The A”allon koneoppimisen sanakirja

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October 10, 2025

please cite as: A. Jung, K. Olioumtsevits, E. Schnoor, T. Ryynänen, J. Gronier ja S. Rastelli, *Aallon koneoppimisen sanakirja*. Käännös Janita Thusberg, Helli Manninen ja Mikko Seesto. 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.

This work was supported by

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

Contents

Lists of Symbols

Sets and Functions

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

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

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

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

See also: gradient, differentiable, function, vector.

Matrices and Vectors

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

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

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

Probability Theory

$\mathbf{x} \sim p(\mathbf{z})$	The random variable (RV) $\mathbf{x}$ is distributed according to the probability distribution $p(\mathbf{z})$ [?], [?]. See also: RV, probability distribution.
$\mathbb{E}_p\{f(\mathbf{z})\}$	The expectation of an RV $f(\mathbf{z})$ that is obtained by applying a deterministic function f to an RV $\mathbf{z}$ whose probability distribution is $\mathbb{P}(\mathbf{z})$. If the probability distribution is clear from context, we just write $\mathbb{E}\{f(\mathbf{z})\}$. See also: expectation, RV, function, probability distribution.
$\mathrm{cov}\,(x, y)$	The covariance between two real-valued RVs defined over a common probability space. See also: covariance, RV, probability distribution.
$\mathbb{P}(\mathbf{x}, y)$	A (joint) probability distribution of an RV whose 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 [?, Sec. 3.5]. See also: probability distribution, RV.
$\mathbb{P}(\mathcal{A})$	The probability of the measurable event $\mathcal{A}$. See also: probability, measurable, event.

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

Machine Learning

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

$\mathbf{z}$	Instead of the symbol $\mathbf{x}$, we sometimes use $\mathbf{z}$ as another symbol to denote a vector whose entries are the individual features of a data point. We need two different symbols to distinguish between raw and learned features [**?**, Ch. 9]. See also: vector, feature, data point.
$\mathbf{x}^{(r)}$	The feature vector of the rth data point within a dataset. See also: feature vector, data point, dataset.
$x_j^{(r)}$	The jth feature of the rth 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 rth data point. See also: label, data point.
$\left(\mathbf{x}^{(r)}, y^{(r)}\right)$	The features and label of the rth data point. See also: feature, label, data point.

$\mathcal{Y}$	The label space $\mathcal{Y}$ of an ML method consists of all potential label values that a data point can carry. The nominal label space might be larger than the set of different label values arising in a given 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 $h : \mathcal{X} \to \mathcal{Y}$. See also: hypothesis, map.
$\mathcal{H}$	A hypothesis space or model used by an ML method. The hypothesis space consists of different hypothesis maps $h : \mathcal{X} \to \mathcal{Y}$, between which the ML method must choose. See also: hypothesis space, model, ML, hypothesis, map.

$d_{\text{eff}}\left(\mathcal{H}\right)$	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 an RV if it is learned from data points being RVs themselves. 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 an RV if it is learned from data points being RVs themselves. 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.
$\widehat{L}\big(h\vert\mathcal{D}\big)$	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). See also: event.
t	An index that enumerates learning tasks within a multitask learning problem. See also: learning task, multitask learning.
α	A regularization parameter that controls the amount of regularization. See also: regularization, parameter.
$\lambda_j(\mathbf{Q})$	The jth eigenvalue (sorted in either ascending or descending order) of a positive semi-definite (psd) matrix $\mathbf{Q}$. We also use the shorthand λ_j if the corresponding matrix is clear from context. See also: eigenvalue, psd, matrix.
$\sigma(\cdot)$	The activation function used by an artificial neuron within an artificial neural network (ANN). See also: activation function, ANN.
$\mathcal{R}_{\hat{y}}$	A decision region within a feature space. See also: decision region, feature space.

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

Federated Learning

$\mathcal{G} = (\mathcal{V}, \mathcal{E})$	An undirected graph whose nodes $i \in \mathcal{V}$ represent 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 the node i in a graph $\mathcal{G}$. See also: neighborhood, graph.
$d^{(i)}$	The weighted node degree $d^{(i)} := \sum_{i' \in \mathcal{N}^{(i)}} A_{i,i'}$ of node i. See also: node degree.
$d^{(\mathcal{G})}_{\max}$	The maximum weighted node degree of a graph $\mathcal{G}$. See also: maximum, node degree, graph.

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

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

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

See also: vector, model parameters.

Tools

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Check the contents of the file `ADictML_Finnish.math-glo`. If it's empty, that means you haven't indexed any of your entries in this glossary (using commands like `\gls` or `\glsadd`) so this list can't be generated. If the file isn't empty, the document build process hasn't been completed.

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- Add `automake` to your package option list when you load `glossaries-extra.sty`. For example:

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  ```

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  ```
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  ```

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  ```
  makeglossaries "ADictML_Finnish"
  ```

Then rerun LaTeX on this document.

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Machine Learning Concepts

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

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

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

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

online algorithm An online algorithm processes input data incrementally, receiving data points sequentially and making decisions or producing outputs (or decisions) immediately without having access to the entire input in advance [**?**], [**?**]. Unlike an offline algorithm, which has the entire input available from the start, an online algorithm must handle uncertainty about future inputs and cannot revise past decisions. Similar to an offline algorithm, we represent an online algorithm formally as a

collection of possible executions. However, the execution sequence for an online algorithm has a distinct structure as follows:

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

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

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

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

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

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 [**?**].

See also: feature map, feature, minimum.

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

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

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

See also: function.

linear map A linear map $f : \mathbb{R}^n \to \mathbb{R}^m$ is a function that satisfies additivity, i.e., $f(\mathbf{x} + \mathbf{y}) = f(\mathbf{x}) + f(\mathbf{y})$, and homogeneity, i.e., $f(c\mathbf{x}) = cf(\mathbf{x})$, for all vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ and scalars $c \in \mathbb{R}$. In particular, $f(\mathbf{0}) = \mathbf{0}$. Any linear map can be represented as a matrix multiplication $f(\mathbf{x}) = \mathbf{A}\mathbf{x}$ for some matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$. The collection of real-valued linear maps for a given dimension n constitute a linear model, which is used in many ML methods.

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

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 [**?**], [**?**]. One precise formulation of this principle is empirical risk minimization (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 [**?**, Ch. 3].

See also: model, data, loss.

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

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

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

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

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

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

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

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.

online learning Some ML methods are designed to process data in a sequential manner, updating their model parameters one at a time, as

new data points become available. A typical example is time-series data, such as daily minimum and maximum temperatures recorded by an Finnish Meteorological Institute (FMI) weather station. These values form a chronological sequence of observations. During each time step t, online learning methods update (or refine) the current hypothesis $h^{(t)}$ (or model parameters $\mathbf{w}^{(t)}$) based on the newly observed data point $\mathbf{z}^{(t)}$. See also: online GD, online algorithm.

multitask learning Multitask learning aims to leverage 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 may be useful to use the same deep net structure for both tasks and only allow the weights of the final output layer to be different. See also: learning task, dataset, deep net, weights, layer.

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

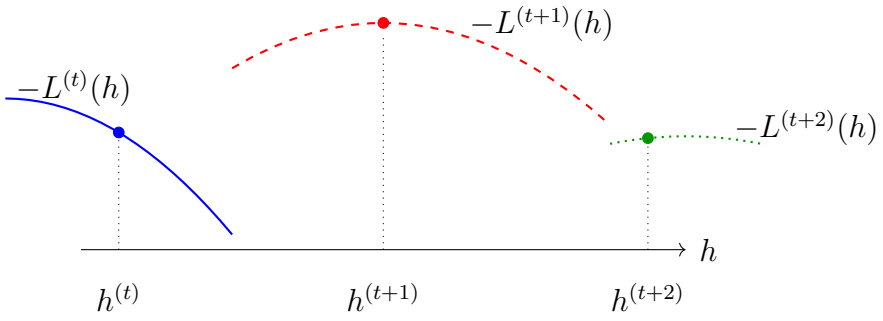


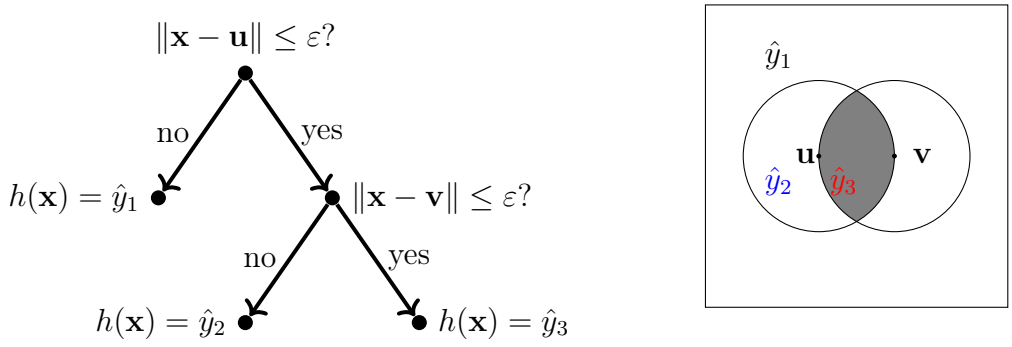
Fig. 1. Three consecutive time steps $t, t+1, t+2$ with corresponding loss functions $L^{(t)}, L^{(t+1)}, L^{(t+2)}$. During time step t, an RL method can evaluate the loss function only for one specific hypothesis $h^{(t)}$, resulting in the reward signal $r^{(t)} = -L^{(t)}(h^{(t)})$.

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

See also: reward, loss function, ML.

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

Fig. **??** for visual illustrations.



(a) (b)

Fig. 2. (a) A decision tree is a flowchart-like representation of a piecewise constant hypothesis $h : \mathcal{X} \to \mathbb{R}$. Each piece is a decision region $\mathcal{R}_{\hat{y}} := \big\{\mathbf{x} \in \mathcal{X} : h(\mathbf{x}) = \hat{y}\big\}$. The depicted decision tree can be applied to numeric feature vectors, i.e., $\mathcal{X} \subseteq \mathbb{R}^d$. It is parameterized by the threshold $\varepsilon > 0$ and the vectors $\mathbf{u}, \mathbf{v} \in \mathbb{R}^d$. (b) A decision tree partitions the feature space $\mathcal{X}$ into decision regions. Each decision region $\mathcal{R}_{\hat{y}} \subseteq \mathcal{X}$ corresponds to a specific leaf node in the decision tree.

See also: decision region.

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 gradient descent (GD).

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

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.

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 within an ML application. Passive attacks, such as privacy attacks, aim to infer sensitive attributes without modifying the system. Depending on their goal, we distinguish among denial-of-service attacks, backdoor attacks, and privacy attacks.

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

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

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

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 artificial intelligence (trustworthy AI), general data protection regulation (GDPR).

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

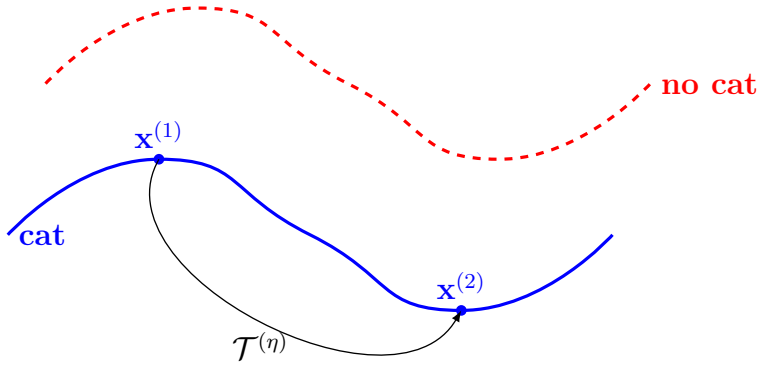


Fig. 3. Data augmentation exploits intrinsic symmetries of data points in some feature space $\mathcal{X}$. We can represent a symmetry by an operator $\mathcal{T}^{(\eta)} : \mathcal{X} \to \mathcal{X}$, parameterized by some number $\eta \in \mathbb{R}$. For example, $\mathcal{T}^{(\eta)}$ might represent the effect of rotating a cat image by η degrees. A data point with feature vector $\mathbf{x}^{(2)} = \mathcal{T}^{(\eta)}\big(\mathbf{x}^{(1)}\big)$ must have the same label $y^{(2)} = y^{(1)}$ as a data point with feature vector $\mathbf{x}^{(1)}$.

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

multiarmed bandit (MAB) An MAB problem is a precise mathematical formulation of a sequential decision-making task under uncertainty. At each discrete time step k, a learner selects one of several possible actions—called arms—from a finite set $\mathcal{A}$. Pulling arm a at time k yields a reward $r^{(a,k)}$ that is drawn from an unknown probability distribution $\mathbb{P}(r^{(a,k)})$. We obtain different classes of MAB problems by placing different restrictions on this probability distribution. In the simplest setting, the probability distribution $\mathbb{P}(r^{(a,k)})$ does not depend on t. Given

an MAB problem, the goal is to construct ML methods that maximize the cumulative reward over time by strategically balancing exploration (i.e., gathering information about uncertain arms) and exploitation (i.e., selecting arms known to perform well). MAB problems form an important special case of reinforcement learning (RL) problems [?], [?]. See also: reward, regret.

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

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

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,

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

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 $B^2 := \big\|\mathbb{E}\{\widehat{\mathbf{w}}\} - \overline{\mathbf{w}}\big\|_2^2$.
See also: i.i.d., RV, probabilistic model, estimation error.

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 [?, Sec. 1.4].

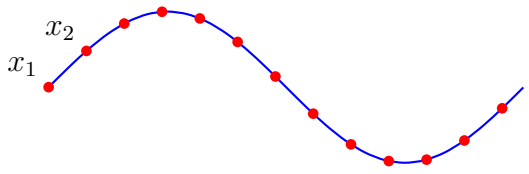


Fig. 4. An audio signal (blue waveform) and its discretized signal samples (red dots) which can be used as its features $x_1, \ldots, x_d$.

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

See also: data point.

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 on values from a finite label space. We might use the function value $h(\mathbf{x})$ itself as a prediction $\hat{y}$ for the label. However, it is customary

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

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

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

See also: hypothesis, classification, decision region.

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 $\mathbb{R}^d$ [**?**, Ch. 2].

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

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 [**?**]. We illustrate one example of a convex set and a convex function in Fig. **??**.

(a) (b)

Fig. 5. (a) A convex set $\mathcal{C} \subseteq \mathbb{R}^d$. (b) A convex function $f : \mathbb{R}^d \to \mathbb{R}$.

See also: Euclidean space, function, epigraph.

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

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

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

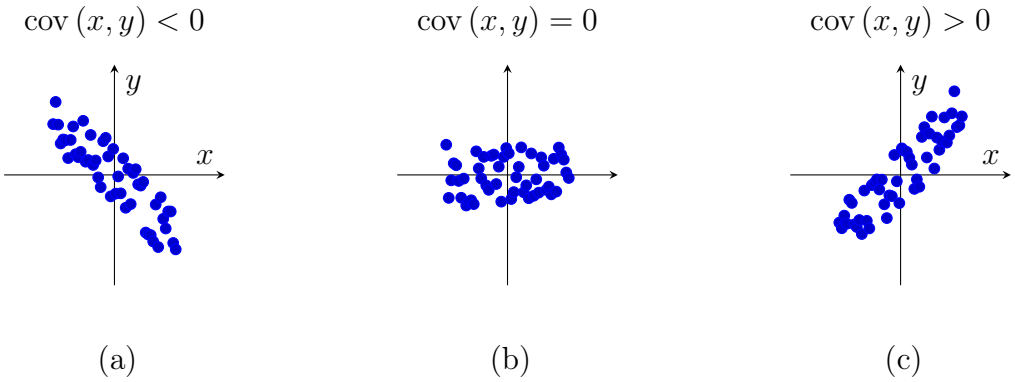


Fig. 6. Scatterplots illustrating realizations from three different probabilistic models for two RVs with different covariance values. (a) Negative. (b) Zero. (c) Positive.

See also: probabilistic model, expectation.

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.

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

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta \nabla f(\mathbf{w}^{(k)}) \tag{2}$$

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

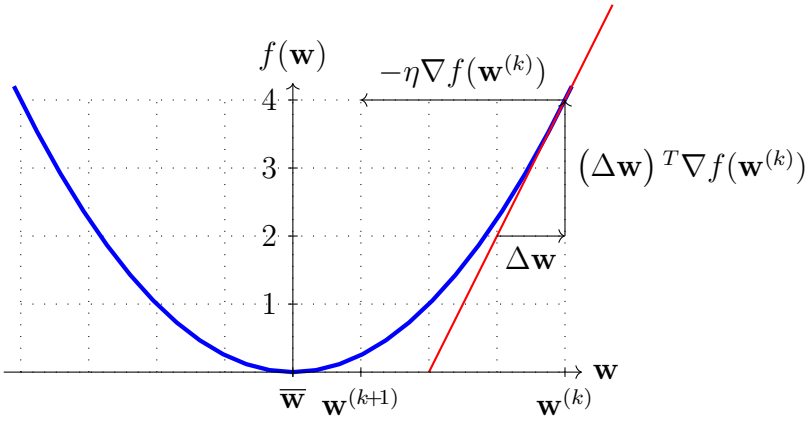


Fig. 7. A single gradient step (**??**) toward the minimizer $\overline{\mathbf{w}}$ of $f(\mathbf{w})$.

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

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

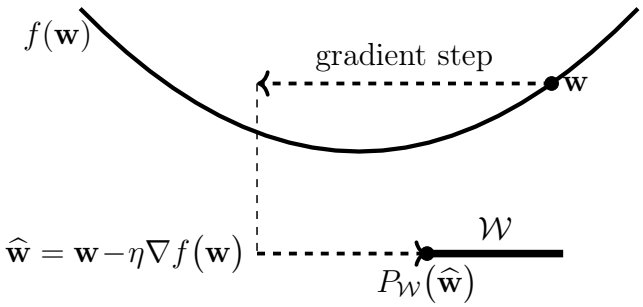


Fig. 8. Projected GD augments a basic gradient step with a projection back onto the constraint set $\mathcal{W}$.

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

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

$$\mathbf{w}^{(t+1)} := P_{\mathcal{W}}\big(\mathbf{w}^{(t)} - \eta_t \nabla_{\mathbf{w}} L\left(\mathbf{z}^{(t)}, \mathbf{w}\right)\big). \tag{3}$$

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

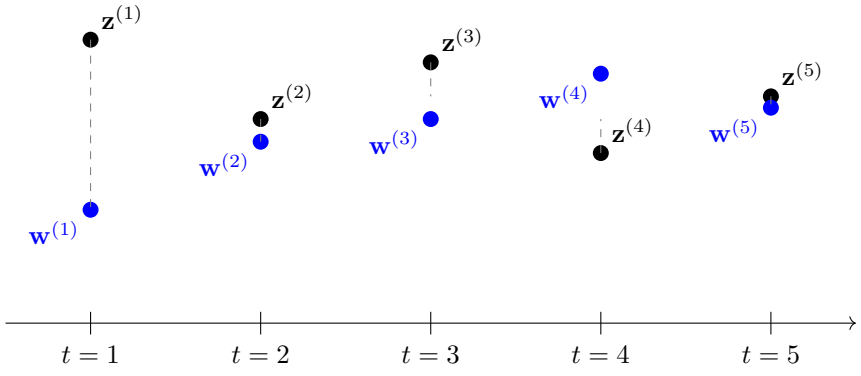


Fig. 9. An instance of online GD that updates the model parameters $\mathbf{w}^{(t)}$ using the data point $\mathbf{z}^{(t)} = x^{(t)}$ arriving at time t. This instance uses the squared error loss $L\left(\mathbf{z}^{(t)}, w\right) = (x^{(t)} - w)^2$.

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

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

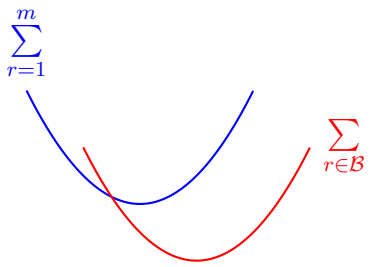


Fig. 10. SGD for ERM approximates the gradient by replacing the sum $\sum_{r=1}^{m} \nabla_{\mathbf{w}} L\left(\mathbf{z}^{(r)}, \mathbf{w}\right)$ over all data points in the training set (indexed by $r = 1, \ldots, m$) with a sum over a randomly chosen subset $\mathcal{B} \subseteq \{1, \ldots, m\}$.

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

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.

discrepancy Consider an federated learning (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.

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.

data In the context of ML, the term data is often used synonymously with dataset [**?**, **?**]. The ISO/IEC 2382:2015 standard defines data as a *re-interpretable representation of information in a formalized manner suitable for communication, interpretation, or processing* [**?**].

See also: dataset, data point, sample.

networked data Networked data consist of local datasets that are related

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

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

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

See also: function, gradient.

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

- Normalized:
$$\det(\mathbf{I}) = 1$$
- Multilinear:
$$\det\big(\mathbf{a}^{(1)}, \ldots, \alpha\mathbf{u} + \beta\mathbf{v}, \ldots, \mathbf{a}^{(d)}\big) = \alpha \det\big(\mathbf{a}^{(1)}, \ldots, \mathbf{u}, \ldots, \mathbf{a}^{(d)}\big) + \beta \det\big(\mathbf{a}^{(1)}, \ldots, \mathbf{v}, \ldots, \mathbf{a}^{(d)}\big)$$
- Antisymmetric:
$$\det\big(\ldots, \mathbf{a}^{(j)}, \ldots, \mathbf{a}^{(j')}, \ldots\big) = -\det\big(\ldots, \mathbf{a}^{(j')}, \ldots, \mathbf{a}^{(j)}, \ldots\big).$$

We can interpret a matrix $\mathbf{A}$ as a linear transformation on $\mathbb{R}^d$. The determinant $\det(\mathbf{A})$ characterizes how volumes in $\mathbb{R}^d$ (and their orientation)

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

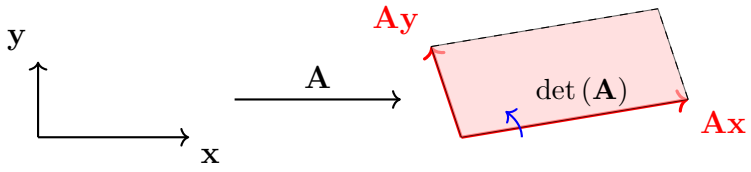


Fig. 11. We can interpret a square matrix $\mathbf{A}$ as a linear transformation of $\mathbb{R}^d$ into itself. The determinant $\det(\mathbf{A})$ characterizes how this transformation alters an oriented volume.

See also: eigenvalue, inverse matrix.

data poisoning Data poisoning refers to the intentional manipulation (or fabrication) of data points to steer the training of an ML model [**?**], [**?**]. Data poisoning attacks take various forms, including backdoor and denial-of-service attacks. A backdoor attack implants triggers into training data, so that the trained model behaves normally on typical feature vectors but misclassifies a feature vector with a trigger pattern. A denial-of-service attack degrades the trained model's overall performance

by injecting mislabeled or adversarial examples to prevent effective learning. Data poisoning is particularly concerning in decentralized or distributed ML settings (such as FL), where training data cannot be centrally verified.

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

training set A training set is a dataset $\mathcal{D}$ that consists of some data points used in ERM to learn a hypothesis $\hat{h}$. The average loss of $\hat{h}$ on the training set is referred to as the training error. The comparison of the training error with the validation error of $\hat{h}$ allows us to diagnose the ML method and informs how to improve the validation error (e.g., using a different hypothesis space or collecting more data points) [**?**, Sec. 6.6].

See also: dataset, data point, ERM, hypothesis, loss, training error, validation error, ML, hypothesis space.

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

See also: data point, model, ERM, validation set.

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 [**?**, 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.

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

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

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

See also: uncertainty, probabilistic model.

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

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

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

See also: uncertainty, probabilistic model.

training error The average loss of a hypothesis when predicting the labels of the data points in a training set. We sometimes also refer to training error as the minimal average loss that is achieved by a solution of ERM.

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

validation error Consider a hypothesis $\hat{h}$ that is obtained by some ML method, e.g., using ERM on a training set. The average loss of $\hat{h}$ on a validation set, which is different from the training set, is referred to as the validation error.

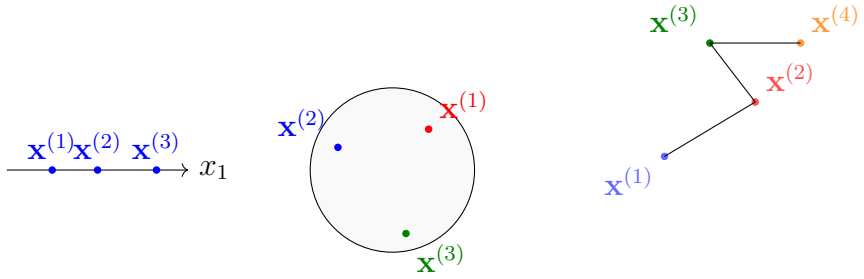
See also: hypothesis, ML, ERM, training set, loss, validation set, validation.

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

See also: vector space, vector, Euclidean space.

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

original (potentially non-numeric) features to ensure a more meaningful arrangement of data points in $\mathbb{R}^d$. Three examples of feature spaces are shown in Fig. **??**.



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

(a) (b) (c)

Fig. 12. Three different feature spaces. (a) A linear space $\mathcal{X}^{(1)} = \mathbb{R}$. (b) A bounded convex set $\mathcal{X}^{(2)} \subseteq \mathbb{R}^2$. (c) A discrete space $\mathcal{X}^{(3)}$ whose elements are nodes of an undirected graph.

See also: feature vector, Euclidean space.

hypothesis space A hypothesis space is a mathematical model that characterizes the learning capacity of an ML method. The goal of such a method is to learn a hypothesis map that maps features of a data point to a prediction of its label. Given a finite amount of computational resources, a practical ML method typically explores only a restricted set of all possible maps from the feature space to the label space. Such a restricted set is referred to as a hypothesis space $\mathcal{H}$ underlying the ML method (see Fig. **??**). For the analysis of a given ML method,

the choice of a hypothesis space $\mathcal{H}$ is not unique, i.e., any superset containing all maps the method can learn is also a valid hypothesis space.

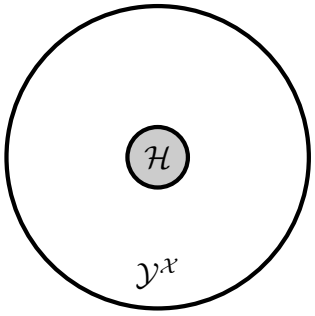


Fig. 13. The hypothesis space $\mathcal{H}$ of an ML method is a (typically very small) subset of the (typically very large) set $\mathcal{Y}^{\mathcal{X}}$ of all possible maps from the feature space $\mathcal{X}$ into the label space $\mathcal{Y}$.

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

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

parameter space The parameter space $\mathcal{W}$ of an ML model $\mathcal{H}$ is the set of all feasible choices for the model parameters (see Fig. **??**). Many important ML methods use a model that is parameterized by vectors of the Euclidean space $\mathbb{R}^d$. Two widely used examples of parameterized

models are linear models and deep nets. The parameter space is then often a subset $\mathcal{W} \subseteq \mathbb{R}^d$, e.g., all vectors $\mathbf{w} \in \mathbb{R}^d$ with a norm smaller than one.

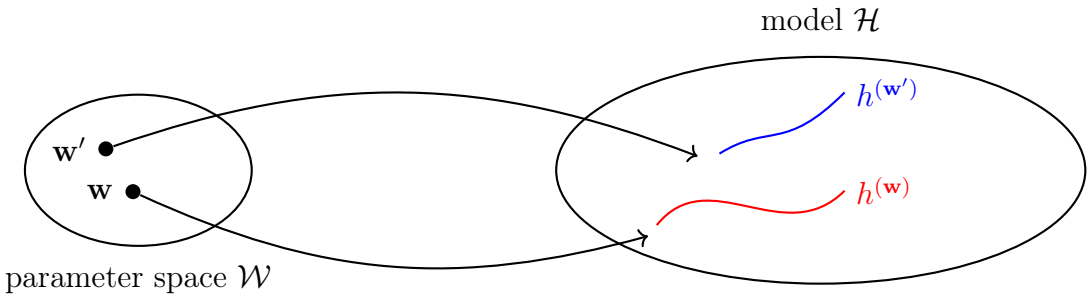
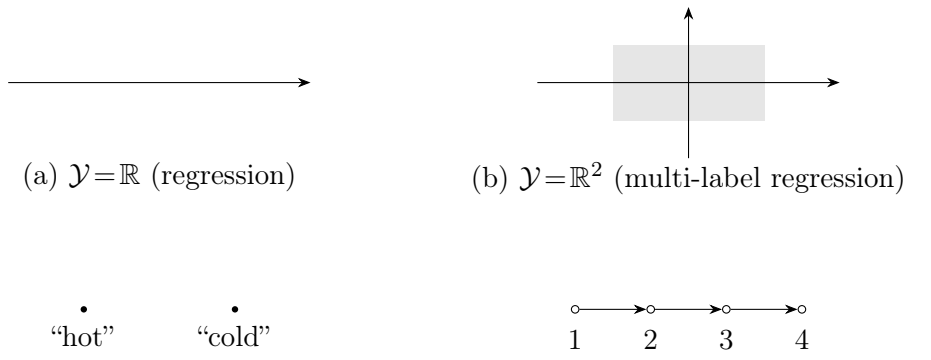


Fig. 14. The parameter space $\mathcal{W}$ of an ML model $\mathcal{H}$ consists of all feasible choices for the model parameters. Each choice $\mathbf{w}$ for the model parameters selects a hypothesis map $h^{(\mathbf{w})} \in \mathcal{H}$.

See also: parameter, model, model parameters.

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



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

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

Fig. 15. Examples of label spaces and corresponding flavours of ML.

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

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

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

See also: vector.

probability space A probability space is a mathematical structure that

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

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

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

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

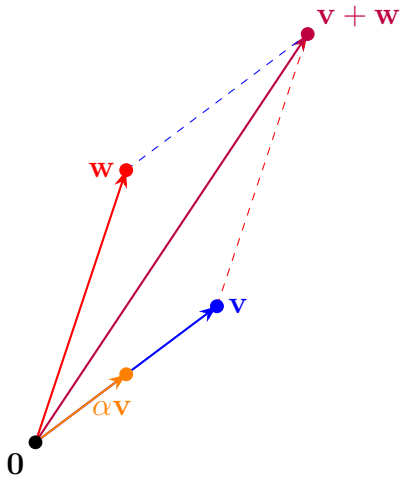


Fig. 16. A vector space $\mathcal{V}$ is a collection of vectors such that scaling and adding them always yields another vector in $\mathcal{V}$.

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

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

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

See also: probability space.

expectation Consider a numeric feature vector $\mathbf{x} \in \mathbb{R}^d$ that we interpret as the realization of an RV with a probability distribution $p(\mathbf{x})$. The

expectation of $\mathbf{x}$ is defined as the integral $\mathbb{E}\{\mathbf{x}\} := \int \mathbf{x} p(\mathbf{x})$. Note that the expectation is only defined if this integral exists, i.e., if the RV is integrable [?], [?], [?]. Fig. ?? illustrates the expectation of a scalar discrete RV x that takes on values from a finite set only.

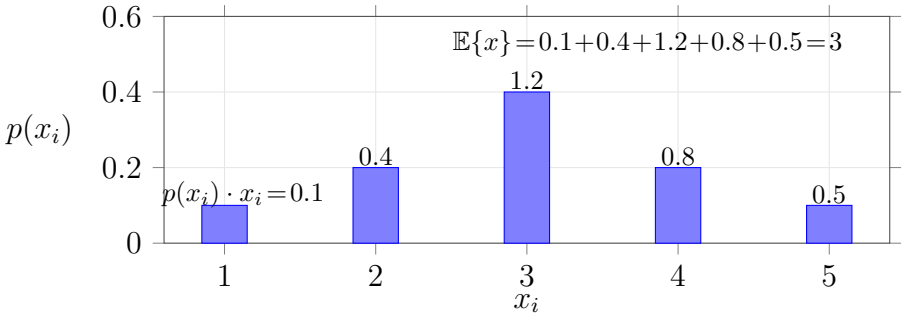


Fig. 17. The expectation of a discrete RV x is obtained by summing its possible values x_i, weighted by the corresponding probability $p(x_i) = \mathbb{P}(x = x_i)$.

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

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

See also: probabilistic model, hypothesis, risk.

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 [**?**]. Regret minimization methods learn a hypothesis that incurs a loss comparable to the best expert [**?**], [**?**].

See also: loss function, baseline, regret.

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

See also: trustworthy AI, regularization.

explanation One approach to enhance the transparency of an ML method for its human user is to provide an explanation alongside the predictions delivered by the method. Explanations can take different forms. For instance, they may consist of human-readable text or quantitative

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

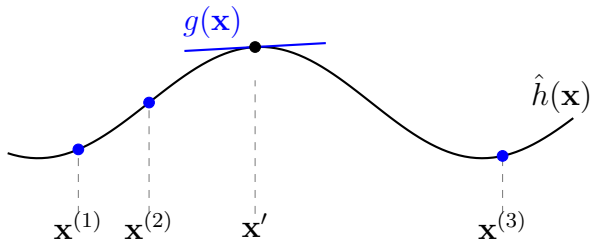


Fig. 18. A trained model $\hat{h}(\mathbf{x})$ can be explained locally at some point $\mathbf{x}'$ by a linear approximation $g(\mathbf{x})$. For a differentiable $\hat{h}(\mathbf{x})$, this approximation is determined by the gradient $\nabla \hat{h}(\mathbf{x}')$. Another form of explanation could be the function values $\hat{h}\big(\mathbf{x}^{(r)}\big)$ for $r = 1, 2, 3$.

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

local interpretable model-agnostic explanations (LIME) Consider a trained model (or learned hypothesis) $\widehat{h} \in \mathcal{H}$, which maps the feature vector of a data point to the prediction $\widehat{y} = \widehat{h}$. LIME is a technique for explaining the behavior of $\widehat{h}$, locally around a data point with

feature vector $\mathbf{x}^{(0)}$ [?]. The explanation is given in the form of a local approximation $g \in \mathcal{H}'$ of $\widehat{h}$ (see Fig. ??). This approximation can be obtained by an instance of ERM with a carefully designed training set. In particular, the training set consists of data points with feature vectors centered around $\mathbf{x}^{(0)}$ and the (pseudo-)label $\widehat{h}(\mathbf{x})$. Note that we can use a different model $\mathcal{H}'$ for the approximation from the original model $\mathcal{H}$. For example, we can use a decision tree to locally approximate a deep net. Another widely used choice for $\mathcal{H}'$ is the linear model.

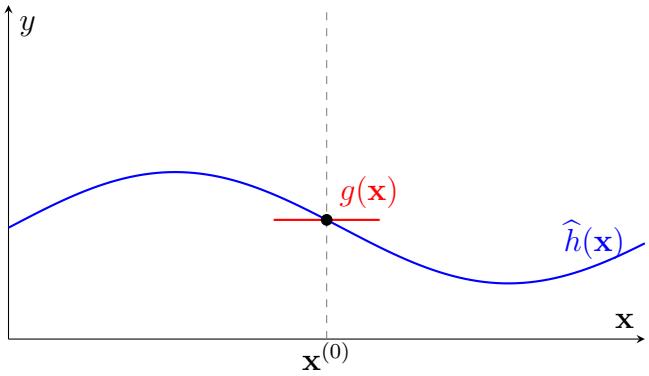


Fig. 19. To explain a trained model $\widehat{h} \in \mathcal{H}$, around a given feature vector $\mathbf{x}^{(0)}$, we can use a local approximation $g \in \mathcal{H}'$.

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

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

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

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

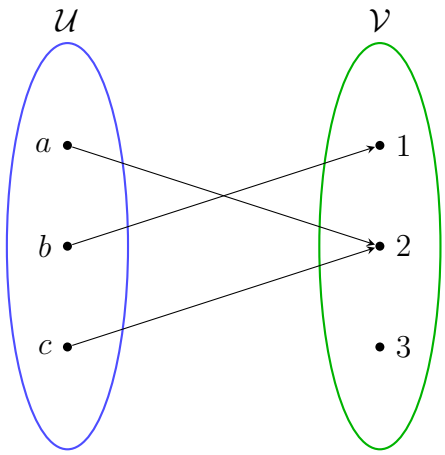


Fig. 20. A function $f\colon \{a, b, c\} \to \{1, 2, 3\}$ mapping each element of the domain to exactly one element of the co-domain.

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

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

The characteristic function uniquely determines the probability distribution of x.

See also: RV, probability distribution.

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

See also: ANN, activation, function, weights.

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 $\mathbb{P}(x \in \mathcal{B}) = \int_{\mathcal{B}} p(x')dx'$ [**?**, 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 $\mathbb{P}(\mathbf{x} \in \mathcal{R}) = \int_{\mathcal{R}} p(\mathbf{x}')dx'_1 \ldots dx'_d$ [**?**, Ch. 3].

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

loss function A loss function is a map

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

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

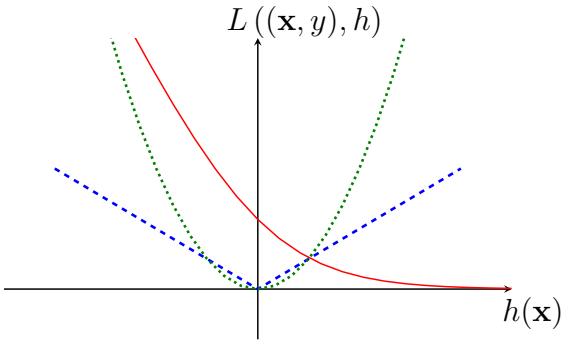


Fig. 21. Some loss function $L\left((\mathbf{x}, y), h\right)$ for a fixed data point, with feature vector $\mathbf{x}$ and label y, and a varying hypothesis h. ML methods try to find (or learn) a hypothesis that incurs minimal loss.

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

objective function An objective function is a map that assigns a numeric objective value $f(\mathbf{w})$ to each choice $\mathbf{w}$ of some variable that we want to optimize (see Fig. **??**). 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.

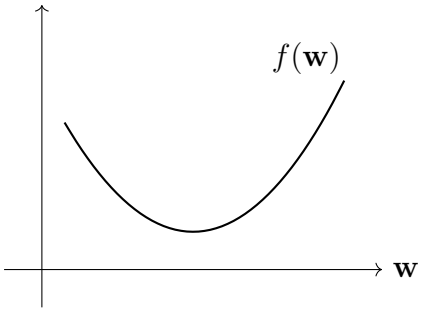


Fig. 22. An objective function maps each possible value $\mathbf{w}$ of an optimization variable, such as the model parameters of an ML model, to a value $f(\mathbf{w})$ that measures the usefulness of $\mathbf{w}$.

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

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

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

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

See also: function, vector.

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

See also: map, weights.

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 parameterized by the number n of nodes and the probability $\mathbb{P}(b^{(\{i,i'\})} = 1)$.

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

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 Fig. **??**.

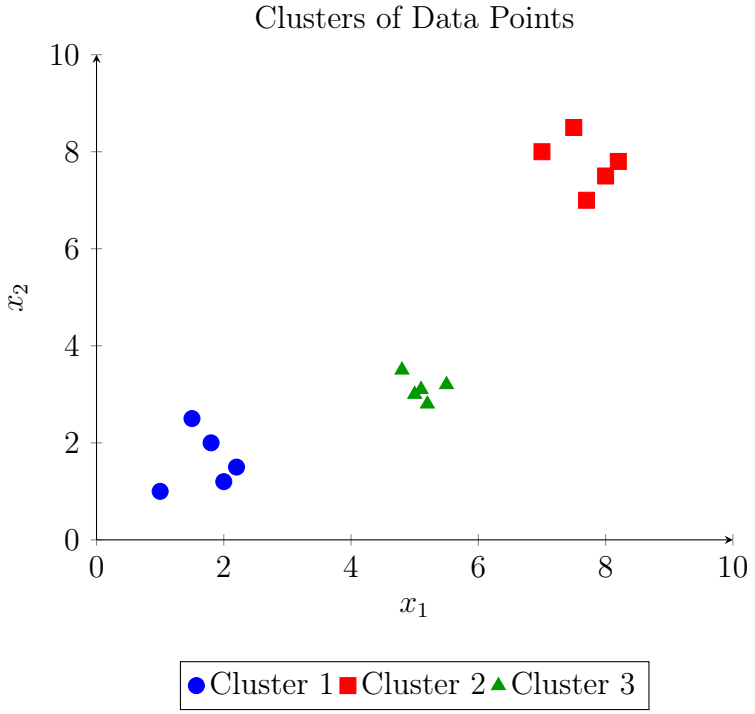


Fig. 23. Illustration of three clusters in a 2-D feature space. Each cluster groups data points that are more similar to each other than to those in other clusters, based on the Euclidean distance.

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

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

discrepancy is the challenge of generalization.

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

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

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

Generalization without probability: Probability theory is one way to study how well a model generalizes beyond the training set, but it is not the only way. Another option is to use simple deterministic changes to the data points in the training set. The basic idea is that a good model $\hat{h}$ should be robust, i.e., its prediction $\hat{h}(\mathbf{x})$ should not change much if we slightly change the features $\mathbf{x}$ of a data point $\mathbf{z}$. For example, an object detector trained on smartphone photos should still detect the object if a few random pixels are masked [**?**]. Similarly, it should deliver the same result if we rotate the object in the image [**?**]. See Fig. **??** for a visual illustration.

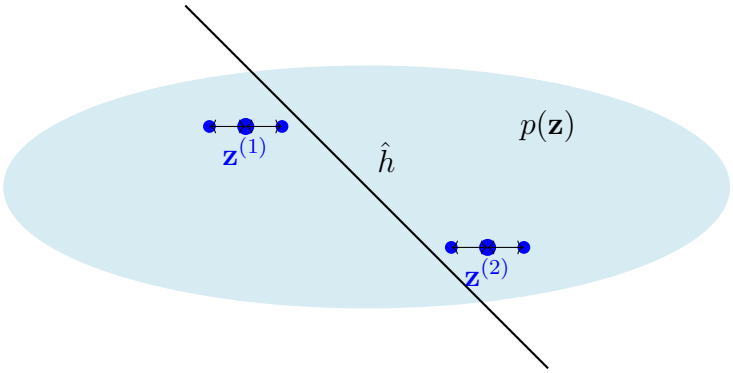


Fig. 24. Two data points $\mathbf{z}^{(1)}, \mathbf{z}^{(2)}$ that are used as a training set to learn a hypothesis $\hat{h}$ via ERM. We can evaluate $\hat{h}$ outside $\mathcal{D}^{(\text{train})}$ either by an i.i.d. assumption with some underlying probability distribution $p(\mathbf{z})$ or by perturbing the data points.

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

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

See also: map, function, prediction, model.

independent and identically distributed assumption (i.i.d. assumption)

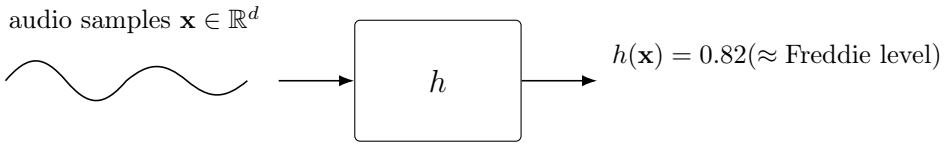


Fig. 25. A hypothesis $h : \mathcal{X} \to \mathcal{Y}$ maps the features $\mathbf{x} \in \mathcal{X}$ of a data point to a prediction $h(\mathbf{x}) \in \mathcal{Y}$ of the label. For example, the ML application `https://freddiemeter.withyoutube.com/` uses the samples of an audio recording as features predict how closely a person's singing resembles that of Freddie Mercury.

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.

uncertainty In the context of ML, uncertainty refers to the presence of multiple plausible outcomes or explanations based on available data. For example, the prediction $\hat{h}(\mathbf{x})$ produced by a trained ML model $\hat{h}$ often reflects a range of possible values for the true label of a given data point. The broader this range, the greater the associated uncertainty. Probability theory allows us to represent, quantify, and reason about uncertainty in a mathematically rigorous manner.

See also: probabilistic model, risk, entropy, variance.

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

any collection of events $\mathcal{A}_1, \ldots, \mathcal{A}_m$, we have

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

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

Finnish Meteorological Institute (FMI) The FMI is a government agency responsible for gathering and reporting weather data in Finland.
See also: data.

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 to predict optimal actions. These predictions are computed from observations about the state of the environment. The choice of loss function sets AI applications apart from more basic ML applications. AI systems rarely have access to a labeled training set that allows the average loss to be measured for any possible choice of model parameters. Instead, AI systems use observed reward signals to estimate the loss incurred by the current choice of model parameters.
See also: ML, RL.

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

1) KR1 – Human agency and oversight;

2) KR2 – Technical robustness and safety;

3) KR3 – Privacy and data governance;

4) KR4 – Transparency;

5) KR5 – Diversity, non-discrimination and fairness;

6) KR6 – Societal and environmental well-being;

7) KR7 – Accountability.

See also: computational aspects, statistical aspects, ML, AI, robustness, data, transparency.

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

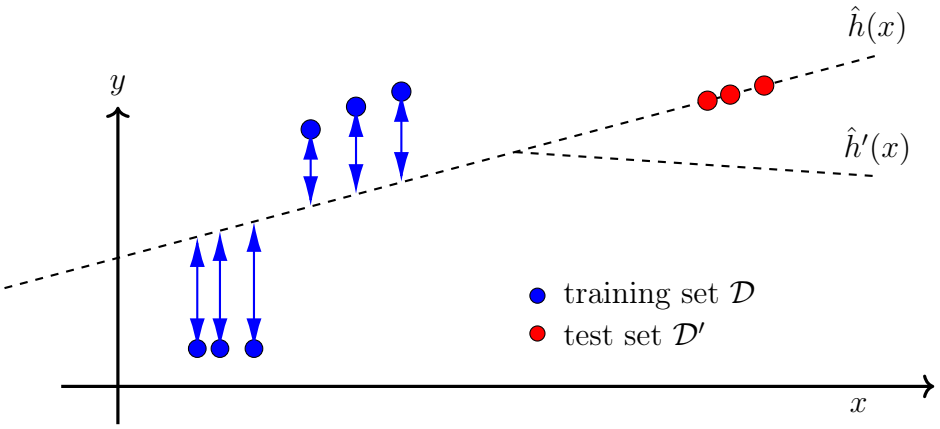


Fig. 26. We can assess the interpretability of trained ML models $\hat{h}$ and $\hat{h}'$ by comparing their predictions to pseudo-labels generated by a human user for $\mathcal{D}'$.

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

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

model inversion A model inversion is a form of privacy attack on an ML system. An adversary seeks to infer sensitive attributes of individual data points by exploiting partial access to a trained model $\hat{h} \in \mathcal{H}$. This

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

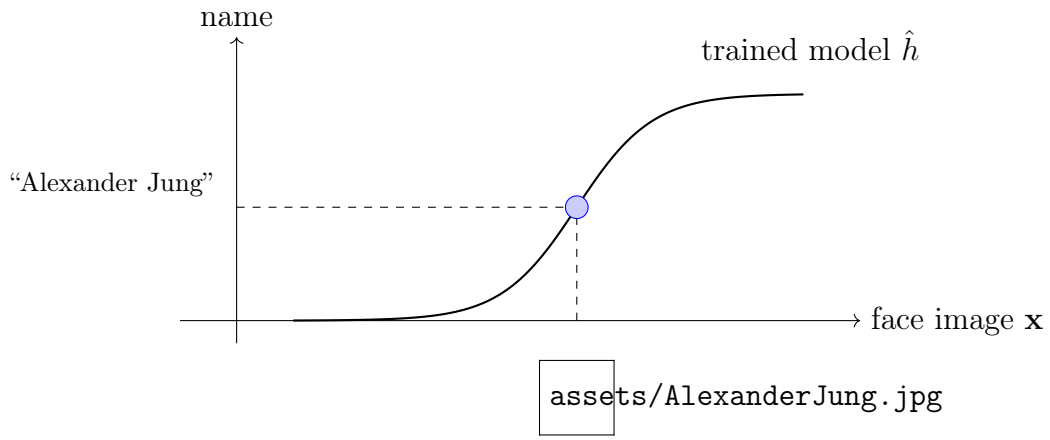


Fig. 27. Model inversion techniques implemented in the context of facial image classification.

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

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

See also: probability, RV, expectation.

dataset A dataset is a set of distinct data points. In contrast to a sample, which is defined as a sequence of data points and may contain repetitions,

a dataset is an unordered collection without duplicates. ML methods use datasets to train and validate models. The notion of a dataset is broad: data points may represent concrete physical entities (such as humans or animals) or abstract objects (such as numbers). For illustration, Fig. **??** depicts a dataset whose data points are cows.

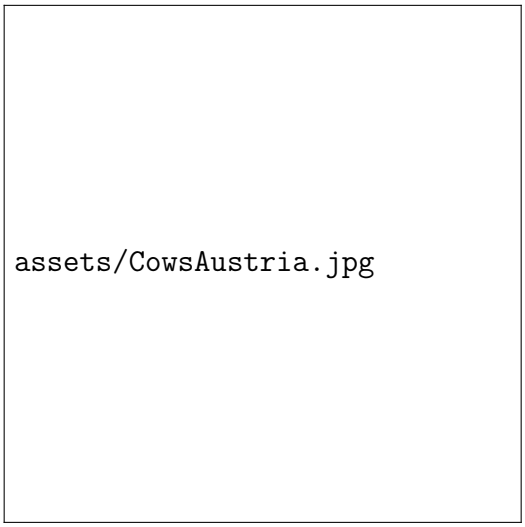


Fig. 28. A cow herd somewhere in the Alps.

Quite often, an ML engineer does not have direct access to the underlying dataset. For instance, accessing the dataset in Fig. **??** would require visiting the cow herd. In practice, we work with a more convenient representation (or approximation) of the dataset. Various mathematical models have been developed for this purpose [**?**], [**?**], [**?**], [**?**]. One of the most widely used is the relational model, which organizes data as a table (or relation) [**?**], [**?**]. A table consists of rows and columns: each row corresponds to a single data point, while each column represents a

specific attribute of a data point. ML methods typically interpret these attributes as features or as a label of a data point. As an illustration, Table **??** shows a relational representation of the dataset from Fig. **??**. In the relational model, the order of rows is immaterial, and each attribute (column) is associated with a domain that specifies the set of admissible values. In ML applications, these attribute domains correspond to the feature space and the label space.

TABLE I

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

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

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

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

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 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.

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

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

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

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

multivariate normal distribution The multivariate normal distribution, which is denoted by $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, is a fundamental probabilistic model for numerical feature vectors of fixed dimension d. It defines a family of probability distributions over vector-valued RVs $\mathbf{x} \in \mathbb{R}^d$ [**?**], [**?**], [**?**].

Each distribution in this family is fully specified by its mean vector $\boldsymbol{\mu} \in \mathbb{R}^d$ and covariance matrix $\boldsymbol{\Sigma} \in \mathbb{R}^{d \times d}$. When the covariance matrix $\boldsymbol{\Sigma}$ is invertible, the corresponding probability distribution is characterized by the following pdf:

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

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

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

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

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

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

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

parameters.

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

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

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

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

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

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

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

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

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

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

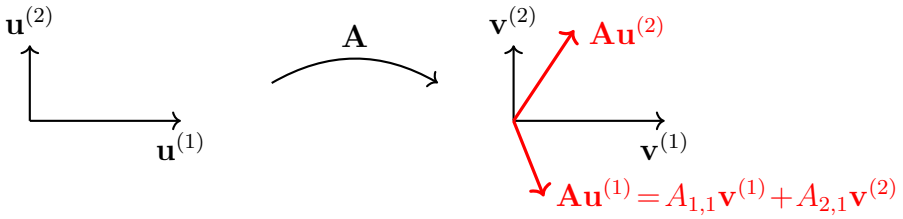


Fig. 29. A matrix $\mathbf{A}$ defines a linear map between two vector spaces.

See also: linear map, dataset, linear model.

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 $\mathbf{X} := \big(\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)}\big)^T$ of size $m \times d$.

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

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: covariance, matrix, RV.

inverse matrix An inverse matrix $\mathbf{A}^{-1}$ is defined for a square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ that is of full rank, meaning its columns are linearly independent. In this case, $\mathbf{A}$ is said to be invertible, and its inverse satisfies

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

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

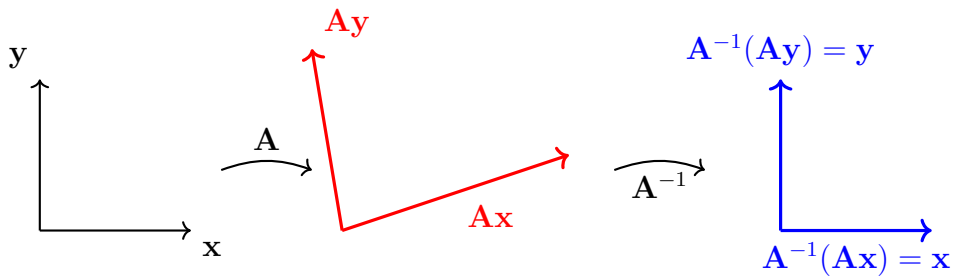


Fig. 30. A matrix $\mathbf{A}$ represents a linear transformation of $\mathbb{R}^2$. The inverse matrix $\mathbf{A}^{-1}$ represents the inverse transformation.

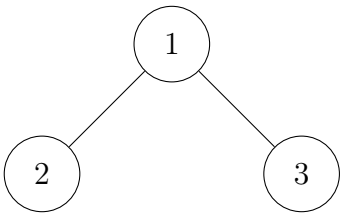
See also: matrix, determinant, linear regression, pseudoinverse.

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

defined elementwise as (see Fig. **??**)

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

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



(a)

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

(b)

Fig. 31. (a) Some undirected graph $\mathcal{G}$ with three nodes $i = 1, 2, 3$. (b) The Laplacian matrix $\mathbf{L}^{(\mathcal{G})} \in \mathbb{R}^{3 \times 3}$ of $\mathcal{G}$.

See also: graph, matrix, edge weight.

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) [**?**, 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, optimization problem, probabilistic model.

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

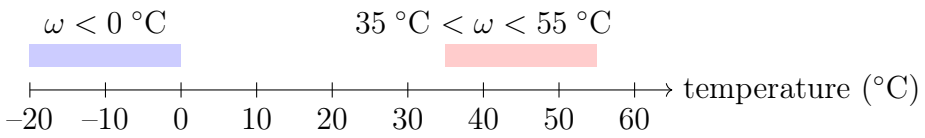


Fig. 32. A sample space constituted by all possible temperature values ω that may be experienced at an FMI station. Two measurable subsets of temperature values, denoted by $\mathcal{A}^{(1)}$ and $\mathcal{A}^{(2)}$, are highlighted. For any actual temperature value ω, it is possible to determine whether $\omega \in \mathcal{A}^{(1)}$ and whether $\omega \in \mathcal{A}^{(2)}$.

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

See also: sample space, probability.

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

See also: RERM, GTV, regularizer.

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

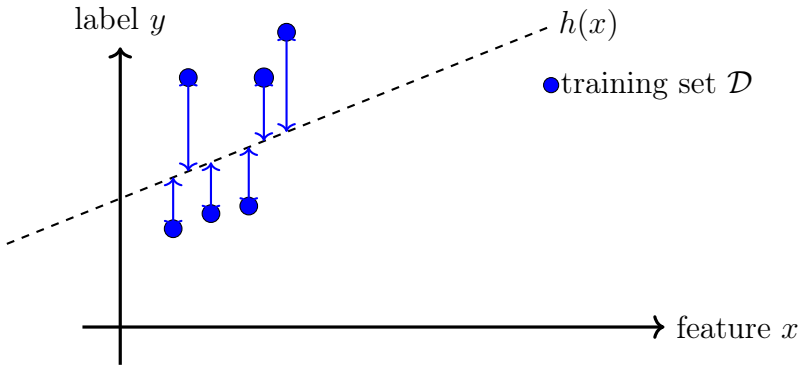


Fig. 33. ERM learns a hypothesis $h \in \mathcal{H}$, out of a model $\mathcal{H}$, by minimizing the average loss (or empirical risk) $1/m \sum_{r=1}^{m} L\left(\left(\mathbf{x}^{(r)}, y^{(r)}\right), h\right)$ incurred on a training set $\mathcal{D}$.

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

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

$$\hat{h} \in \arg\min_{h \in \mathcal{H}} \widehat{L}\big(h|\mathcal{D}\big) + \alpha \mathcal{R}\big\{h\big\}. \tag{4}$$

The parameter $\alpha \geq 0$ controls the regularization strength. For $\alpha = 0$, we recover standard ERM without regularization. As α increases, the learned hypothesis is increasingly biased toward small values of $\mathcal{R}\big\{h\big\}$. The component $\alpha \mathcal{R}\big\{h\big\}$ in the objective function of (**??**) can be intuitively understood as a surrogate for the increased average loss that may occur when predicting labels for data points outside the training set. This intuition can be made precise in various ways. For example, consider a linear model trained using squared error loss and the regularizer $\mathcal{R}\big\{h\big\} = \|\mathbf{w}\|_2^2$. In this setting, $\alpha \mathcal{R}\big\{h\big\}$ corresponds to the expected increase in loss caused by adding Gaussian RVs to the feature vectors in the training set [**?**, Ch. 3]. A principled construction for the regularizer $\mathcal{R}\big\{h\big\}$ arises from approximate upper bounds on the generalization error. The resulting RERM instance is known as structural risk minimization (SRM) [**?**, Sec. 7.2].

See also: ERM, regularization, loss, SRM.

structural risk minimization (SRM) SRM is an instance of RERM, with which the model $\mathcal{H}$ can be expressed as a countable union of submodels such that $\mathcal{H} = \bigcup_{n=1}^{\infty} \mathcal{H}^{(n)}$. Each submodel $\mathcal{H}^{(n)}$ permits the derivation of an approximate upper bound on the generalization error incurred when applying ERM to train $\mathcal{H}^{(n)}$. These individual bounds—one for each submodel—are then combined to form a regularizer used in the RERM objective. These approximate upper bounds (one for each $\mathcal{H}^{(n)}$) are then combined to construct a regularizer for RERM [**?**, Sec. 7.2]. See also: RERM, model, generalization, ERM, regularizer, risk.

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.

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

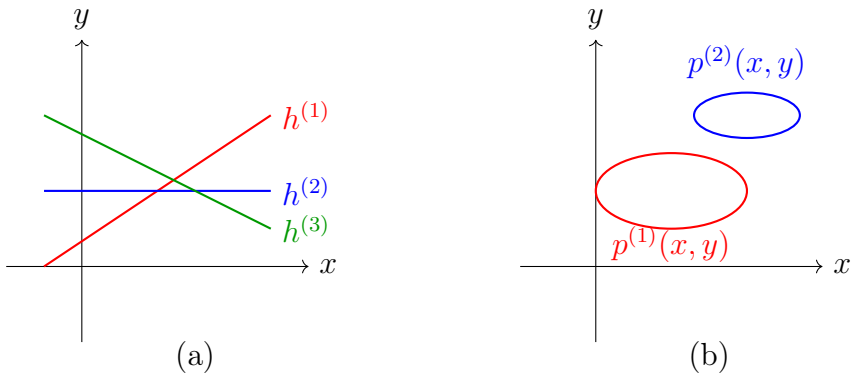


Fig. 34. Two types of mathematical models used in ML. (a) A hypothesis space consisting of three linear maps. (b) A probabilistic model consisting of probability distribution over the plane spanned by the feature and label values of a data point.

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

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

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

Each value of d defines a different hypothesis space, corresponding to the number of features used to compute the prediction $h(\mathbf{x})$. The choice of d is often guided not only by computational aspects (e.g., fewer features reduce computation) and statistical aspects (e.g., more features typically reduce bias and risk), but also by interpretability. A linear model using a small number of well-chosen features is generally considered more

interpretable [**?**], [**?**]. The linear model is attractive because it can typically be trained using scalable convex optimization methods [**?**], [**?**]. Moreover, linear models often permit rigorous statistical analysis, including fundamental limits on the minimum achievable risk [**?**]. They are also useful for analyzing more complex nonlinear models such as 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 $g(\mathbf{x})$. Fig. **??** illustrates such a local linear approximation, defined by the gradient $\nabla \hat{h}(\mathbf{x}')$. Note that the gradient is only defined where $\hat{h}$ is differentiable. To ensure robustness in the context of trustworthy AI, one may prefer models whose associated map $\hat{h}$ is Lipschitz continuous. A classic result in mathematical analysis—Rademacher's Theorem—states that if $\hat{h}$ is Lipschitz continuous with some constant L over an open set $\Omega \subseteq \mathbb{R}^d$, then $\hat{h}$ is differentiable almost everywhere in Ω [**?**, Th. 3.1].

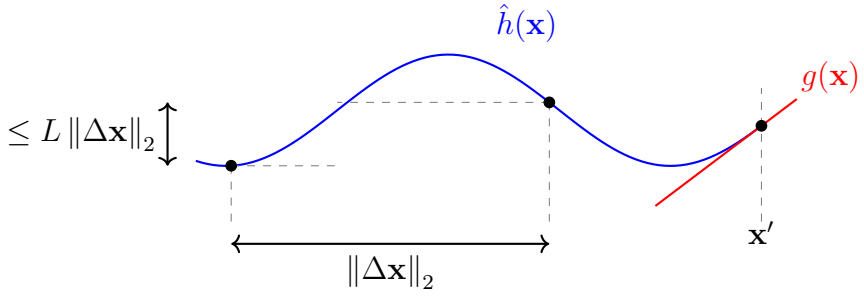


Fig. 35. A trained model $\hat{h}(\mathbf{x})$ that is differentiable at a point $\mathbf{x}'$ can be locally approximated by a linear map $g \in \mathcal{H}^{(d)}$. This local approximation is determined by the gradient $\nabla \hat{h}(\mathbf{x}')$.

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

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

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

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

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

stochastic block model (SBM) The SBM is a probabilistic generative

model for an undirected graph $\mathcal{G} = \big(\mathcal{V}, \mathcal{E}\big)$ with a given set of nodes $\mathcal{V}$ [?]. In its most basic variant, the SBM generates a graph by first randomly assigning each node $i \in \mathcal{V}$ to a 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.

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

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

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

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

$$\mathbb{E}\{\mathbf{x}\} = \operatorname*{arg\,min}_{\mathbf{c} \in \mathbb{R}^d} \mathbb{E}\big\{ \left\|\mathbf{x} - \mathbf{c}\right\|_2^2 \big\}.$$

We also use the term to refer to the average of a finite sequence $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)} \in \mathbb{R}^d$. However, these two definitions are essentially

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

See also: RV, expectation, probability distribution.

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

See also: algorithm, optimization problem.

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

$$\mathbf{w}^{(k+1)} = \mathcal{F}\mathbf{w}^{(k)}, \text{ for } k = 0, 1, \ldots. \tag{5}$$

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 (**??**) that reduces the distance to a solution such that

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

Thus, we require $\mathcal{F}$ to be at least non-expansive, i.e., the iteration (**??**) should not result in worse model parameters that have a larger distance

to a solution $\widehat{\mathbf{w}}$. Furthermore, each iteration (**??**) should also make some progress, i.e., reduce the distance to a solution $\widehat{\mathbf{w}}$. This requirement can be made precise using the notion of a contraction operator [**?**], [**?**]. The operator $\mathcal{F}$ is a contraction operator if, for some $\kappa \in [0, 1)$,

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

For a contraction operator $\mathcal{F}$, the fixed-point iteration (**??**) generates a sequence $\mathbf{w}^{(k)}$ that converges quite rapidly. In particular [**?**, 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 (**??**) with a firmly non-expansive operator $\mathcal{F}$ is guaranteed to converge to a fixed-point of $\mathcal{F}$ [**?**, Corollary 5.16]. Fig. **??** depicts examples of a firmly non-expansive operator, a non-expansive operator, and a contraction operator. All of these operators are defined on the 1-D space $\mathbb{R}$. Another example of a firmly non-expansive operator is the proximal operator of a convex function [**?**], [**?**].

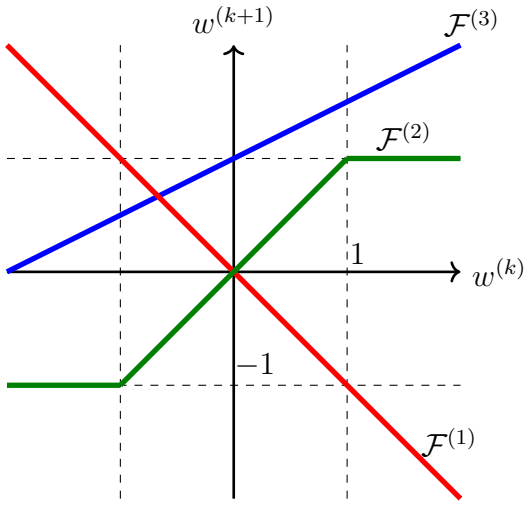


Fig. 36. Example of a non-expansive operator $\mathcal{F}^{(1)}$, a firmly non-expansive operator $\mathcal{F}^{(2)}$, and a contraction operator $\mathcal{F}^{(3)}$.

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

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 $\mathbf{z} = K\big(\mathbf{x}, \cdot\big)$ [?], [?]. 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 Fig. **??**).

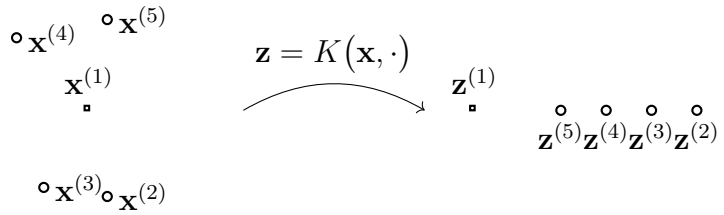


Fig. 37. Five data points characterized by feature vectors $\mathbf{x}^{(r)}$ and labels $y^{(r)} \in \{\circ, \square\}$, for $r = 1, \ldots, 5$. With these feature vectors, there is no way to separate the two classes by a straight line (representing the decision boundary of a linear classifier). In contrast, the transformed feature vectors $\mathbf{z}^{(r)} = K\big(\mathbf{x}^{(r)}, \cdot\big)$ allow us to separate the data points using a linear classifier.

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

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.

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

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

This minimum achievable risk (referred to as the Bayes risk) is the risk of the Bayes estimator for the label y of a data point, given its features $\mathbf{x}$. Note that, for a given choice of loss function, the Bayes estimator (if it exists) is completely determined by the probability distribution $p(\mathbf{x}, y)$ [**?**, Ch. 4]. However, computing the Bayes estimator and Bayes risk presents two main challenges. First, the probability distribution

$p(\mathbf{x}, y)$ is unknown and must be estimated from observed data. Second, even if $p(\mathbf{x}, y)$ were known, computing the Bayes risk exactly may be computationally infeasible [**?**]. A widely used probabilistic model is the multivariate normal distribution $(\mathbf{x}, y) \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ for data points characterized by numeric features and labels. Here, for the squared error loss, the Bayes estimator is given by the posterior mean $\mu_{y|\mathbf{x}}$ of the label y, given the features $\mathbf{x}$ [**?**], [**?**]. The corresponding Bayes risk is given by the posterior variance $\sigma^2_{y|\mathbf{x}}$ (see Fig. **??**).

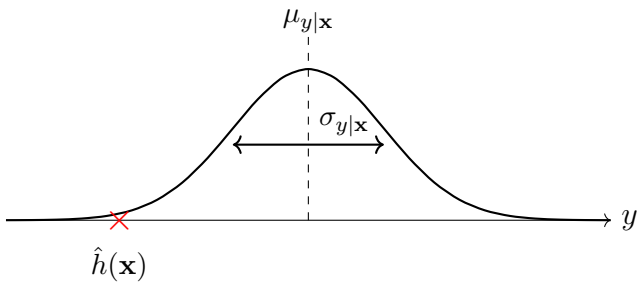


Fig. 38. If the features and the label of a data point are drawn from a multivariate normal distribution, we can achieve the minimum risk (under squared error loss) by using the Bayes estimator $\mu_{y|\mathbf{x}}$ to predict the label y of a data point with features $\mathbf{x}$. The corresponding minimum 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.

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

See also: function, smooth.

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

See also: function, vector, vector space.

kernel Consider a set of data points, each represented by a feature vector $\mathbf{x} \in \mathcal{X}$, where $\mathcal{X}$ denotes the feature space. A (real-valued) kernel is a function $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ that assigns to every pair of feature vectors $\mathbf{x}, \mathbf{x}' \in \mathcal{X}$ a real number $K\big(\mathbf{x}, \mathbf{x}'\big)$. This value is typically interpreted as a similarity measure between $\mathbf{x}$ and $\mathbf{x}'$. The defining property of a kernel is that it is symmetric, i.e., $K\big(\mathbf{x}, \mathbf{x}'\big) = K\big(\mathbf{x}', \mathbf{x}\big)$, and that for any finite set of feature vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathcal{X}$, the matrix

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

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

that assigns a real value to each index $j \in \{1, \ldots, d\}$.

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

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

$$\mathbf{An} = \mathbf{0}.$$

Consider a feature learning method that uses the matrix $\mathbf{A}$ to transform a feature vector $\mathbf{x} \in \mathbb{R}^d$ of a data point into a new feature vector $\mathbf{z} = \mathbf{Ax} \in \mathbb{R}^{d'}$. The nullspace null($\mathbf{A}$) characterizes all directions in the original feature space $\mathbb{R}^d$ along which the transformation $\mathbf{Ax}$ remains unchanged. In other words, adding any vector from the nullspace to a feature vector $\mathbf{x}$ does not affect the transformed representation $\mathbf{z}$. This property can be exploited to enforce invariances in the predictions (computed from $\mathbf{Ax}$). Fig. **??** illustrates one such invariance. It shows rotated versions of two handwritten digits, which approximately lie along 1-D curves in the original feature space. These curves are aligned with a direction vector $\mathbf{n} \in \mathbb{R}^d$. To ensure that the trained model is invariant to such rotations, we can choose the transformation matrix $\mathbf{A}$ such that $\mathbf{n} \in$ null($\mathbf{A}$). This ensures that $\mathbf{Ax}$, and hence the resulting prediction, is approximately insensitive to rotations of the input image.

Fig. 39. Rotated handwritings of two different digits. The rotations are approximately aligned along straight lines parallel to the vector $\mathbf{n}$. For a binary classifier distinguishing between these digits, a natural choice is a linear feature map $\mathbf{x} \mapsto \mathbf{A}\mathbf{x}$ with a matrix $\mathbf{A}$ whose nullspace contains $\mathbf{n}$, i.e., $\mathbf{n} \in \text{null}(\mathbf{A})$.

See also: matrix, feature map, feature learning.

Python demo: click me

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

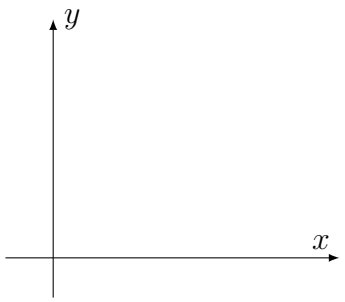


Fig. 40. A scatterplot with circle markers, where the data points represent daily weather conditions in Finland. Each data point is characterized by its minimum daytime temperature x as the feature and its maximum daytime temperature y as the label. The temperatures have been measured at the FMI weather station Helsinki Kaisaniemi during 1 September 2024—28 October 2024.

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

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

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

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

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

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

As illustrated in Fig. **??**, 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 $\rho = 1/\eta$.

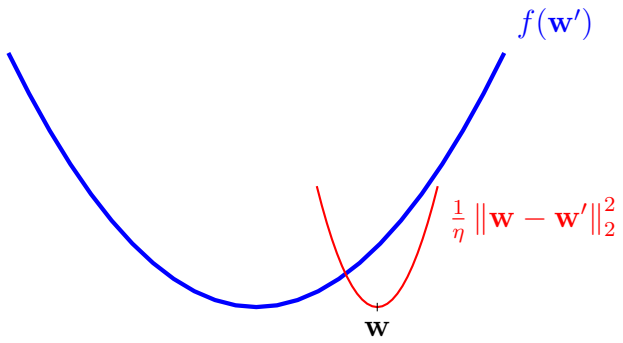


Fig. 41. The proximal operator updates a vector $\mathbf{w}$ by minimizing a penalized version of the function $f(\cdot)$. The penalty term is the scaled squared Euclidean distance between the optimization variable $\mathbf{w}'$ and the given vector $\mathbf{w}$.

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

parameter The parameter of an ML model is a tunable (i.e., learnable or adjustable) quantity that allows us to choose between different hypothesis maps. For example, the linear model $\mathcal{H} := \{h^{(\mathbf{w})} : h^{(\mathbf{w})}(x) =$

$w_1 x + w_2\}$ consists of all hypothesis maps $h^{(\mathbf{w})}(x) = w_1 x + w_2$ with a particular choice for the parameters $\mathbf{w} = \big(w_1, w_2\big)^T \in \mathbb{R}^2$. Another example of a model parameter is the weights assigned to a connection between two neurons of an ANN.

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

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.

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

$$\widehat{\mathbf{w}} := \mathbf{w} - \eta \nabla f(\mathbf{w}). \tag{6}$$

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

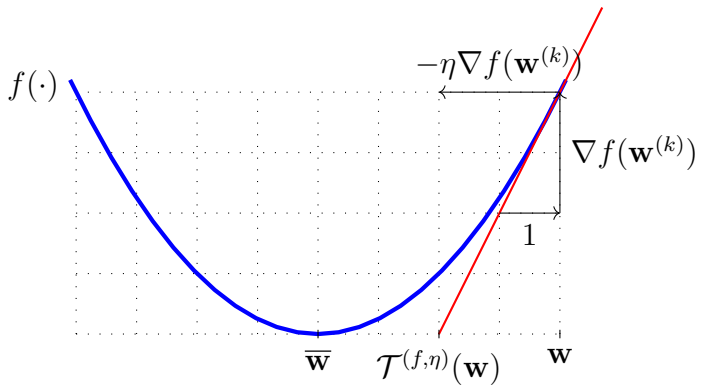


Fig. 42. The basic gradient step (**??**) maps a given vector $\mathbf{w}$ to the updated vector $\mathbf{w}'$. It defines an operator $\mathcal{T}^{(f,\eta)}(\cdot) : \mathbb{R}^d \to \mathbb{R}^d : \mathbf{w} \mapsto \widehat{\mathbf{w}}$.

Note that the gradient step (**??**) 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 (**??**) is to locally optimize the function itself—instead of its linear approximation—such that

$$\widehat{\mathbf{w}} = \operatorname*{arg\,min}_{\mathbf{w}' \in \mathbb{R}^d} f(\mathbf{w}') + \frac{1}{\eta} \|\mathbf{w} - \mathbf{w}'\|_2^2 . \tag{7}$$

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

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

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

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

See also: loss function, empirical risk.

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

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

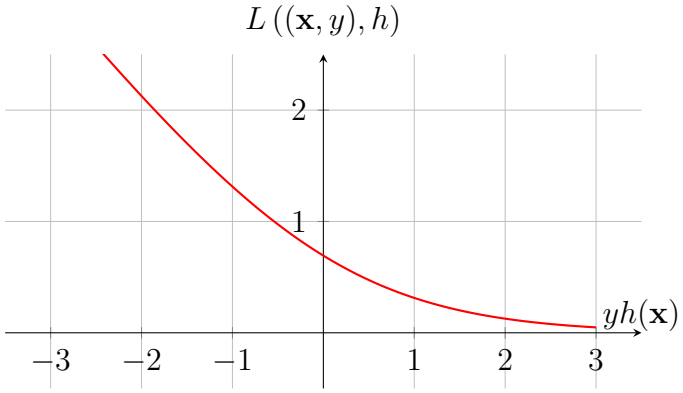


Fig. 43. The logistic loss incurred by the prediction $h(\mathbf{x}) \in \mathbb{R}$ for a data point with label $y \in \{-1, 1\}$.

Note that the expression (**??**) for the logistic loss applies only for the label space $\mathcal{Y} = \{-1, 1\}$ and when using the thresholding rule (**??**).
See also: data point, feature, label, hypothesis, loss, prediction, label space.

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.

weights Consider a parameterized hypothesis space $\mathcal{H}$. We use the term weights for numeric model parameters that are used to scale features or their transformations in order to compute $h^{(\mathbf{w})} \in \mathcal{H}$. A linear model uses weights $\mathbf{w} = \big(w_1, \ldots, w_d\big)^T$ to compute the linear combination $h^{(\mathbf{w})}(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$. Weights are also used in ANNs to form linear combinations of features or the outputs of neurons in hidden layers (see Fig. **??**).

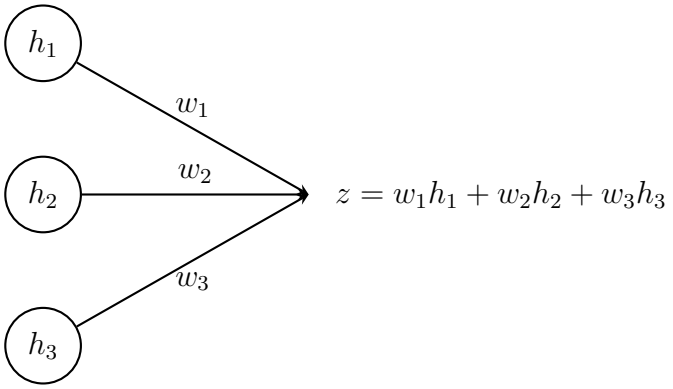


Fig. 44. A section of an ANN that contains a hidden layer with outputs (or activations) h_1,h_2, and h_3. These outputs are combined linearly to compute z, which can be used either as output of the ANN or as input to another layer.

See also: hypothesis space, model parameters, feature, linear model, ANN, layer, activation.

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

See also: FL network.

data point A data point is any object that conveys information [**?**]. Examples include students, radio signals, trees, images, RVs, real numbers, or proteins. We describe data points of the same type by two categories of properties. The first category includes features that are measurable or computable properties of a data point. These attributes can be automatically extracted or computed using sensors, computers, or other data collection systems. For a data point that represents a patient,

one feature could be the body weight. The second category includes labels that are higher level facts (or quantities of interest)—that is, facts which typically require human expertise or domain knowledge to determine, rather than being directly measurable—associated with the data point. Determining the labels of a data point usually requires human expertise or domain knowledge. For a data point that represents a patient, a cancer diagnosis provided by a physician would serve as the label. Fig. **??** depicts an image as an example of a data point along with its features and labels. Importantly, what constitutes a feature or a label is not inherent to the data point itself—it is a design choice that depends on the specific ML application.

A single data point.

Features:

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

Labels:

- y_1: Number of cows depicted.[104]
- y_2: Number of wolves depicted.
- y_3: Condition of the pasture (e.g., healthy, overgrazed).

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

See also: data, feature, label, dataset.

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

See also: data point, label.

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

See also: ML, training set, data poisoning, algorithm, ERM, hypothesis, prediction, feature.

data minimization principle European data protection regulation includes a data minimization principle. This principle requires a data controller to limit the collection of personal information to what is directly relevant

and necessary to accomplish a specified purpose. The data should be retained only for as long as necessary to fulfill that purpose [**?**, Article 5(1)(c)], [**?**].

See also: data.

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

See also: event, random experiment.

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

See also: objective function.

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

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

For a fixed input space $\mathcal{X}$, a GP is fully specified (or parameterized) by: 1) a mean function $\mu(\mathbf{x}) = \mathbb{E}\{f(\mathbf{x})\}$; and 2) a covariance function $K\left(\mathbf{x}, \mathbf{x}'\right) = \mathbb{E}\{\left(f(\mathbf{x}) - \mu(\mathbf{x})\right)\left(f(\mathbf{x}') - \mu(\mathbf{x}')\right)\}$.

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

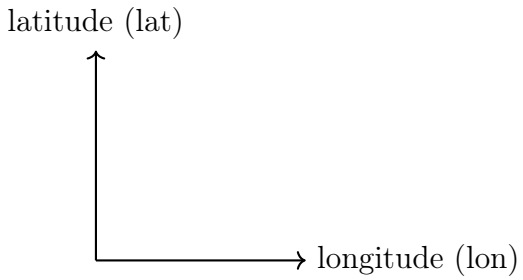


Fig. 46. For a given point in time, we can interpret the current temperature distribution over Finland as a realization of a GP indexed by geographic coordinates and sampled at FMI weather stations. The weather stations are indicated by blue dots.

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

stochastic process A stochastic process is a collection of RVs defined on a common probability space and indexed by some set $\mathcal{I}$ [**?**], [**?**], [**?**]. The index set $\mathcal{I}$ typically represents time or space, allowing us to represent

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

See also: RV, SBM, SGD, uncertainty, probabilistic model.

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

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

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

See also: matrix, ML, model, vector.

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

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

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

See also: Euclidean space, vector, minimum.

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.

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.

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 [?]. The pseudoinverse arises naturally within ridge regression when applied to a dataset with arbitrary labels $\mathbf{y}$ and a feature matrix $\mathbf{X} = \mathbf{A}$ [?, Ch. 3]. The model parameters learned by ridge regression are given by

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

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

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

See also: matrix, inverse matrix, ridge regression.

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' [?]. The baseline hypothesis h' is also referred to as an expert.

See also: baseline, loss, expert.

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

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

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 $h : \mathcal{X} \to \mathcal{Y}$. Any hypothesis that achieves the Bayes risk is referred to as a Bayes estimator [**?**].

See also: probabilistic model, risk, Bayes estimator.

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.

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

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

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

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

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

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

See also: RV, probability space, measurable.

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

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

See also: loss, MAB, RL.

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

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

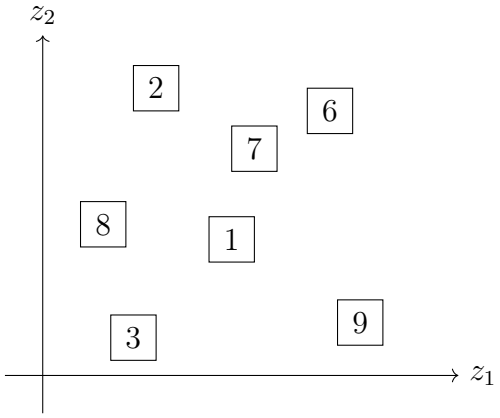


Fig. 47. Example of dimensionality reduction: High-dimensional image data (e.g., high-resolution images of handwritten digits) embedded into 2-D using learned features (z_1, z_2) and visualized in a scatterplot.

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

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.

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

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

linear regression Linear regression aims to learn a linear hypothesis map to predict a numeric label based on the numeric features of a data point.

The quality of a linear hypothesis map is measured using the average squared error loss incurred on a set of labeled data points, which we refer to as the training set.

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

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 data points (i.e., the training set).

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

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

See also: regression, ERM, squared error loss.

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

squared error loss is measured on a set of labeled data points (i.e., the training set)

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

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

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

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

1) Model pruning: We prune the original model $\mathcal{H}$ to obtain a smaller

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

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

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

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

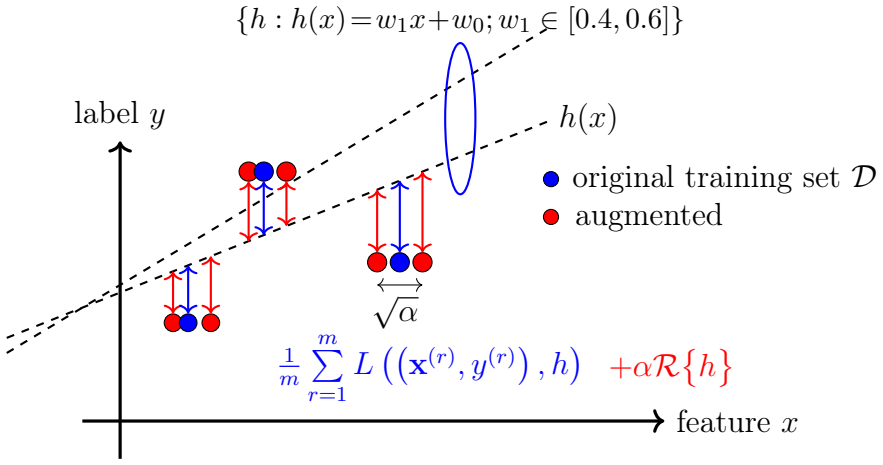


Fig. 48. Three approaches to regularization: 1) data augmentation; 2) loss penalization; and 3) model pruning (via constraints on model parameters).

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

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

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

The constant β quantifies the smoothness of the function f: the smaller the β, the smoother f is. Optimization problems with a smooth objective function can be solved effectively by gradient-based methods. Indeed, gradient-based methods approximate the objective function locally around a current choice $\mathbf{w}$ using its gradient. This approximation works well if the gradient does not change too rapidly. We can make this

informal claim precise by studying the effect of a single gradient step with step size $\eta = 1/\beta$ (see Fig. **??**).

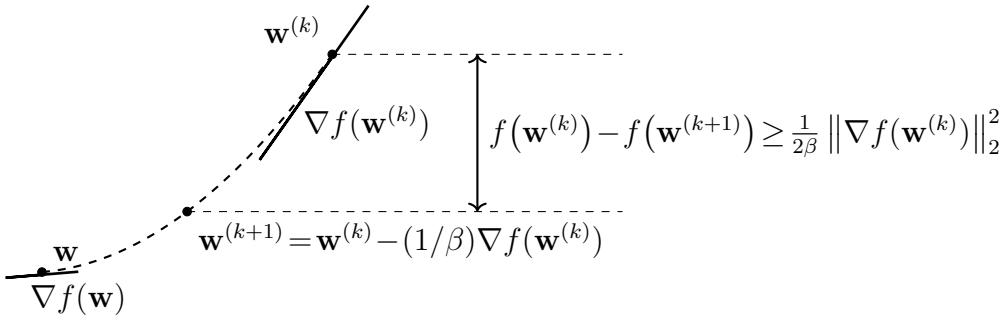


Fig. 49. Consider an objective function $f(\mathbf{w})$ that is β-smooth. Taking a gradient step, with step size $\eta = 1/\beta$, decreases the objective by at least $1/2\beta \left\|\nabla f(\mathbf{w}^{(k)})\right\|_2^2$ [**?**], [**?**], [**?**]. Note that the step size $\eta = 1/\beta$ becomes larger for smaller β. Thus, for smoother objective functions (i.e., those with smaller β), we can take larger steps.

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

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, layer.

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

See also: ANN, layer, ML, model.

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 generalized total variation minimization (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.

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

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

underfitting Consider an ML method that uses ERM to learn a hypothesis with the minimum empirical risk on a given training set. Such a method is underfitting the training set if it is not able to learn a hypothesis

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

See also: ML, ERM, hypothesis, minimum, empirical risk, training set, risk.

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 [**?**, Ch. 13]). To build intuition, consider the three datasets depicted in Fig. **??**, 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.

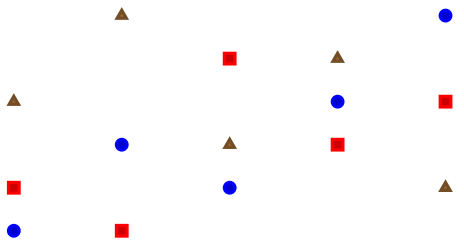


Fig. 50. Three datasets $\mathcal{D}^{(*)}$, $\mathcal{D}^{(\square)}$, and $\mathcal{D}^{(\triangle)}$, each sampled independently from the same data-generating probability distribution. A stable ML method should return similar outputs when trained on any of these datasets.

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

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

See also: SGD, uncertainty, probabilistic model.

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

set.

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

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 [**?**, Ch. 6].

See also: ML, model, validation error.

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

See also: data point, dataset.

step size See learning rate.

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 [**?**, Ch. 5].

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

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

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

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

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

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

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

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

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

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

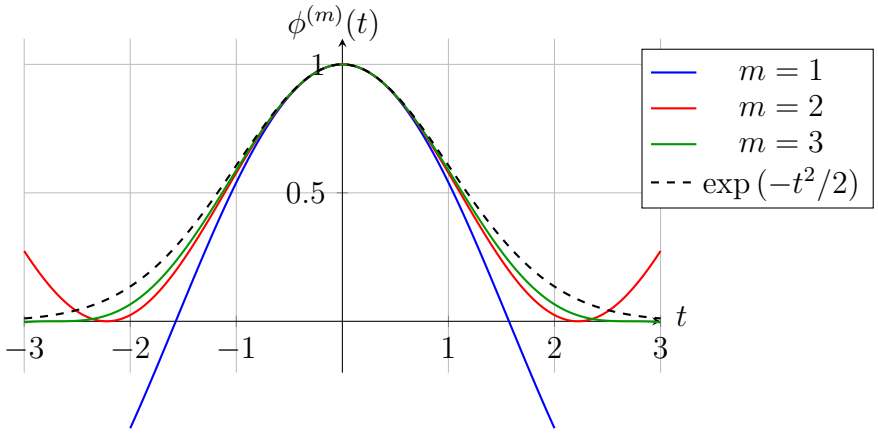


Fig. 51. Characteristic functions of normalized sums of i.i.d. RVs $x^{(r)} \in \{-1, 1\}$ for $r = 1, \ldots, m$ compared to the Gaussian limit.

See also: RV, Gaussian RV.

feature map A feature map refers to a function

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

that transforms a feature vector $\mathbf{x} \in \mathcal{X}$ of a data point into a new feature vector $\mathbf{x}' \in \mathcal{X}'$, where $\mathcal{X}'$ is typically different from $\mathcal{X}$. The transformed representation $\mathbf{x}'$ is often more useful than the original $\mathbf{x}$. For instance, the geometry of data points may become more linear in $\mathcal{X}'$, allowing the application of a linear model to $\mathbf{x}'$. This idea is central to the design of kernel methods [**?**]. Other benefits of using a feature

map include reducing overfitting and improving interpretability [**?**]. A common use case is data visualization, where a feature map with two output dimensions allows the representation of data points in a 2-D scatterplot. Some ML methods employ trainable feature maps, whose parameters are learned from data. An example is the use of hidden layers in a deep net, which act as successive feature maps [**?**]. A principled way to train a feature map is through ERM, using a loss function that measures reconstruction quality, e.g., $L = \|\mathbf{x} - r(\mathbf{x}')\|^2$, where $r(\cdot)$ is a trainable map that attempts to reconstruct $\mathbf{x}$ from the transformed feature vector $\mathbf{x}'$.

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

transparency Transparency is a fundamental requirement for trustworthy AI [**?**]. In the context of ML methods, transparency is often used interchangeably with explainability [**?**], [**?**]. However, in the broader scope of AI systems, transparency extends beyond explainability and includes providing information about the system's limitations, reliability, and intended use. In medical diagnosis systems, transparency requires disclosing the confidence level for the predictions delivered by a trained model. In credit scoring, AI-based lending decisions should be accompanied by explanations of contributing factors, such as income level or credit history. These explanations allow humans (e.g., a loan applicant) to understand and contest automated decisions. Some ML methods inherently offer transparency. For example, logistic regression provides a quantitative measure of classification reliability through the value $|h(\mathbf{x})|$. Decision trees are another example, as they allow human-

readable decision rules [**?**]. Transparency also requires a clear indication when a user is engaging with an AI system. For example, AI-powered chatbots should notify users that they are interacting with an automated system rather than a human. Furthermore, transparency encompasses comprehensive documentation detailing the purpose and design choices underlying the AI system. For instance, model datasheets [**?**] and AI system cards [**?**] help practitioners understand the intended use cases and limitations of an AI system [**?**].

See also: trustworthy AI, explainability.

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

An image showing cows grazing in the Austrian countryside.

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

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

Fig. 52. Two learning tasks constructed from a single image dataset. These tasks differ in feature selection and choice of label (i.e., the objective), but are both derived from the same dataset.

Different learning tasks arising from the same underlying dataset are often coupled. For example, when a probabilistic model is used to generate data points, statistical dependencies among different labels induce dependencies among the corresponding learning tasks. In general, solving learning tasks jointly, e.g., using multitask learning methods, tends to be more effective than solving them independently (thereby ignoring dependencies among learning tasks) [**?**], [**?**], [**?**].

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

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

See also: matrix, vector.

validation Consider a hypothesis $\hat{h}$ that has been learned via some ML method, e.g., by solving ERM on a training set $\mathcal{D}$. Validation refers to the process of evaluating the loss incurred by the hypothesis $\hat{h}$ on a set of data points that are not contained in the training set $\mathcal{D}$. This set of data points is called the validation set. The average loss of $\hat{h}$ on the validation set is referred to as the validation error.

See also: training set, overfitting, generalization, validation error, validation set.

random variable (RV) An RV is a function that maps the outcomes of a random experiment to a value space [**?**], [**?**]. Mathematically, an RV

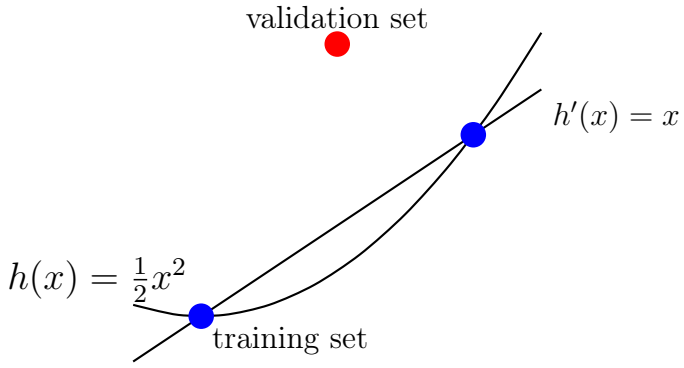


Fig. 53. Illustration of validation. The blue points represent the data points in the training set, while the red point represents a data point in the validation set. The hypothesis $\hat{h}$ (black curve) fits the data points in the training set perfectly, but incurs a large loss on the data point in the validation set.

is a function $x : \Omega \to \mathcal{X}$ that is defined on the sample space Ω of a probability space. Different types of RVs include

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

Probability theory uses the concept of measurable spaces to rigorously define and study the properties of collections of RVs [**?**].

See also: function, random experiment, sample space, probability space, vector, Euclidean space, probability, measurable.

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

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

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

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

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

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

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

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

Gaussian RVs are widely used probabilistic models in the statistical analysis of ML methods. Their significance arises partly from the central limit theorem (CLT), which is a mathematically precise formulation of the following rule of thumb: The average of many independent RVs (not necessarily Gaussian themselves) tends toward a Gaussian RV [?]. The multivariate normal distribution is also distinct in that it represents maximum uncertainty. Among all vector-valued RVs with a

given covariance matrix $\mathbf{C}$, the RV $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{C})$ maximizes differential entropy [?, 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, differential entropy.

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

See also: RV, expectation, vector.

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 $\{i, i'\} \in \mathcal{E}$.

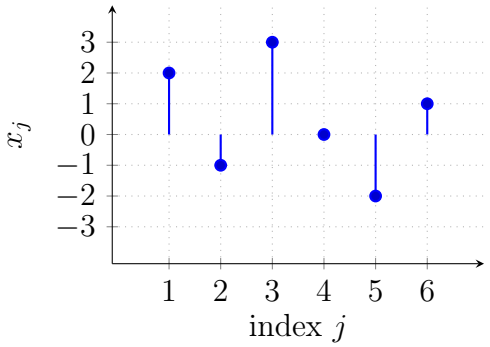
See also: local model, model parameters, graph, discrepancy, hypothesis, map.

vector A vector is an element of a vector space. In the context of ML, a particularly important example of a vector space is the Euclidean space $\mathbb{R}^d$, where $d \in \mathbb{N}$ is the (finite) dimension of the space. A vector $\mathbf{x} \in \mathbb{R}^d$ can be represented as a list or one-dimensional (1-D) array of

real numbers, i.e., $x_1, \ldots, x_d$ with $x_j \in \mathbb{R}$ for $j = 1, \ldots, d$. The value x_j is the jth entry of the vector $\mathbf{x}$. It can also be useful to view a vector $\mathbf{x} \in \mathbb{R}^d$ as a function that maps each index $j \in \{1, \ldots, d\}$ to a value $x_j \in \mathbb{R}$, i.e., $\mathbf{x} : j \mapsto x_j$. This perspective is particularly useful for the study of kernel methods. See Fig. **??** for the two views of a vector.

2, –1, 3, 0, –2, 1

(a)



(b)

Fig. 54. Two equivalent views of a vector $\mathbf{x} = \big(2, -1, 3, 0, -2, 1\big)^T \in \mathbb{R}^6$. (a) As a numeric array. (b) As a map $j \mapsto x_j$.

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

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

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

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

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

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

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

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

See also: neighbors, metric.

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

See also: FL network.

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

of a validation set, which is different from the training set, to estimate the generalization gap.

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

sample In the context of ML, a sample is a finite sequence (of length m) of data points, $\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(m)}$. The number m is called the sample size. ERM-based methods use a sample to train a model (or learn a hypothesis) by minimizing the average loss (the empirical risk) over that sample. Since a sample is defined as a sequence, the same data point may appear more than once. By contrast, some authors in statistics define a sample as a set of data points, in which case duplicates are not allowed [**?**, **?**]. These two views can be reconciled by regarding a sample as a sequence of feature–label pairs, $\left(\mathbf{x}^{(1)}, y^{(1)}\right), \ldots, \left(\mathbf{x}^{(m)}, y^{(m)}\right)$. The r-th pair consists of the features $\mathbf{x}^{(r)}$ and the label $y^{(r)}$ of an unique underlying data point $\widetilde{\mathbf{z}}^{(r)}$. While the underlying data points $\widetilde{\mathbf{z}}^{(1)}, \ldots, \widetilde{\mathbf{z}}^{(m)}$ are unique, some of them can have identical features and labels. For the analysis of ML methods, it is common to interpret a sample as the realization of a stochastic process indexed by $\{1, \ldots, m\}$. A widely used assumption is the i.i.d. assumption, where sample elements $\left(\mathbf{x}^{(r)}, y^{(r)}\right)$, for $r = 1, \ldots, m$, are i.i.d. RVs with common probability distribution $p(\mathbf{x}, y)$.

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

epigraph The epigraph of a real-valued function $f : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is the

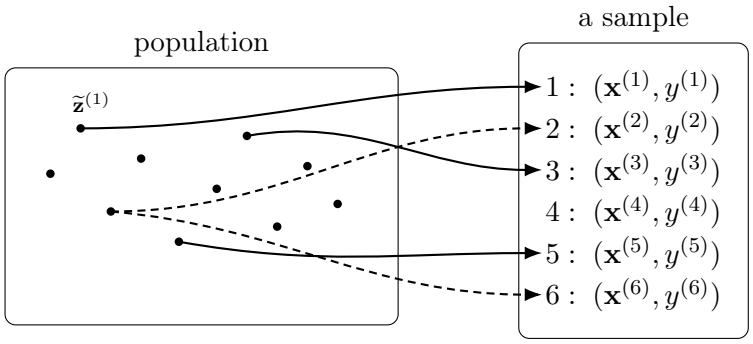


Fig. 55. Illustration of a sample as a finite sequence. Each sequence element consists of the feature vector and the label of some data point which belongs to an underlying population. Depending on the application, the same data point is used to obtain multiple sample elements.

set of points lying on or above its graph (see Fig. **??**), i.e.,

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

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

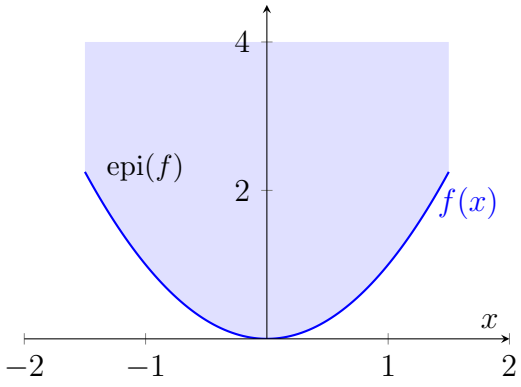


Fig. 56. Epigraph of the function $f(x) = x^2$ (i.e., the shaded area).

See also: function, convex.

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

See also: data point, label space.

event Consider an RV $\mathbf{x}$, defined on some probability space $\mathcal{P}$, which takes values in a measurable space $\mathcal{X}$. An event $\mathcal{A} \subseteq \mathcal{X}$ is a subset of $\mathcal{X}$ such that the probability $\mathbb{P}(\mathbf{x} \in \mathcal{A})$ is well defined. In other words, the preimage $\mathbf{x}^{-1}(\mathcal{A})$ of an event belongs to the σ-algebra of $\mathcal{P}$.

See also: RV, data point, i.i.d. assumption, probabilistic model.

Machine Learning Systems

This document is incomplete. The external file associated with the glossary 'systems' (which should be called `ADictML_Finnish.systems-gls`) hasn't been created.

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