The A”alto

Dictionary of Machine Learning

Alexander Jung[1], Konstantina Olioumtsevits[1], and Juliette Gronier[2]
[1]Aalto University [2]ENS Lyon

June 24, 2025

please cite as: A. Jung, K. Olioumtsevits, and J. Gronier, *The Aalto Dictionary of Machine Learning*. Espoo, Finland: Aalto University, 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. Some of the figures in the dictionary have been prepared with the help of Salvatore Rastelli.

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 $\mathcal{B}$.
$\mathbb{N}$	The natural numbers $1, 2, \ldots$.
$\mathbb{R}$	The real numbers x [1].
$\mathbb{R}_+$	The non-negative 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 $0 \leq x \leq 1$.

$\underset{\mathbf{w}}{\operatorname{argmin}} f(\mathbf{w})$	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.
$\exp(a)$	The exponential function evaluated at the real number $a \in \mathbb{R}$.
$\log(a)$	The logarithm of the positive number $a \in \mathbb{R}_{++}$.
$f(\cdot)\!:\!\mathcal{A}\!\rightarrow\!\mathcal{B} : a\!\mapsto\! f(a)$	A function (or map) from a set $\mathcal{A}$ to a set $\mathcal{B}$, assigning 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 codomain of f. Machine learning (ML) aims to learn a function h that maps features $\mathbf{x}$ of a data point to a prediction $h(\mathbf{x})$ for its label y. See also: function, map, ML, hypothesis, feature, data point, prediction, label.
$\operatorname{epi}(f)$	The epigraph of a real-valued function $f : \mathbb{R}^d \rightarrow \mathbb{R}$. See also: epigraph, function.
$\dfrac{\partial f(w_1, \ldots, w_d)}{\partial w_j}$	The partial derivative (if it exists) of a real-valued function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ with respect to w_j [2, Ch. 9]. See also: function.

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

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

See also: gradient, differentiable, function.

Matrices and Vectors

$\mathbf{x} = \big(x_1, \ldots, x_d\big)^T$ A vector of length d, with its j-th entry being x_j.

$\mathbb{R}^d$ The set of vectors $\mathbf{x} = \big(x_1, \ldots, x_d\big)^T$ consisting of d real-valued entries $x_1, \ldots, x_d \in \mathbb{R}$.

$\mathbf{I}_{l \times d}$ 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 equal to 0 otherwise.

$\mathbf{I}_d, \mathbf{I}$ A square identity matrix of size $d \times d$. If the size is clear from context, we drop the subscript.

$\|\mathbf{x}\|_2$ The Euclidean (or ℓ_2) norm of the vector $\mathbf{x} = \big(x_1, \ldots, x_d\big)^T \in \mathbb{R}^d$ defined as $\|\mathbf{x}\|_2 := \sqrt{\sum_{j=1}^{d} x_j^2}$.
See also: norm.

$\|\mathbf{x}\|$ Some norm of the vector $\mathbf{x} \in \mathbb{R}^d$ [3]. Unless specified otherwise, we mean the Euclidean norm $\|\mathbf{x}\|_2$.
See also: norm.

$\mathbf{x}^T$ The transpose of a matrix that has the vector $\mathbf{x} \in \mathbb{R}^d$ as its single column.

$\mathbf{X}^T$ 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 $\mathbf{X} = \mathbf{X}^T$.

$\mathbf{X}^{-1}$ The inverse matrix of a matrix $\mathbf{X} \in \mathbb{R}^{d \times d}$.
See also: inverse matrix.

$\mathbf{0} = \big(0, \ldots, 0\big)^T$	The vector in $\mathbb{R}^d$ with each entry equal to zero.
$\mathbf{1} = \big(1, \ldots, 1\big)^T$	The vector in $\mathbb{R}^d$ with each entry equal to one.
$\big(\mathbf{v}^T, \mathbf{w}^T\big)^T$	The vector of length $d + d'$ obtained by concatenating the entries of vector $\mathbf{v} \in \mathbb{R}^d$ with the entries of $\mathbf{w} \in \mathbb{R}^{d'}$.
$\mathrm{span}\{\mathbf{B}\}$	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 $\mathrm{span}\{\mathbf{B}\} = \big\{\mathbf{Ba} : \mathbf{a} \in \mathbb{R}^b\big\} \subseteq \mathbb{R}^a$.
$\det(\mathbf{C})$	The determinant of the matrix $\mathbf{C}$. See also: determinant.
$\mathbf{A} \otimes \mathbf{B}$	The Kronecker product of $\mathbf{A}$ and $\mathbf{B}$ [4].

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 a 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.

$\text{cov}\,(x, y)$

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 realizations 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.

$\mathbb{P}(\mathbf{x}; \mathbf{w})$

A parametrized 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 covariance matrix $\mathbb{E}\Big\{\big(\mathbf{x} - \mathbb{E}\{\mathbf{x}\}\big)\big(\mathbf{x} - \mathbb{E}\{\mathbf{x}\}\big)^T\Big\}$.

See also: probability distribution, RV, parameter, multivariate normal distribution, mean, covariance matrix.

$\mathcal{N}(\mu, \sigma^2)$ 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, mean, expectation, variance.

$\mathcal{N}(\boldsymbol{\mu}, \mathbf{C})$ 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 covariance matrix $\mathbf{C} = \mathbb{E}\big\{\big(\mathbf{x}-\boldsymbol{\mu}\big)\big(\mathbf{x}-\boldsymbol{\mu}\big)^T\big\}$.

See also: multivariate normal distribution, Gaussian RV, mean, expectation, covariance matrix.

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 dataset.

See also: data point, dataset.

$\mathcal{D}$

A dataset $\mathcal{D} = \{\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(m)}\}$ is a list of individual data points $\mathbf{z}^{(r)}$, for $r = 1, \ldots, m$.

See also: dataset, data point.

d

The number of features that characterize a data point.

See also: feature, data point.

x_j

The j-th feature of a data point. The first feature is denoted 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, 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: feature, data point.
$\mathbf{x}^{(r)}$	The feature vector of the r-th data point within a dataset. See also: feature, data point, dataset.
$x_j^{(r)}$	The j-th feature of the r-th data point within a dataset. See also: feature, data point, dataset.
$\mathcal{B}$	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 r-th data point. See also: label, data point.
$\big(\mathbf{x}^{(r)}, y^{(r)}\big)$	The features and label of the r-th 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 dataset (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 classification problems (or methods).

See also: label space, ML, label, data point, dataset, training set, regression, classification.

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 $h : \mathcal{X} \rightarrow \mathcal{Y}$.

See also: hypothesis, map.

$\mathcal{H}$

A hypothesis space or model used by an ML method. The hypothesis space consists of different hypothesis maps $h : \mathcal{X} \rightarrow \mathcal{Y}$, between which the ML method must choose.

See also: hypothesis space, model, ML, hypothesis, map.

$d_{\text{eff}}\left(\mathcal{H}\right)$

The effective dimension of a hypothesis space $\mathcal{H}$.

See also: effective dimension, hypothesis space.

B^2

The squared bias of a learned hypothesis $\hat{h}$, or its parameters. Note that $\hat{h}$ becomes a RV if it is learned from data points being RVs.

See also: bias, hypothesis, parameter, RV, data point.

V

The variance of a learned hypothesis $\hat{h}$, or its parameters. Note that $\hat{h}$ becomes a RV if it is learned from data points being RVs.

See also: variance, hypothesis, parameter, RV, data point.

$L\left((\mathbf{x}, y), h\right)$

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 dataset $\mathcal{D}$.

See also: empirical risk, loss, hypothesis, dataset.

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).

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 j-th 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.

$\sigma(\cdot)$

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 in an ANN. See also: parameter, 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.
$\phi(\cdot)$	A feature map $\phi : \mathcal{X} \rightarrow \mathcal{X}' : \mathbf{x} \mapsto \mathbf{x}' := \phi\big(\mathbf{x}\big) \in \mathcal{X}'$. See also: feature map.
$K\big(\cdot, \cdot\big)$	Given some feature space $\mathcal{X}$, a kernel is a map $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{C}$ that is psd. See also: feature space, kernel, map, psd.

Federated Learning

$\mathcal{G} = (\mathcal{V}, \mathcal{E})$

An undirected graph whose nodes $i \in \mathcal{V}$ represent devices within a federated learning network (FL network). The undirected weighted edges $\mathcal{E}$ represent connectivity between devices and statistical similarities between their datasets and learning tasks.

See also: graph, device, FL network, dataset, 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 a node i in a graph $\mathcal{G}$.

See also: neighborhood, graph.

$d^{(i)}$

The weighted degree $d^{(i)} := \sum_{i' \in \mathcal{N}^{(i)}} A_{i,i'}$ of a node i in a graph $\mathcal{G}$.

See also: graph.

$d_{\max}^{(\mathcal{G})}$	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 r-th data point in the local dataset $\mathcal{D}^{(i)}$. See also: feature, data point, local dataset.
$y^{(i,r)}$	The label of the r-th 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.

$\mathrm{stack}\big\{\mathbf{w}^{(i)}\big\}_{i=1}^{n}$

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

See also: model parameters.

Machine Learning Concepts

k-fold cross-validation (k-fold CV) k-fold CV is a method for learning and validating a hypothesis using a given dataset. This method divides the dataset evenly into k subsets or folds and then executes k repetitions of model training (e.g., via empirical risk minimization (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 algorithm is a hard clustering method which assigns each data point of a dataset to precisely one of k different clusters. The method alternates between updating the cluster assignments (to the cluster with the nearest mean) and, given the updated cluster assignments, re-calculating the cluster means [8, Ch. 8].

See also: mean, algorithm, hard clustering, data point, dataset, cluster.

absolute error loss Consider a data point with features $\mathbf{x} \in \mathcal{X}$ and numeric label $y \in \mathbb{R}$. The absolute error loss incurred by a hypothesis $h : \mathcal{X} \rightarrow \mathbb{R}$ is defined as $|y - h(\mathbf{x})|$, i.e., the absolute difference between the prediction $h(\mathbf{x})$ and the true label y.

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

accuracy Consider data points characterized by features $\mathbf{x} \in \mathcal{X}$ and a

categorical label y which takes on values from a finite label space $\mathcal{Y}$. The accuracy of a hypothesis $h : \mathcal{X} \rightarrow \mathcal{Y}$, when applied to the data points in a dataset $\mathcal{D} = \big\{ \big(\mathbf{x}^{(1)}, y^{(1)}\big), \ldots, \big(\mathbf{x}^{(m)}, y^{(m)}\big) \big\}$, 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: loss, 0/1 loss, metric.

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 parametrized by the weights $w_1, \ldots, w_d$.
See also: ANN, 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.

algorithm An algorithm is a precise, step-by-step specification for how to produce an output from a given input within a finite number of computational steps [9]. For example, an algorithm for training 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 [10]. One approach is to represent an algorithm as a collection of possible executions. Each individual execution is 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 [11]. In the context of ML, APIs are commonly used to provide access to a trained ML model. Users—whether humans or machines—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:

- The server can centralize computational resources which are required to compute predictions.
- 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 on carefully selected feature vectors.
See also: ML, model, feature vector, data point, prediction, feature, model inversion.

artificial intelligence (AI) 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 for predicting 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 obtain a (point-wise) estimate for the loss incurred by the current choice of model parameters.
See also: reward, ML, model, loss function, training set, loss, model parameters.

artificial neural network (ANN) 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.

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 datasets (via data poisoning) or communication links between devices in a federated learning (FL) setting. Passive attacks, such as privacy attacks, aim to infer sensitive attributes without modifying the system. Depending on their goal, we distinguish between denial-of-service attacks, backdoor attacks, and privacy attacks.
See also: data poisoning, privacy attack, sensitive attribute, denial-of-service attack, backdoor.

autoencoder 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 $\mathbf{x} - h^{*}\big(h(\mathbf{x})\big)$.
See also: ML, map, ERM, loss.

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 $\hat{h}$ towards 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.

bagging (or bootstrap aggregation) Bagging (or bootstrap aggregation) is a generic technique to improve (the robustness of) a given ML method. The idea is to use the bootstrap to generate perturbed copies of a given dataset and then 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.
See also: robustness, ML, bootstrap, dataset, hypothesis, label, data point, prediction, map.

baseline 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 and 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 [12]. 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 $\mathcal{H}$) [13]. 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 $p(\mathbf{x}, y)$ [13, Ch. 4]. However, computing the Bayes estimator and Bayes risk presents two main challenges:

1) The probability distribution $p(\mathbf{x}, y)$ is unknown and needs to be estimated.
2) Even if $p(\mathbf{x}, y)$ is known, it can be computationally too expensive to compute the Bayes risk exactly [14].

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 $\mathbf{x}$ [13], [15]. The corresponding Bayes risk is given by the posterior variance $\sigma^2_{y|\mathbf{x}}$

(see Figure 1).

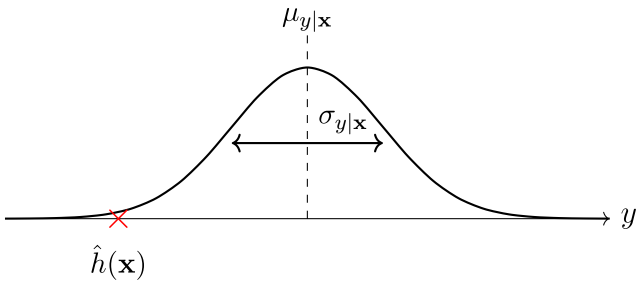


Fig. 1. If the features and the label of a data point are drawn from a multivariate normal distribution, we can achieve the minimum risk (under squared error loss) by using the Bayes estimator $\mu_{y|\mathbf{x}}$ to predict the label y of a data point with features $\mathbf{x}$. The corresponding minimum 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 stochastic gradient descent (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.

Bayes estimator 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. For a given loss function $L(\cdot, \cdot)$, we refer to a hypothesis h as a Bayes estimator if its risk $\mathbb{E}\{L\left((\mathbf{x},y),h\right)\}$ is the minimum [13]. Note that the property of a hypothesis being a Bayes estimator depends on the underlying probability distribution and the choice for the loss function $L\left(\cdot,\cdot\right)$.

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 [13].

See also: probabilistic model, risk, Bayes estimator.

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

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

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: ML, hypothesis space, model parameters, dataset, data point, realization, i.i.d., RV, ERM.

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) [16, Ch. 10]. For example, weak learners are shallow decision trees which 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 functions [17]. Just like gradient descent (GD) iteratively updates model parameters to reduce the empirical risk, boosting iteratively combines (e.g., by summation) hypothesis maps to reduce the empirical risk. 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 [17].

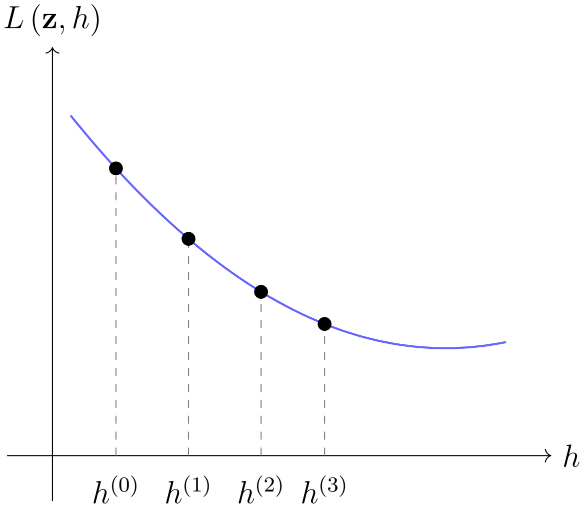


Fig. 2. Boosting methods construct a sequence of hypothesis maps $h^{(0)}, h^{(1)}, \ldots$ that are increasingly strong learners (i.e., incurring a smaller loss).

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.

bootstrap For the analysis of ML methods, it is often useful to interpret a given set of data points $\mathcal{D} = \big\{\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(m)}\big\}$ as realizations of i.i.d. RVs with a common probability distribution $p(\mathbf{z})$. In general, we do not know $p(\mathbf{z})$ exactly, but we need to estimate it. The bootstrap uses the histogram of $\mathcal{D}$ as an estimator for the underlying probability distribution $p(\mathbf{z})$.

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 $m \to \infty$ [18, Proposition 2.17]. One elegant way to derive the CLT is via the characteristic function of the normalized sum $s^{(m)}$. Let $\phi(t) = \mathbb{E}\big\{ \exp\big(jtx\big)\big\}$ (with the imaginary unit $j = \sqrt{-1}$) be the common characteristic function of each summand $x^{(r)}$, and let $\phi^{(m)}(t)$ denote the characteristic function of $s^{(m)}$. Define an operator $\mathcal{T}$ acting on characteristic functions such that

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

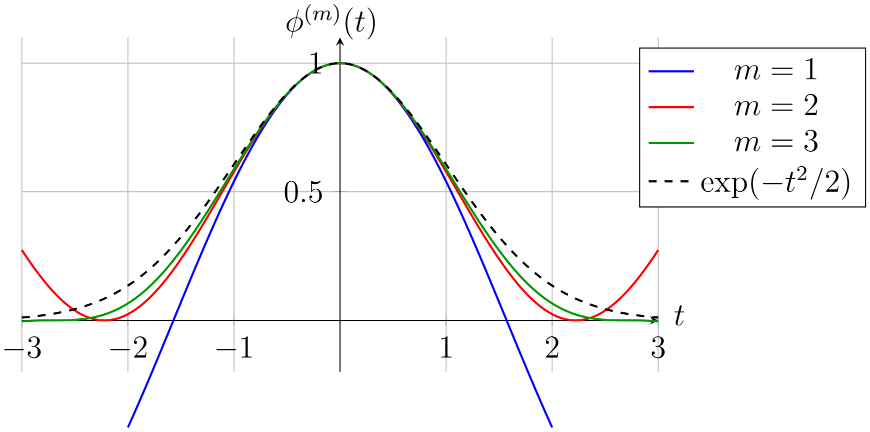


Fig. 3. Characteristic functions of normalized sums of i.i.d. RVs $x^{(r)} \in \{-1, 1\}$ for $r = 1, \ldots, m$ compared to the Gaussian limit.

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

$$\phi^*(t) = e^{-t^2\sigma^2/2},$$

which is the characteristic function of a Gaussian RV with mean zero and variance σ^2. Generalizations of the CLT allow for dependent or non-identically distributed RVs [18, Section 2.8].

See also: RV, Gaussian RV.

characteristic function The characteristic function of a real-valued RV x is the function [6, Section 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: probability distribution, RV.

classification 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.

classifier A classifier is a hypothesis (i.e., a map) $h(\mathbf{x})$ used to predict a label taking 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 classification problem with 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, map, label, label space, function, prediction, classification, decision region.

cluster 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 Figure 4.

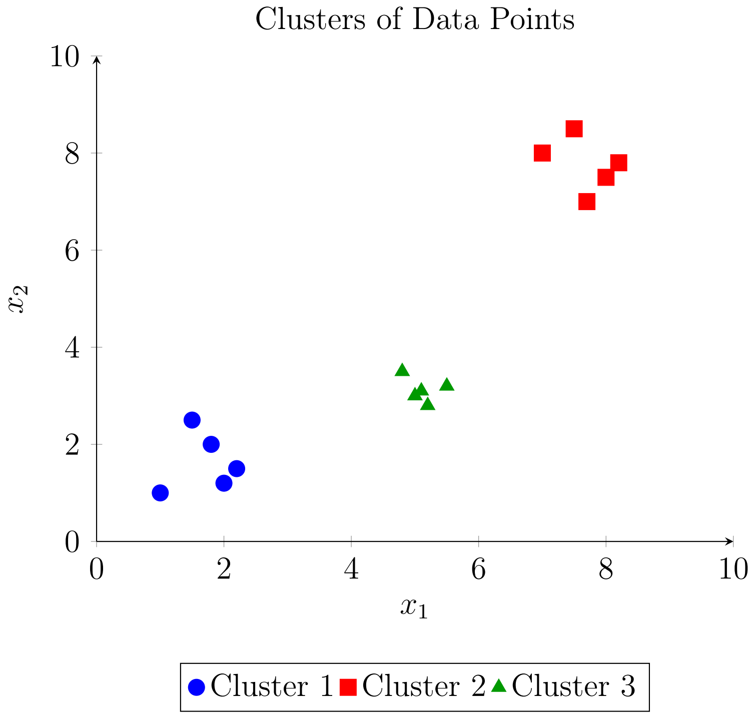


Fig. 4. Illustration of three clusters in a two-dimensional feature space. Each cluster groups data points that are more similar to each other than to those in other clusters, based on the Euclidean distance.

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

clustered federated learning (CFL) CFL trains local models for the devices in a FL application by using a clustering assumption, i.e., the devices of an FL network form clusters. Two devices in the same cluster

generate local datasets with similar statistical properties. CFL pools the local datasets of devices in the same cluster to obtain a training set for a cluster-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, cluster, graph clustering.

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

clustering assumption The clustering assumption postulates that data points in a dataset form a (small) number of groups or clusters. Data points in the same cluster are more similar to each other than those outside the cluster [19]. We obtain different clustering methods by using different notions of similarity between data points.
See also: clustering, data point, dataset, cluster.

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 [20].

See also: probability, RV, expectation.

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

confusion matrix Consider data points, which are characterized by features $\mathbf{x}$ and label y, having values from the finite label space $\mathcal{Y} = \{1, \ldots, k\}$. For a given hypothesis h, the confusion matrix is a $k \times k$ matrix with rows representing the elements of $\mathcal{Y}$. The columns of a confusion matrix correspond to the prediction $h(\mathbf{x})$. The (c, c')-th entry of the confusion matrix is the fraction of data points with label $y = c$ and resulting in a prediction $h(\mathbf{x}) = c'$.

See also: label, label space, hypothesis, classification.

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

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

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 $f : \mathbb{R}^d \rightarrow \mathbb{R}$ 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 [21]. We illustrate one example of a convex set and a convex function in Figure 5.

$\mathbf{w}$
$\mathbf{w}'$
$\mathcal{C}$
$f(\mathbf{w})$

Fig. 5. Left: A convex set $\mathcal{C} \subseteq \mathbb{R}^d$. Right: A convex function $f : \mathbb{R}^d \rightarrow \mathbb{R}$.

See also: Euclidean space, function, epigraph.

convex clustering Consider a dataset $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)} \in \mathbb{R}^d$. Convex clustering 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 cluster then consists of those data points $r \in \{1, \ldots, m\}$ with identical $\widehat{\mathbf{w}}^{(r)}$ [22], [23].

See also: dataset, convex, clustering, norm, cluster, 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),

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

Here, we use the ordered (in increasing fashion) 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, 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 defined as

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

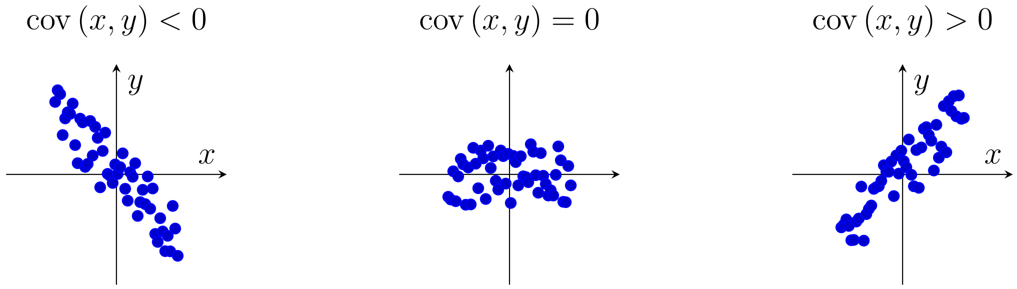


Fig. 6. Scatterplots illustrating realizations from three different probabilistic models for two RVs with different covariance values: negative (left), zero (center), and positive (right).

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 $\text{cov}\,(x, y) = 0$, the RVs are said to be uncorrelated, though not necessarily statistically independent. See Figure 6 for visual illustrations.

covariance matrix 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: RV.

data Data refers to objects that carry information. These objects can be either concrete physical objects (such as persons or animals) or abstract concepts (such as numbers). We often use representations (or approximations) of the original data that are more convenient for data processing. These approximations use different mathematical structures such as relations that are used in relational databases [24, 25].
See also: model, dataset, data point.

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 Figure 7). Data augmentation can be an efficient form of regularization.

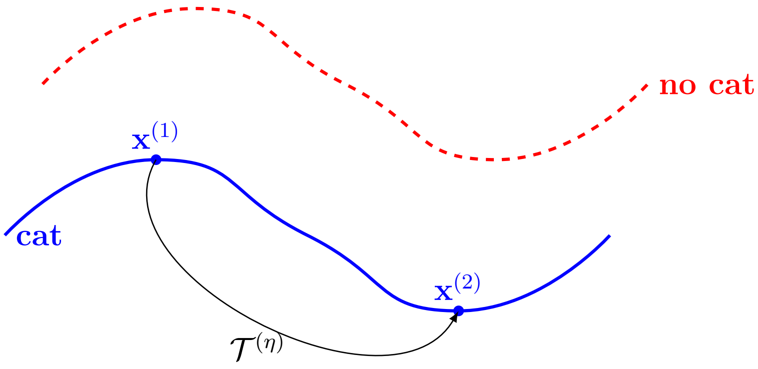


Fig. 7. Data augmentation exploits intrinsic symmetries of data points in some feature space $\mathcal{X}$. We can represent a symmetry by an operator $\mathcal{T}^{(\eta)} : \mathcal{X} \to \mathcal{X}$, parametrized by some number $\eta \in \mathbb{R}$. For example, $\mathcal{T}^{(\eta)}$ might represent 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 [26, Article 5(1)(c)], [27].
See also: data.

data normalization 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, norm, training set.

data point A data point is any object that conveys information [28]. Data points might be students, radio signals, trees, forests, images, RVs, real numbers, or proteins. We characterize data points using two types of properties. One type of property is referred to as a feature. Features are properties of a data point that can be measured or computed in an automated fashion. A different kind of property is referred to as a label. The label of a data point represents some higher-level fact (or quantity of interest). In contrast to features, determining the label of a data point typically requires human experts (or domain experts). Roughly speaking, ML aims to predict the label of a data point based solely on its features.

See also: data, RV, feature, label, ML.

data poisoning Data poisoning refers to the intentional manipulation (or fabrication) of data points to steer the training of an ML model [29], [30]. Data poisoning attacks take various forms, including:

- Backdoor attacks : implanting triggers into training data so that the trained model behaves normally on typical feature vectors but misclassifies a feature vector with a trigger pattern.
- denial-of-service attack: degrading overall performance of the trained model 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: backdoor, attack, denial-of-service attack, trustworthy artificial intelligence (trustworthy AI).

dataset A dataset refers to a collection of data points. These data points carry information about some quantity of interest (or label) within an ML application. ML methods use datasets for model training (e.g., via ERM) and model validation. Note that our notion of a dataset is very flexible, as it allows for very different types of data points. Indeed, data points can be concrete physical objects (such as humans or animals) or abstract objects (such as numbers). As a case in point, Figure 8 depicts a dataset that consists of cows as data points.

Fig. 8. A cow herd somewhere in the Alps.

Quite often, an ML engineer does not have direct access to a dataset. Indeed, accessing the dataset in Figure 8 would require us to visit the cow herd in the Alps. Instead, we need to use an approximation (or representation) of the dataset which is more convenient to work with. Different mathematical models have been developed for the representation (or approximation) of datasets [24], [31], [32], [33]. One of the most widely adopted data model is the relational model, which organizes data as a table (or relation) [25], [24]. A table consists of rows and columns:

- Each row of the table represents a single data point.
- Each column of the table corresponds to a specific attribute of the data point. ML methods can use attributes as features and labels of the data point.

For example, Table 1 shows a representation of the dataset in Figure 8. In the relational model, the order of rows is irrelevant, and each attribute (i.e., column) must be precisely defined with a domain, which specifies the set of possible values. In ML applications, these attribute domains become the feature space and the label space.

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

Table 1: A relation (or table) that represents the dataset in Figure **??**.

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 [34].

See also: data point, data, feature, feature space, label space, trustworthy AI.

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, 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 flow-chart-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 itself child nodes, 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.

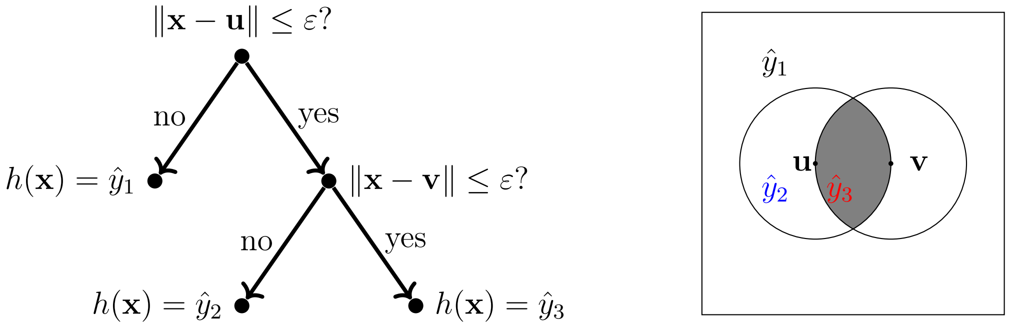

$\|\mathbf{x}-\mathbf{u}\| \leq \varepsilon$?
no
yes
$h(\mathbf{x}) = \hat{y}_1$
$\|\mathbf{x}-\mathbf{v}\| \leq \varepsilon$?
no
yes
$h(\mathbf{x}) = \hat{y}_2$
$h(\mathbf{x}) = \hat{y}_3$
$\hat{y}_1$
$\mathbf{u}$
$\mathbf{v}$
$\hat{y}_2$
$\hat{y}_3$

Fig. 9. Left: A decision tree is a flow-chart-like representation of a piece-wise constant hypothesis $h : \mathcal{X} \rightarrow \mathbb{R}$. Each piece is a decision region $\mathcal{R}_{\hat{y}} := \big\{\mathbf{x} \in \mathcal{X} : h(\mathbf{x}) = \hat{y}\big\}$. The depicted decision tree can be applied to numeric feature vectors, i.e., $\mathcal{X} \subseteq \mathbb{R}^d$. It is parametrized by the threshold $\varepsilon > 0$ and the vectors $\mathbf{u}, \mathbf{v} \in \mathbb{R}^d$. Right: 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 [35].

See also: ANN, ML, model.

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

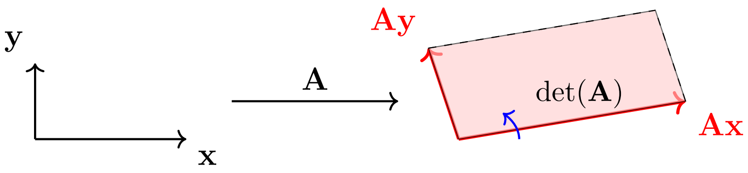
denial-of-service attack A denial-of-service attack aims (e.g., via data poisoning) to steer the training of a model such that it performs poorly for typical data points.

See also: data poisoning, model, data point.

density-based spatial clustering of applications with noise (DBSCAN) DBSCAN refers to a clustering algorithm for data points that are characterized by numeric feature vectors. Like k-means and soft clustering via GMM, also DBSCAN uses the Euclidean distances between feature vectors to determine the clusters. 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 close-by 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: clustering, graph, k-means, GMM, cluster.

determinant The determinant $\det(\mathbf{A})$ of a square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ is a scalar that characterizes how (the orientation of) volumes in $\mathbb{R}^n$ are altered by applying $\mathbf{A}$ [3], [36]. Note that a matrix $\mathbf{A}$ represents a linear transformation on $\mathbb{R}^n$. 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 $\lambda_1, \ldots, \lambda_n$, then $\det(\mathbf{A}) = \prod_{i=1}^{n} \lambda_i$ [37]. For the special cases $n = 2$ (2D) and $n = 3$ (3D), the determinant can be interpreted as an oriented area or volume spanned by the column vectors of $\mathbf{A}$.



See also: eigenvalue, inverse matrix.

device Any physical system that can be used to store and process data. In the context of ML, we typically mean a computer that is able to read in data points from different sources and, in turn, to train an ML model using these data points.
See also: data, ML, data point, model.

differentiable A real-valued function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is differentiable if it can, at any point, be approximated locally 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 probability density function (pdf) $p(x)$, the differential entropy is defined as [28]

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

Differential entropy can be negative and lacks some properties of entropy for discrete-valued RVs, such as invariance under change of variables [28].

Among all RVs with given mean $\boldsymbol{\mu}$ and covariance matrix $\boldsymbol{\Sigma}$, $h(\mathbf{x})$ 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 dataset (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 $\mathcal{A}(\mathcal{D})$ does not change too much 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: ML, dataset, training set, ERM, model parameters, prediction, data point, privacy leakage, probability distribution, sensitive attribute, probabilistic model, realization, RV.

dimensionality reduction Dimensionality reduction refers to methods that learn a transformation $h : \mathbb{R}^d \rightarrow \mathbb{R}^{d'}$ 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. Figure 10 depicts the scatterplot of hand-written digits that are placed according transformed features. Here, the data points are naturally represented by a large number of grayscale values (one value for each pixel).

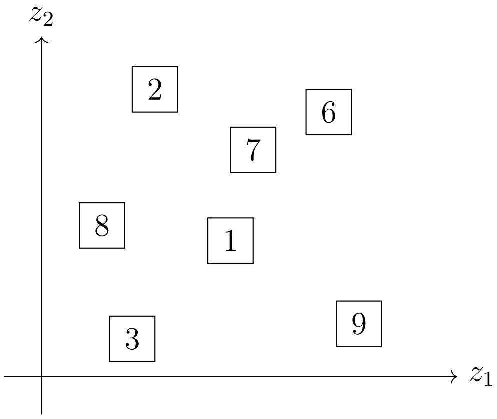


Fig. 10. Example of dimensionality reduction: High-dimensional image data (e.g., high-resolution images of hand-written digits) embedded into 2D using learned features (z_1, z_2) and visualized in a scatterplot.

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 [38], [39]. 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:

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

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 algorithms is in FL where a network of devices collaboratively trains a personal model for each device.

See also: algorithm, device, FL, model.

dual norm Every norm $\|\cdot\|$ defined on an Euclidean space $\mathbb{R}^d$ has an associated dual norm, which is denoted $\|\cdot\|_*$ 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 [21, Sec. A.1.6].

See also: norm, Euclidean space.

edge weight Each edge $\{i, i'\}$ of an FL network is assigned a non-negative 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 bias 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 is a non-zero vector $\mathbf{x} \in \mathbb{R}^d \setminus \{\mathbf{0}\}$ such that $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$.

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 eigenvectors of the matrix $\mathbf{V}$. The diagonal matrix $\mathbf{\Lambda} = \mathrm{diag}\big\{\lambda_1, \ldots, \lambda_d\big\}$ 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: eigenvector, eigenvalue.

eigenvector An eigenvector of a matrix $\mathbf{A} \in \mathbb{R}^{d \times d}$ is a non-zero 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: eigenvalue.

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

empirical risk minimization (ERM) ERM is the optimization problem of finding a hypothesis (out of a model) with the minimum average loss (or empirical risk) on a given dataset $\mathcal{D}$ (i.e., the training set). Many ML methods are obtained from empirical risk via specific design choices for the dataset, model, and loss [8, Ch. 3].
See also: optimization problem, hypothesis, model, minimum, loss, empirical risk, dataset, training set, ML.

entropy Entropy quantifies the uncertainty or unpredictability associated with a RV [28]. For a discrete RV x taking values in a finite set

$\mathcal{S} = \{x_1, \ldots, x_n\}$ with 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 $f : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{+\infty\}$ is the set of points lying on or above its graph:

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

A function is convex if and only if its epigraph is a convex set [21], [40].

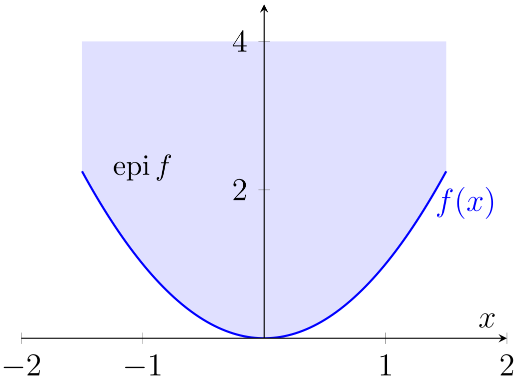


Fig. 11. Epigraph of the function $f(x) = x^2$ (i.e., shaded area).

See also: function, graph, convex.

Erdős-Rényi graph (ER graph) An ER graph is a probabilistic model for graphs 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 parametrized 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 $\Delta\mathbf{w} = \widehat{\mathbf{w}} - \overline{\mathbf{w}}$ [16], [41].

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 an 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].

expectation Consider a numeric feature vector $\mathbf{x} \in \mathbb{R}^d$ which 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], [42]. Figure 12 illustrates the expectation of a scalar discrete RV x which takes on values from a finite set only.

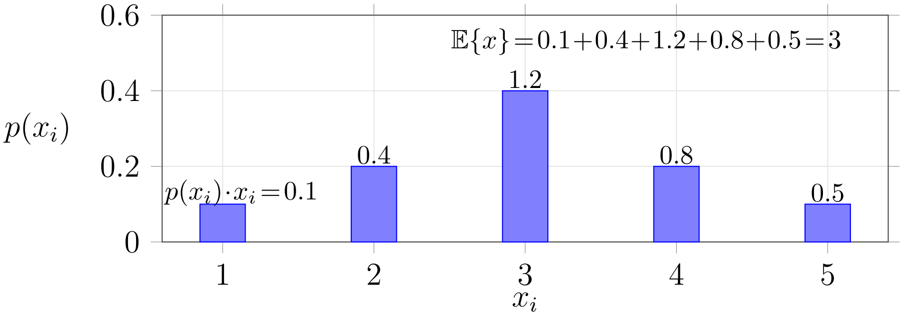


Fig. 12. The expectation of a discrete RV x is obtained by summing up its possible values x_i, weighted by the corresponding probability $p(x_i) = \mathbb{P}(x = x_i)$.

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 [16], [43], [44]. Since we do not observe $\mathbf{z}$, we need to

estimate it from the observed dataset $\mathcal{D}$ 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 re-calculate $\widehat{\mathbf{z}}$, 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 independent and identically distributed assumption (i.i.d. assumption) and by using the Bayes risk as the baseline for the (average) loss of a hypothesis. An alternative approach to obtaining a baseline is to use the hypothesis h' learned by an existing ML method. We refer to this hypothesis h' as an expert [45]. Regret minimization methods learn a hypothesis that incurs a loss comparable to the best expert [45], [46].
See also: loss function, baseline, regret.

explainability We define the (subjective) explainability of an ML method as the level of simulatability [47] 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 [47], [48]. 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 predictions [49], [50].
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 [48].
See also: SRM, regularization, loss, objective function, ERM, hypothesis, map, prediction, data point, training set.

explainable machine learning (XML) XML methods aim at complementing 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 [51].
See also: prediction, explanation, ML, model.

explanation One approach to make ML methods transparent is to provide an explanation along with the prediction delivered by an ML method. Explanations can take on many different forms. An explanation could

be some natural text or some quantitative measure for the importance of individual features of a data point [52]. We can also use visual forms of explanations, such as intensity plots for image classification [53].
See also: ML, prediction, feature, data point, classification.

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 could use the red-green-blue intensities of its pixels as features. Domain-specific synonyms for the term feature are "covariate," "explanatory variable," "independent variable," "input (variable)," "predictor (variable)," or "regressor" [54], [55], [56].
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 raw 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

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

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 dataset 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: ML, data point, feature, map, feature space, hypothesis space, PCA, minimum, dataset.

feature map Feature map refers to a map that transforms the original features of a data point into new features. The so-obtained new features might be preferable over the original features for several reasons. For example, the arrangement of data points might become simpler (or more linear) in the new feature space, allowing the use of linear models in the new features. This idea is a main driver for the development of kernel methods [57]. Moreover, the hidden layers of a deep net can be interpreted as a trainable feature map followed by a linear model in the form of the output layer. Another reason for learning a feature map could be that learning a small number of new features helps to avoid overfitting and ensures interpretability [58]. The special case of a feature map delivering two numeric features is particularly useful for data visualization. Indeed, we can depict data points in a scatterplot by using two features as the coordinates of a data point.
See also: feature, map, data point, feature space, linear model, kernel method, deep net, overfitting, interpretability, data, scatterplot.

feature matrix Consider a dataset $\mathcal{D}$ 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 $\mathbf{X} := \left(\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)}\right)^T$ of size $m \times d$.

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

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. A widely used choice for the feature space is the Euclidean space $\mathbb{R}^d$, with the dimension d being the number of individual features of a data point.

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

feature vector Feature vector refers to a vector $\mathbf{x} = \left(x_1, \ldots, x_d\right)^T$ 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, ML, Euclidean space, vector space, kernel method.

FedAvg FedAvg refers to a family of iterative FL algorithms. It uses a server-client setting and alternates between client-wise local models re-training, followed by the aggregation of updated model parameters at the server [59]. 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). Figure 13 illustrates the execution of a single iteration of FedAvg.

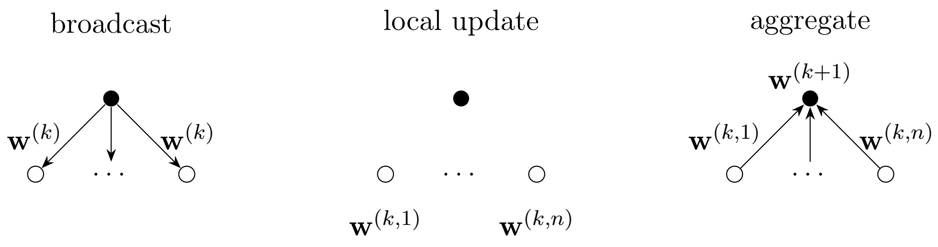


Fig. 13. Illustration of a single iteration of FedAvg which consists of broadcasting model parameters by the server, local updates at clients, and their aggregation by the server.

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

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.

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.

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 [60].

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

FedRelax An FL distributed algorithm.

See also: FL, distributed algorithm.

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 $\mathbf{w}^{(0)}, \mathbf{w}^{(1)}, \ldots$ 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 $\widehat{\mathbf{w}}$. What is more, 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 [61], [62]. 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 $\mathcal{F}$ [61, Cor. 5.16]. Figure 14 depicts examples of a firmly non-expansive operator, a non-expansive operator, and a contraction operator. All these operators are defined on the one-dimensional space $\mathbb{R}$. Another example of a firmly non-expansive operator is the proximal operator of a convex function [61], [63].

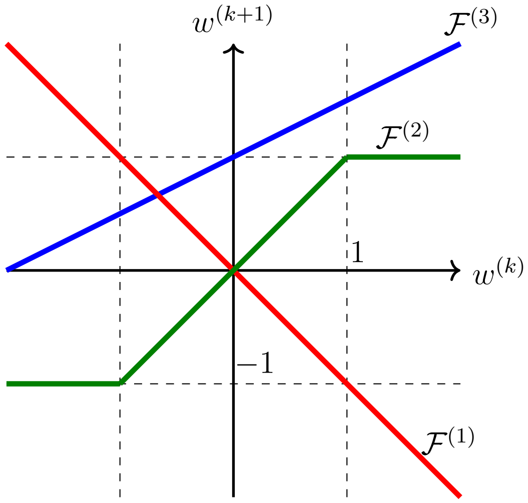


Fig. 14. Example of a non-expansive operator $\mathcal{F}^{(1)}$, a firmly non-expansive operator $\mathcal{F}^{(2)}$, and a contraction operator $\mathcal{F}^{(3)}$.

See also: optimization problem, differentiable, convex function, model parameters, contraction operator, proximal operator.

flow-based clustering Flow-based clustering groups the nodes of an undirected graph by applying k-means clustering to node-wise feature vectors. These feature vectors are built from network flows between carefully selected sources and destination nodes [64].

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

function A function is a mathematical rule that assigns each element $u \in \mathcal{U}$ exactly one element $v \in \mathcal{V}$ [2]. We write this as $f : \mathcal{U} \rightarrow \mathcal{V}$, 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 $u \in \mathcal{U}$.

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 parametrized by the probability p_c, the mean vector $\boldsymbol{\mu}^{(c)}$, and the covariance matrix $\mathbf{C}^{(c)}$ for each $c = 1, \ldots, k$. GMMs are widely used for clustering, density estimation, and as a generative model.
See also: probabilistic model, feature, data point, multivariate normal distribution, RV, mean, covariance matrix, clustering, model.

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 Gaussian distribution:

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

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

- a mean function $\mu(\mathbf{x}) = \mathbb{E}\{f(\mathbf{x})\}$
- and 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 $\mathbf{x} = (\mathrm{lat}, \mathrm{lon})$ denotes a geographic location. Temperature observations from Finnish Meteorological Institute (FMI) weather stations provide samples of $f(\mathbf{x})$ at specific locations (see Figure 15). A GP allows us to predict the temperature nearby FMI weather stations and to quantify the uncertainty of these predictions.

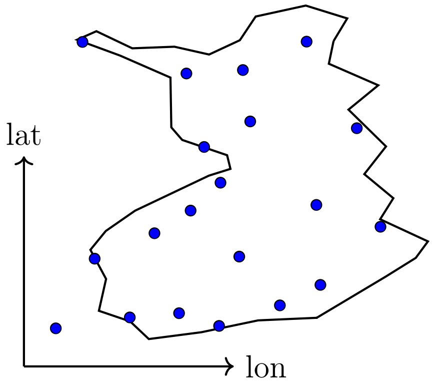


Fig. 15. We can interpret the temperature distribution over Finland as a realization of a GP indexed by geographic coordinates and sampled at FMI weather stations (indicated by blue dots).

See also: RV, mean, function, realization, FMI, sample, uncertainty.

Gaussian random variable (Gaussian RV) A standard Gaussian RV is a real-valued RV x with pdf [7], [15], [65]

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

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 $\mathcal{N}(\mu, \sigma^2)$.

A Gaussian random vector $\mathbf{x} \in \mathbb{R}^d$ with covariance matrix $\mathbf{C}$ and mean $\boldsymbol{\mu}$ can be constructed as [15], [65], [66]

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

where $\mathbf{z} := \big(z_1, \ldots, z_d\big)^T$ 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 $\mathcal{N}(\boldsymbol{\mu}, \mathbf{C})$.

Gaussian random vectors arise as finite-dimensional marginals of GPs, which define consistent joint Gaussian distributions over arbitrary (potentially infinite) index sets [67].

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 a large number of independent RVs (not necessarily Gaussian themselves) tends towards a Gaussian RV [68].

Compared to other probability distributions, the multivariate normal distribution is also distinct in that—in a mathematically precise sense—represents maximum uncertainty. Among all vector-valued RVs with a given covariance matrix $\mathbf{C}$, the RV $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{C})$ maximizes differential entropy [28, Th. 8.6.5]. This makes GPs 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, entropy.

general data protection regulation (GDPR) The GDPR was enacted by the European Union (EU), effective from May 25, 2018 [26]. It safeguards the privacy and data rights of individuals in the EU. The GDPR has significant implications for how data is 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 $\mathcal{D}^{(\rm train)}$. 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 $\widehat{L}\big(\hat{h}|\mathcal{D}^{(\rm train)}\big)$ 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 [69].

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 [70]. Similarly, it should deliver the same result if we rotate the object in the image [71].

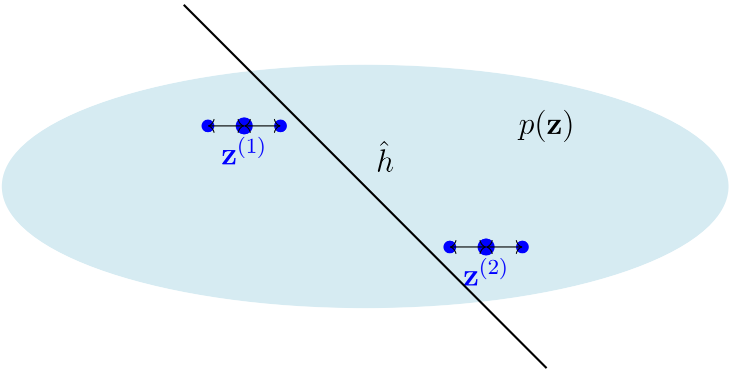


Fig. 16. Two data points $\mathbf{z}^{(1)}, \mathbf{z}^{(2)}$ that are used as a training set to learn a hypothesis $\hat{h}$ via ERM. We can evaluate $\hat{h}$ outside $\mathcal{D}^{(\text{train})}$ either by an i.i.d. assumption with some underlying probability distribution $p(\mathbf{z})$ or by perturbing the data points.

See also: model, training set, prediction, data point, ML, AI, ERM, hypothesis, loss, data, probabilistic model, i.i.d. assumption, RV, probability distribution, risk, empirical risk, generalization gap, probability, concentration inequality, feature.

generalization gap The difference between the performance of a trained model on the training set and its performance on other data points (such as those in a validation set).

See also: model, training set, data point, validation set, hypothesis, decision tree, generalization, gradient-based methods, ERM, smooth, loss function, GD, model parameters, empirical risk, gradient, loss, gradient step.

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 [72].
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 [21] such that

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

Figure 17 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 of (??). It turns out that the solution to (3) cannot be arbitrarily pulled away from trustworthy input vectors as long as they are the majority [73, Th. 2.2].

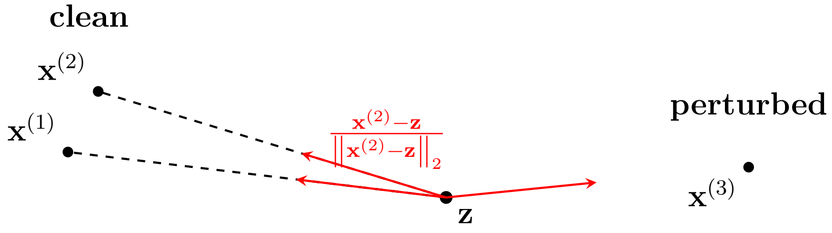


Fig. 17. Consider a solution $\mathbf{z}$ of (??) that does not coincide with any of the input vectors. The optimality condition for (??) requires that the unit vectors from $\mathbf{z}$ to the input vectors sum to zero.

See also: subgradient.

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

See also: function.

gradient descent (GD) GD is an iterative method for finding the minimum of a differentiable function $f(\mathbf{w})$ of a vector-valued argument $\mathbf{w} \in \mathbb{R}^d$. Consider a current guess or approximation $\mathbf{w}^{(k)}$ for the minimum of the function $f(\mathbf{w})$. We would like to find a new (better) vector $\mathbf{w}^{(k+1)}$ that has a smaller objective value $f(\mathbf{w}^{(k+1)}) < f\big(\mathbf{w}^{(k)}\big)$ than the current guess $\mathbf{w}^{(k)}$. We can achieve this typically by using a gradient step

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

with a sufficiently small step size $\eta > 0$. Figure 18 illustrates the effect of a single GD step (4).

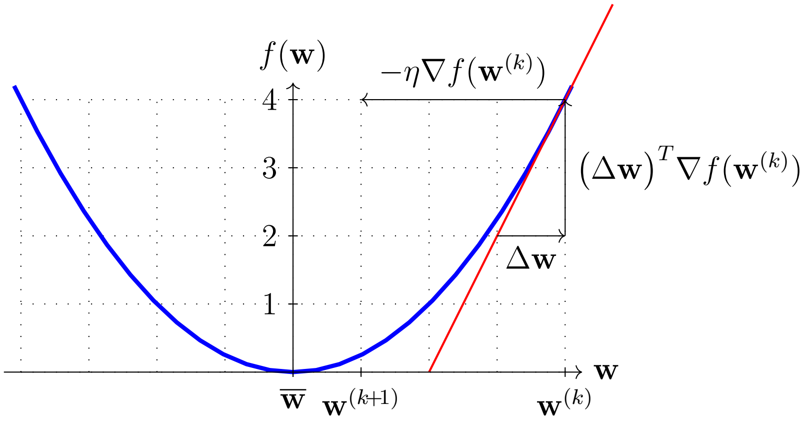


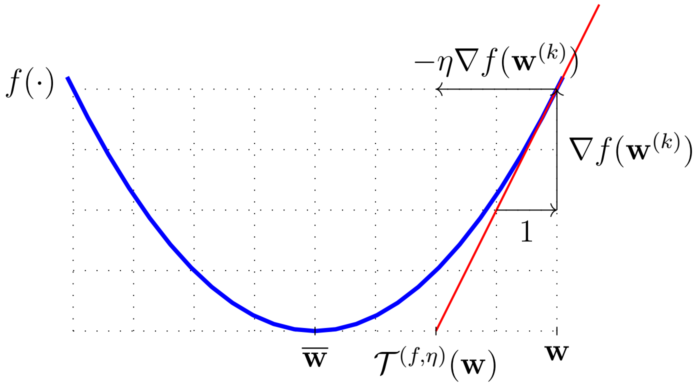
Fig. 18. A single gradient step (4) towards the minimizer $\overline{\mathbf{w}}$ of $f(\mathbf{w})$.

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

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 Figure 19)

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

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



$f(\cdot)$
$-\eta\nabla f(\mathbf{w}^{(k)})$
$\nabla f(\mathbf{w}^{(k)})$
1
$\overline{\mathbf{w}}$
$\mathcal{T}^{(f,\eta)}(\mathbf{w})$
$\mathbf{w}$

Fig. 19. 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

$$\widehat{\mathbf{w}} = \operatorname*{argmin}_{\mathbf{w}' \in \mathbb{R}^d} f(\mathbf{w}') + (1/\eta) \left\| \mathbf{w} - \mathbf{w}' \right\|_2^2 . \tag{6}$$

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 towards reducing the function value $f(\widehat{\mathbf{w}})$. Note that, much like the gradient step (5), also the update (6) defines an operator that is parametrized 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 $f(\cdot)$ [63].

See also: differentiable, function, gradient, step size, neighborhood, 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 [74]. 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 clustering aims at clustering data points that are represented as the nodes of a graph $\mathcal{G}$. The edges of $\mathcal{G}$ represent pairwise similarities between data points. Sometimes we can quantify the extent of these similarities by an edge weight [64], [75].

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

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

See also: clustering, data point, cluster, 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 ANNs, 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 [20], [76].

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

Hilbert space A Hilbert space is a complete inner product space [77]. 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, 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

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

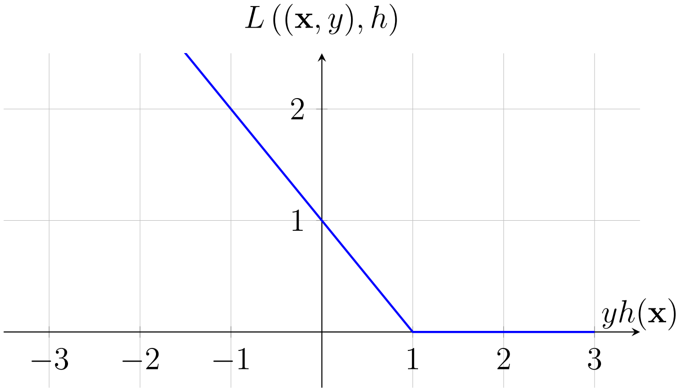


Fig. 20. The hinge loss incurred by the prediction $h(\mathbf{x}) \in \mathbb{R}$ for a data point with label $y \in \{-1, 1\}$. A regularized variant of the hinge loss is used by the support vector machine (SVM) [78].

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

histogram Consider a dataset $\mathcal{D}$ 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

Figure 21.

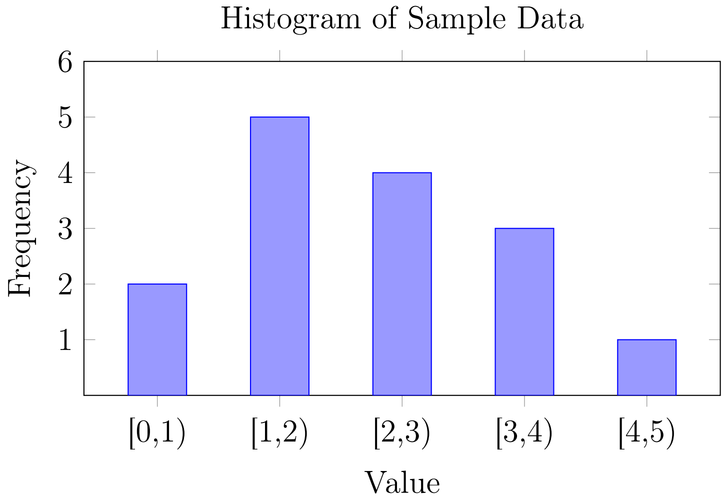


Fig. 21. A histogram representing the frequency of data points falling within discrete value ranges (i.e., bins). Each bar height shows the count of samples in the corresponding interval.

See also: dataset, data point, sample.

horizontal federated learning (HFL) HFL uses local datasets constituted by different data points but uses the same features to characterize them [79]. 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 charac-

terized 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 (having features $\mathbf{x}$ and label y).
See also: map, function, feature space, label space, data point, feature, label, prediction, ML.

hypothesis space Every practical ML method uses a hypothesis space (or model) $\mathcal{H}$. The hypothesis space of an ML method is a subset of all possible maps from the feature space to the label space. The design choice of the hypothesis space should take into account available computational resources and statistical aspects. If the computational infrastructure allows for efficient matrix operations, and there is an (approximately) linear relation between a set of features and a label, a useful choice for the hypothesis space might be the linear model.

See also: ML, hypothesis, model, map, feature space, label space, statistical aspects, feature, label, linear model.

independent and identically distributed (i.i.d.) It can be useful to interpret data points $\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(m)}$ as realizations of i.i.d. RVs with a common probability distribution. If these RVs are continuous-valued, their joint pdf is $p\big(\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(m)}\big) = \prod_{r=1}^{m} p\big(\mathbf{z}^{(r)}\big)$, with $p(\mathbf{z})$ being the common marginal pdf of the underlying RVs.

See also: data point, realization, RV, probability distribution, pdf.

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

See also: i.i.d., data point, dataset, 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 via the concept of simulatbility is via the concept of simulatability, i.e., the ability of a human to mentally simulate the model behavior [50, 80–83]. The idea is as follows: if a human user understands a ML method then they should

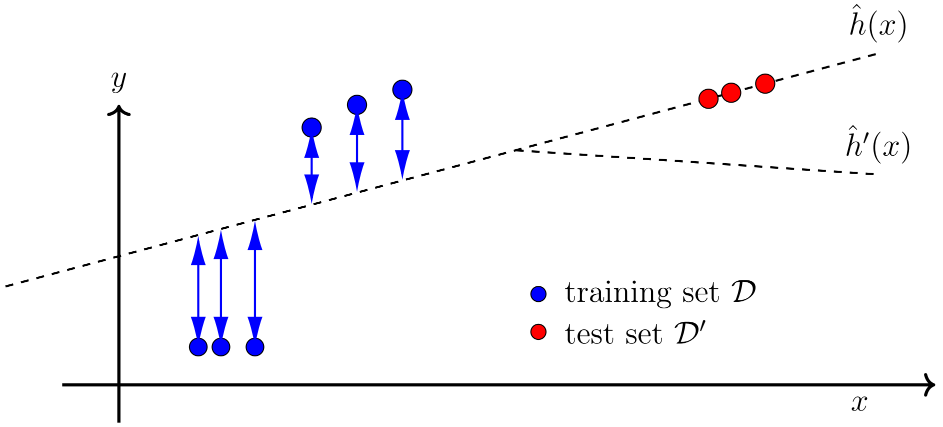


Fig. 22. We can assess the interpretability of trained ML models $\hat{h}$ and $\hat{h}'$ by comparing their predictions to pseudo-labels generated by a human user for $\mathcal{D}'$.

be able to anticipate its predictions on a test set. We illustrate such a test set in Figure 22 which also depicts two learned hypothesiss $\hat{h}$ 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. 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 Figure 22, interpretability of a ML method $\hat{h}$ requires that the human user can anticiapte 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 form 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 non-zero. Inverse matrices are fundamental in solving systems of linear equations and in the closed-form solution of linear regression [36], [84]. 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 generalized inverse matrix [3].

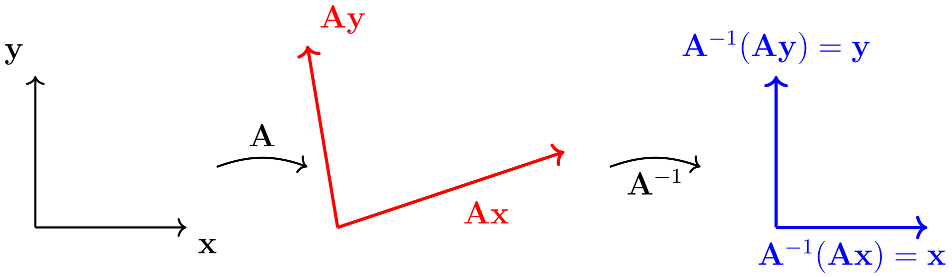

$\mathbf{y}$
$\mathbf{x}$
$\mathbf{A}$
$\mathbf{Ay}$
$\mathbf{Ax}$
$\mathbf{A}^{-1}$
$\mathbf{A}^{-1}(\mathbf{Ay}) = \mathbf{y}$
$\mathbf{A}^{-1}(\mathbf{Ax}) = \mathbf{x}$

Fig. 23. A matrix $\mathbf{A}$ represents a linear transformation of $\mathbb{R}^2$. The inverse matrix $\mathbf{A}^{-1}$ represents the inverse transformation.

See also: 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 non-zero main diagonal entries. The method constructs a sequence $\mathbf{x}^{(0)}, \mathbf{x}^{(1)}, \ldots$ by updating each entry of $\mathbf{x}^{(k)}$ according to

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

Carefully note that all entries $x_1^{(k)}, \ldots, x_d^{(k)}$ 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], [84], [85]. Jacobi-type methods are appealing for large linear systems due to their parallelizable structure [39]. 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 $\mathbf{x}^{(k+1)} = \mathbf{D}^{-1}(\mathbf{b} - \mathbf{R}\mathbf{x}^{(k)})$.

For example, for the linear equation

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

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, fixed-point iteration, optimization method.

kernel Consider data points characterized by a feature vector $\mathbf{x} \in \mathcal{X}$ with a generic feature space $\mathcal{X}$. A (real-valued) kernel $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ assigns each pair of feature vectors $\mathbf{x}, \mathbf{x}' \in \mathcal{X}$ a real number $K\big(\mathbf{x}, \mathbf{x}'\big)$. The value $K\big(\mathbf{x}, \mathbf{x}'\big)$ is often interpreted as a measure for the similarity between $\mathbf{x}$ and $\mathbf{x}'$. Kernel methods use a kernel to transform the feature vector $\mathbf{x}$ to a new feature vector $\mathbf{z} = K\big(\mathbf{x}, \cdot\big)$. This new feature vector belongs to a linear feature space $\mathcal{X}'$ which is (in general) different from the original feature space $\mathcal{X}$. The feature space $\mathcal{X}'$ has a specific mathematical structure, i.e., it is a reproducing kernel Hilbert space [57], [78].

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

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 $\mathbf{z} = K\big(\mathbf{x}, \cdot\big)$ [57], [78]. 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 classification 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 Figure 24).

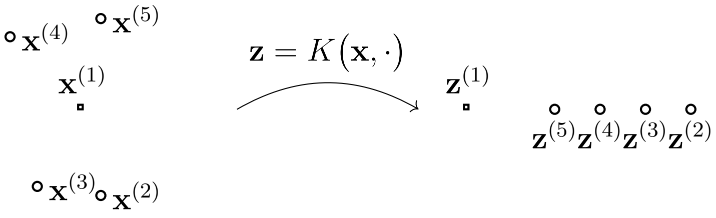

$\mathbf{x}^{(4)}$
$\mathbf{x}^{(5)}$
$\mathbf{x}^{(1)}$
$\mathbf{x}^{(3)}$
$\mathbf{x}^{(2)}$
$\mathbf{z} = K\big(\mathbf{x}, \cdot\big)$
$\mathbf{z}^{(1)}$
$\mathbf{z}^{(5)}\mathbf{z}^{(4)}\mathbf{z}^{(3)}\mathbf{z}^{(2)}$

Fig. 24. Five data points characterized by feature vectors $\mathbf{x}^{(r)}$ and labels $y^{(r)} \in \{\circ, \Box\}$, 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 $\mathbf{z}^{(r)} = K\big(\mathbf{x}^{(r)}, \cdot\big)$ 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 between two matries **A** and **B** as defined as...

Kullback-Leibler divergence (KL divergence) The KL divergence is a quantitative measure of how much one probability distribution is different from another probability distribution [28].
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" [54], [55], [56].
See also: data point.

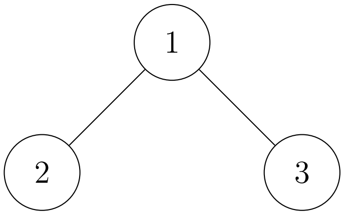
label space Consider an ML application that involves data points characterized by features and labels. The label space is constituted by all potential values that the label of a data point can take on. Regression methods, aiming at predicting numeric labels, often use the label space $\mathcal{Y} = \mathbb{R}$. Binary classification methods use a label space that consists of two different elements, e.g., $\mathcal{Y} = \{-1, 1\}$, $\mathcal{Y} = \{0, 1\}$, or $\mathcal{Y} = \{\text{“cat image”}, \text{“no cat image”}\}$.
See also: ML, data point, feature, label, regression, classification.

labeled datapoint A data point whose label is known or has been determined by some means which 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 [75], [86]. It is defined element-wise as (see Figure 25)

$$L^{(\mathcal{G})}_{i,i'} := \begin{cases} -A_{i,i'} & \text{for } i \neq i', \{i, i'\} \in \mathcal{E}, \\ \sum_{i'' \neq i} A_{i,i''} & \text{for } i = i', \\ 0 & \text{else.} \end{cases} \tag{8}$$

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



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

Fig. 25. Left: Some undirected graph $\mathcal{G}$ with three nodes $i = 1, 2, 3$. Right: The Laplacian matrix $\mathbf{L}^{(\mathcal{G})} \in \mathbb{R}^{3\times 3}$ of $\mathcal{G}$.

See also: graph, edge weight.

large language model (LLM) LLMs is an umbrella term for ML methods that process and generate human-like 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 [87]. 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 datapoints simply by selecting some words of a 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 datapoint.

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 [65].

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

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 dataset $\mathcal{D}$ constituted by several data points, each of them characterized by features $\mathbf{x}$. For example, the dataset $\mathcal{D}$ might be constituted by the images of a particular database. Sometimes it might be useful to represent a dataset $\mathcal{D}$, along with the choice of features, by a probability distribution $p(\mathbf{x})$. A learning task associated with $\mathcal{D}$ consists of a specific choice for the label of a data point and the corresponding label space. Given a choice for the loss function and model, a learning task gives rise to an instance of ERM. Thus, we could define a learning task also via an instance of ERM, i.e., via an objective function. Note that, for the same dataset, we obtain different learning tasks by using different choices for the features and label of a data point. These learning tasks are related, as they are based on the same dataset, and solving them jointly (via multitask learning methods) is typically preferable over solving them separately [88], [89], [90].

See also: dataset, data point, feature, probability distribution, label, label space, loss function, model, ERM, objective function, multitask learning.

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 $h(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$ based on a training set. Lasso is obtained from linear regression by adding the scaled ℓ_1-norm $\alpha \left\|\mathbf{w}\right\|_1$ 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 classifier 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, classifier, 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, 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

$$\mathcal{H}^{(d)} := \left\{ h : \mathbb{R}^d \to \mathbb{R} \mid h(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} \text{ for some } \mathbf{w} \in \mathbb{R}^d \right\}. \tag{9}$$

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 by computational aspects (e.g., fewer features reduce computation), statistical aspects (e.g., more features typically reduce bias, risk) but also interpretability. A linear model using a small number of well-chosen features is generally considered more interpretable [51], [58]. The linear model is attractive because it can typically be trained using scalable convex optimization methods [16], [91]. Moreover, linear models often permit rigorous statistical analysis, including fundamental limits on the minimum achievable risk [20]. They are also useful for analyzing more complex, non-linear models such as ANNs.

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 $g(\mathbf{x})$. Figure 26 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 [92, Th. 3.1].

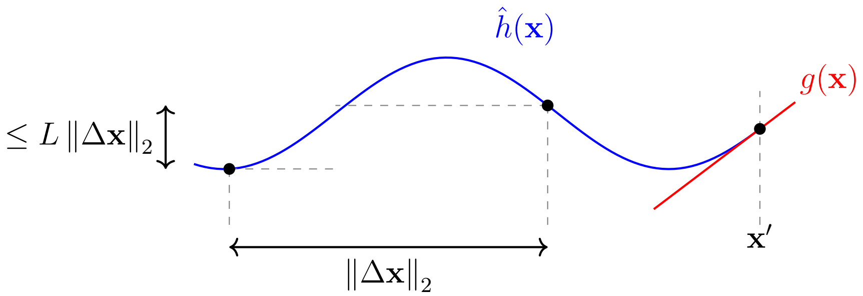


Fig. 26. A trained model $\hat{h}(\mathbf{x})$ that is differentiable at a point $\mathbf{x}'$ can be locally approximated by a linear map $g \in \mathcal{H}^{(d)}$. This local approximation is determined by the gradient $\nabla \hat{h}(\mathbf{x}')$.

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 datapoints, which we refer to as the training set.

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

local dataset The concept of a local dataset is in between the concept of a data point and a dataset. A local dataset consists of several individual data points, which are characterized by features and labels. In contrast to a single dataset used in basic ML methods, a local dataset is also related to other local datasets 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: dataset, 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 $\mathbf{x}^{(0)}$ [58]. The explanation is given in the form of a local approximation $g \in \mathcal{H}'$ of $\widehat{h}$ (see Figure 27). 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 vector $\mathbf{x}$ close to $\mathbf{x}^{(0)}$ 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.

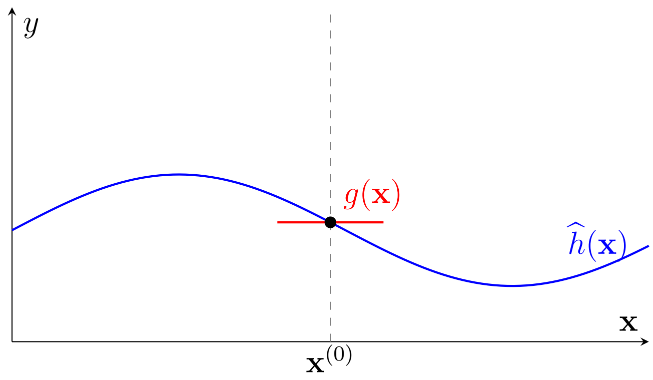


Fig. 27. To explain a trained model $\widehat{h} \in \mathcal{H}$, around a given feature vector $\mathbf{x}^{(0)}$, we can use a local approximation $g \in \mathcal{H}'$.

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 might be assigned 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

$$L\left((\mathbf{x}, y), h\right) := \log(1 + \exp(-yh(\mathbf{x}))). \tag{10}$$

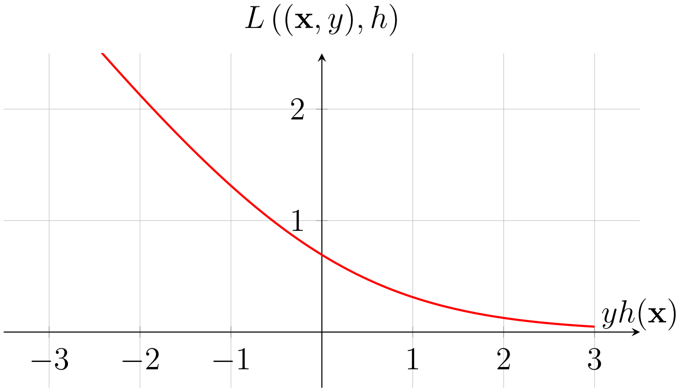


Fig. 28. The logistic loss incurred by the prediction $h(\mathbf{x}) \in \mathbb{R}$ for a data point with label $y \in \{-1, 1\}$.

Carefully note that the expression (10) 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 classifier) $h(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$ 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 datapoints (i.e., the training set).

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

loss ML methods use a loss function $L(\mathbf{z}, h)$ 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 $L(\mathbf{z}, h)$, for a data point $\mathbf{z}$ and hypothesis h.

See also: ML, loss function, hypothesis, data point.

loss function A loss function is a map

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

It assigns a non-negative real number (i.e., the loss) $L((\mathbf{x}, y), h)$ 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 $L((\mathbf{x}, y), h)$ quantifies the discrepancy between the true label y and the prediction $h(\mathbf{x})$. Lower (closer to zero) values $L((\mathbf{x}, y), h)$ indicate a smaller discrepancy between prediction $h(\mathbf{x})$ and label y. Figure 29 depicts a loss function for a given data point, with features $\mathbf{x}$ and label y, as a function of the hypothesis $h \in \mathcal{H}$.

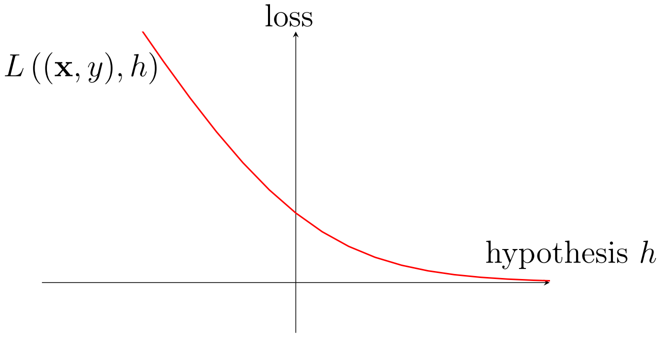


Fig. 29. Some loss function $L((\mathbf{x}, y), h)$ for a fixed data point, with feature vector $\mathbf{x}$ and label y, and a varying hypothesis h. ML methods try to find (or learn) a hypothesis that incurs minimal loss.

See also: loss, function, map, data point, feature, label, hypothesis, prediction, feature vector, ML.

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], [93]. 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: label, feature, data point, hypothesis, hypothesis space, model, loss function, ERM.

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

See also: function.

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 $\mathcal{D} = \{\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(m)}\}$ 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 dataset. 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, probabilistic model, optimization problem.

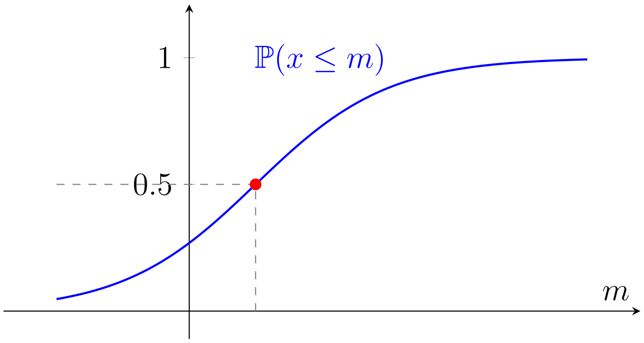
mean The mean of an RV $\mathbf{x}$, taking values in an Euclidean space $\mathbb{R}^d$, is its expectation $\mathbb{E}\{\mathbf{x}\}$. It is defined as the Lebesgue integral of $\mathbf{x}$ with respect to the underlying probability distribution P (e.g., see [2] or [6]), i.e.,

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

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

$$\mathbb{E}\{\mathbf{x}\} = \operatorname*{argmin}_{\mathbf{c} \in \mathbb{R}^d} \mathbb{E}\big\{ \|\mathbf{x} - \mathbf{c}\|_2^2 \big\}.$$

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



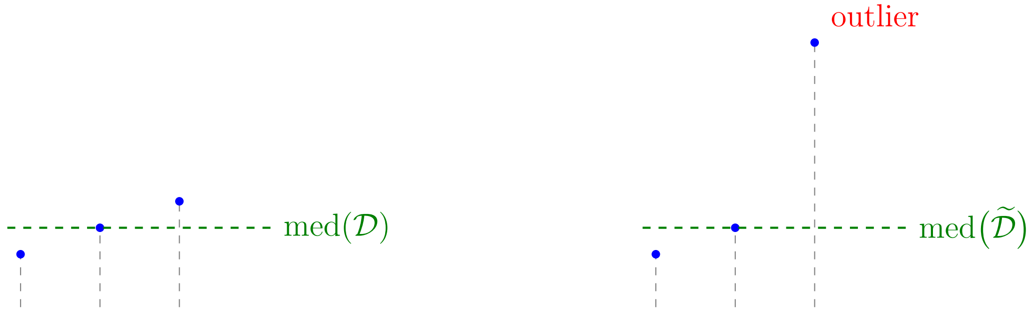
same. Indeed, we can use the sequence $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)} \in \mathbb{R}^d$ to construct a discrete RV $\widetilde{\mathbf{x}} = \mathbf{x}^{(I)}$, with the index I being chosen uniformly at random from the set $\{1, \ldots, m\}$. The mean of $\widetilde{\mathbf{x}}$ is precisely the average $\frac{1}{m}\sum_{r=1}^{m} \mathbf{x}^{(r)}$.

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 dataset $\mathcal{D}$. 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 [13], [41].

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

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 $\mathbb{P}(x \geq m) \geq 1/2$ [13]. We can define the median $\mathrm{med}(\mathcal{D})$ of a dataset $\mathcal{D} = \{x^{(1)}, \ldots, x^{(m)} \in \mathbb{R}\}$ via a specific RV $\tilde{x}$ that is naturally associated with $\mathcal{D}$. In particular, this RV is constructed



(a) Original dataset $\mathcal{D}$.

(b) Noisy dataset $\widetilde{\mathcal{D}}$ including an outlier.

Fig. 30. The median is robust against outlier contamination.

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

See also: mean, robustness, outlier.

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 non-negative, 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 accuracy, precision, and the average 0/1 loss on a test set [35], [43]. A loss function is used to train models, while a metric is used to compare trained models.
See also: ML, model, accuracy, 0/1 loss, test set, loss function, loss, model selection.

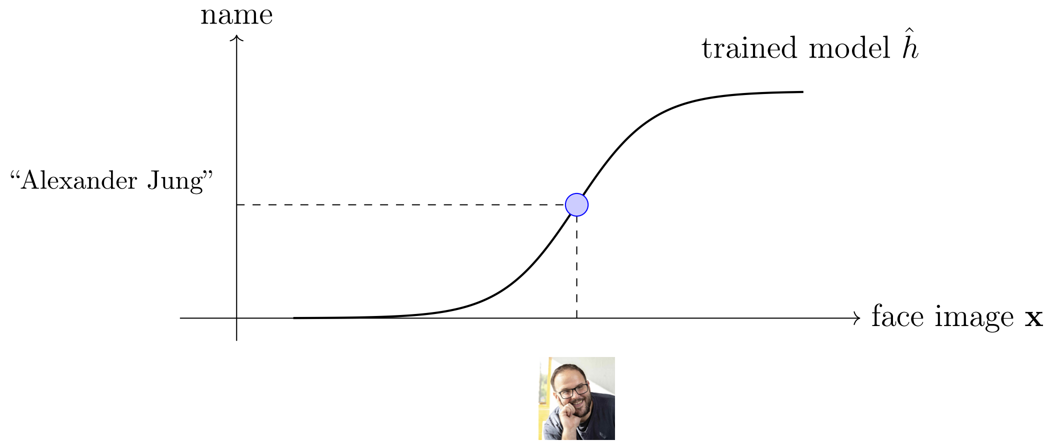
minimum Given a set of real numbers, the minimum is the smallest of those numbers. Note that for some sets, such as the set of negative real numbers, the minimum does not exist.

missing data Consider a dataset 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 at estimating these missing values [94]. 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: dataset, data point, device, feature, label, data, ML.

model In the context of ML, the term model typically refers to the hypothesis space underlying an ML method [8], [69]. However, the term is also used in other fields but with a different meaning. For example, a probabilistic model refers to a parametrized set of probability distributions.
See also: ML, hypothesis space, probabilistic model, probability distri-

bution.

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 $\hat{h}(\mathbf{x})$ on carefully chosen inputs. Basic model inversion techniques have been demonstrated in the context of facial image classification, where images are reconstructed using the (gradient of) model outputs combined with auxiliary information such as a person's name [95].



See also: model, privacy attack, ML, sensitive attribute, data point, prediction, classification, 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-armed bandit (MAB) A MAB problem models a repeated decision-making scenario in which, at each time step k, a learner must choose one out of several possible actions, often referred to as arms, from a finite set $\mathcal{A}$. Each arm $a \in \mathcal{A}$ yields a stochastic reward $r^{(a)}$ drawn from an unknown probability distribution with mean $\mu^{(a)}$. The learner's goal is to 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). This balance is quantified by the notion of regret, which measures the performance gap between the learner's strategy and the optimal strategy that always selects the best arm. MAB problems form a foundational model in online learning, reinforcement learning, and sequential experimental design [96].

See also: stochastic, reward, probability distribution, mean, regret, model.

multi-label classification Multi-label classification 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, classification, data point.

multitask learning Multitask learning aims at leveraging relations between different learning tasks. Consider two learning tasks obtained from the same dataset 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 might 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, dataset, deep net, weights.

multivariate normal distribution The multivariate normal distribution, which is denoted $\mathcal{N}(\boldsymbol{\mu}, \mathbf{\Sigma})$, 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], [15], [66]. Each distribution in this family is fully specified by its mean vector $\boldsymbol{\mu} \in \mathbb{R}^d$ and covariance matrix $\mathbf{\Sigma} \in \mathbb{R}^{d \times d}$. When the covariance matrix $\mathbf{\Sigma}$ is invertible, its probability distribution is fully characterized by the following pdf:

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

Note that the pdf is only defined when $\mathbf{\Sigma}$ is invertible. More generally, any RV $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{\Sigma})$ admits the following innovation 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 $\mathbf{A}\mathbf{A}^T = \mathbf{\Sigma}$. This innovation representation is valid even when the covariance matrix $\mathbf{\Sigma}$ is singular, in which case $\mathbf{A}$ is not necessarily full-rank [97, 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.,

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

Second, the probability distribution $\mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$ maximizes the differential entropy among all distributions with the same covariance matrix $\mathbf{\Sigma}$ [28].

See also: probabilistic model, feature vector, probability distribution, RV, covariance matrix, pdf, standard normal vector, Gaussian RV, mean, entropy.

mutual information (MI) The MI $I(\mathbf{x}; y)$ between two RVs $\mathbf{x}$, y defined on the same probability space is given by [28]

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

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 $h : \mathcal{X} \rightarrow \mathcal{Y}$ whose function value $h(\mathbf{x})$ is solely determined by the NNs within a given dataset. 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, dataset, data point, feature vector, neighbors.

neighborhood The neighborhood of a node $i \in \mathcal{V}$ is the subset of nodes constituted by the neighbors of i.

See also: neighbors.

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 consists 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 edges encode pairwise similarities. One example of networked data arises 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 [98].

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 [99].

See also: function, smooth.

norm A norm is a function that maps each (vector) element of a vector space to a non-negative real number. This function must be homogeneous and definite, and it must satisfy the triangle inequality [37].

See also: function, vector space.

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 Figure 31). 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.

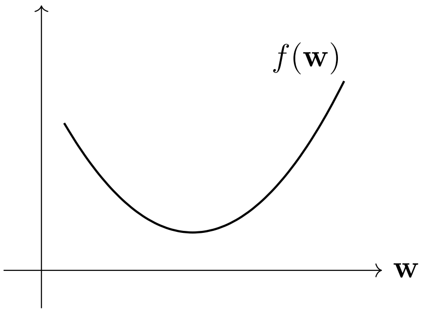


Fig. 31. An objective function maps each possible value $\mathbf{w}$ of an optimization variable, such as the model parameters of an ML model, to a value that measures the usefulness of $\mathbf{w}$.

See also: function, map, ML, model parameters, hypothesis, risk, loss, empirical risk, training set, gradient-based methods, minimum, maximum, model, loss function.

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 [45], [46]. 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 also represent an online algorithm formally as a collection of possible executions. However, the execution sequence for an online algorithm has a distinct structure:

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

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

$$\mathbf{w}^{(t+1)} := P_{\mathcal{W}}\big(\mathbf{w}^{(t)} - \eta_t \nabla_{\mathbf{w}} L\left(\mathbf{z}^{(t)}, \mathbf{w}\right)\big). \tag{11}$$

Note that (11) is a gradient step for the current component $L\left(\mathbf{z}^{(t)}, \cdot\right)$ of the risk. The update (11) ignores all the previous components $L\left(\mathbf{z}^{(t')}, \cdot\right)$, for $t' < t$. It might therefore happen that, compared to $\mathbf{w}^{(t)}$, 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 [46], [100].

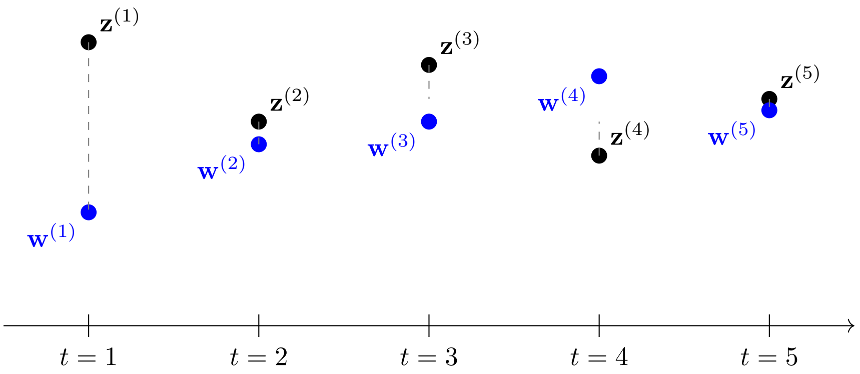


Fig. 32. An instance of online GD that updates the model parameters $\mathbf{w}^{(t)}$ using the data point $\mathbf{z}^{(t)} = x^{(t)}$ arriving at time t. This instance uses the squared error loss $L\left(\mathbf{z}^{(t)}, w\right) = (x^{(t)} - w)^2$.

See also: ML, model parameters, parameter space, data point, i.i.d., RV, risk, hypothesis, objective function, GD, gradient step, loss, learning rate, squared error loss.

online learning Some ML methods are designed to process data in a sequential manner, updating their model parameters as new data points become available—one at a time. A typical example is time series data, such as daily minimum and maximum temperatures recorded by a FMI weather station. These values form a chronological sequence of observations. In online learning, the hypothesis (or its model parameters) is refined incrementally with each newly observed data point, without revisiting past data.

See also: ML, data, model parameters, data point, FMI, hypothesis, 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 approximation) $f(\mathbf{w})$ of $\bar{f}(\mathbf{w})$. As a case in point, ERM-based methods use the average loss on a given dataset (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. Two examples of ML methods that use such an optimistic construction of an objective function are SRM [69, Ch. 11] and upper confidence bound (UCB) methods for sequential decision making [96, Sec. 2.2].

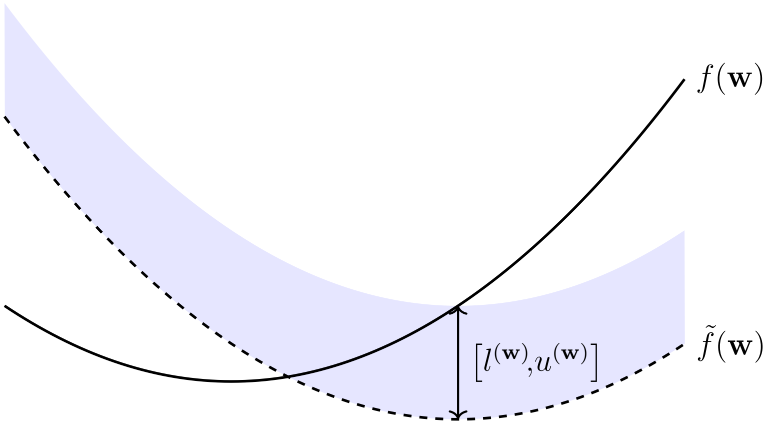


Fig. 33. ML methods learn model parameters $\mathbf{w}$ by using some estimate of $f(\mathbf{w})$ for the ultimate performance criterion $\bar{f}(\mathbf{w})$. Using a probabilistic model, one can use $f(\mathbf{w})$ to construct confidence intervals $\left[l^{(\mathbf{w})}, u^{(\mathbf{w})}\right]$ 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, dataset, 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 [21], [99], [91].

See also: algorithm, optimization problem.

optimization problem An optimization problem is a mathematical structure consisting of an objective function $f : \mathcal{U} \rightarrow \mathcal{V}$ 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 [21], [99], [91].

See also: objective function.

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) [101]. However, in some applications the data consists of a majority of regular data points that conform with an i.i.d. assumption as well as a small number of data points that have fundamentally different statistical properties compared to 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 [102], [103].

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

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 small empirical risk on the training set but a significantly larger loss outside the training set.

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

parameter The parameter of an ML model is a tunable (i.e., learnable or adjustable) quantity that allowa 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 Figure 34). Many important ML methods use a model that is parametrized by vectors of the Euclidean space $\mathbb{R}^d$. Two widely used examples of parametrized 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.

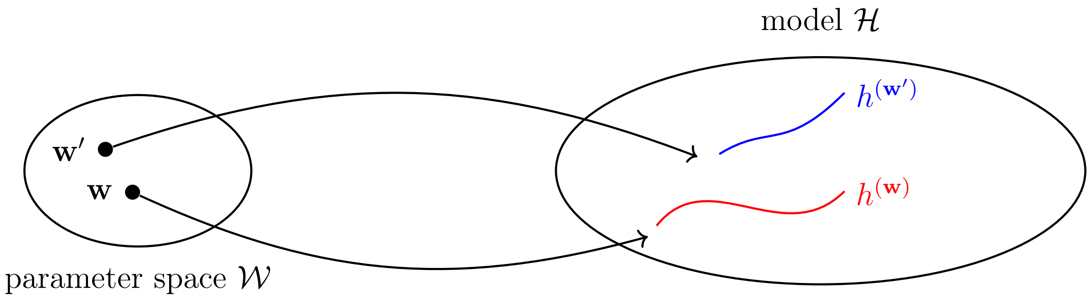


Fig. 34. The parameter space $\mathcal{W}$ of an ML model $\mathcal{H}$ consists of all feasible choices for the model parameters. Each choice $\mathbf{w}$ for the model parameters selects a hypothesis map $h^{(\mathbf{w})} \in \mathcal{H}$.

See also: parameter, model, model parameters.

polynomial regression Polynomial regression is an ERM-based methods 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 $\mathcal{H}_d^{(\mathrm{poly})} := \{h(x) = \sum_{j=0}^{d-1} x^j w_j\}$. The quality of a polynomial hypothesis map is measured using the average squared error loss incurred on a set of labeled datapoints (which we refer to as the training set).
See also: regression, squared error loss, ERM.

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 $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ (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 [57].

See also: 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.

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 [104].

See also: feature, data point.

privacy leakage Consider an ML application that processes a dataset $\mathcal{D}$ 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 (which might be a human) of $\mathcal{D}$. 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 [105]).

See also: ML, dataset, prediction, data point, feature, probabilistic model, data, MI, DP.

privacy protection Consider some ML method $\mathcal{A}$ that reads in a dataset $\mathcal{D}$ 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, dataset, 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 which have to be manually chosen or learned via statistical inference methods such as maximum likelihood estimation [13].

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 reduces the task of dimensionality reduction to an estimation problem that can be solved using EM [106].

See also: PCA, probabilistic model, EM.

probability We assign a probability value, typically chosen in the interval $[0, 1]$, to each event that might occur in a random experiment [6], [7], [42], [107].

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.

probability distribution To analyze ML methods, it can be useful to in-

terpret 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], [15].
See also: i.i.d., realization, RV, probability, pdf.

probability space A probability space is a mathematical model of a physical process (i.e., a random experiment) with an uncertain outcome. Formally, a probability space $\mathcal{P}$ is a triplet $(\Omega, \mathcal{F}, P)$ where

- Ω is a sample space containing all possible elementary outcomes of a random experiment;
- $\mathcal{F}$ is a sigma-algebra, i.e., a collection of subsets of Ω (called events) that satisfies certain closure properties under set operations;
- P is a probability measure, i.e., a function that assigns a probability $P(\mathcal{A}) \in [0, 1]$ to each event $\mathcal{A} \in \mathcal{F}$. The function must satisfy $P(\Omega) = 1$ and $P\left(\bigcup_{i=1}^{\infty} \mathcal{A}_i\right) = \sum_{i=1}^{\infty} P(\mathcal{A}_i)$ for any countable sequence of pairwise disjoint events $\mathcal{A}_1, \mathcal{A}_2, \ldots$ in $\mathcal{F}$.

Probability spaces provide the foundation for defining RVs and to reason about uncertainty in ML applications [6], [15], [68].
See also: probability, model, sample, function, RV, uncertainty, ML.

projected gradient descent (projected GD) Consider an ERM-based method that uses a parametrized 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 contraints on the optimization variable (i.e., the model parameters). Projected GD extends basic GD to handle constraints on the optimization variable (i.e., the model parameters). A single iteration of projected GD consists of first taking a gradient step and then projecting the result back onto the parameter space.

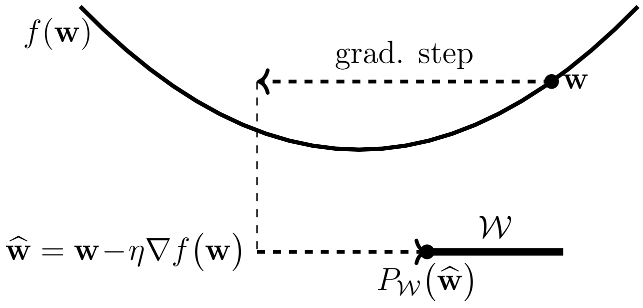

$f(\mathbf{w})$
grad. step
$\mathbf{w}$
$\widehat{\mathbf{w}} = \mathbf{w} - \eta \nabla f(\mathbf{w})$
$\mathcal{W}$
$P_{\mathcal{W}}(\widehat{\mathbf{w}})$

Fig. 35. 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

$$P_{\mathcal{W}}(\mathbf{w}) = \underset{\mathbf{w}' \in \mathcal{W}}{\operatorname{argmin}} \|\mathbf{w} - \mathbf{w}'\|_2 \,. \tag{12}$$

In other words, $P_{\mathcal{W}}(\mathbf{w})$ is the vector in $\mathcal{W}$ which is closest to $\mathbf{w}$. The projection is only well-defined for subsets $\mathcal{W}$ for which the above minimum exists [21].

See also: Euclidean space, minimum.

proximable A convex function for which the proximal operator can be computed efficiently is sometimes referred to as proximable or simple [108].

See also: convex, function, proximal operator.

proximal operator Given a convex function $f(\mathbf{w}')$, we define its proximal operator as [63], [61]

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

As illustrated in Figure 36, 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 $\rho = 1/\eta$.

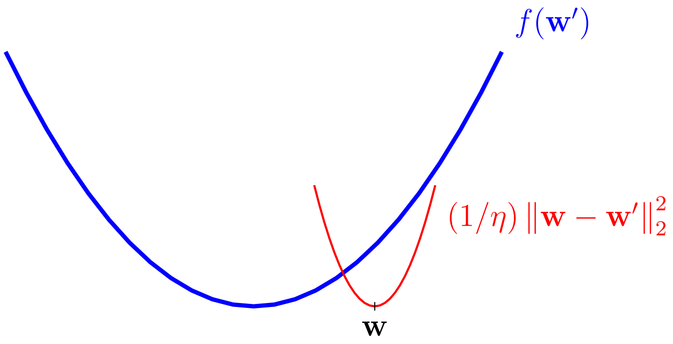


Fig. 36. A generalized gradient step updates a vector $\mathbf{w}$ by minimizing a penalized version of the function $f(\cdot)$. The penalty term is the scaled squared Euclidean distance between the optimization variable $\mathbf{w}'$ and the given vector $\mathbf{w}$.

See also: convex, function, 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 dataset with arbitrary labels $\mathbf{y}$ and a feature matrix $\mathbf{X} = \mathbf{A}$ [16, 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 [109, Ch. 3]

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

See also: inverse matrix, ridge regression, dataset, label, feature matrix, model parameters, ridge regression.

quadratic function A function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ 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.

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 dataset.
See also: decision tree, dataset.

random variable (RV) An RV is a function that maps from a probability space $\mathcal{P}$ to a value space [6], [15]. The probability space consists of elementary events and is equipped with a probability measure that assigns probabilities to subsets of $\mathcal{P}$. Different types of RVs include

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

Probability theory uses the concept of measurable spaces to rigorously define and study the properties of (large) collections of RVs [6].

See also: function, probability space, probability, Euclidean space.

realization Consider an RV x which maps each element (i.e., outcome or elementary event) $\omega \in \mathcal{P}$ of a probability space $\mathcal{P}$ to an element a of a measurable space $\mathcal{N}$ [2], [6], [42]. A realization of x is any element $a' \in \mathcal{N}$ such that there is an element $\omega' \in \mathcal{P}$ with $x(\omega') = a'$.

See also: RV, probability space.

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 baseline, is the difference between the loss incurred by h and the loss incurred by h' [45]. The baseline hypothesis h' is also referred to as an expert.

See also: baseline, 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 performs not 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 larger the expected loss (or risk) is compared to 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.

Figure 37 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.

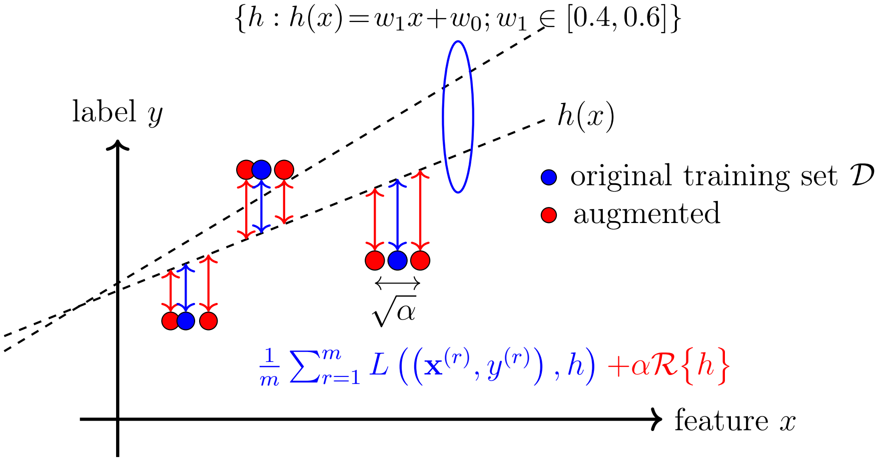

$\{h : h(x)=w_1x+w_0; w_1 \in [0.4, 0.6]\}$
label y
$h(x)$
● original training set $\mathcal{D}$
● augmented
$\sqrt{\alpha}$
$\frac{1}{m}\sum_{r=1}^{m} L\left(\left(\mathbf{x}^{(r)}, y^{(r)}\right), h\right) + \alpha\mathcal{R}\{h\}$
feature x

Fig. 37. 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 $\mathcal{R}\{h\}$ in the learning objective. This leads to RERM such that

$$\hat{h} \in \operatorname*{argmin}_{h \in \mathcal{H}} \widehat{L}\big(h|\mathcal{D}\big) + \alpha\mathcal{R}\{h\}. \tag{13}$$

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 $\mathcal{R}\{h\}$. The component $\alpha\mathcal{R}\{h\}$ in the objective function of (13) 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 $\mathcal{R}\{h\} = \|\mathbf{w}\|_2^2$. In this setting, $\alpha\mathcal{R}\{h\}$ 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 $\mathcal{R}\{h\}$ arises from approximate upper bounds on the generalization error. The resulting RERM instance is known as SRM [110, Sec. 7.2].

See also: ERM, hypothesis, model, empirical risk, training set, overfitting, regularization, regularizer, parameter, objective function, loss, label, data point, linear model, squared error loss, Gaussian RV, feature vector, generalization, SRM.

regularized loss minimization (RLM) See RERM.

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

See also: hypothesis, hypothesis space, prediction, training set, data point, ridge regression, map, Lasso.

Rényi divergence The Rényi divergence measures the (dis)similarity between two probability distributions [111].

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 towards an obstacle. We define a low reward for the steering direction $h(\mathbf{x})$ if the vehicle moves dangerously towards an obstacle.

See also: loss, prediction, hypothesis, ML.

ridge regression Ridge regression learns the weights $\mathbf{w}$ of a linear hypothesis map $h^{(\mathbf{w})}(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$. The quality of a particular choice for the model parameters $\mathbf{w}$ is measured by the sum of two components. The first component is the average squared error loss incurred by $h^{(\mathbf{w})}$ on a set of labeled datapoints (i.e., the training set). The second component is the scaled squared Euclidean norm $\alpha\|\mathbf{w}\|_2^2$ with a regularization parameter $\alpha > 0$. Adding $\alpha\|\mathbf{w}\|_2^2$ to the average squared error loss is equivalent to replacing original data points by the realizations of (infinitely many) i.i.d. RVs centered around these data points (see regularization).

See also: regression, weights, hypothesis, map, model parameters, squared error loss, labeled datapoint, training set, norm, regularization, parameter, data point, realization, i.i.d., RV.

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, also the $L\left((\mathbf{x}, y), h\right)$ 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 can be to 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, ML, feature, data point, prediction, model, stability, ERM, training set, data poisoning, attack.

sample A finite sequence (or list) of data points $\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(m)}$ that is obtained or interpreted as the realization of m i.i.d. RVs with a common probability distribution $p(\mathbf{z})$. The length m of the sequence is referred to as the sample size.

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

sample covariance matrix The sample covariance matrix $\widehat{\mathbf{\Sigma}} \in \mathbb{R}^{d \times d}$ for a given set of feature vectors $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)} \in \mathbb{R}^{d}$ is defined as

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

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

See also: sample, covariance matrix, feature vector, sample mean.

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

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

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

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

See also: data point, dataset.

scatterplot A visualization technique that depicts data points by markers in a two-dimensional plane. Figure 38 depicts an example of a scatterplot.

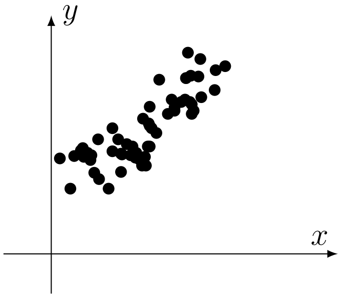


Fig. 38. A scatterplot with circle markers, where the data points represent daily weather conditions in Finland. Each data point is characterized by its minimum daytime temperature x as the feature and its maximum daytime temperature y as the label. The temperatures have been measured at the FMI weather station Helsinki Kaisaniemi during 1.9.2024 - 28.10.2024.

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 datapoints [19]. This approach is particularly useful for ML applications that offer a large amount of unlabeled data points, but only a limited number of labeled datapoints.
See also: data point, hypothesis, labeled datapoint, 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 r-th 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 non-zero along the main diagonal, whose entries $\Lambda_{j,j}$ are non-negative and referred to as singular values.

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 $\mathbf{w} \in \mathbb{R}^{d}$ [99], [112]. 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 amount of 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 Figure 39).

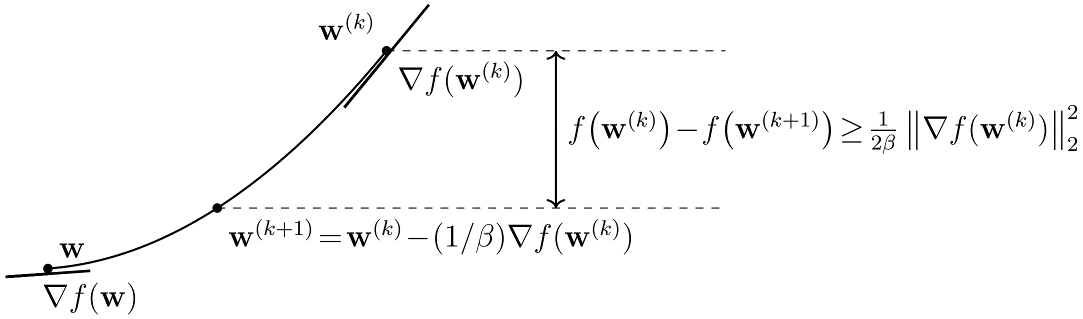

$\mathbf{w}^{(k)}$
$\nabla f(\mathbf{w}^{(k)})$
$f\big(\mathbf{w}^{(k)}\big) - f\big(\mathbf{w}^{(k+1)}\big) \geq \frac{1}{2\beta} \left\|\nabla f(\mathbf{w}^{(k)})\right\|_2^2$
$\mathbf{w}$
$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - (1/\beta)\nabla f(\mathbf{w}^{(k)})$
$\nabla f(\mathbf{w})$

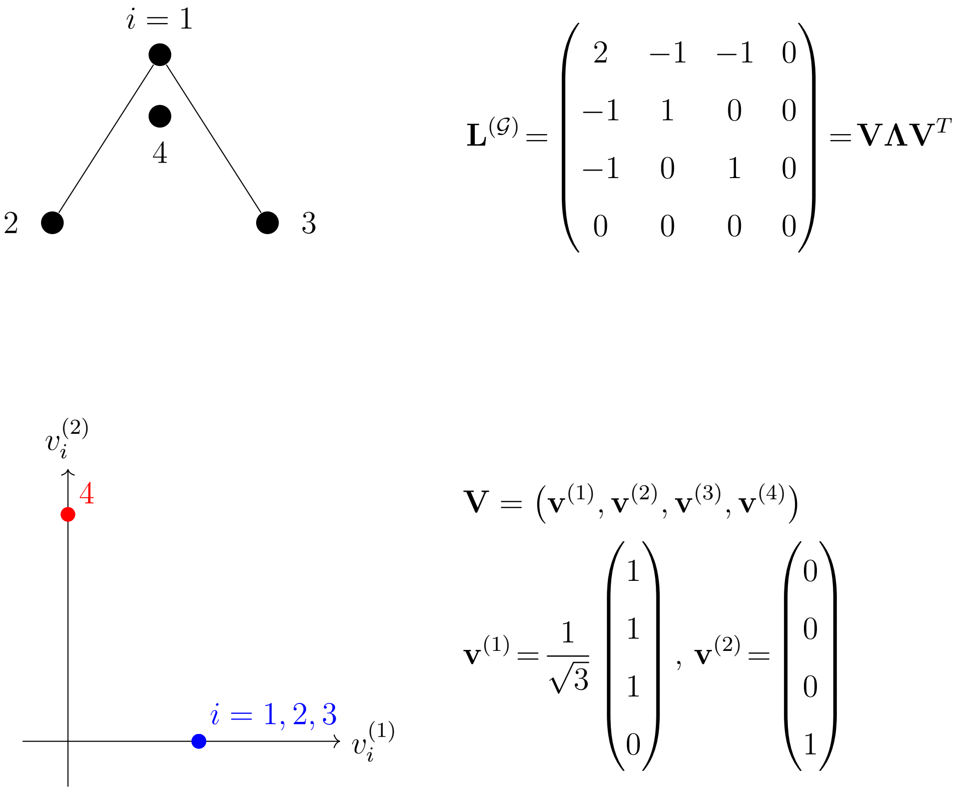
Fig. 39. Consider an objective function $f(\mathbf{w})$ that is β-smooth. Taking a gradient step, with step size $\eta = 1/\beta$, decreases the objective by at least $\frac{1}{2\beta} \left\|\nabla f(\mathbf{w}^{(k)})\right\|_2^2$ [99], [112], [113]. Note that the step size $\eta = 1/\beta$ becomes 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, optimization problem, objective function, gradient-based methods, gradient step, step size.

soft clustering Soft clustering refers to the task of partitioning a given set of data points into (a few) overlapping clusters. Each data point is

assigned to several different clusters with varying degrees of belonging. Soft clustering methods determine the degree of belonging (or soft cluster assignment) for each data point and each cluster. A principled approach to soft clustering is by interpreting data points as i.i.d. realizations of a GMM. We then obtain a natural choice for the degree of belonging as the conditional probability of a data point belonging to a specific mixture component.
See also: clustering, data point, cluster, degree of belonging, i.i.d., realization, GMM, probability.

spectral clustering Spectral clustering 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 clustering 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 clustering methods, such as k-means or soft clustering via GMM. Roughly speaking, the feature vectors of nodes belonging to a well-connected subset (or cluster) of nodes in $\mathcal{G}$ are located nearby in the Euclidean space $\mathbb{R}^d$ (see Figure 40).



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

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

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

Fig. 40. **Top.** Left: An undirected graph $\mathcal{G}$ with four nodes $i = 1, 2, 3, 4$, each representing a data point. Right: The Laplacian matrix $\mathbf{L}^{(\mathcal{G})} \in \mathbb{R}^{4 \times 4}$ and its EVD. **Bottom.** Left: A scatterplot of data points using the feature vectors $\mathbf{x}^{(i)} = \left(v_i^{(1)}, v_i^{(2)}\right)^T$. Right: 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: clustering, 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) [114]. Figure 41 depicts a time signal along with its spectrogram.

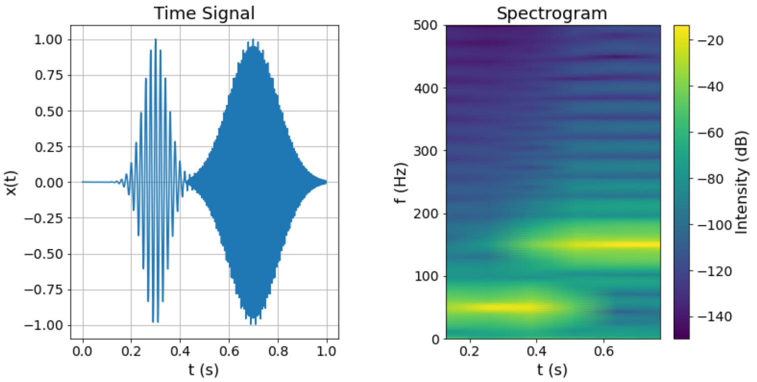


Fig. 41. Left: A time signal consisting of two modulated Gaussian pulses. Right: An intensity plot of the spectrogram.

The intensity plot of its spectrogram can serve as an image of a signal. A simple recipe for audio signal classification is to feed this signal image into deep nets originally developed for image classification and object detection [115]. It is worth noting that, beyond the spectrogram, several alternative representations exist for the time-frequency distribution of signal energy [116], [117].

See also: classification, 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 dataset $\mathcal{D}$ (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 dataset $\mathcal{D}$ 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 [69, Ch. 13]). To build intuition, consider the three datasets depicted in Figure 42, 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 datasets. 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.

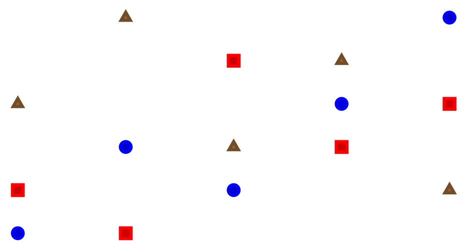


Fig. 42. Three datasets $\mathcal{D}^{(*)}$, $\mathcal{D}^{(\square)}$, and $\mathcal{D}^{(\triangle)}$, each sampled independently from the same data-generating probability distribution. A stable ML method should return similar outputs when trained on any of these datasets.

See also: ML, dataset, 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: 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 reducing computational complexity (see, e.g., SGD) or to capture uncertainty in probabilistic models.

See also: uncertainty, probabilistic model, SGD.

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 process, i.e., the possible execution sequence is the possible outcomes of a random experiment [7], [118], [119].

See also: stochastic, algorithm, SGD, data point, gradient, objective function, 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 $\mathcal{V}$ [120]. In its most basic variant, the SBM generates a graph by first randomly assigning each node $i \in \mathcal{V}$ to a cluster 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, cluster, 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 parametrized 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 all over the planet). 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 Figure 43). 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 [121].

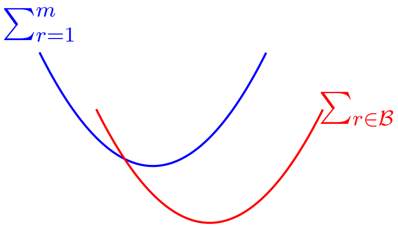


Fig. 43. SGD for ERM approximates the gradient $\sum_{r=1}^{m} \nabla_{\mathbf{w}} L\left(\mathbf{z}^{(r)}, \mathbf{w}\right)$ by replacing the sum over all data points in the training set (indexed by $r = 1, \ldots, m$) with a sum over a randomly chosen subset $\mathcal{B} \subseteq \{1, \ldots, m\}$.

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

stochastic process A stochastic process is a collection of RVs defined over a common probability space. These RVs are indexed by time or space,

which are used to model random phenomena evolving over time (e.g., noise in sensors or financial time series). Random graphs, such as stochastic block model (SBM) or Erdős-Rényi (ER) graph, are another example of stochastic processes. These processes use pairs of nodes in a graph as the index set. We can also use stochastic processes to represent stochastic algorithms such as SGD.
See also: SGD, uncertainty, probabilistic model, RV, SBM.

stopping criterion Many ML methods use iterative algorithms 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 $f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^T(\mathbf{y}-\mathbf{x}) + (\sigma/2)\left\|\mathbf{y}-\mathbf{x}\right\|_2^2$ [99], [113, 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 [69, 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 $f(\mathbf{w}) \geq f(\mathbf{w}') + \big(\mathbf{w} - \mathbf{w}'\big)^T \mathbf{a}$ is referred to as a subgradient of f at $\mathbf{w}'$ [40], [91].
See also: function.

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, also 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 classification 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 Figure 44, 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) [43], [78], [122].

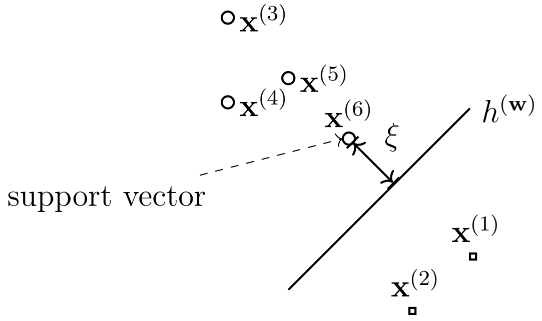


Fig. 44. The SVM learns a hypothesis (or classifier) $h^{(\mathbf{w})}$ with minimal average soft-margin hinge loss. Minimizing this loss is equivalent to maximizing the margin ξ between the decision boundary of $h^{(\mathbf{w})}$ and each class of the training set.

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: classification, hypothesis, map, linear regression, logistic regression, ERM, linear model, loss function, data point, feature space, maximum, hinge loss, SVM, classifier, loss, decision boundary, training set, ML, kernel.

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].

test set A set of data points that have been used neither to train a model (e.g., via ERM) nor in a validation set to choose between different models.
See also: data point, model, ERM, validation set.

total variation See GTV.

training error The average loss of a hypothesis when predicting the labels of the data points in a training set. We sometimes refer by training error also to minimal average loss which is achieved by a solution of ERM.
See also: loss, hypothesis, label, data point, training set, ERM.

training set A training set is a dataset $\mathcal{D}$ which 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: dataset, data point, ERM, hypothesis, loss, training error, validation error, ML, hypothesis space.

transparency Transparency is a fundamental requirement for trustworthy AI [123]. In the context of ML methods, transparency is often used

interchangeably with explainability [49], [124]. 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 classification reliability through the value $|h(\mathbf{x})|$. Decision trees are another example, as they allow human-readable decision rules [51]. 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 [34] and AI system cards [125] help practitioners understand the intended use cases and limitations of an AI system [126].
See also: trustworthy AI, ML, explainability, AI, prediction, model, logistic regression, classification, decision tree.

trustworthy artificial intelligence (trustworthy AI) Besides the computational aspects and statistical aspects, a third main design aspect of ML methods is their trustworthiness [127]. The EU has put forward seven key requirements (KRs) for trustworthy AI (that typically build on ML methods) [128]:

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 Uncertainty refers to the degree of confidence—or lack thereof—associated with a quantity such as a model prediction, parameter estimate, or observed data point. In ML, uncertainty arises from various sources, including noisy data, limited training samples, or ambiguity in model assumptions. Probability theory offers a principled framework for representing and quantifying such uncertainty.
See also: model, prediction, parameter, data point, ML, data, sample, probability.

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 small empirical risk on the training set. If a method is underfitting, it will typically also not be able to learn a hypothesis with a small 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 [96]. 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 [96].

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 practice of evaluating the loss incurred by the hypothesis $\hat{h}$ on a set of data points that are not contained in the training set $\mathcal{D}$.

See also: hypothesis, ML, ERM, training set, loss, data point.

validation error Consider a hypothesis $\hat{h}$ which is obtained by some ML method, e.g., using ERM on a training set. The average loss of $\hat{h}$ on a 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 VC dimension of an infinite hypothesis space is a widely-used measure for its size. We refer to the literature (see [69]) for a precise definition of VC dimension as well as a discussion of its basic properties and use in ML.

See also: hypothesis space, ML.

variance The variance of a real-valued RV x is defined as the expectation $\mathbb{E}\{\big(x-\mathbb{E}\{x\}\big)^2\}$ of the squared difference between x and its expectation $\mathbb{E}\{x\}$. We extend this definition to vector-valued RVs $\mathbf{x}$ as $\mathbb{E}\{\big\|\mathbf{x}-\mathbb{E}\{\mathbf{x}\}\big\|_2^2\}$.

See also: RV, expectation.

vector space A vector space (also called linear space) is a collection of elements (called vectors) closed under vector addition and scalar multiplication, i.e.,

- If $\mathbf{x}, \mathbf{y} \in \mathcal{V}$, then $\mathbf{x} + \mathbf{y} \in \mathcal{V}$.
- If $\mathbf{x} \in \mathcal{V}$ and $c \in \mathbb{R}$, then $c\mathbf{x} \in \mathcal{V}$.
- In particular, $\mathbf{0} \in \mathcal{V}$.

The Euclidean space $\mathbb{R}^n$ is a vector space. Linear models and linear maps operate within such spaces.

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

vertical federated learning (VFL) VFL refers to FL applications where devices have access to different features of the same set of data points [129]. Formally, the underlying global dataset is

$$\mathcal{D}^{(\mathrm{global})} := \left\{\left(\mathbf{x}^{(1)}, y^{(1)}\right), \ldots, \left(\mathbf{x}^{(m)}, y^{(m)}\right)\right\}.$$

We denote by $\mathbf{x}^{(r)} = \big(x_1^{(r)}, \ldots, x_{d'}^{(r)}\big)^T$, 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

$$\mathbf{x}^{(i,r)} = \big(x_{j_1}^{(r)}, \ldots, x_{j_d}^{(r)}\big)^T.$$

Some of the devices might also have access to the labels $y^{(r)}$, for $r = 1, \ldots, m$, of the global dataset. 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.

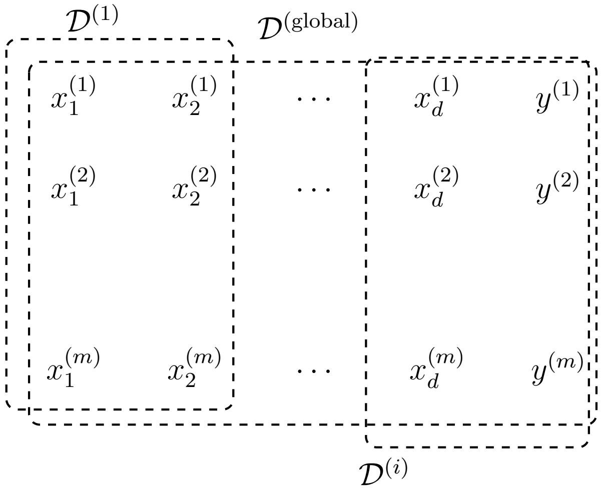

$\mathcal{D}^{(1)}$
$\mathcal{D}^{(\mathrm{global})}$
$x_1^{(1)}$ $x_2^{(1)}$ $\cdots$ $x_d^{(1)}$ $y^{(1)}$
$x_1^{(2)}$ $x_2^{(2)}$ $\cdots$ $x_d^{(2)}$ $y^{(2)}$
$x_1^{(m)}$ $x_2^{(m)}$ $\cdots$ $x_d^{(m)}$ $y^{(m)}$
$\mathcal{D}^{(i)}$

Fig. 45. VFL uses local datasets that are derived from the data points of a common global dataset. The local datasets differ in the choice of features used to characterize the data points.

See also: FL, privacy protection.

weights Consider a parametrized 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 ANNs to form linear combinations of features or the outputs of neurons in hidden layers.
See also: hypothesis space, model parameters, feature, linear model, ANN.

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, gradient.

0/1 loss The 0/1 loss $L^{(0/1)}\left((\mathbf{x}, y), h\right)$ measures the quality of a classifier $h(\mathbf{x})$ 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, classifier, prediction, label, data point, feature.

Index

References

[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.

[9] T. H. Cormen, C. E. Leiserson, R. L. Rivest, and C. Stein, *Introduction to Algorithms*. Cambridge, MA, USA: MIT Press, 2022. [Online]. Available: http://ebookcentral.proquest.com/lib/aalto-ebooks/detail.action?docID=6925615

[10] M. Sipser, *Introduction to the Theory of Computation*, 3rd ed. Andover, U.K.: Cengage Learning, 2013.

[11] L. Richardson and M. Amundsen, *RESTful Web APIs.* Sebastopol, CA, USA: O'Reilly Media, 2013.

[12] M. P. Salinas et al., "A systematic review and meta-analysis of artificial intelligence versus clinicians for skin cancer diagnosis," *npj Digit. Med.*, vol. 7, no. 1, May 2024, Art. no. 125, doi: 10.1038/s41746-024-01103-x.

[13] E. L. Lehmann and G. Casella, *Theory of Point Estimation*, 2nd ed. New York, NY, USA: Springer-Verlag, 1998.

[14] G. F. Cooper, "The computational complexity of probabilistic inference using bayesian belief networks," *Artif. Intell.*, vol. 42, no. 2–3, pp. 393–405, Mar. 1990, doi: 10.1016/0004-3702(90)90060-D.

[15] R. M. Gray, *Probability, Random Processes, and Ergodic Properties*, 2nd ed. New York, NY, USA: Springer Science+Business Media, 2009.

[16] T. Hastie, R. Tibshirani, and J. Friedman, *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*, 2nd ed. New York, NY, USA: Springer Science+Business Media, 2009.

[17] J. H. Friedman, "Greedy function approximation: A gradient boosting machine," *Ann. Statist.*, vol. 29, no. 5, pp. 1189–1232, Oct. 2001, doi: 10.1214/aos/1013203451.

[18] A. van der Vaart, *Asymptotic Statistics.* Cambridge, UK: Cambridge Univ. Press, 1998.

[19] O. Chapelle, B. Schölkopf, and A. Zien, Eds., *Semi-Supervised Learning.* Cambridge, MA, USA: MIT Press, 2006.

[20] M. J. Wainwright, *High-Dimensional Statistics: A Non-Asymptotic Viewpoint.* Cambridge, U.K.: Cambridge Univ. Press, 2019.

[21] S. Boyd and L. Vandenberghe, *Convex Optimization.* Cambridge, U.K.: Cambridge Univ. Press, 2004.

[22] D. Sun, K.-C. Toh, and Y. Yuan, "Convex clustering: Model, theoretical guarantee and efficient algorithm," *J. Mach. Learn. Res.*, vol. 22, no. 9, pp. 1–32, Jan. 2021. [Online]. Available: http://jmlr.org/papers/v22/18-694.html

[23] K. Pelckmans, J. De Brabanter, J. A. K. Suykens, and B. De Moor, "Convex clustering shrinkage," presented at the PASCAL Workshop Statist. Optim. Clustering Workshop, 2005.

[24] A. Silberschatz, H. F. Korth, and S. Sudarshan, *Database System Concepts*, 7th ed. New York, NY, USA: McGraw-Hill Education, 2019. [Online]. Available: https://db-book.com/

[25] E. F. Codd, "A relational model of data for large shared data banks," *Commun. ACM*, vol. 13, no. 6, pp. 377–387, Jun. 1970, doi: 10.1145/362384.362685.

[26] European Union, "Regulation (EU) 2016/679 of the European Parliament and of the Council of 27 April 2016 on the protection of natural persons with regard to the processing of personal data and on the free

movement of such data, and repealing Directive 95/46/EC (General Data Protection Regulation) (Text with EEA relevance)," L 119/1, May 4, 2016. [Online]. Available: https://eur-lex.europa.eu/eli/reg/2016/679/oj

[27] European Union, "Regulation (EU) 2018/1725 of the European Parliament and of the Council of 23 October 2018 on the protection of natural persons with regard to the processing of personal data by the Union institutions, bodies, offices and agencies and on the free movement of such data, and repealing Regulation (EC) No 45/2001 and Decision No 1247/2002/EC (Text with EEA relevance)," L 295/39, Nov. 21, 2018. [Online]. Available: https://eur-lex.europa.eu/eli/reg/2018/1725/oj

[28] T. M. Cover and J. A. Thomas, *Elements of Information Theory*, 2nd ed. Hoboken, NJ, USA: Wiley, 2006.

[29] X. Liu, H. Li, G. Xu, Z. Chen, X. Huang, and R. Lu, "Privacy-enhanced federated learning against poisoning adversaries," *IEEE Trans. Inf. Forensics Security*, vol. 16, pp. 4574–4588, 2021, doi: 10.1109/TIFS.2021.3108434.

[30] J. Zhang, B. Chen, X. Cheng, H. T. T. Binh, and S. Yu, "PoisonGAN: Generative poisoning attacks against federated learning in edge computing systems," *IEEE Internet Things J.*, vol. 8, no. 5, pp. 3310–3322, Mar. 2021, doi: 10.1109/JIOT.2020.3023126.

[31] S. Abiteboul, R. Hull, and V. Vianu, *Foundations of Databases*. Reading, MA, USA: Addison-Wesley, 1995.

[32] S. Hoberman, *Data Modeling Made Simple: A Practical Guide for Business and IT Professionals*, 2nd ed. Basking Ridge, NJ, USA: Technics Publications, 2009.

[33] R. Ramakrishnan and J. Gehrke, *Database Management Systems*, 3rd ed. New York, NY, USA: McGraw-Hill, 2002.

[34] T. Gebru et al., "Datasheets for datasets," *Commun. ACM*, vol. 64, no. 12, pp. 86–92, Nov. 2021, doi: 10.1145/3458723.

[35] I. Goodfellow, Y. Bengio, and A. Courville, *Deep Learning.* Cambridge, MA, USA: MIT Press, 2016.

[36] G. Strang, *Computational Science and Engineering.* Wellesley-Cambridge Press, MA, 2007.

[37] R. A. Horn and C. R. Johnson, *Matrix Analysis*, 2nd ed. New York, NY, USA: Cambridge Univ. Press, 2013.

[38] G. Tel, *Introduction to Distributed Algorithms*, 2nd ed. Cambridge, U.K.: Cambridge Univ. Press, 2000.

[39] D. P. Bertsekas and J. N. Tsitsiklis, *Parallel and Distributed Computation: Numerical Methods.* Belmont, MA, USA: Athena Scientific, 2015.

[40] D. P. Bertsekas, A. Nedic, and A. E. Ozdaglar, *Convex Analysis and Optimization.* Belmont, MA, USA: Athena Scientific, 2003.

[41] S. M. Kay, *Fundamentals of Statistical Signal Processing: Estimation Theory.* Upper Saddle River, NJ, USA: Prentice Hall PTR, 1993.

[42] P. R. Halmos, *Measure Theory.* New York, NY, USA: Springer-Verlag, 1974.

[43] C. M. Bishop, *Pattern Recognition and Machine Learning.* New York, NY, USA: Springer Science+Business Media, 2006.

[44] M. J. Wainwright and M. I. Jordan, "Graphical models, exponential families, and variational inference," *Found. Trends Mach. Learn.*, vol. 1, no. 1–2, pp. 1–305, Nov. 2008, doi: 10.1561/2200000001.

[45] N. Cesa-Bianchi and G. Lugosi, *Prediction, Learning, and Games.* New York, NY, USA: Cambridge Univ. Press, 2006.

[46] E. Hazan, "Introduction to online convex optimization," *Found. Trends Optim.*, vol. 2, no. 3–4, pp. 157–325, Aug. 2016, doi: 10.1561/2400000013.

[47] J. Colin, T. Fel, R. Cadène, and T. Serre, "What I cannot predict, I do not understand: A human-centered evaluation framework for explainability methods," in *Adv. Neural Inf. Process. Syst.*, 2022.

[48] L. Zhang, G. Karakasidis, A. Odnoblyudova, L. Dogruel, Y. Tian, and A. Jung, "Explainable empirical risk minimization," *Neural Comput. Appl.*, vol. 36, no. 8, pp. 3983–3996, Mar. 2024, doi: 10.1007/s00521-023-09269-3.

[49] A. Jung and P. H. J. Nardelli, "An information-theoretic approach to personalized explainable machine learning," *IEEE Signal Process. Lett.*, vol. 27, pp. 825–829, 2020, doi: 10.1109/LSP.2020.2993176.

[50] J. Chen, L. Song, M. J. Wainwright, and M. I. Jordan, "Learning to explain: An information-theoretic perspective on model interpretation," in *Proc. 35th Int. Conf. Mach. Learn.*, J. Dy and A. Krause, Eds. vol. 80, 2018, pp. 883–892. [Online]. Available: https://proceedings.mlr.press/v80/chen18j.html

[51] C. Rudin, "Stop explaining black box machine learning models for high-stakes decisions and use interpretable models instead," *Nature Mach. Intell.*, vol. 1, no. 5, pp. 206–215, May 2019, doi: 10.1038/s42256-019-0048-x.

[52] C. Molnar, *Interpretable Machine Learning: A Guide for Making Black Box Models Explainable*, 3rd ed., 2025. [Online]. Available: https://christophm.github.io/interpretable-ml-book/

[53] R. R. Selvaraju, M. Cogswell, A. Das, R. Vedantam, D. Parikh, and D. Batra, "Grad-CAM: Visual explanations from deep networks via gradient-based localization," in *2017 IEEE Int. Conf. Comput. Vis.*, 2017, pp. 618–626, doi: 10.1109/ICCV.2017.74.

[54] D. N. Gujarati and D. C. Porter, *Basic Econometrics*, 5th ed. New York, NY, USA: McGraw-Hill/Irwin, 2009.

[55] Y. Dodge, Ed., *The Oxford Dictionary of Statistical Terms.* New York, NY, USA: Oxford Univ. Press, 2003.

[56] B. S. Everitt, *The Cambridge Dictionary of Statistics*, 2nd ed. Cambridge, U.K.: Cambridge Univ. Press, 2002.

[57] B. Schölkopf and A. J. Smola, *Learning with Kernels: Support Vector Machines, Regularization, Optimization, and Beyond.* Cambridge, MA, USA: MIT Press, 2002.

[58] M. T. Ribeiro, S. Singh, and C. Guestrin, "Why should i trust you?: Explaining the predictions of any classifier," in *Proc. 22nd ACM SIGKDD Int. Conf. Knowl. Discovery Data Mining*, Aug. 2016, pp. 1135–1144, doi: 10.1145/2939672.2939778.

[59] H. B. McMahan, E. Moore, D. Ramage, S. Hampson, and B. A. y Arcas, "Communication-efficient learning of deep networks from decentralized data," in *Proc. 20th Int. Conf. Artif. Intell. Statist.*, 2017, A. Singh and J. Zhu, Eds. vol. 54, 2017, pp. 1273–1282. [Online]. Available: https://proceedings.mlr.press/v54/mcmahan17a.html

[60] T. Li, A. K. Sahu, M. Zaheer, M. Sanjabi, A. Talwalkar, and V. Smith, "Federated optimization in heterogeneous networks," in *Proc. Mach. Learn. Syst.*, 2020, I. Dhillon, D. Papailiopoulos, and V. Sze, Eds. vol. 2, 2020. [Online]. Available: https://proceedings.mlsys.org/paper_files/paper/2020/hash/1f5fe83998a09396ebe6477d9475ba0c-Abstract.html

[61] H. H. Bauschke and P. L. Combettes, *Convex Analysis and Monotone Operator Theory in Hilbert Spaces*, 2nd ed. New York, NY, USA: Springer Science+Business Media, 2017.

[62] V. I. Istrăţescu, *Fixed Point Theory: An Introduction.* Dordrecht, The Netherlands: D. Reidel, 1981.

[63] N. Parikh and S. Boyd, "Proximal algorithms," *Found. Trends Optim.*, vol. 1, no. 3, pp. 127–239, Jan. 2014, doi: 10.1561/2400000003.

[64] Y. SarcheshmehPour, Y. Tian, L. Zhang, and A. Jung, "Flow-based clustering and spectral clustering: A comparison," in *2021 55th Asilomar Conf. Signals, Syst., Comput.*, 2021.

[65] A. Papoulis and S. U. Pillai, *Probability, Random Variables, and Stochastic Processes*, 4th ed. New York, NY, USA: McGraw-Hill Higher Education, 2002.

[66] A. Lapidoth, *A Foundation in Digital Communication.* Cambridge, U.K.: Cambridge Univ. Press, 2009.

[67] C. E. Rasmussen and C. K. I. Williams, *Gaussian Processes for Machine Learning.* Cambridge, MA, USA: MIT Press, 2006.

[68] S. Ross, *A First Course in Probability*, 9th ed. Boston, MA, USA: Pearson Education, 2014.

[69] S. Shalev-Shwartz and S. Ben-David, *Understanding Machine Learning: From Theory to Algorithms.* New York, NY, USA: Cambridge Univ. Press, 2014.

[70] J. Su, D. V. Vargas, and K. Sakurai, "One pixel attack for fooling deep neural networks," *IEEE Trans. Evol. Comput.*, vol. 23, no. 5, pp. 828–841, Oct. 2019, doi: 10.1109/TEVC.2019.2890858.

[71] S. Mallat, "Understanding deep convolutional networks," *Philos. Trans.*

Roy. Soc. A, vol. 374, no. 2065, Apr. 2016, Art. no. 20150203, doi: 10.1098/rsta.2015.0203.

[72] Y. SarcheshmehPour, Y. Tian, L. Zhang, and A. Jung, "Clustered federated learning via generalized total variation minimization," *IEEE Trans. Signal Process.*, vol. 71, pp. 4240–4256, 2023, doi: 10.1109/TSP.2023.3322848.

[73] H. P. Lopuhaä and P. J. Rousseeuw, "Breakdown points of affine equivariant estimators of multivariate location and covariance matrices," *Ann. Statist.*, vol. 19, no. 1, pp. 229–248, Mar. 1991, doi: 10.1214/aos/1176347978.

[74] R. T. Rockafellar, *Network Flows and Monotropic Optimization.* Belmont, MA, USA: Athena Scientific, 1998.

[75] U. von Luxburg, "A tutorial on spectral clustering," *Statist. Comput.*, vol. 17, no. 4, pp. 395–416, Dec. 2007, doi: 10.1007/s11222-007-9033-z.

[76] P. Bühlmann and S. van de Geer, *Statistics for High-Dimensional Data: Methods, Theory and Applications.* Berlin, Germany: Springer-Verlag, 2011.

[77] N. Young, *An Introduction to Hilbert Space.* New York, NY, USA: Cambridge Univ. Press, 1988.

[78] C. H. Lampert, "Kernel methods in computer vision," *Found. Trends Comput. Graph. Vis.*, vol. 4, no. 3, pp. 193–285, Sep. 2009, doi: 10.1561/0600000027.

[79] Q. Yang, Y. Liu, Y. Cheng, Y. Kang, T. Chen, and H. Yu, "Horizontal federated learning," in *Federated Learning*. Cham, Switzerland: Springer Nature, 2020, ch. 4, pp. 49–67.

[80] F. Doshi-Velez and B. Kim, "Towards a rigorous science of interpretable machine learning," *arXiv preprint arXiv:1702.08608*, 2017.

[81] P. Hase and M. Bansal, "Evaluating explainable AI: Which algorithmic explanations help users predict model behavior?" in *Proc. 58th Annual Meeting of the Association for Comp. Ling.* Online: Association for Computational Linguistics, July 2020, pp. 5540–5552. [Online]. Available: https://aclanthology.org/2020.acl-main.491

[82] J. Colin, T. Fel, R. Cadène, and T. Serre, "What I Cannot Predict, I Do Not Understand: A Human-Centered Evaluation Framework for Explainability Methods." *Advances in Neural Information Processing Systems*, vol. 35, pp. 2832–2845, 2022.

[83] Z. C. Lipton, "The mythos of model interpretability: In machine learning, the concept of interpretability is both important and slippery." *Queue*, vol. 16, no. 3, p. 31–57, June 2018. [Online]. Available: https://doi.org/10.1145/3236386.3241340

[84] R. A. Horn and C. R. Johnson, *Topics in Matrix Analysis.* Cambridge, UK: Cambridge Univ. Press, 1991.

[85] G. Strang, *Introduction to Linear Algebra*, 5th ed. Wellesley-Cambridge Press, MA, 2016.

[86] A. Y. Ng, M. I. Jordan, and Y. Weiss, “On spectral clustering: Analysis and an algorithm,” in *Adv. Neural Inf. Process. Syst.*, 2001. [Online]. Available: https://papers.nips.cc/paper_files/paper/2001/hash/801272ee79cfde7fa5960571fee36b9b-Abstract.html

[87] A. Vaswani et al., “Attention is all you need,” in *Adv. Neural Inf. Process. Syst.*, 2017, I. Guyon, U. von Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, Eds. vol. 30, 2017, pp. 5998–6008. [Online]. Available: https://papers.nips.cc/paper_files/paper/2017/hash/3f5ee243547dee91fbd053c1c4a845aa-Abstract.html

[88] R. Caruana, “Multitask learning,” *Mach. Learn.*, vol. 28, pp. 41–75, Jul. 1997, doi: 10.1023/A:1007379606734.

[89] A. Jung, G. Hannak, and N. Goertz, “Graphical lasso based model selection for time series,” *IEEE Signal Process. Lett.*, vol. 22, no. 10, pp. 1781–1785, Oct. 2015, doi: 10.1109/LSP.2015.2425434.

[90] A. Jung, “Learning the conditional independence structure of stationary time series: A multitask learning approach,” *IEEE Trans. Signal Process.*, vol. 63, no. 21, Nov. 2015, doi: 10.1109/TSP.2015.2460219.

[91] D. P. Bertsekas, *Nonlinear Programming*, 2nd ed. Belmont, MA, USA: Athena Scientific, 1999.

[92] J. Heinonen, “Lectures on lipschitz analysis,” University of Jyväskylä, Jyväskylä, Finland, Report 100, 2005, lecture notes from the 14th Jyväskylä Summer School, August 2004. [Online]. Available: http://www.math.jyu.fi/research/reports/rep100.pdf

[93] T. Hastie, R. Tibshirani, and M. Wainwright, *Statistical Learning with Sparsity: The Lasso and Generalizations.* Boca Raton, FL, USA: CRC Press, 2015.

[94] K. Abayomi, A. Gelman, and M. Levy, "Diagnostics for multivariate imputations," *J. Roy. Statist. Soc.: Ser. C (Appl. Statist.)*, vol. 57, no. 3, pp. 273–291, Jun. 2008, doi: 10.1111/j.1467-9876.2007.00613.x.

[95] M. Fredrikson, S. Jha, and T. Ristenpart, "Model inversion attacks that exploit confidence information and basic countermeasures," in *Proc. 22nd ACM SIGSAC Conf. Comput. Commun. Secur.*, Oct. 2015, pp. 1322–1333, doi: 10.1145/2810103.2813677.

[96] S. Bubeck and N. Cesa-Bianchi, "Regret analysis of stochastic and non-stochastic multi-armed bandit problems," *Found. Trends Mach. Learn.*, vol. 5, no. 1, pp. 1–122, Dec. 2012, doi: 10.1561/2200000024.

[97] A. Lapidoth, *A Foundation in Digital Communication*, 2nd ed. Cambridge, U.K.: Cambridge Univ. Press, 2017.

[98] A. Jung, "Networked exponential families for big data over networks," *IEEE Access*, vol. 8, pp. 202 897–202 909, Nov. 2020, doi: 10.1109/ACCESS.2020.3033817.

[99] Y. Nesterov, *Introductory Lectures on Convex Optimization: A Basic Course.* Boston, MA, USA: Kluwer Academic, 2004.

[100] A. Rakhlin, O. Shamir, and K. Sridharan, "Making gradient descent optimal for strongly convex stochastic optimization," in

Proc. 29th Int. Conf. Mach. Learn., 2012, J. Langford and J. Pineau, Eds. 2012, pp. 449–456. [Online]. Available: https://icml.cc/Conferences/2012/papers/261.pdf

[101] P. J. Brockwell and R. A. Davis, *Time Series: Theory and Methods*, 2nd ed. New York, NY, USA: Springer-Verlag, 1991.

[102] M. Kearns and M. Li, "Learning in the presence of malicious errors," *SIAM J. Comput.*, vol. 22, no. 4, pp. 807–837, Aug. 1993, doi: 10.1137/0222052.

[103] G. Lugosi and S. Mendelson, "Robust multivariate mean estimation: The optimality of trimmed mean," *Ann. Statist.*, vol. 49, no. 1, pp. 393–410, Feb. 2021, doi: 10.1214/20-AOS1961.

[104] A. Makhdoumi, S. Salamatian, N. Fawaz, and M. Médard, "From the information bottleneck to the privacy funnel," in *2014 IEEE Inf. Theory Workshop*, 2014, pp. 501–505, doi: 10.1109/ITW.2014.6970882.

[105] A. Ünsal and M. Önen, "Information-theoretic approaches to differential privacy," *ACM Comput. Surv.*, vol. 56, no. 3, Oct. 2023, Art. no. 76, doi: 10.1145/3604904.

[106] M. E. Tipping and C. M. Bishop, "Probabilistic principal component analysis," *J. Roy. Stat. Soc. Ser. B*, vol. 61, pp. 611–622, 1999.

[107] O. Kallenberg, *Foundations of Modern Probability.* New York, NY, USA: Springer-Verlag, 1997.

[108] L. Condat, "A primal–dual splitting method for convex optimization involving lipschitzian, proximable and linear composite terms," *J. Optim. Theory Appl.*, vol. 158, no. 2, pp. 460–479, Aug. 2013, doi: 10.1007/s10957-012-0245-9.

[109] A. Ben-Israel and T. N. E. Greville, *Generalized Inverses: Theory and Applications*, 2nd ed., ser. CMS Books in Mathematics. New York, NY: Springer, 2003, originally published by Wiley-Interscience, 1974. [Online]. Available: https://doi.org/10.1007/b97366

[110] S. Shalev-Shwartz and A. Tewari, "Stochastic methods for ℓ_1 regularized loss minimization," in *Proc. 26th Annu. Int. Conf. Mach. Learn.*, 2009, L. Bottou and M. Littman, Eds. Jun. 2009, pp. 929–936.

[111] I. Csiszar, "Generalized cutoff rates and Renyi's information measures," *IEEE Trans. Inf. Theory*, vol. 41, no. 1, pp. 26–34, Jan. 1995, doi: 10.1109/18.370121.

[112] S. Bubeck, "Convex optimization: Algorithms and complexity," *Found. Trends Mach. Learn.*, vol. 8, no. 3–4, pp. 231–357, Nov. 2015, 10.1561/2200000050.

[113] D. P. Bertsekas, *Convex Optimization Algorithms.* Belmont, MA, USA: Athena Scientific, 2015.

[114] L. Cohen, *Time-Frequency Analysis.* Upper Saddle River, NJ, USA: Prentice Hall PTR, 1995.

[115] J. Li, L. Han, X. Li, J. Zhu, B. Yuan, and Z. Gou, "An evaluation of deep neural network models for music classification using spectrograms,"

Multimedia Tools Appl., vol. 81, no. 4, pp. 4621–4647, Feb. 2022, doi: 10.1007/s11042-020-10465-9.

[116] B. Boashash, Ed., *Time Frequency Signal Analysis and Processing: A Comprehensive Reference.* Oxford, U.K.: Elsevier, 2003.

[117] S. Mallat, *A Wavelet Tour of Signal Processing: The Sparse Way*, 3rd ed. Burlington, MA, USA: Academic, 2009.

[118] R. Motwani and P. Raghavan, *Randomized Algorithms.* Cambridge, U.K.: Cambridge Univ. Press, 1995.

[119] R. G. Gallager, *Stochastic Processes: Theory for Applications.* New York, NY, USA: Cambridge Univ. Press, 2013.

[120] E. Abbe, "Community detection and stochastic block models: Recent developments," *J. Mach. Learn. Res.*, vol. 18, no. 177, pp. 1–86, Apr. 2018. [Online]. Available: http://jmlr.org/papers/v18/16-480.html

[121] L. Bottou, "On-line learning and stochastic approximations," in *On-Line Learning in Neural Networks*, D. Saad, Ed. New York, NY, USA: Cambridge Univ. Press, 1999, ch. 2, pp. 9–42.

[122] N. Cristianini and J. Shawe-Taylor, *An Introduction to Support Vector Machines and Other Kernel-based Learning Methods.* New York, NY, USA: Cambridge Univ. Press, 2000.

[123] High-Level Expert Group on Artificial Intelligence, "Ethics guidelines for trustworthy AI," European Commission, Apr. 8, 2019.

[Online]. Available: https://digital-strategy.ec.europa.eu/en/library/ethics-guidelines-trustworthy-ai

[124] C. Gallese, "“the AI act proposal: A new right to technical interpretability?," *SSRN Electron. J.*, feb. 2023," *SSRN Electronic Journal*, 2023. [Online]. Available: https://ssrn.com/abstract=4398206

[125] M. Mitchell et al., "Model cards for model reporting," in *Proc. Conf. Fairness, Accountability, Transparency*, 2019, pp. 220–229, doi: 10.1145/3287560.3287596.

[126] K. Shahriari and M. Shahriari, "IEEE standard review — Ethically aligned design: A vision for prioritizing human wellbeing with artificial intelligence and autonomous systems," in *2017 IEEE Canada Int. Humanitarian Technol. Conf.*, pp. 197–201, doi: 10.1109/IHTC.2017.8058187.

[127] D. Pfau and A. Jung, "Engineering trustworthy AI: A developer guide for empirical risk minimization," Nov. 2024. [Online]. Available: https://arxiv.org/abs/2410.19361

[128] High-Level Expert Group on Artificial Intelligence, "The assessment list for trustworthy artificial intelligence (ALTAI): For self assessment," European Commission, Jul. 17, 2020. [Online]. Available: https://digital-strategy.ec.europa.eu/en/library/assessment-list-trustworthy-artificial-intelligence-altai-self-assessment

[129] Q. Yang, Y. Liu, Y. Cheng, Y. Kang, T. Chen, and H. Yu, "Vertical federated learning," in *Federated Learning.* Cham, Switzerland: Springer Nature, 2020, ch. 5, pp. 69–81.