objective function are SRM [**?**, Ch. 11] and upper confidence bound (UCB) methods for sequential decision making [**?**, Sec. 2.2].

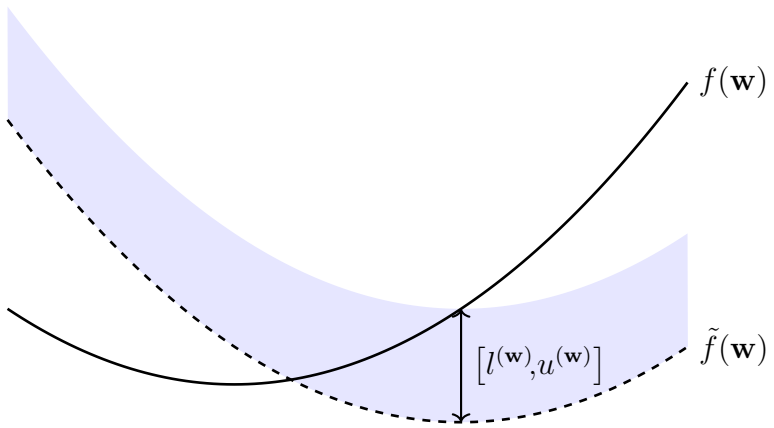


Fig. 59. ML methods learn model parameters $\mathbf{w}$ by using some estimate of $f(\mathbf{w})$ for the ultimate performance criterion $\bar{f}(\mathbf{w})$. Using a probabilistic model, one can use $f(\mathbf{w})$ to construct confidence intervals $\left[l^{(\mathbf{w})}, u^{(\mathbf{w})}\right]$, which contain $\bar{f}(\mathbf{w})$ with a high probability. The best plausible performance measure for a specific choice $\mathbf{w}$ of model parameters is $\tilde{f}(\mathbf{w}) := l^{(\mathbf{w})}$.

See also: ML, model parameters, ERM, loss, tietoaineisto, training set, risk, hypothesis, probabilistic model, probability, objective function, SRM, UCB.

optimization method An optimization method is an algorithm that reads in a representation of an optimization problem and delivers an (approximate) solution as its output [**?**], [**?**], [**?**].

See also: algorithm, optimization problem.

outlier Many ML methods are motivated by the i.i.d. assumption, which interprets data points as realizations of i.i.d. RVs with a common probability distribution. The i.i.d. assumption is useful for applications

where the statistical properties of the data generation process are stationary (or time-invariant) [?]. However, in some applications, the data consist of a majority of regular data points that conform with the i.i.d. assumption as well as a small number of data points that have fundamentally different statistical properties compared with the regular data points. We refer to a data point that substantially deviates from the statistical properties of most data points as an outlier. Different methods for outlier detection use different measures for this deviation. Statistical learning theory studies fundamental limits on the ability to mitigate outliers reliably [?], [?].

See also: robustness, stability, Huber regression, probabilistic model.

overfitting Consider an ML method that uses ERM to learn a hypothesis with the minimum empirical risk on a given training set. Such a method is overfitting the training set if it learns a hypothesis with a low empirical risk on the training set but a significantly higher loss outside the training set.

See also: ERM, generalization, validation, generalization gap.

parameter The parameter of an ML model is a tunable (i.e., learnable or adjustable) quantity that allows us to choose between different hypothesis maps. For example, the linear model $\mathcal{H} := \{h^{(\mathbf{w})} : h^{(\mathbf{w})}(x) = w_1 x + w_2\}$ consists of all hypothesis maps $h^{(\mathbf{w})}(x) = w_1 x + w_2$ with a particular choice for the parameters $\mathbf{w} = \big(w_1, w_2\big)^T \in \mathbb{R}^2$. Another example of a model parameter is the weights assigned to a connection between two neurons of an ANN.

See also: ML, model, hypothesis, map, linear model, weights, ANN.

parameter space The parameter space $\mathcal{W}$ of an ML model $\mathcal{H}$ is the set of all feasible choices for the model parameters (see Fig. 60). Many important ML methods use a model that is parameterized by vectors of the Euclidean space $\mathbb{R}^d$. Two widely used examples of parameterized models are linear models and deep nets. The parameter space is then often a subset $\mathcal{W} \subseteq \mathbb{R}^d$, e.g., all vectors $\mathbf{w} \in \mathbb{R}^d$ with a norm smaller than one.

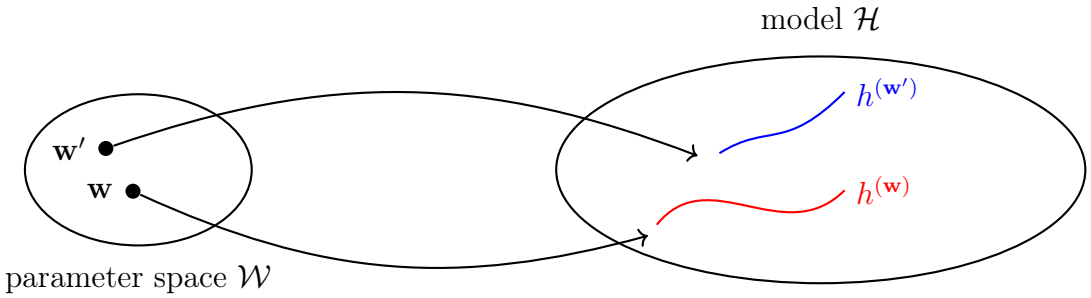


Fig. 60. The parameter space $\mathcal{W}$ of an ML model $\mathcal{H}$ consists of all feasible choices for the model parameters. Each choice $\mathbf{w}$ for the model parameters selects a hypothesis map $h^{(\mathbf{w})} \in \mathcal{H}$.

See also: parameter, model, model parameters.

parametric model A parametric model $\mathcal{H}$ is a model that is parameterized by a finite number of model parameters. In particular, each hypothesis $h \in \mathcal{H}$ is uniquely identified by a list of model parameters $w_1, w_2, \ldots$ (see Fig. 60). For many important ML methods , this list has a fixed length d which we refer to as the number of model parameters. We then

stack the model parameters into a vector $\mathbf{w} \in \mathbb{R}^d$. Two widely used examples of a paramtric model are a linear model and a neuroverkot. The parameter space is then often a subset $\mathcal{W} \subseteq \mathbb{R}^d$, e.g., all vectors $\mathbf{w} \in \mathbb{R}^d$ with a norm smaller than one.

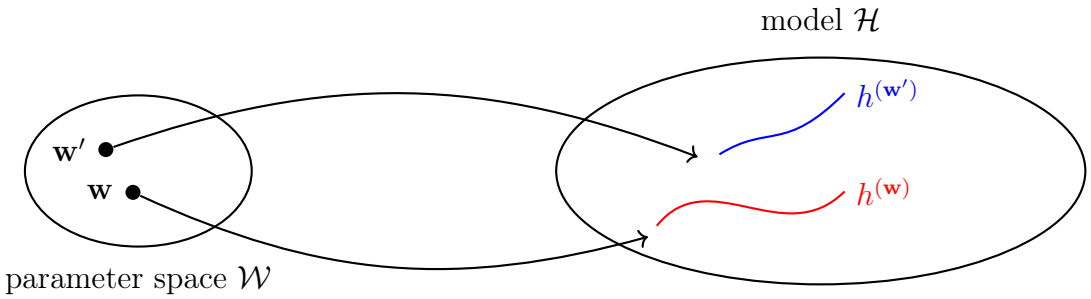


Fig. 61. The parameter space $\mathcal{W}$ of an ML model $\mathcal{H}$ consists of all feasible choices for the model parameters. Each choice $\mathbf{w}$ for the model parameters selects a hypothesis map $h^{(\mathbf{w})} \in \mathcal{H}$.

See also: parameter space, model, model parameters.

polynomial regression Polynomial regression is an instance of ERM that learns a polynomial hypothesis map to predict a numeric label based on the numeric features of a data point. For data points characterized by a single numeric feature, polynomial regression uses the hypothesis space $\mathcal{H}_d^{(\text{poly})} := \{h(x) = \sum_{j=0}^{d-1} x^j w_j\}$. The quality of a polynomial hypothesis map is measured using the average squared error loss incurred on a set of labeled data points (which we refer to as the training set).

See also: regression, ERM, squared error loss.

positive semi-definite (psd) A (real-valued) symmetric matrix $\mathbf{Q} = \mathbf{Q}^T \in$

$\mathbb{R}^{d \times d}$ is referred to as psd if $\mathbf{x}^T \mathbf{Q} \mathbf{x} \geq 0$ for every vector $\mathbf{x} \in \mathbb{R}^d$. The property of being psd can be extended from matrices to (real-valued) symmetric kernel maps $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ (with $K(\mathbf{x}, \mathbf{x}') = K(\mathbf{x}', \mathbf{x})$) as follows: For any finite set of feature vectors $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)}$, the resulting matrix $\mathbf{Q} \in \mathbb{R}^{m \times m}$ with entries $Q_{r,r'} = K\big(\mathbf{x}^{(r)}, \mathbf{x}^{(r')}\big)$ is psd [**?**].

See also: matrix, vector, kernel, map, feature vector.

prediction A prediction is an estimate or approximation for some quantity of interest. ML revolves around learning or finding a hypothesis map h that reads in the features $\mathbf{x}$ of a data point and delivers a prediction $\widehat{y} := h(\mathbf{x})$ for its label y.

See also: ML, hypothesis, map, feature, data point, label.

predictor A predictor is a real-valued hypothesis map. Given a data point with features $\mathbf{x}$, the value $h(\mathbf{x}) \in \mathbb{R}$ is used as a prediction for the true numeric label $y \in \mathbb{R}$ of the data point.

See also: hypothesis, map, data point, feature, prediction, label.

preimage Consider a function $f : \mathcal{U} \to \mathcal{V}$ between two sets. The preimage $f^{-1}(\mathcal{B})$ of a subset $\mathcal{B} \subseteq \mathcal{V}$ is the set of all inputs $u \in \mathcal{U}$ that are mapped into $\mathcal{B}$ by f, i.e.,

$$f^{-1}(\mathcal{B}) := \{u \in \mathcal{U} \mid f(u) \in \mathcal{B}\}.$$

The preimage is well defined even if the function f is non-invertible [2].

See also: function.

principal component analysis (PCA) PCA determines a linear feature map such that the new features allow us to reconstruct the original

features with the minimum reconstruction error [8].

See also: feature map, feature, minimum.

privacy attack A privacy attack on an ML system aims to infer sensitive attributes of individuals by exploiting partial access to a trained ML model. One form of a privacy attack is model inversion.

See also: attack, sensitive attribute, model inversion, trustworthy AI, general data protection regulation (GDPR).

privacy funnel The privacy funnel is a method for learning privacy-friendly features of data points [**?**].

See also: feature, data point.

privacy leakage Consider an ML application that processes a tietoaineisto $\mathcal{D}$ and delivers some output, such as the predictions obtained for new data points. Privacy leakage arises if the output carries information about a private (or sensitive) feature of a data point of $\mathcal{D}$ (such as a human). Based on a probabilistic model for the data generation, we can measure the privacy leakage via the MI between the output and the sensitive feature. Another quantitative measure of privacy leakage is DP. The relations between different measures of privacy leakage have been studied in the literature (see [**?**]).

See also: MI, DP, privacy attack, GDPR.

privacy protection Consider some ML method $\mathcal{A}$ that reads in a tietoaineisto $\mathcal{D}$ and delivers some output $\mathcal{A}(\mathcal{D})$. The output could be the learned model parameters $\widehat{\mathbf{w}}$ or the prediction $\hat{h}(\mathbf{x})$ obtained for a specific data point with features $\mathbf{x}$. Many important ML applications involve

data points representing humans. Each data point is characterized by features $\mathbf{x}$, potentially a label y, and a sensitive attribute s (e.g., a recent medical diagnosis). Roughly speaking, privacy protection means that it should be impossible to infer, from the output $\mathcal{A}(\mathcal{D})$, any of the sensitive attributes of data points in $\mathcal{D}$. Mathematically, privacy protection requires non-invertibility of the map $\mathcal{A}(\mathcal{D})$. In general, just making $\mathcal{A}(\mathcal{D})$ non-invertible is typically insufficient for privacy protection. We need to make $\mathcal{A}(\mathcal{D})$ sufficiently non-invertible.

See also: ML, tietoaineisto, model parameters, prediction, data point, feature, label, sensitive attribute, map.

probabilistic model A probabilistic model interprets data points as realizations of RVs with a joint probability distribution. This joint probability distribution typically involves parameters that have to be manually chosen or learned via statistical inference methods such as maximum likelihood estimation [**?**].

See also: model, data point, realization, RV, probability distribution, parameter, maximum likelihood.

probabilistic principal component analysis (PPCA) PPCA extends basic PCA by using a probabilistic model for data points. The probabilistic model of PPCA frames the task of dimensionality reduction as an estimation problem that can be solved using EM [**?**].

See also: PCA, probabilistic model, dimensionality reduction, EM.

probability We assign a probability value, typically chosen in the interval $[0, 1]$, to each event that can occur in a random experiment [6], [7], [**?**], [**?**].

See also: event, random experiment.

probability density function (pdf) The pdf $p(x)$ of a real-valued RV $x \in \mathbb{R}$ is a particular representation of its probability distribution. If the pdf exists, it can be used to compute the probability that x takes on a value from a measurable set $\mathcal{B} \subseteq \mathbb{R}$ via $\mathbb{P}(x \in \mathcal{B}) = \int_{\mathcal{B}} p(x')dx'$ [7, Ch. 3]. If the pdf of a vector-valued RV $\mathbf{x} \in \mathbb{R}^d$ exists, it allows us to compute the probability of $\mathbf{x}$ belonging to a measurable region $\mathcal{R}$ via $\mathbb{P}(\mathbf{x} \in \mathcal{R}) = \int_{\mathcal{R}} p(\mathbf{x}')dx'_1 \ldots dx'_d$ [7, Ch. 3].

See also: RV, probability distribution, probability, measurable, vector.

probability distribution To analyze ML methods, it can be useful to interpret data points as i.i.d. realizations of an RV. The typical properties of such data points are then governed by the probability distribution of this RV. The probability distribution of a binary RV $y \in \{0, 1\}$ is fully specified by the probabilities $\mathbb{P}(y = 0)$ and $\mathbb{P}(y = 1) = 1 - \mathbb{P}(y = 0)$. The probability distribution of a real-valued RV $x \in \mathbb{R}$ might be specified by a pdf $p(x)$ such that $\mathbb{P}(x \in [a, b]) \approx p(a)|b - a|$. In the most general case, a probability distribution is defined by a probability measure [6], [**?**].

See also: i.i.d., realization, RV, probability, pdf.

probability space A probability space is a mathematical structure that allows us to reason about a random experiment, e.g., the observation of a physical phenomenon. Formally, a probability space $\mathcal{P}$ is a triplet $(\Omega, \mathcal{F}, \mathbb{P}(\cdot))$ where

- Ω is a sample space containing all possible outcomes of a random experiment;

- $\mathcal{F}$ is a σ-algebra, i.e., a collection of subsets of Ω (called events) that satisfies certain closure properties under set operations;
- $\mathbb{P}(\cdot)$ is a probability distribution, i.e., a function that assigns a probability $P(\mathcal{A}) \in [0, 1]$ to each event $\mathcal{A} \in \mathcal{F}$. This function must satisfy $\mathbb{P}(\Omega) = 1$ and $\mathbb{P}(\bigcup_{i=1}^{\infty} \mathcal{A}_i) = \sum_{i=1}^{\infty} \mathbb{P}(\mathcal{A}_i)$ for any countable sequence of pairwise disjoint events $\mathcal{A}_1$, $\mathcal{A}_2$, ... in $\mathcal{F}$.

Probability spaces provide the foundation of probabilistic models that can be used to study the behavior of ML methods [6], [?], [?].
See also: probability, random experiment, sample space, event, probability distribution, function, probabilistic model, ML.

projected gradient descent (projected GD) Consider an ERM-based method that uses a parameterized model with parameter space $\mathcal{W} \subseteq \mathbb{R}^d$. Even if the objective function of ERM is smooth, we cannot use basic GD, as it does not take into account constraints on the optimization variable (i.e., the model parameters). Projected GD extends basic GD to address this issue. A single iteration of projected GD consists of first taking a gradient step and then projecting the result back onto the parameter space. See Fig. 62 for a visual illustration.

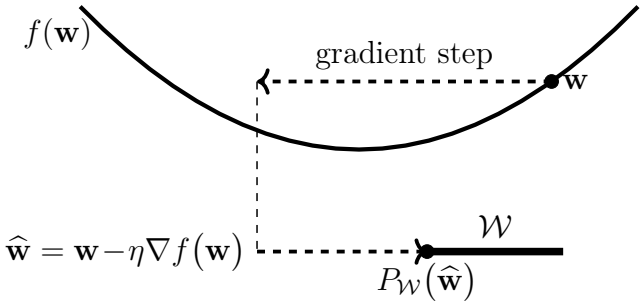


Fig. 62. Projected GD augments a basic gradient step with a projection back onto the constraint set $\mathcal{W}$.

See also: ERM, model, parameter space, objective function, smooth, GD, model parameters, gradient step, projection.

projection Consider a subset $\mathcal{W} \subseteq \mathbb{R}^d$ of the d-dimensional Euclidean space. We define the projection $P_{\mathcal{W}}(\mathbf{w})$ of a vector $\mathbf{w} \in \mathbb{R}^d$ onto $\mathcal{W}$ as

$$P_{\mathcal{W}}(\mathbf{w}) = \operatorname*{arg\,min}_{\mathbf{w}' \in \mathcal{W}} \|\mathbf{w} - \mathbf{w}'\|_2 .$$

In other words, $P_{\mathcal{W}}(\mathbf{w})$ is the vector in $\mathcal{W}$ that is closest to $\mathbf{w}$. The projection is only well defined for subsets $\mathcal{W}$ for which the above minimum exists [**?**].

See also: Euclidean space, vector, minimum.

proximable A convex function for which the proximal operator can be computed efficiently is sometimes referred to as proximable or simple [**?**].

See also: convex, function, proximal operator.

proximal operator Given a convex function $f(\mathbf{w}')$, we define its proximal

operator as [?], [?]

$$\mathbf{prox}_{f(\cdot),\rho}(\mathbf{w}) := \underset{\mathbf{w}' \in \mathbb{R}^d}{\arg\min} \left[f(\mathbf{w}') + \frac{\rho}{2} \|\mathbf{w} - \mathbf{w}'\|_2^2 \right] \text{ with } \rho > 0.$$

As illustrated in Fig. 63, evaluating the proximal operator amounts to minimizing a penalized variant of $f(\mathbf{w}')$. The penalty term is the scaled squared Euclidean distance to a given vector $\mathbf{w}$ (which is the input to the proximal operator). The proximal operator can be interpreted as a generalization of the gradient step, which is defined for a smooth convex function $f(\mathbf{w}')$. Indeed, taking a gradient step with step size η at the current vector $\mathbf{w}$ is the same as applying the proximal operator of the function $\tilde{f}(\mathbf{w}') = \big(\nabla f(\mathbf{w})\big)^T(\mathbf{w}' - \mathbf{w})$ and using $\rho = 1/\eta$.

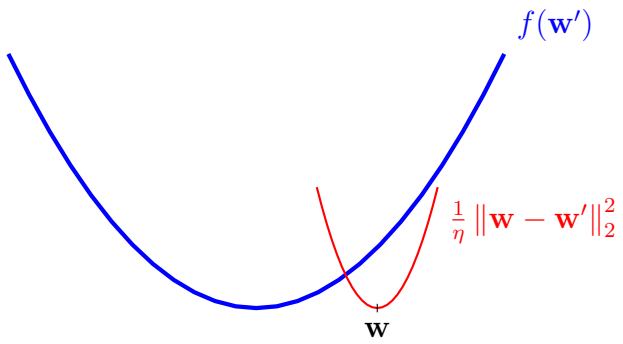


Fig. 63. The proximal operator updates a vector $\mathbf{w}$ by minimizing a penalized version of the function $f(\cdot)$. The penalty term is the scaled squared Euclidean distance between the optimization variable $\mathbf{w}'$ and the given vector $\mathbf{w}$.

See also: convex, function, vector, generalization, gradient step, smooth, step size.

pseudoinverse The Moore–Penrose pseudoinverse $\mathbf{A}^{+}$ of a matrix $\mathbf{A} \in \mathbb{R}^{m \times d}$ generalizes the notion of an inverse matrix [3]. The pseudoinverse arises naturally within ridge regression when applied to a tietoaineisto with arbitrary labels $\mathbf{y}$ and a feature matrix $\mathbf{X} = \mathbf{A}$ [**?**, Ch. 3]. The model parameters learned by ridge regression are given by

$$\widehat{\mathbf{w}}^{(\alpha)} = \left(\mathbf{A}^{T}\mathbf{A} + \alpha \mathbf{I}\right)^{-1} \mathbf{A}^{\top}\mathbf{y}, \quad \alpha > 0.$$

We can then define the pseudoinverse $\mathbf{A}^{+} \in \mathbb{R}^{d \times m}$ via the limit [**?**, Ch. 3]

$$\lim_{\alpha \to 0^{+}} \widehat{\mathbf{w}}^{(\alpha)} = \mathbf{A}^{+}\mathbf{y}.$$

See also: matrix, inverse matrix, ridge regression.

quadratic function A function $f : \mathbb{R}^{d} \to \mathbb{R}$ of the form

$$f(\mathbf{w}) = \mathbf{w}^{T}\mathbf{Q}\mathbf{w} + \mathbf{q}^{T}\mathbf{w} + a$$

with some matrix $\mathbf{Q} \in \mathbb{R}^{d \times d}$, vector $\mathbf{q} \in \mathbb{R}^{d}$, and scalar $a \in \mathbb{R}$.

See also: function, matrix, vector.

Rademacher complexity TBD.

See also: hypothesis space, generalization, ML, effective dimension, VC dimension.

random experiment A random experiment is a physical (or abstract) process that produces an outcome ω from a set of possibilities Ω. This set of all possible outcomes is referred to as the sample space of the

experiment. The key characteristic of a random experiment is that its outcome is unpredictable (or uncertain). Any measurement or observation of the outcome is an RV, i.e., a function of the outcome $\omega \in \Omega$. Probability theory uses a probability space as a mathematical structure for the study of random experiments. A key conceptual property of a random experiment is that it can be repeated under identical conditions. Strictly speaking, repeating a random experiment a given number of m times defines a new random experiment. The outcomes of this new experiment are length-m sequences of outcomes from the original experiment (see Fig. 64). While the outcome of a single experiment is uncertain, the long-run behavior of the outcomes of repeated experiments tends to become increasingly predictable. This informal claim can be made precise via fundamental results of probability theory, such as the law of large numbers and the CLT.

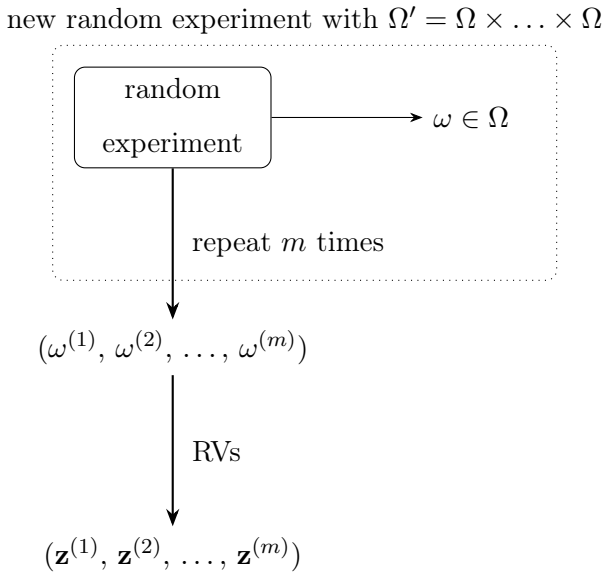


Fig. 64. A random experiment produces an outcome $\omega \in \Omega$ from a set of possibilities (or sample space) *ga*. Repeating the experiment m times yields another random experiment, whose outcomes are sequences $(\omega^{(1)}, \omega^{(2)}, \ldots, \omega^{(m)}) \in \Omega \times \ldots \times \Omega$. One example of a random experiment arising in many ML applications is the gathering of a training set $\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(m)}$.

Examples for random experiments arising in ML applications include the following:

- Data collection: The data points collected in ERM-based methods can be interpreted as RVs, i.e., as functions of the outcome $\omega \in \Omega$ of a random experiment.
- SGD uses a random experiment at each iteration to select a subset of the training set.

- Privacy protection methods use random experiments to generate noise that is added to the outputs of an ML method to ensure DP.

See also: sample space, RV, function, probability, probability space, law of large numbers, CLT, sample space, ML, training set, data, data point, ERM, SGD, privacy protection, DP.

random forest A random forest is a set of different decision trees. Each of these decision trees is obtained by fitting a perturbed copy of the original tietoaineisto.
See also: decision tree, tietoaineisto.

random variable (RV) An RV is a function that maps the outcomes of a random experiment to a value space [6], [**?**]. Mathematically, an RV is a function $x : \Omega \to \mathcal{X}$ that is defined on the sample space Ω of a probability space. Different types of RVs include

- binary RVs, which map each outcome to an element of a binary set (e.g., $\{-1, 1\}$ or $\{\text{cat}, \text{no cat}\}$);
- real-valued RVs, which take on values in the real numbers $\mathbb{R}$;
- vector-valued RVs, which map outcomes to the Euclidean space $\mathbb{R}^d$.

Probability theory uses the concept of measurable spaces to rigorously define and study the properties of collections of RVs [6].
See also: function, random experiment, sample space, probability space, vector, Euclidean space, probability, measurable.

realization Consider an RV $\mathbf{x}$ that maps each outcome $\omega \in \mathcal{P}$ of a probability space $\mathcal{P}$ to an element a of a measurable space $\mathcal{N}$ [2], [6], [?]. A realization of $\mathbf{x}$ is any element $\mathbf{a} \in \mathcal{N}$ such that there exists an element $\omega' \in \mathcal{P}$ with $\mathbf{x}(\omega') = \mathbf{a}$.

See also: RV, probability space, measurable.

rectified linear unit (ReLU) The ReLU is a popular choice for the activation function of a neuron within an ANN. It is defined as $\sigma(z) = \max\{0, z\}$, with z being the weighted input of the artificial neuron.

See also: activation function, ANN.

regression Regression problems revolve around the prediction of a numeric label solely from the features of a data point [8, Ch. 2].

See also: prediction, label, feature, data point.

regret The regret of a hypothesis h relative to another hypothesis h', which serves as a vertailutaso, is the difference between the loss incurred by h and the loss incurred by h' [?]. The vertailutaso hypothesis h' is also referred to as an expert.

See also: vertailutaso, loss, expert.

regularization A key challenge of modern ML applications is that they often use large models, which have an effective dimension in the order of billions. Training a high-dimensional model using basic ERM-based methods is prone to overfitting, i.e., the learned hypothesis performs well on the training set but poorly outside the training set. Regularization refers to modifications of a given instance of ERM in order to avoid overfitting, i.e., to ensure that the learned hypothesis does not

perform much worse outside the training set. There are three routes for implementing regularization:

1) Model pruning: We prune the original model $\mathcal{H}$ to obtain a smaller model $\mathcal{H}'$. For a parametric model, the pruning can be implemented via constraints on the model parameters (such as $w_1 \in [0.4, 0.6]$ for the weight of feature x_1 in linear regression).

2) Loss penalization: We modify the objective function of ERM by adding a penalty term to the training error. The penalty term estimates how much higher the expected loss (or risk) is compared with the average loss on the training set.

3) Data augmentation: We can enlarge the training set $\mathcal{D}$ by adding perturbed copies of the original data points in $\mathcal{D}$. One example for such a perturbation is to add the realization of an RV to the feature vector of a data point.

Fig. 65 illustrates the above three routes to regularization. These routes are closely related and sometimes fully equivalent. Data augmentation using Gaussian RVs to perturb the feature vectors in the training set of linear regression has the same effect as adding the penalty $\lambda \|\mathbf{w}\|_2^2$ to the training error (which is nothing but ridge regression). The decision on which route to use for regularization can be based on the available computational infrastructure. For example, it might be much easier to implement data augmentation than model pruning.

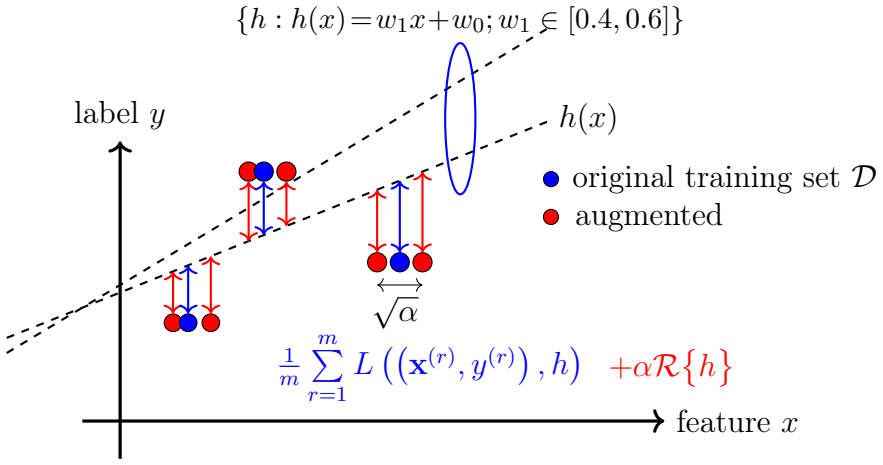


Fig. 65. Three approaches to regularization: 1) data augmentation; 2) loss penalization; and 3) model pruning (via constraints on model parameters).

See also: overfitting, data augmentation, validation, model selection.

regularized empirical risk minimization (RERM) Basic ERM learns a hypothesis (or trains a model) $h \in \mathcal{H}$ based solely on the empirical risk $\widehat{L}\big(h|\mathcal{D}\big)$ incurred on a training set $\mathcal{D}$. To make ERM less prone to overfitting, we can implement regularization by including a (scaled) regularizer $\mathcal{R}\big\{h\big\}$ in the learning objective. This leads to RERM such that

$$\hat{h} \in \arg\min_{h \in \mathcal{H}} \widehat{L}\big(h|\mathcal{D}\big) + \alpha\mathcal{R}\big\{h\big\}. \tag{10}$$

The parameter $\alpha \geq 0$ controls the regularization strength. For $\alpha = 0$, we recover standard ERM without regularization. As α increases, the learned hypothesis is increasingly biased toward small values of $\mathcal{R}\big\{h\big\}$. The component $\alpha\mathcal{R}\big\{h\big\}$ in the objective function of (10) can

be intuitively understood as a surrogate for the increased average loss that may occur when predicting labels for data points outside the training set. This intuition can be made precise in various ways. For example, consider a linear model trained using squared error loss and the regularizer $\mathcal{R}\big\{h\big\} = \|\mathbf{w}\|_2^2$. In this setting, $\alpha\mathcal{R}\big\{h\big\}$ corresponds to the expected increase in loss caused by adding Gaussian RVs to the feature vectors in the training set [8, Ch. 3]. A principled construction for the regularizer $\mathcal{R}\big\{h\big\}$ arises from approximate upper bounds on the generalization error. The resulting RERM instance is known as SRM [**?**, Sec. 7.2].

See also: ERM, regularization, loss, SRM.

regularized loss minimization (RLM) See RERM.

regularizer A regularizer assigns each hypothesis h from a hypothesis space $\mathcal{H}$ a quantitative measure $\mathcal{R}\big\{h\big\}$ conveying to what extent its prediction errors might differ on data points on and outside a training set. Ridge regression uses the regularizer $\mathcal{R}\big\{h\big\} := \|\mathbf{w}\|_2^2$ for linear hypothesis maps $h^{(\mathbf{w})}(\mathbf{x}) := \mathbf{w}^T\mathbf{x}$ [8, Ch. 3]. Lasso uses the regularizer $\mathcal{R}\big\{h\big\} := \|\mathbf{w}\|_1$ for linear hypothesis maps $h^{(\mathbf{w})}(\mathbf{x}) := \mathbf{w}^T\mathbf{x}$ [8, Ch. 3].

See also: ridge regression, Lasso, loss, objective function.

reinforcement learning (RL) RL refers to an online learning setting where we can only evaluate the usefulness of a single hypothesis (i.e., a choice of model parameters) at each time step t. In particular, RL methods apply the current hypothesis $h^{(t)}$ to the feature vector $\mathbf{x}^{(t)}$ of the newly received data point. The usefulness of the resulting prediction $h^{(t)}(\mathbf{x}^{(t)})$

is quantified by a reward signal $r^{(t)}$ (see Fig. 66).

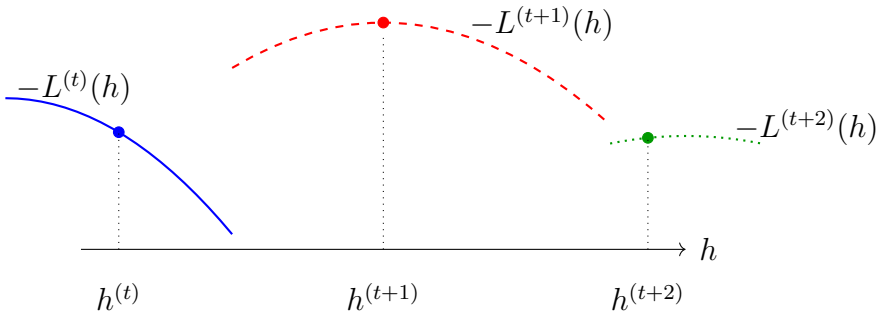


Fig. 66. Three consecutive time steps $t, t+1, t+2$ with corresponding loss functiont $L^{(t)}, L^{(t+1)}, L^{(t+2)}$. During time step t, an RL method can evaluate the loss function only for one specific hypothesis $h^{(t)}$, resulting in the reward signal $r^{(t)} = -L^{(t)}(h^{(t)})$.

In general, the reward depends also on the previous predictions $h^{(t')}\big(\mathbf{x}^{(t')}\big)$ for $t' < t$. The goal of RL is to learn $h^{(t)}$, for each time step t, such that the (possibly discounted) cumulative reward is maximized [8], [**?**].

See also: reward, loss function, ML.

Rényi divergence The Rényi divergence measures the (dis)similarity between two probability distributions [**?**].

See also: probability distribution.

reward A reward refers to some observed (or measured) quantity that allows us to estimate the loss incurred by the prediction (or decision) of a hypothesis $h(\mathbf{x})$. For example, in an ML application to self-driving vehicles, $h(\mathbf{x})$ could represent the current steering direction of a vehicle.

We could construct a reward from the measurements of a collision sensor that indicate if the vehicle is moving toward an obstacle. We define a low reward for the steering direction $h(\mathbf{x})$ if the vehicle moves dangerously toward an obstacle.

See also: loss, MAB, RL.

ridge regression Consider a regression problem where the goal is to learn a hypothesis $h^{(\mathbf{w})}$ for predicting the numeric label of a data point based on its feature vector. Ridge regression learns the parameters $\mathbf{w}$ by minimizing the penalized average squared error loss. The average squared error loss is measured on a set of labeled data points (i.e., the training set)

$$\left(\mathbf{x}^{(1)}, y^{(1)}\right), \ldots, \left(\mathbf{x}^{(m)}, y^{(m)}\right).$$

The penalty term is the scaled squared Euclidean norm $\alpha\|\mathbf{w}\|_2^2$ with a regularization parameter $\alpha > 0$. The purpose of the penalty term is regularization, i.e., to prevent overfitting in the high-dimensional regime, where the number of features d exceeds the number of data points m in the training set. Adding $\alpha\|\mathbf{w}\|_2^2$ to the average squared error loss is equivalent to computing the average squared error loss on an augmented training set. This augmented training set is obtained by replacing each data point $\left(\mathbf{x}^{(r)}, y^{(r)}\right)$ in the original training set by the realization of infinitely many i.i.d. RVs whose probability distribution is centered at $\left(\mathbf{x}^{(r)}, y^{(r)}\right)$.

See also: regression, regularization, map, data augmentation.

risk Consider a hypothesis h used to predict the label y of a data point based

on its features $\mathbf{x}$. We measure the quality of a particular prediction using a loss function $L\left((\mathbf{x}, y), h\right)$. If we interpret data points as the realizations of i.i.d. RVs, the $L\left((\mathbf{x}, y), h\right)$ also becomes the realization of an RV. The i.i.d. assumption allows us to define the risk of a hypothesis as the expected loss $\mathbb{E}\big\{L\left((\mathbf{x}, y), h\right)\big\}$. Note that the risk of h depends on both the specific choice for the loss function and the probability distribution of the data points.

See also: hypothesis, label, data point, feature, prediction, loss function, realization, i.i.d. RV, i.i.d. assumption, loss, probability distribution.

robustness Robustness is a key requirement for trustworthy AI. It refers to the property of an ML system to maintain acceptable performance even when subjected to different forms of perturbations. These perturbations may affect the features of a data point in order to manipulate the prediction delivered by a trained ML model. Robustness also includes the stability of ERM-based methods against perturbations of the training set. Such perturbations can occur within data poisoning attacks.

See also: trustworthy AI,stability,data poisoning, attack.

sample In the context of ML, a sample is a finite sequence (of length m) of data points, $\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(m)}$. The number m is called the sample size. ERM-based methods use a sample to train a model (or learn a hypothesis) by minimizing the average loss (the empirical risk) over that sample. Since a sample is defined as a sequence, the same data point may appear more than once. By contrast, some authors in statistics define a sample as a set of data points, in which case duplicates are not

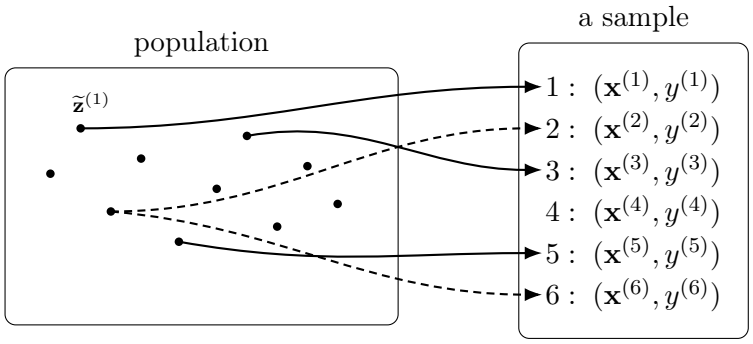


Fig. 67. Illustration of a sample as a finite sequence. Each sequence element consists of the feature vector and the label of some data point which belongs to an underlying population. Depending on the application, the same data point is used to obtain multiple sample elements.

allowed [**?**,**?**]. These two views can be reconciled by regarding a sample as a sequence of feature–label pairs, $\left(\mathbf{x}^{(1)}, y^{(1)}\right), \ldots, \left(\mathbf{x}^{(m)}, y^{(m)}\right)$. The r-th pair consists of the features $\mathbf{x}^{(r)}$ and the label $y^{(r)}$ of an unique underlying data point $\widetilde{\mathbf{z}}^{(r)}$. While the underlying data points $\widetilde{\mathbf{z}}^{(1)}, \ldots, \widetilde{\mathbf{z}}^{(m)}$ are unique, some of them can have identical features and labels. For the analysis of ML methods, it is common to interpret a sample as the realization of a stochastic process indexed by $\{1, \ldots, m\}$. A widely used assumption is the i.i.d. assumption, where sample elements $\left(\mathbf{x}^{(r)}, y^{(r)}\right)$, for $r = 1, \ldots, m$, are i.i.d. RVs with common probability distribution $p(\mathbf{x}, y)$.

See also: data point, realization, i.i.d., RV, probability distribution, sample size, ERM.

sample covariance matrix The sample kovarianssimatriisi $\widehat{\mathbf{\Sigma}} \in \mathbb{R}^{d \times d}$ for a

given set of feature vectors $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)} \in \mathbb{R}^d$ is defined as

$$\widehat{\mathbf{\Sigma}} = \frac{1}{m} \sum_{r=1}^{m} (\mathbf{x}^{(r)} - \widehat{\mathbf{m}})(\mathbf{x}^{(r)} - \widehat{\mathbf{m}})^T.$$

Here, we use the sample mean $\widehat{\mathbf{m}}$.

See also: sample, kovarianssimatriisi, feature vector, sample mean.

sample mean The sample mean $\mathbf{m} \in \mathbb{R}^d$ for a given tietoaineisto, with feature vectors $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)} \in \mathbb{R}^d$, is defined as

$$\mathbf{m} = \frac{1}{m} \sum_{r=1}^{m} \mathbf{x}^{(r)}.$$

See also: sample, mean, tietoaineisto, feature vector.

sample size The number of individual data points contained in a sample.

See also: data point, tietoaineisto.

sample space A sample space is the set of all possible outcomes of a random experiment [6], [7], [**?**], [**?**].

See also: probability space.

scatterplot A visualization technique that depicts data points using markers in a 2-D plane. Fig. 68 depicts an example of a scatterplot.

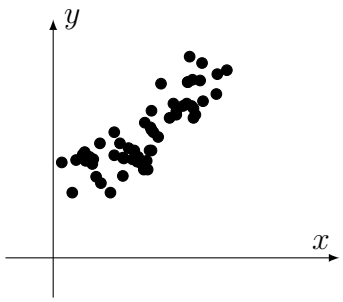


Fig. 68. A scatterplot with circle markers, where the data points represent daily weather conditions in Finland. Each data point is characterized by its minimum daytime temperature x as the feature and its maximum daytime temperature y as the label. The temperatures have been measured at the FMI weather station Helsinki Kaisaniemi during 1 September 2024—28 October 2024.

A scatterplot can enable the visual inspection of data points that are naturally represented by feature vectors in high-dimensional spaces.

See also: data point, minimum, feature, maximum, label, FMI, feature vector, dimensionality reduction.

semi-supervised learning (SSL) SSL methods use unlabeled data points to support the learning of a hypothesis from labeled data points [**?**]. This approach is particularly useful for ML applications that offer a large number of unlabeled data points, but only a limited number of labeled data points.

See also: data point, hypothesis, labeled data point, ML.

sensitive attribute ML revolves around learning a hypothesis map that allows us to predict the label of a data point from its features. In some

applications, we must ensure that the output delivered by an ML system does not allow us to infer sensitive attributes of a data point. Which part of a data point is considered a sensitive attribute is a design choice that varies across different application domains.

See also: ML, hypothesis, map, label, data point, feature.

similarity graph Some ML applications generate data points that are related by a domain-specific notion of similarity. These similarities can be represented conveniently using a similarity graph $\mathcal{G} = \big(\mathcal{V} := \{1, \ldots, m\}, \mathcal{E}\big)$. The node $r \in \mathcal{V}$ represents the rth data point. Two nodes are connected by an undirected edge if the corresponding data points are similar.

See also: ML, data point, graph.

singular value decomposition (SVD) The SVD for a matrix $\mathbf{A} \in \mathbb{R}^{m \times d}$ is a factorization of the form

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

with orthonormal matrices $\mathbf{V} \in \mathbb{R}^{m \times m}$ and $\mathbf{U} \in \mathbb{R}^{d \times d}$ [3]. The matrix $\mathbf{\Lambda} \in \mathbb{R}^{m \times d}$ is only nonzero along the main diagonal, whose entries $\Lambda_{j,j}$ are nonnegative and referred to as singular values.

See also: matrix.

smooth A real-valued function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is smooth if it is differentiable and its gradient $\nabla f(\mathbf{w})$ is continuous at all $\mathbf{w} \in \mathbb{R}^d$ [?], [?]. A smooth function f is referred to as β-smooth if the gradient $\nabla f(\mathbf{w})$ is Lipschitz

continuous with Lipschitz constant β, i.e.,

$$\|\nabla f(\mathbf{w}) - \nabla f(\mathbf{w}')\| \leq \beta \|\mathbf{w} - \mathbf{w}'\|, \text{ for any } \mathbf{w}, \mathbf{w}' \in \mathbb{R}^d.$$

The constant β quantifies the smoothness of the function f: the smaller the β, the smoother f is. Optimization problems with a smooth objective function can be solved effectively by gradient-based methods. Indeed, gradient-based methods approximate the objective function locally around a current choice $\mathbf{w}$ using its gradient. This approximation works well if the gradient does not change too rapidly. We can make this informal claim precise by studying the effect of a single gradient step with step size $\eta = 1/\beta$ (see Fig. 69).

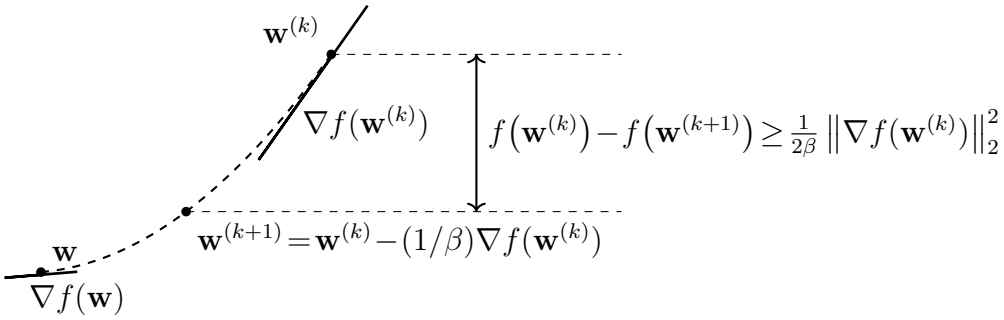


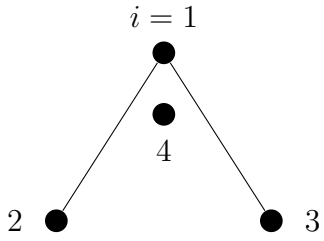
Fig. 69. Consider an objective function $f(\mathbf{w})$ that is β-smooth. Taking a gradient step, with step size $\eta = 1/\beta$, decreases the objective by at least $1/2\beta \left\|\nabla f(\mathbf{w}^{(k)})\right\|_2^2$ [?], [?], [?]. Note that the step size $\eta = 1/\beta$ becomes larger for smaller β. Thus, for smoother objective functions (i.e., those with smaller β), we can take larger steps.

See also: function, differentiable, gradient, gradient-based methods.

soft clustering Soft klusterointi refers to the task of partitioning a given set of data points into (a few) overlapping ryppäät. Each data point is assigned to several different ryppäät with varying degrees of belonging. Soft klusterointi methods determine the degree of belonging (or soft rypäs assignment) for each data point and each rypäs. A principled approach to soft klusterointi is by interpreting data points as i.i.d. realizations of a GMM. The conditional probability of a data point belonging to a specific mixture component is then a natural choice for the degree of belonging.

See also: klusterointi, data point, rypäs, degree of belonging, i.i.d., realization, GMM, probability.

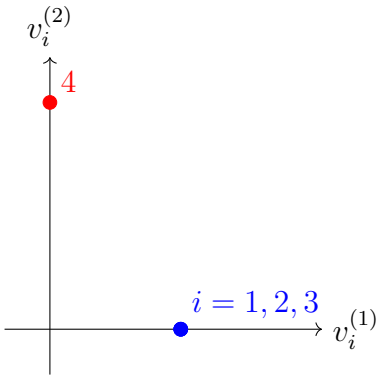
spectral clustering Spectral klusterointi is a particular instance of graph clustering, i.e., it clusters data points represented as the nodes $i = 1, \ldots, n$ of a graph $\mathcal{G}$. Spectral klusterointi uses the eigenvectors of the Laplacian matrix $\mathbf{L}^{(\mathcal{G})}$ to construct feature vectors $\mathbf{x}^{(i)} \in \mathbb{R}^d$ for each node (i.e., for each data point) $i = 1, \ldots, n$. We can feed these feature vectors into Euclidean space-based klusterointi methods, such as k-means or soft clustering via GMM. Roughly speaking, the feature vectors of nodes belonging to a well-connected subset (or rypäs) of nodes in $\mathcal{G}$ are located nearby in the Euclidean space $\mathbb{R}^d$ (see Fig. 70).



(a)

$$\mathbf{L}^{(\mathcal{G})} = \begin{pmatrix} 2 & -1 & -1 & 0 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$$

(b)



(c)

$$\mathbf{V} = \left(\mathbf{v}^{(1)}, \mathbf{v}^{(2)}, \mathbf{v}^{(3)}, \mathbf{v}^{(4)}\right)$$

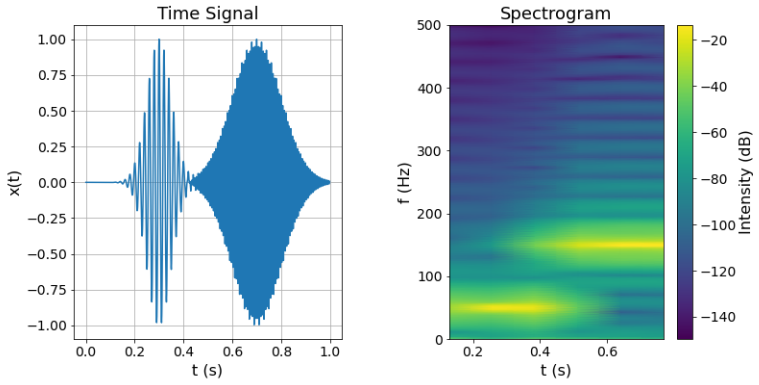
$$\mathbf{v}^{(1)} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 0 \end{pmatrix}, \; \mathbf{v}^{(2)} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

(d)

Fig. 70. (a) An undirected graph $\mathcal{G}$ with four nodes $i = 1, 2, 3, 4$, each representing a data point. (b) The Laplacian matrix $\mathbf{L}^{(\mathcal{G})} \in \mathbb{R}^{4\times 4}$ and its EVD. (c) A scatterplot of data points using the feature vectors $\mathbf{x}^{(i)} = \left(v_i^{(1)}, v_i^{(2)}\right)^T$. (d) Two eigenvectors $\mathbf{v}^{(1)}, \mathbf{v}^{(2)} \in \mathbb{R}^d$ corresponding to the eigenvalue $\lambda = 0$ of the Laplacian matrix $\mathbf{L}^{(\mathcal{G})}$.

See also: klusterointi, graph clustering, Laplacian matrix, eigenvalue.

spectrogram A spectrogram represents the time-frequency distribution of the energy of a time signal $x(t)$. Intuitively, it quantifies the amount of signal energy present within a specific time segment $[t_1, t_2] \subseteq \mathbb{R}$ and frequency interval $[f_1, f_2] \subseteq \mathbb{R}$. Formally, the spectrogram of a signal is defined as the squared magnitude of its short-time Fourier transform (STFT) [**?**]. Fig. 71 depicts a time signal along with its spectrogram.



(a) (b)

Fig. 71. (a) A time signal consisting of two modulated Gaussian pulses. (b) An intensity plot of the spectrogram.

The intensity plot of its spectrogram can serve as an image of a signal. A simple recipe for audio signal luokittelu is to feed this signal image into deep nets originally developed for image luokittelu and object detection [**?**]. It is worth noting that, beyond the spectrogram, several alternative representations exist for the time-frequency distribution of signal energy [**?**], [**?**].

See also: luokittelu, deep net.

squared error loss The squared error loss measures the prediction error of a hypothesis h when predicting a numeric label $y \in \mathbb{R}$ from the features $\mathbf{x}$ of a data point. It is defined as

$$L\left((\mathbf{x}, y), h\right) := \big(y - \underbrace{h(\mathbf{x})}_{=\hat{y}}\big)^2.$$

See also: loss, prediction, hypothesis, label, feature, data point.

stability Stability is a desirable property of an ML method $\mathcal{A}$ that maps a tietoaineisto $\mathcal{D}$ (e.g., a training set) to an output $\mathcal{A}(\mathcal{D})$. The output $\mathcal{A}(\mathcal{D})$ can be the learned model parameters or the prediction delivered by the trained model for a specific data point. Intuitively, $\mathcal{A}$ is stable if small changes in the input tietoaineisto $\mathcal{D}$ lead to small changes in the output $\mathcal{A}(\mathcal{D})$. Several formal notions of stability exist that enable bounds on the generalization error or risk of the method (see [**?**, Ch. 13]). To build intuition, consider the three tietoaineistot depicted in Fig. 72, each of which is equally likely under the same data-generating probability distribution. Since the optimal model parameters are determined by this underlying probability distribution, an accurate ML method $\mathcal{A}$ should return the same (or very similar) output $\mathcal{A}(\mathcal{D})$ for all three tietoaineistot. In other words, any useful $\mathcal{A}$ must be robust to variability in sample realizations from the same probability distribution, i.e., it must be stable.

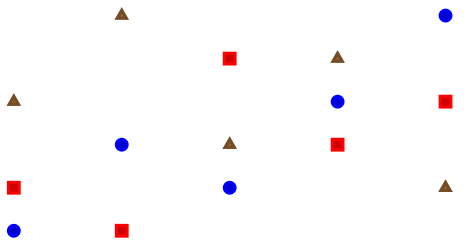


Fig. 72. Three tietoaineistot $\mathcal{D}^{(*)}$, $\mathcal{D}^{(\square)}$, and $\mathcal{D}^{(\triangle)}$, each sampled independently from the same data-generating probability distribution. A stable ML method should return similar outputs when trained on any of these tietoaineistot.

See also: ML, tietoaineisto, training set, model parameters, prediction, model, data point, generalization, risk, data, probability distribution, sample, realization.

standard normal vector A standard normal vector is a random vector $\mathbf{x} = \big(x_1, \ldots, x_d\big)^T$ whose entries are i.i.d. Gaussian RVs $x_j \sim \mathcal{N}(0,1)$. It is a special case of a multivariate normal distribution, $\mathbf{x} \sim (\mathbf{0}, \mathbf{I})$.

See also: vector, i.i.d., Gaussian RV, multivariate normal distribution, RV.

statistical aspects By statistical aspects of an ML method, we refer to (properties of) the probability distribution of its output under a probabilistic model for the data fed into the method.

See also: ML, probability distribution, probabilistic model, data.

step size See learning rate.

stochastic We refer to a method as stochastic if it involves a random component or is governed by probabilistic laws. ML methods use randomness to reduce computational complexity (e.g., see SGD) or to capture uncertainty in probabilistic models.

See also: SGD, uncertainty, probabilistic model.

stochastic algorithm A stochastic algorithm uses a random mechanism during its execution. For example, SGD uses a randomly selected subset of data points to compute an approximation for the gradient of an objective function. We can represent a stochastic algorithm by a stochastic processes, i.e., the possible execution sequence is the possible outcomes of a random experiment [7], [?], [?].

See also: stochastic, algorithm, SGD, data point, gradient, objective function, stochastic process, random experiment, optimization method, gradient-based methods.

stochastic block model (SBM) The SBM is a probabilistic generative model for an undirected graph $\mathcal{G} = \big(\mathcal{V}, \mathcal{E}\big)$ with a given set of nodes $\mathcal{V}$ [?]. In its most basic variant, the SBM generates a graph by first randomly assigning each node $i \in \mathcal{V}$ to a rypäs index $c_i \in \{1, \ldots, k\}$. A pair of different nodes in the graph is connected by an edge with probability $p_{i,i'}$ that depends solely on the labels $c_i, c_{i'}$. The presence of edges between different pairs of nodes is statistically independent.

See also: model, graph, rypäs, probability, label.

stochastic gradient descent (SGD) SGD is obtained from GD by replacing

the gradient of the objective function with a stochastic approximation. A main application of SGD is to train a parameterized model via ERM on a training set $\mathcal{D}$ that is either very large or not readily available (e.g., when data points are stored in a database distributed globally). To evaluate the gradient of the empirical risk (as a function of the model parameters $\mathbf{w}$), we need to compute a sum $\sum_{r=1}^{m} \nabla_{\mathbf{w}} L\left(\mathbf{z}^{(r)}, \mathbf{w}\right)$ over all data points in the training set. We obtain a stochastic approximation to the gradient by replacing the sum $\sum_{r=1}^{m} \nabla_{\mathbf{w}} L\left(\mathbf{z}^{(r)}, \mathbf{w}\right)$ with a sum $\sum_{r \in \mathcal{B}} \nabla_{\mathbf{w}} L\left(\mathbf{z}^{(r)}, \mathbf{w}\right)$ over a randomly chosen subset $\mathcal{B} \subseteq \{1, \ldots, m\}$ (see Fig. 73). We often refer to these randomly chosen data points as a batch. The batch size $|\mathcal{B}|$ is an important parameter of SGD. SGD with $|\mathcal{B}| > 1$ is referred to as mini-batch SGD [**?**].

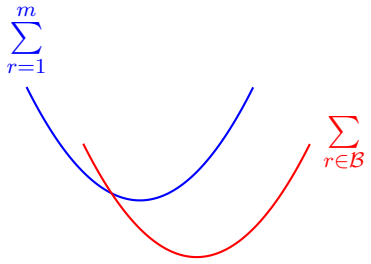


Fig. 73. SGD for ERM approximates the gradient by replacing the sum $\sum_{r=1}^{m} \nabla_{\mathbf{w}} L\left(\mathbf{z}^{(r)}, \mathbf{w}\right)$ over all data points in the training set (indexed by $r = 1, \ldots, m$) with a sum over a randomly chosen subset $\mathcal{B} \subseteq \{1, \ldots, m\}$.

See also: GD, gradient, objective function, stochastic, model, ERM, training set, data point, empirical risk, function, model parameters, batch, parameter.

stopping criterion Many ML methods use iterative algoritmit that construct a sequence of model parameters in order to minimize the training error. For example, gradient-based methods iteratively update the parameters of a parametric model, such as a linear model or a deep net. Given a finite amount of computational resources, we need to stop updating the parameters after a finite number of iterations. A stopping criterion is any well-defined condition for deciding when to stop updating.

See also: algorithm, gradient-based methods.

strongly convex A continuously differentiable real-valued function $f(\mathbf{x})$ is strongly convex with coefficient σ if $f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^{T}(\mathbf{y}-\mathbf{x}) + (\sigma/2)\left\|\mathbf{y}-\mathbf{x}\right\|_{2}^{2}$ [?], [?, Sec. B.1.1].

See also: differentiable, function, convex.

structural risk minimization (SRM) SRM is an instance of RERM, with which the model $\mathcal{H}$ can be expressed as a countable union of submodels such that $\mathcal{H} = \bigcup_{n=1}^{\infty} \mathcal{H}^{(n)}$. Each submodel $\mathcal{H}^{(n)}$ permits the derivation of an approximate upper bound on the generalization error incurred when applying ERM to train $\mathcal{H}^{(n)}$. These individual bounds—one for each submodel—are then combined to form a regularizer used in the RERM objective. These approximate upper bounds (one for each $\mathcal{H}^{(n)}$) are then combined to construct a regularizer for RERM [?, Sec. 7.2].

See also: RERM, model, generalization, ERM, regularizer, risk.

subgradient For a real-valued function $f : \mathbb{R}^{d} \rightarrow \mathbb{R} : \mathbf{w} \mapsto f(\mathbf{w})$, a vector $\mathbf{a}$ such that $f(\mathbf{w}) \geq f(\mathbf{w}') + \left(\mathbf{w}-\mathbf{w}'\right)^{T}\mathbf{a}$ is referred to as a subgradient

of f at $\mathbf{w}'$ [?], [?].

See also: function, vector.

subgradient descent Subgradient descent is a generalization of GD that does not require differentiability of the function to be minimized. This generalization is obtained by replacing the concept of a gradient with that of a subgradient. Similar to gradients, subgradients allow us to construct local approximations of an objective function. The objective function might be the empirical risk $\widehat{L}\big(h^{(\mathbf{w})}\big|\mathcal{D}\big)$ viewed as a function of the model parameters $\mathbf{w}$ that select a hypothesis $h^{(\mathbf{w})} \in \mathcal{H}$.

See also: subgradient, generalization, GD, function, gradient, objective function, empirical risk, model parameters, hypothesis.

support vector machine (SVM) The SVM is a binary luokittelu method that learns a linear hypothesis map. Thus, like linear regression and logistic regression, it is also an instance of ERM for the linear model. However, the SVM uses a different loss function from the one used in those methods. As illustrated in Fig. 74, it aims to maximally separate data points from the two different classes in the feature space (i.e., maximum margin principle). Maximizing this separation is equivalent to minimizing a regularized variant of the hinge loss (7) [?], [?], [?].

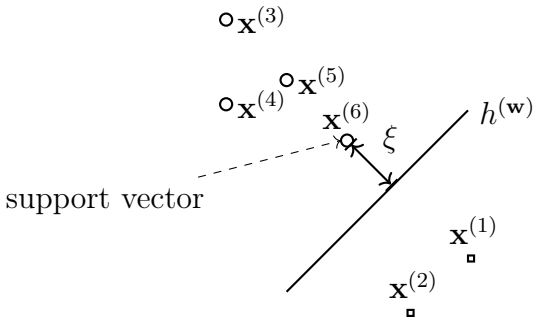


Fig. 74. The SVM learns a hypothesis (or luokitin) $h^{(\mathbf{w})}$ with minimal average soft-margin hinge loss. Minimizing this loss is equivalent to maximizing the margin ξ between the decision boundary of $h^{(\mathbf{w})}$ and each class of the training set.

The above basic variant of SVM is only useful if the data points from different categories can be (approximately) linearly separated. For an ML application where the categories are not derived from a kernel.
See also: luokittelu, linear model, luokitin, hinge loss.

supremum (or least upper bound) The supremum of a set of real numbers is the smallest number that is greater than or equal to every element in the set. More formally, a real number a is the supremum of a set $\mathcal{A} \subseteq \mathbb{R}$ if: 1) a is an upper bound of $\mathcal{A}$; and 2) no number smaller than a is an upper bound of $\mathcal{A}$. Every non-empty set of real numbers that is bounded above has a supremum, even if it does not contain its supremum as an element [2, Sec. 1.4].

tarkkuus Consider data points characterized by features $\mathbf{x} \in \mathcal{X}$ and a

categorical label y that takes on values from a finite label space $\mathcal{Y}$. The accuracy of a hypothesis $h : \mathcal{X} \to \mathcal{Y}$, when applied to the data points in a tietoaineisto $\mathcal{D} = \big\{\big(\mathbf{x}^{(1)}, y^{(1)}\big), \ldots, \big(\mathbf{x}^{(m)}, y^{(m)}\big)\big\}$, is then defined as $1 - (1/m) \sum_{r=1}^{m} L^{(0/1)} \big(\big(\mathbf{x}^{(r)}, y^{(r)}\big), h\big)$ using the 0/1 loss $L^{(0/1)}(\cdot, \cdot)$.
See also: 0/1 loss, loss, metric.

test set A set of data points that have been used neither to train a model (e.g., via ERM) nor to choose between different models in a validation set.
See also: data point, model, ERM, validation set.

total variation See GTV.

training In the context of ML, training refers to the process of learning a useful hypothesis $\hat{h}$ out of a model $\mathcal{H}$. The training of a model $\mathcal{H}$ is guided by the loss incurred on a set of data points, which serve as the training set. For parametric models, where each hypothesis $h^{(\mathbf{w})}$ is characterized by a specific choice for the model parameters, training amounts to finding an optimal choice for the model parameterst $\mathbf{w}$. A widely-used approach to training is ERM, which learns a hypothesis by minimizing the average loss incurred on a training set. One of the main challenges in ML is to control the discrepancy between the loss incurred on the training set and the loss incurred on other (unseen) data points.
See also: ERM, loss, model.

training error The average loss of a hypothesis when predicting the labels of the data points in a training set. We sometimes also refer to training

error as the minimal average loss that is achieved by a solution of ERM.

See also: loss, hypothesis, label, data point, training set, ERM.

training set A training set is a tietoaineisto $\mathcal{D}$ that consists of some data points used in ERM to learn a hypothesis $\hat{h}$. The average loss of $\hat{h}$ on the training set is referred to as the training error. The comparison of the training error with the validation error of $\hat{h}$ allows us to diagnose the ML method and informs how to improve the validation error (e.g., using a different hypothesis space or collecting more data points) [8, Sec. 6.6].

See also: tietoaineisto, data point, ERM, hypothesis, loss, training error, validation error, ML, hypothesis space.

transfer learning Transfer learning aims at leveraging information obtained while solving an existing learning task to solve another learning task.

See also: learning task, multitask learning

transparency Transparency is a fundamental requirement for trustworthy AI [**?**]. In the context of ML methods, transparency is often used interchangeably with explainability [**?**], [**?**]. However, in the broader scope of AI systems, transparency extends beyond explainability and includes providing information about the system's limitations, reliability, and intended use. In medical diagnosis systems, transparency requires disclosing the confidence level for the predictions delivered by a trained model. In credit scoring, AI-based lending decisions should be accompanied by explanations of contributing factors, such as income level or credit history. These explanations allow humans (e.g., a loan

applicant) to understand and contest automated decisions. Some ML methods inherently offer transparency. For example, logistic regression provides a quantitative measure of luokittelu reliability through the value $|h(\mathbf{x})|$. Decision trees are another example, as they allow human-readable decision rules [**?**]. Transparency also requires a clear indication when a user is engaging with an AI system. For example, AI-powered chatbots should notify users that they are interacting with an automated system rather than a human. Furthermore, transparency encompasses comprehensive documentation detailing the purpose and design choices underlying the AI system. For instance, model datasheets [**?**] and AI system cards [**?**] help practitioners understand the intended use cases and limitations of an AI system [**?**].

See also: trustworthy AI, explainability.

trustworthy artificial intelligence (trustworthy AI) Besides the computational aspects and statistical aspects, a third main design aspect of ML methods is their trustworthiness [**?**]. The EU has put forward seven key requirements (KRs) for trustworthy AI (which typically build on ML methods) [**?**]:

1) KR1 – Human agency and oversight;
2) KR2 – Technical robustness and safety;
3) KR3 – Privacy and data governance;
4) KR4 – Transparency;
5) KR5 – Diversity, non-discrimination and fairness;
6) KR6 – Societal and environmental well-being;

7) KR7 – Accountability.

See also: computational aspects, statistical aspects, ML, AI, robustness, data, transparency.

uncertainty In the context of ML, uncertainty refers to the presence of multiple plausible outcomes or explanations based on available data. For example, the prediction $\hat{h}(\mathbf{x})$ produced by a trained ML model $\hat{h}$ often reflects a range of possible values for the true label of a given data point. The broader this range, the greater the associated uncertainty. Probability theory allows us to represent, quantify, and reason about uncertainty in a mathematically rigorous manner.

See also: probabilistic model, risk, entropy, variance.

underfitting Consider an ML method that uses ERM to learn a hypothesis with the minimum empirical risk on a given training set. Such a method is underfitting the training set if it is not able to learn a hypothesis with a sufficiently low empirical risk on the training set. If a method is underfitting, it will typically also not be able to learn a hypothesis with a low risk.

See also: ML, ERM, hypothesis, minimum, empirical risk, training set, risk.

upper confidence bound (UCB) Consider an ML application that requires selecting, at each time step k, an action a_k from a finite set of alternatives $\mathcal{A}$. The utility of selecting action a_k is quantified by a numeric reward signal $r^{(a_k)}$. A widely used probabilistic model for this type

of sequential decision-making problem is the stochastic MAB setting [**?**]. In this model, the reward $r^{(a)}$ is viewed as the realization of an RV with unknown mean $\mu^{(a)}$. Ideally, we would always choose the action with the largest expected reward $\mu^{(a)}$, but these means are unknown and must be estimated from observed data. Simply choosing the action with the largest estimate $\widehat{\mu}^{(a)}$ can lead to suboptimal outcomes due to estimation uncertainty. The UCB strategy addresses this by selecting actions not only based on their estimated means but also by incorporating a term that reflects the uncertainty in these estimates—favoring actions with a high-potential reward and high uncertainty. Theoretical guarantees for the performance of UCB strategies, including logarithmic regret bounds, are established in [**?**].

See also: ML, reward, probabilistic model, stochastic, MAB, model, realization, RV, mean, data, uncertainty, regret.

validation Consider a hypothesis $\hat{h}$ that has been learned via some ML method, e.g., by solving ERM on a training set $\mathcal{D}$. Validation refers to the process of evaluating the loss incurred by the hypothesis $\hat{h}$ on a set of data points that are not contained in the training set $\mathcal{D}$. This set of data points is called the validation set. The average loss of $\hat{h}$ on the validation set is referred to as the validation error.

See also: training set, overfitting, generalization, validation error, validation set.

validation error Consider a hypothesis $\hat{h}$ that is obtained by some ML method, e.g., using ERM on a training set. The average loss of $\hat{h}$ on a

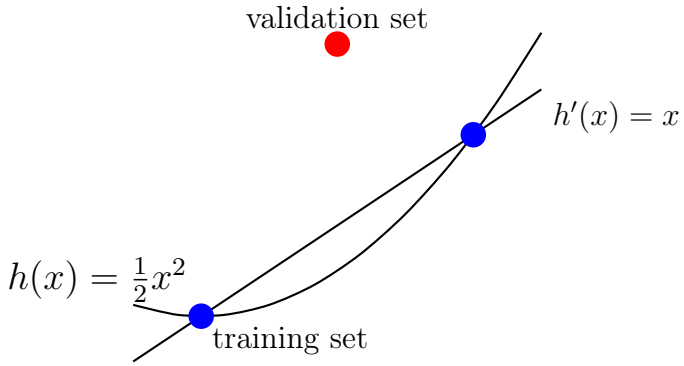


Fig. 75. Illustration of validation. The blue points represent the data points in the training set, while the red point represents a data point in the validation set. The hypothesis $\hat{h}$ (black curve) fits the data points in the training set perfectly, but incurs a large loss on the data point in the validation set.

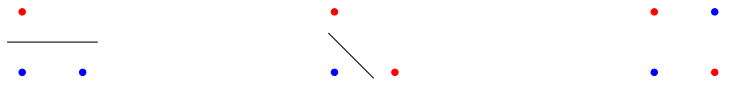
validation set, which is different from the training set, is referred to as the validation error.

See also: hypothesis, ML, ERM, training set, loss, validation set, validation.

validation set A set of data points used to estimate the risk of a hypothesis $\hat{h}$ that has been learned by some ML method (e.g., solving ERM). The average loss of $\hat{h}$ on the validation set is referred to as the validation error and can be used to diagnose an ML method (see [8, Sec. 6.6]). The comparison between training error and validation error can inform directions for the improvement of the ML method (such as using a different hypothesis space).

See also: data point, risk, hypothesis, ML, ERM, loss, validation, validation error, training error, hypothesis space.

Vapnik–Chervonenkis dimension (VC dimension) The statistical properties of an ERM-based method depends critically on the expressive capacity of its hypothesis space (or model) $\mathcal{H}$. A standard measure of this capacity is the VC dimension $\text{VCdim}(\mathcal{H})$ [**?**]. Formally, it is the largest integer m such that there exists a tietoaineisto $\mathcal{D} = \mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)} \subseteq \mathcal{X}$ that can be perfectly classified (or shattered) by some $h \in \mathcal{H}$. In particular, for every one of the 2^m possible assignments of binary labels to each feature vector in $\mathcal{D}$, there exists some hypothesis $h \in \mathcal{H}$ that realizes this labeling. Intuitively, the VC dimension quantifies how well $\mathcal{H}$ can fit arbitrary label assignments, and thus captures its approximate power. It plays a central role in deriving bounds on the generalization gap. Fig. 76 illustrates the definition of the VC dimension for a linear model $\mathcal{H}^{(2)}$ with $d = 2$ features. Fig. 76(a) and 76(b) show the same set of three noncollinear feature vectors under two different binary labelings. In both cases, a separating hyperplane exists that realizes the labeling. Since this holds for all $2^3 = 8$ possible binary labelings of the three feature vectors, the set is shattered. Fig. 76(c) depicts four feature vectors with a specific labeling. No linear separator can correctly classify all data points in this case. Thus, $\text{VCdim}\left(\mathcal{H}^{(2)}\right) = 3$.



(a) (b) (c)

Fig. 76. Illustration of the VC dimension for a linear model $\mathcal{H}^{(2)}$ that is used to learn a linear classifier in the feature space $\mathbb{R}^2$.

More generally, for a linear model $\mathcal{H}^{(d)}$, the VC dimension equals $d+1$. In other words, for linear models, the VC dimension essentially matches the dimension of the underlying feature space $\mathbb{R}^d$. For more complex hypothesis spaces, such as decision trees or neuroverkot, the relation between VC dimension and the dimension of the feature space is far less direct. In these cases, alternative complexity measures, such as the Rademacher complexity, can be more useful for analyzing ERM-based methods.

See also: hypothesis space, Rademacher complexity, generalization, ML, effective dimension.

variance The variance of a real-valued RV x is defined as the expectation $\mathbb{E}\big\{\big(x-\mathbb{E}\{x\}\big)^2\big\}$ of the squared difference between x and its expectation $\mathbb{E}\{x\}$. We extend this definition to vector-valued RVs $\mathbf{x}$ as $\mathbb{E}\big\{\big\|\mathbf{x}-\mathbb{E}\{\mathbf{x}\}\big\|_2^2\big\}$.

See also: RV, expectation, vector.

vertical federated learning (VFL) VFL refers to FL applications where devices have access to different features of the same set of data points [**?**].

Formally, the underlying global tietoaineisto is

$$\mathcal{D}^{(\text{global})} := \left\{ \left(\mathbf{x}^{(1)}, y^{(1)}\right), \ldots, \left(\mathbf{x}^{(m)}, y^{(m)}\right) \right\}.$$

We denote by $\mathbf{x}^{(r)} = \left(x_1^{(r)}, \ldots, x_{d'}^{(r)}\right)^T$, for $r = 1, \ldots, m$, the complete feature vectors for the data points. Each device $i \in \mathcal{V}$ observes only a subset $\mathcal{F}^{(i)} \subseteq \{1, \ldots, d'\}$ of features, resulting in a local dataset $\mathcal{D}^{(i)}$ with feature vectors

$$\mathbf{x}^{(i,r)} = \left(x_{j_1}^{(r)}, \ldots, x_{j_d}^{(r)}\right)^T.$$

Some of the devices may also have access to the labels $y^{(r)}$, for $r = 1, \ldots, m$, of the global tietoaineisto (see Fig. 77).

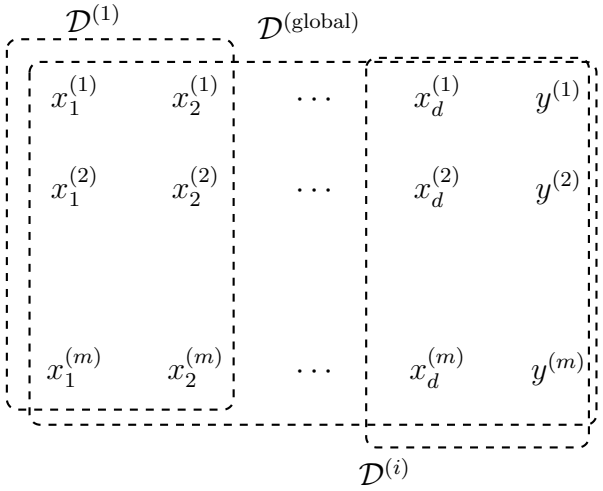


Fig. 77. VFL uses local datasets that are derived from the data points of a common global tietoaineisto. The local datasets differ in the choice of features used to characterize the data points.

One potential application of VFL is to enable collaboration between

different healthcare providers. Each provider collects distinct types of measurements—such as blood values, electrocardiography, and lung X-rays—for the same patients. Another application is a national social insurance system, where health records, financial indicators, consumer behavior, and mobility data are collected by different institutions. VFL enables joint learning across these parties while allowing well-defined levels of privacy protection.

See also: FL, privacy protection.

weights Consider a parameterized hypothesis space $\mathcal{H}$. We use the term weights for numeric model parameters that are used to scale features or their transformations in order to compute $h^{(\mathbf{w})} \in \mathcal{H}$. A linear model uses weights $\mathbf{w} = \big(w_1, \ldots, w_d\big)^T$ to compute the linear combination $h^{(\mathbf{w})}(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$. Weights are also used in neuroverkot to form linear combinations of features or the outputs of neurons in hidden layers (see Fig. 78).

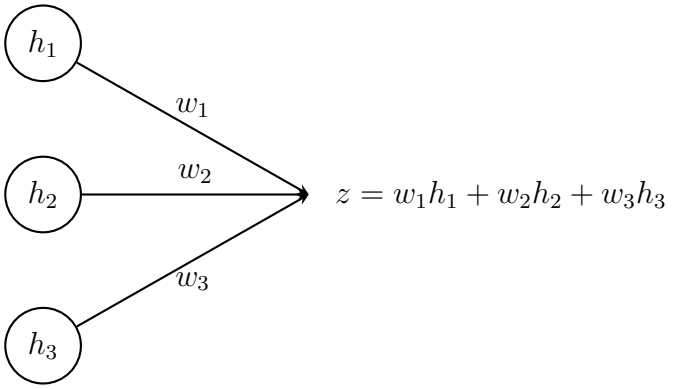


Fig. 78. A section of an ANN that contains a hidden layer with outputs (or activations) h_1,h_2, and h_3. These outputs are combined linearly to compute z, which can be used either as output of the ANN or as input to another layer.

See also: hypothesis space, model parameters, feature, linear model, ANN, layer, activation.

zero-gradient condition Consider the unconstrained optimization problem $\min_{\mathbf{w} \in \mathbb{R}^d} f(\mathbf{w})$ with a smooth and convex objective function $f(\mathbf{w})$. A necessary and sufficient condition for a vector $\widehat{\mathbf{w}} \in \mathbb{R}^d$ to solve this problem is that the gradient $\nabla f\big(\widehat{\mathbf{w}}\big)$ is the zero vector such that

$$\nabla f\big(\widehat{\mathbf{w}}\big) = \mathbf{0} \Leftrightarrow f\big(\widehat{\mathbf{w}}\big) = \min_{\mathbf{w} \in \mathbb{R}^d} f(\mathbf{w}).$$

See also: optimization problem, smooth, convex, objective function, vector, gradient.

0/1 loss The 0/1 loss $L^{(0/1)}\left((\mathbf{x}, y), h\right)$ measures the quality of a luokitin $h(\mathbf{x})$ that delivers a prediction $\hat{y}$ (e.g., via thresholding (1)) for the label y of

a data point with features $\mathbf{x}$. It is equal to 0 if the prediction is correct, i.e., $L^{(0/1)}\left((\mathbf{x}, y), h\right) = 0$ when $\hat{y} = y$. It is equal to 1 if the prediction is wrong, i.e., $L^{(0/1)}\left((\mathbf{x}, y), h\right) = 1$ when $\hat{y} \neq y$.

See also: loss, luokitin, prediction, label, data point, feature.

Hakemisto

Viitteet

[1] W. Rudin, *Real and Complex Analysis*, 3rd ed. New York, NY, USA: McGraw-Hill, 1987.

[2] W. Rudin, *Principles of Mathematical Analysis*, 3rd ed. New York, NY, USA: McGraw-Hill, 1976.

[3] G. H. Golub and C. F. Van Loan, *Matrix Computations*, 4th ed. Baltimore, MD, USA: The Johns Hopkins Univ. Press, 2013.

[4] G. H. Golub and C. F. Van Loan, "An analysis of the total least squares problem," *SIAM J. Numer. Anal.*, vol. 17, no. 6, pp. 883–893, Dec. 1980, doi: 10.1137/0717073.

[5] A. Klenke, *Probability Theory: A Comprehensive Course*, 3rd ed. Cham, Switzerland: Springer Nature, 2020.

[6] P. Billingsley, *Probability and Measure*, 3rd ed. New York, NY, USA: Wiley, 1995.

[7] D. P. Bertsekas and J. N. Tsitsiklis, *Introduction to Probability*, 2nd ed. Belmont, MA, USA: Athena Scientific, 2008.

[8] A. Jung, *Machine Learning: The Basics*. Singapore, Singapore: Springer Nature, 2022.