The A”alto Dictionary of Machine Learning

Dipl.-Ing. Dr.techn. Alexander Jung

4. Januar 2025

please cite as: A. Jung, “The Aalto Dictionary of Machine Learning,” Aalto University, 2024.

Zusammenfassung

This dictionary of machine learning evolved during the design and implementation of the courses 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** offered to Finnish university students via **Aalto University** `https://www.aalto.fi/en`, to Finnish adult learners via **The Finnish Institute of Technology (FITech)** `fitech.io` and to international students via the **European University Alliance Unite!** `https://www.aalto.fi/en/unite`.

Lists of Symbols

Sets and Functions

$a \in \mathcal{A}$	This statement indicates that the object a is an element of the set $\mathcal{A}$.
$a := b$	This statement defines a to be shorthand for b.
$\lvert\mathcal{A}\rvert$	The cardinality (number of elements) of a finite set $\mathcal{A}$.
$\mathcal{A} \subseteq \mathcal{B}$	$\mathcal{A}$ is a subset of $\mathcal{B}$.
$\mathcal{A} \subset \mathcal{B}$	$\mathcal{A}$ is a strict subset of $\mathcal{B}$.
$\mathbb{N}$	The natural numbers $1, 2, \ldots$.
$\mathbb{R}$	The real numbers x [1].
$\mathbb{R}_+$	The non-negative real numbers $x \geq 0$.
$\mathbb{R}_{++}$	The positive real numbers $x > 0$.

$\{0,1\}$	The set that consists of the two real numbers 0 and 1.
$[0,1]$	The closed interval of real numbers x with $0 \leq x \leq 1$.
$\operatorname*{argmin}_{\mathbf{w}} f(\mathbf{w})$	The set of minimizers for a real-valued function $f(\mathbf{w})$.
$\mathbb{S}^{(n)}$	The set of unit-norm vectors in $\mathbb{R}^{n+1}$.
$\log a$	The logarithm of the positive number $a \in \mathbb{R}_{++}$.
$h(\cdot): \mathcal{A} \rightarrow \mathcal{B} : a \mapsto h(a)$	A function (map) that accepts any element $a \in \mathcal{A}$ from a set $\mathcal{A}$ as input and delivers a well-defined element $h(a) \in \mathcal{B}$ of a set $\mathcal{B}$. The set $\mathcal{A}$ is the domain of the function h and the set $\mathcal{B}$ is the codomain of h. ML aims at finding (or learning) a function h (*hypothesis*) that reads in the features $\mathbf{x}$ of a data point and delivers a prediction $h(\mathbf{x})$ for its label y.
$\nabla f(\mathbf{w})$	The gradient of a differentiable real-valued function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is the vector $\nabla f(\mathbf{w}) = \left(\frac{\partial f}{\partial w_1}, \ldots, \frac{\partial f}{\partial w_d}\right)^T \in \mathbb{R}^d$ [2, Ch. 9].

Matrices and Vectors

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

$\left(\mathbf{v}^T, \mathbf{w}^T\right)^T$	The vector of length $d + d'$ obtained by concatenating the entries of vector $\mathbf{v} \in \mathbb{R}^d$ with the entries of $\mathbf{w} \in \mathbb{R}^{d'}$.
$\text{span}\{\mathbf{B}\}$	The span of a matrix $\mathbf{B} \in \mathbb{R}^{a \times b}$, which is the subspace of all linear combinations of columns of $\mathbf{B}$, $\text{span}\{\mathbf{B}\} = \left\{\mathbf{B}\mathbf{a} : \mathbf{a} \in \mathbb{R}^b\right\} \subseteq \mathbb{R}^a$.
$\mathbb{S}_+^d$	The set of all positive semi-definite (psd) matrices of size $d \times d$.
$\det(\mathbf{C})$	The determinant of the matrix $\mathbf{C}$.
$\mathbf{A} \otimes \mathbf{B}$	The Kronecker product of $\mathbf{A}$ and $\mathbf{B}$ [4].

Probability Theory

$\mathbb{E}_p\{f(\mathbf{z})\}$	The expectation of a function $f(\mathbf{z})$ of a RV $\mathbf{z}$ whose probability distribution is $p(\mathbf{z})$. If the probability distribution is clear from context we just write $\mathbb{E}\{f(\mathbf{z})\}$.
$p(\mathbf{x}, y)$	A (joint) probability distribution of a RV whose realizations are data points with features $\mathbf{x}$ and label y.
$p(\mathbf{x}\|y)$	A conditional probability distribution of a RV $\mathbf{x}$ given the value of another RV y [5, Sec. 3.5].
$p(\mathbf{x}; \mathbf{w})$	A parametrized probability distribution of a RV $\mathbf{x}$. The probability distribution depends on a parameter vector $\mathbf{w}$. For example, $p(\mathbf{x}; \mathbf{w})$ 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 $\mathbb{E}\left\{\big(\mathbf{x} - \mathbb{E}\{\mathbf{x}\}\big)\big(\mathbf{x} - \mathbb{E}\{\mathbf{x}\}\big)^T\right\}$.
$\mathcal{N}(\mu, \sigma^2)$	The probability distribution of a Gaussian RV $x \in \mathbb{R}$ with mean (or expectation) $\mu = \mathbb{E}\{x\}$ and variance $\sigma^2 = \mathbb{E}\big\{(x - \mu)^2\big\}$.
$\mathcal{N}(\boldsymbol{\mu}, \mathbf{C})$	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 $\mathbf{C} = \mathbb{E}\big\{\big(\mathbf{x} - \boldsymbol{\mu}\big)\big(\mathbf{x} - \boldsymbol{\mu}\big)^T\big\}$.

Machine Learning

r	An index $r = 1, 2, \ldots,$ that enumerates data points.
m	The number of data points in (the size of) a 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 $r = 1, \ldots, m$.
d	Number of features that characterize a data point.
x_j	The j-th feature of a data point. The first feature of a given data point is denoted x_1, the second feature x_2 and so on.
$\mathbf{x}$	The feature vector $\mathbf{x} = \big(x_1, \ldots, x_d\big)^T$ of a data point whose entries are the individual features of a data point.
$\mathcal{X}$	The feature space $\mathcal{X}$ is the set of all possible values that the features $\mathbf{x}$ of a data point can take on.
$\mathbf{z}$	Beside the symbol $\mathbf{x}$, we sometimes use $\mathbf{z}$ as another symbol to denote a vector whose entries are individual features of a data point. We need two different symbols to distinguish between *raw* and learnt features [6, Ch. 9].
$\mathbf{x}^{(r)}$	The feature vector of the r-th data point within a dataset.
$x_j^{(r)}$	The j-th feature of the r-th data point within a dataset.

$\mathcal{B}$	A mini-batch (subset) of randomly chosen data points.
B	The size of (the number of data points in) a mini-batch.
y	The label (quantity of interest) of a data point.
$y^{(r)}$	The label of the r-th data point.
$\left(\mathbf{x}^{(r)}, y^{(r)}\right)$	The features and label of the r-th data point.
$\mathcal{Y}$	The label space $\mathcal{Y}$ of a 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). We refer to ML problems (methods) using a numeric label space, such as $\mathcal{Y} = \mathbb{R}$ or $\mathcal{Y} = \mathbb{R}^3$, as regression problems (methods). ML problems (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 (methods).
η	Learning rate (step-size) used by gradient-based methods.
$h(\cdot)$	A hypothesis map that reads in features $\mathbf{x}$ of a data point and delivers a prediction $\hat{y} = h(\mathbf{x})$ for its label y.
$\mathcal{Y}^{\mathcal{X}}$	Given two sets $\mathcal{X}$ and $\mathcal{Y}$, we denote by $\mathcal{Y}^{\mathcal{X}}$ the set of all possible hypothesis maps $h : \mathcal{X} \to \mathcal{Y}$.

$\mathcal{H}$	A hypothesis space or model used by a ML method. The hypothesis space consists of different hypothesis maps $h : \mathcal{X} \rightarrow \mathcal{Y}$ between which the ML method has to choose .
$d_{\text{eff}}(\mathcal{H})$	The effective dimension of a hypothesis space $\mathcal{H}$.
B^2	The squared bias of a learnt hypothesis $\hat{h}$ delivered by a ML algorithm that is fed with data points which are modelled as realizations of RVs. If data is modelled as realizations of RVs, also the delivered hypothesis $\hat{h}$ is the realization of a RV.
V	The variance of the (parameters of the) hypothesis delivered by a ML algorithm. If the input data for this algorithm is interpreted as realizations of RVs, so is the delivered hypothesis a realization of a RV.
$L((\mathbf{x}, y), h)$	The loss incurred by predicting the label y of a data point using the prediction $\hat{y} = h(\mathbf{x})$. The prediction $\hat{y}$ is obtained from evaluating the hypothesis $h \in \mathcal{H}$ for the feature vector $\mathbf{x}$ of the data point.
E_v	The validation error of a hypothesis h, which is its average loss incurred over a validation set.
$\widehat{L}\big(h\vert\mathcal{D}\big)$	The empirical risk or average loss incurred by the hypothesis h on a dataset $\mathcal{D}$.

E_t	The training error of a hypothesis h, which is its average loss incurred over a training set.
t	A discrete-time index $t = 0, 1, \ldots$ used to enumerate sequential events (or time instants).
t	An index that enumerates learning tasks within a multi-task learning problem.
α	A regularization parameter that controls the amount of regularization.
$\lambda_j\big(\mathbf{Q}\big)$	The j-th eigenvalue (sorted either ascending or descending) of a psd matrix $\mathbf{Q}$. We also use the shorthand λ_j if the corresponding matrix is clear from context.
$\sigma(\cdot)$	The activation function used by an artificial neuron within an artificial neural network (ANN).
$\mathcal{R}_{\hat{y}}$	A decision region within a feature space.
$\mathbf{w}$	A parameter vector $\mathbf{w} = \big(w_1, \ldots, w_d\big)^T$ of a model, e.g, the weights of a linear model or in a ANN.
$h^{(\mathbf{w})}(\cdot)$	A hypothesis map that involves tunable model parameters $w_1, \ldots, w_d$, stacked into the vector $\mathbf{w} = \big(w_1, \ldots, w_d\big)^T$.
$\phi(\cdot)$	A feature map $\phi : \mathcal{X} \rightarrow \mathcal{X}' : \mathbf{x} \mapsto \mathbf{x}' := \phi\big(\mathbf{x}\big) \in \mathcal{X}'$.
$K\big(\cdot, \cdot\big)$	Given an arbitrary feature space, a kernel is a map $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{C}$ that is psd.

Federated Learning

$\mathcal{G} = (\mathcal{V}, \mathcal{E})$	Federated learning (FL) network whose nodes $i \in \mathcal{V}$ carry local datasets and local models.
$i \in \mathcal{V}$	A node in the FL network that represents a local dataset and a corresponding local model. It might also be useful to think of node i as a small computer that can collect data and execute computations to train ML models.
$\mathcal{G}^{(\mathcal{C})}$	The induced sub-graph of $\mathcal{G}$ using the nodes in $\mathcal{C} \subseteq \mathcal{V}$.
$\mathbf{L}^{(\mathcal{G})}$	The Laplacian matrix of a graph $\mathcal{G}$.
$\mathbf{L}^{(\mathcal{C})}$	The Laplacian matrix of the induced graph $\mathcal{G}^{(\mathcal{C})}$.
$\mathcal{D}^{(i)}$	The local dataset $\mathcal{D}^{(i)}$ at node $i \in \mathcal{V}$ of an FL network.
m_i	The number of data points (sample size) contained in the local dataset $\mathcal{D}^{(i)}$ at node $i \in \mathcal{V}$.
$\mathcal{N}^{(i)}$	The neighbourhood of the node i in an FL network.
$\mathbf{x}^{(i,r)}$	The features of the r-th data point in the local dataset $\mathcal{D}^{(i)}$.
$y^{(i,r)}$	The label of the r-th data point in the local dataset $\mathcal{D}^{(i)}$.

$L^{(\mathrm{d})}\left(\mathbf{x}, h\left(\mathbf{x}\right), h'\left(\mathbf{x}\right)\right)$	The loss incurred by a hypothesis h' on a data point with features $\mathbf{x}$ and label $h\left(\mathbf{x}\right)$ that is obtained from another hypothesis.
$\mathrm{stack}\left\{\mathbf{w}^{(i)}\right\}_{i=1}^{n}$	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 $\mathbf{w}^{(i)} \in \mathbb{R}^{d}$.

Glossar

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

k-means The k-means algorithm is a hard clustering method which assigns each data point of a dataset to precisely one of k different clusters. The method alternates between updating the cluster assignments (to the cluster with nearest cluster mean) and, given the updated cluster assignments, re-calculating the cluster means [6, Ch. 8].

absolute error loss Consider a data point with features $\mathbf{x} \in \mathcal{X}$ and numeric label $y \in \mathbb{R}$. The absolute error loss incurred by a hypothesis $h : \mathcal{X} \to \mathbb{R}$ is defined as $|y - h(\mathbf{x})|$.

accuracy Consider data points characterized by features $\mathbf{x} \in \mathcal{X}$ and a categorical label y which takes on values from a finite label space $\mathcal{Y}$. The accuracy of a hypothesis $h : \mathcal{X} \to \mathcal{Y}$, when applied to the data

points in a dataset $\mathcal{D} = \left\{ \left(\mathbf{x}^{(1)}, y^{(1)}\right), \ldots, \left(\mathbf{x}^{(m)}, y^{(m)}\right) \right\}$ is then defined as $1 - (1/m) \sum_{r=1}^{m} L\left(\left(\mathbf{x}^{(r)}, y^{(r)}\right), h\right)$ using the 0/1 loss.

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

Application Programming Interface (API) An application programming interface (API) is a precise specification of the services and resources offered by software or hardware implementing that API.

artificial intelligence Artificial intelligence refers to systems that behave rational in the sense of maximizing a long-term reward. The ML-based approach to AI is to train a model that allows to predict optimal actions for a given observed state of the environment. What sets AI applications apart from more basic ML applications is the choice of loss function. AI systems rarely have access to a labeled training set that allows to measure the average loss for a given choice of model parameters. Rather, AI systems typically use a loss function that can only be estimated from observed reward signals.

artificial neural network An artificial neural network is a graphical (signal-flow) representation of a map from features of a data point at its input to a prediction for the label as its output.

autoencoder An autoencoder is a ML method that jointly learns an encoder map $h(\cdot) \in \mathcal{H}$ and a decoder map $h^{*}(\cdot) \in \mathcal{H}^{*}$. It is an instance of ERM

using a loss computed from the reconstruction error $\mathbf{x} - h^{*}\big(h\big(\mathbf{x}\big)\big)$.

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

bagging Bagging (or *bootstrap aggregation*) is a generic technique to improve (the robustness of) a given ML method. The idea is to use the bootstrap to generate perturbed copies of a given dataset and then to learn a separate hypothesis for each copy. We then predict the label of a data point by combining or aggregating the individual predictions of each separate hypothesis. For hypothesis maps delivering numeric label values, this aggregation could be implemented by computing the average of individual predictions.

baseline Consider some ML method that delivers a learnt 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 do we know that the resulting test set performance is good (enough)? How can we determine if the trained model performs close to optimal and there is little point in investing more resources (for data collection or computation) to improve

it? To this end, it is useful to have a reference (or baseline) level against which we can compare the performance of the trained model. Such a reference value might be obtained from human performance, e.g., the misclassification rate of dermatologists who diagnose cancer from visual inspection of skin. 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. However, we might still use its test set error as a baseline. Another, somewhat more principled, approach to constructing a baseline is via a probabilistic model. For a wide range of probabilistic models $p(\mathbf{x}, y)$ we can precisely determine the minimum achievable risk among *any* hypothesis (not even required to belong to the hypothesis space $\mathcal{H}$) [7]. 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 $p(\mathbf{x}, y)$ [7, Chapter 4]. However, there are two challenges to computing the Bayes estimator and Bayes risk: i) the probability distribution $p(\mathbf{x}, y)$ is unknown and needs to be estimated but (ii) even if we know $p(\mathbf{x}, y)$ it might be computationally too expensive to compute the Bayes risk exactly. A widely used probabilistic model is the multivariate normal distribution $(\mathbf{x}, y) \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ for data points characterised 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 $\mathbf{x}$ [7, 8]. The corresponding Bayes risk is given by

the posterior variance $\sigma^2_{y|\mathbf{x}}$ (see Figure 1).

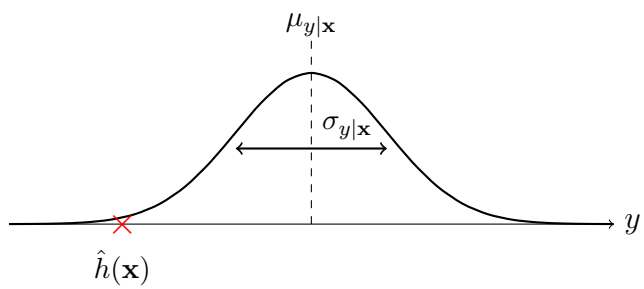


Abbildung 1: If features and label of a data point are drawn from a multivariate normal distribution, we can achievive minimum risk (under squared error loss) by using the Bayes estimator $\mu_{y|\mathbf{x}}$ to predict the label y of a data point with features $\mathbf{x}$. The corresponding minimum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

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

Bayes estimator Consider a probabilistic model with joint probability distribution $p(\mathbf{x}, y)$ for the features $\mathbf{x}$ and label y of a data point. For a given loss function $L(\cdot,\cdot)$, we refer to a hypothesis h as a Bayes estimator if its risk $\mathbb{E}\{L((\mathbf{x}, y), h)\}$ is minimum [7]. Note that the property of a hypothesis being a Bayes estimator depends on the underlying probability distribution and the choice for the loss function $L(\cdot,\cdot)$.

Bayes risk Consider a probabilistic model with joint probability distribution $p(\mathbf{x}, y)$ for the features $\mathbf{x}$ and label y of a data point. The Bayes risk is the minimum possible risk that can be achieved by any hypothesis $h : \mathcal{X} \rightarrow \mathcal{Y}$. Any hypothesis that achieves the Bayes risk is referred to as a Bayes estimator [7].

bias Consider a ML method using a parameterized hypothesis space $\mathcal{H}$. It learns the model parameters $\mathbf{w} \in \mathbb{R}^d$ using the dataset $\mathcal{D} = \left\{ \left(\mathbf{x}^{(r)}, y^{(r)}\right) \right\}_{r=1}^{m}$. To analyze the properties of the ML method, we typically interpret the data points as realizations of independent and identically distributed (i.i.d.) RVs,

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

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

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

classification Classification is the task of determining a discrete-valued label y of a 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

a category to which the corresponding data point belongs to. Some classification problems involve a countably infinite label space.

classifier A classifier is a hypothesis (map) $h(\mathbf{x})$ used to predict a label taking values from a finite label space. We might use the function value $h(\mathbf{x})$ itself as a prediction $\hat{y}$ for the label. However, it is customary to use a map $h(\cdot)$ that delivers a numeric quantity. The prediction is then obtained by a simple thresholding step. For example, in a binary classification problem with $\mathcal{Y} \in \{-1, 1\}$, we might use real-valued hypothesis map $h(\mathbf{x}) \in \mathbb{R}$ as 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 $a \in \mathcal{Y}$.

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.

clustered federated learning (CFL) Clustered federated learning (FL) (CFL) assumes that local datasets form clusters. The local datasets belonging to the same cluster have similar statistical properties. CFL pools local datasets in the same cluster to obtain a training set for

training a cluster-specific model. GTV minimization (GTVMin) implements this pooling implicitly by forcing the local model parameters to be approximately identical over well-connected subsets of the FL network.

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

clustering assumption The clustering assumption postulates that data points in a dataset form a (small) number of groups or clusters. Data points in the same cluster are more similar with each other than with those outside the cluster [9]. We obtain different clustering methods by using different notions of similarity between data points.

computational aspects By computational aspects of a ML method, we mainly refer to the computational resources required for its implementation. For example, if a ML method uses iterative optimization techniques to solve ERM, then its computational aspects include (i) how many arithmetic operations are needed to implement a single iteration (gradient step) and (ii) how many iterations are needed to obtain useful

model parameters. One important example of an iterative optimization technique is gradient descent (GD).

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

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

connected graph A undirected graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is connected if it does not contain a (non-empty) subset $\mathcal{V}' \subset \mathcal{V}$ with no edges leaving $\mathcal{V}'$.

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 of that set. We define a function as convex if its epigraph is a convex set [10].

convex clustering Consider a dataset $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)} \in \mathbb{R}^d$. Convex cluste-

ring learns vectors $\mathbf{w}^{(1)}, \ldots, \mathbf{w}^{(m)}$ by minimizing

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

Here, $\|\mathbf{u}\|_p := \left(\sum_{j=1}^{d} |u_j|^p \right)^{1/p}$ denotes the p-norm (for $p \geq 1$). It turns out that many of the optimal vectors $\widehat{\mathbf{w}}^{(1)}, \ldots, \widehat{\mathbf{w}}^{(m)}$ coincide. A cluster then consists of those data points $r \in \{1, \ldots, m\}$ with identical $\widehat{\mathbf{w}}^{(r)}$ [11, 12].

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

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

Here, we used the ordered (in increasing fashion) eigenvalues

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

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

covariance matrix The covariance matrix of a RV $\mathbf{x} \in \mathbb{R}^d$ is defined as $\mathbb{E}\left\{ \left(\mathbf{x} - \mathbb{E}\{\mathbf{x}\} \right) \left(\mathbf{x} - \mathbb{E}\{\mathbf{x}\} \right)^T \right\}$.

data See dataset.

data augmentation Data augmentation methods add synthetic data points to an existing set of data points. These synthetic data points are

obtained by perturbations (e.g., adding noise to physical measurements) or transformations (e.g., rotations of images) of the original data points. These perturbations and transformations are such that the resulting synthetic data points should still have the same label. As a case in point, a rotated cat image is still a cat image even if their feature vectors (obtained by stacking pixel color intensities) are very different (see Figure 2). Data augmentation can be an efficient form of regularization.

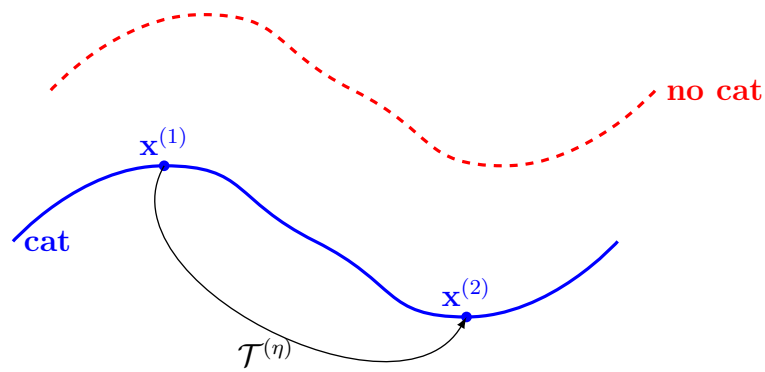


Abbildung 2: Data augmentation exploits intrinsic symmetries of data points in some feature space $\mathcal{X}$. We can represent a symmetry by an operator $\mathcal{T}^{(\eta)} : \mathcal{X} \rightarrow \mathcal{X}$, parametrized by some number $\eta \in \mathbb{R}$. For example, $\mathcal{T}^{(\eta)}$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

data minimization principle European data protection regulation inclu-

des 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 [13, Article 5(1)(c)] [14].

data normalization Data normalization refers to basic transformations of the feature vectors of data points. Data normalization ensures that the new feature vectors $\mathbf{x}'$ have properties that are benefetial for the statistical aspects or the computational aspects of the overal ML method. For example, consider linear regression using gradient-based methods with a fixed learning rate. To ensure convergence of gradient-based methods, we need to ensure that the feature vectors in the training set have not too large norm. We can ensure this by normalizing the feature vectors such that $\|\mathbf{x}'\|_2 \leq 1$.

data point A data point is any object that conveys information [15]. Data points might be students, radio signals, trees, forests, images, RVs, real numbers or proteins. We characterize data points using two types of properties. One type of property is referred to as a feature. Features are properties of a data point that can be measured or computed in an automated fashion. A different kind of property is referred to as labels. The label of a data point represents some higher-level fact (or quantity of interest). In contrast to features, determining the label of a data point typically requires human experts (domain experts). Roughly speaking, ML aims to predict the label of a data point based solely on

its features.

data poisoning Data poisoning refers to the intentional manipulation (or fabrication) of data points to steer the training of a ML model [16, 17]. The protection against data poisoning is particularly important in distributed ML applications where datasets are de-centralized.

dataset With a slight abuse of language we use the term *dataset* or *set of data points* to refer to an indexed list of data points $\mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \ldots$. Thus, there is a first data point $\mathbf{z}^{(1)}$, a second data point $\mathbf{z}^{(2)}$ and so on. Strictly speaking, a dataset is a list and not a set [18]. We need to keep track of the order of data points in order to cope with several data points having the same features and labels. Database theory studies formal languages for defining, structuring, and reasoning about datasets [19].

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 neighbourhood $\{\mathbf{x}' : \|\mathbf{x} - \mathbf{x}'\| \leq \varepsilon\}$, for any $\varepsilon > 0$, contains at least two vectors with different function values.

decision region Consider a hypothesis map h that delivers values from a finite set $\mathcal{Y}$. For each label value (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.

decision tree A decision tree is a flow-chart-like representation of a hypothesis map h. More formally, a decision tree is a directed graph containing a root node that reads in the feature vector $\mathbf{x}$ of a data point. The root node then forwards the data point to one of its children nodes based on some elementary test on the features $\mathbf{x}$. If the receiving children node is not a leaf node, i.e., it has itself children nodes, it represents another test. Based on the test result, the data point is further pushed 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 (having no children nodes).

deep net A deep net is a 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 [20].

degree of belonging A number that indicates the extent by which a data point belongs to a cluster [6, Ch. 8]. The degree of belonging can be interpreted as a soft cluster assignment. Soft clustering methods can encode the degree of belonging by a real number in the interval $[0, 1]$. Hard clustering is obtained as the extreme case when the degree of belonging only takes on values 0 or 1.

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

density-based spatial clustering of applications with noise A clustering algorithm for data points that are characterized by numeric feature

vectors. Like k-means and soft clustering via GMM, also DBSCAN uses the Euclidean distances between feature vectors to determine the clusters. However, in contrast to k-means and GMM, DBSCAN uses a different notion of similarity between data points. DBSCAN considers two data points as similar if they are *connected* via a sequence (path) of close-by intermediate data points. Thus, DBSCAN might consider two data points as similar (and therefore belonging to the same cluster) even if their feature vectors have a large Euclidean distance.

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

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

differential privacy Consider some ML method $\mathcal{A}$ that reads in a dataset (e.g., the training set used for ERM) and delivers some output $\mathcal{A}(\mathcal{D})$. The output could be either the learnt model parameters or the predictions for specific data points. Differential privacy is a precise measure of privacy leakage incurred by revealing the output. Roughly speaking, a ML method is differentially private if the probability distribution of the output $\mathcal{A}(\mathcal{D})$ does not change too much if the sensitive attribute of one data point in the training set is changed. Note that differential privacy

builds on a probabilistic model for a ML method, i.e., we interpret its output $\mathcal{A}(\mathcal{D})$ as the realization of a RV. The randomness in the output can be ensured by intentionally adding the realization of an auxiliary RV (*noise*) to the output of the ML method.

dimensionality reduction Dimensionality reduction methods map (typically many) raw features to a (relatively small) set of new features. These methods can be used to visualize data points by learning two features that can be used as the coordinates of a depiction in a scatterplot.

discrepancy Consider a FL application with networked data represented by a 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.

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

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 parameters of the model. These parameters might be the coefficients used in a linear map or the weights and bias terms of an ANN.

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

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

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

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

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

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 $\mathcal{D}$.

empirical risk minimization Empirical risk minimization is the optimization problem of finding a hypothesis (out of a model) with minimum average loss (or empirical risk) on a given dataset $\mathcal{D}$ (the training set). Many ML methods are obtained from empirical risk via specific design choices for the dataset, model and loss [6, Ch. 3].

estimation error Consider data points with feature vectors $\mathbf{x}$ and label y. In some applications we can model the relation between the features and the label of a data point as $y = \bar{h}(\mathbf{x}) + \varepsilon$. Here, we used some true underlying hypothesis $\bar{h}$ and a noise term ε which summarized any modelling or labelling errors. The estimation error incurred by a ML method that learns a hypothesis $\widehat{h}$, e.g., using ERM, is defined as $\widehat{h}(\mathbf{x}) - \bar{h}(\mathbf{x})$, for some feature vector. For a parameterized hypothesis

space, consisting of hypothesis maps that are determined by a model parameters $\mathbf{w}$, we can define the estimation error as $\Delta\mathbf{w} = \widehat{\mathbf{w}} - \overline{\mathbf{w}}$ [21,22].

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

expectation Consider a numeric feature vector $\mathbf{x} \in \mathbb{R}^d$ which we interpret as the realization of a RV with probability distribution $p(\mathbf{x})$. The expectation of $\mathbf{x}$ is defined as the integral $\mathbb{E}\{\mathbf{x}\} := \int \mathbf{x} p(\mathbf{x})$ [2, 23, 24]. Note that the expectation is only defined if this integral exists, i.e., if the RV is integrable.

expectation-maximization Consider a probabilistic model $p(\mathbf{z}; \mathbf{w})$ for the data points $\mathcal{D}$ generated in some ML application. The maximum likelihood estimator for the model parameters $\mathbf{w}$ is obtained by maximizing $p(\mathcal{D}; \mathbf{w})$. However, the resulting oprimtization problem might be computationally challenging. Expectation-maximization approximates the maximum likelihood estimator by introducing a latent RV $\mathbf{z}$ such that maximizing $p(\mathcal{D}, \mathbf{z}; \mathbf{w})$ would be easier [22, 25, 26]. Since we do not observe $\mathbf{z}$, we need to estimate it from the observed dataset $\mathcal{D}$ using a conditional expectation. The resulting estimate $\widehat{\mathbf{z}}$ is then used to compute a new estimate $\widehat{\mathbf{w}}$ by solving $\max_{\mathbf{w}} p(\mathcal{D}, \widehat{\mathbf{z}}; \mathbf{w})$. The crux is that the conditional expectation $\widehat{\mathbf{z}}$ depends on the model parameters $\widehat{\mathbf{w}}$ which we have updated based on $\widehat{\mathbf{z}}$. Thus, we have to re-calculate $\widehat{\mathbf{z}}$ which, in turn, results in a new choice $\widehat{\mathbf{w}}$ for the model parameters.

In practice, we repeat the computation of the conditional expectation (the E step) and the update of the model parameters (the M step) until some stopping criterion is met.

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 minimum loss on any data point. We can make this informal goal precise via the i.i.d. assumption and using the Bayes risk as the baseline for the (average) loss of a hypothesis. An alternative approach to obtain a baseline is to use the hypothesis h' learnt by an existing ML method. We refer to this hypothesis h' as an expert [27]. Regret minimization methods learn a hypothesis that incurs a loss comparable to the best expert [27, 28].

explainability We define the (subjective) explainability of a ML method as the level of simulatability [29] of the predictions delivered by a 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 [29, 30]. Alternatively, we can use probabilistic models for data and measure explainability of a trained ML model via the conditional (differential) entropy of its predictions, given the user predictions [31, 32].

explainable empirical risk minimization An instance of structural risk minimization that adds a regularization term to the average loss in the objective function of ERM. The regularization term is chosen to favour

hypothesis maps that are intrinsically explainable for a specific user. This user is characterized by their predictions provided for the data points in a training set [30].

explainable ML Explainable ML methods aim at complementing each prediction with an explanation for how the prediction has been obtained. The construction of an explicit explanation might not be necessary if the ML method uses a sufficiently simple (or interpretable) model [33].

explanation One approach to make ML methods transparent, is to provide an explanation along with the prediction delivered by an ML method. Explanations can take on many different forms. An explanation could be some natural text or some quantitative measure for the importance of individual features of a data point [34]. We can also use visual forms of explanations such as intensity plots for image classification [35].

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 in as a jpeg file), then we could use the red-green-blue intensities of its pixels as features. Domain-specific synonyms for the term feature are *covariate*, *explanatory variable*, *independent variable*, *input (variable)*, *predictor (variable)* or *regressor* [36–38].

feature learning Feature learning refers to the task of learning a map $\mathbf{\Phi}$ that reads in raw features of a data point and delivers new features. Different feature learning methods are obtained for different quantitative

measures for the usefulness of the new features.

feature map A map that transforms the original features of a data point into new features. The so-obtained new features might be preferable over the original features for several reasons. For example, the arrangement of data points might become simpler (of *more linear*) in the new feature space, allowing to use linear models in the new features. This idea is a main driver for the development of kernel methods [39]. Moreover, the hidden layers of a deep net can be interpreted as a trainable feature map followed by a linear model in the form of the output layer. Another reason for learning a feature map could be that learning a small number of new features helps to avoid overfitting and ensure interpretability [40]. The special case of a feature map delivering two numeric features is particularly useful for data visualization. Indeed, we can depict data points in a scatterplot by using two features as the coordinates of a data point.

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

feature space The feature space of a given ML application or method is constituted by all potential values that the feature vector of a data point can take on. A widely used choice for the feature space is the Euclidean space $\mathbb{R}^d$ with dimension d being the number of individual features of a data point.

feature vector A vector $\mathbf{x} = \left(x_1, \ldots, x_d\right)^T$ whose entries are individual features $x_1, \ldots, x_d$. Many ML methods use feature vectors that belong to some finite-dimensional Euclidean space $\mathbb{R}^d$. However, for some ML methods it is more convenient to work with feature vectors that belong to an infinite-dimensional vector space (see, e.g., kernel method).

federated averaging (FedAvg) Federated averaging is an iterative FL algorithm that alternates between local model trainings and averaging the resulting local model parameters. Different variants of this algorithm are obtained by different techniques for the model training. The authors of [41] consider federated averaging methods where the local model training is implemented by running several GD steps.

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

federated learning (FL) network A federated network is an undirected weighted graph whose nodes represent data generators that aim to train a local (or personalized) model. Each node in a federated network represents some device, capable to collect a local dataset and, in turn, train a local model. FL methods learn a local hypothesis $h^{(i)}$, for each node $i \in \mathcal{V}$, such that it incurs small loss on the local datasets.

Finnish Meteorological Institute The Finnish Meteorological Institute is a government agency responsible for gathering and reporting weather data in Finland.

flow-based clustering Flow-basted clustering groups the nodes of an undirected graph by applying k-means clustering to node-wise feature vectors. These feature vectors are built from networks flows between carefully selected source and destination nodes [42].

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

Gaussian random variable A standard Gaussian RV is a real-valued random variable x with probability density function (pdf) [5, 8, 43]

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

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

A Gaussian random vector $\mathbf{x} \in \mathbb{R}^d$ with covariance matrix $\mathbf{C}$ and mean $\boldsymbol{\mu}$ can be constructed via $\mathbf{x} := \mathbf{A}\big(\mathbf{z} + \boldsymbol{\mu}\big)$. Here, $\mathbf{A}$ is any matrix that satisfies $\mathbf{A}\mathbf{A}^T = \mathbf{C}$ and $\mathbf{z} := \big(z_1, \ldots, z_d\big)^T$ is a vector whose entries

are i.i.d. standard Gaussian RVs $z_1, \ldots, z_d$. Gaussian random processes generalize Gaussian random vectors by applying linear transformations to infinite sequences of standard Gaussian RVs [44].

Gaussian RVs are widely used probabilistic models for the statistical analysis of machine learning methods. Their significance arises partly from the central limit theorem which states that the sum of many independent RVs (not necessarily Gaussian themselves) tends to a Gaussian RV [45].

General Data Protection Regulation The General Data Protection Regulation (GDPR) was enacted by the European Union (EU), effective from May 25, 2018 [13]. It safeguards the privacy and data rights of individuals in the EU. The GDPR has significant implications for how data is collected, stored, and used in ML applications. Key provisions include:

- Data minimization principle: ML systems should only use necessary amount of personal data for their purpose.
- Transparency and Explainability: ML systems should enable their users to understand how they make decisions that impact them.
- Data Subject Rights: Including the rights to access, rectify, and delete 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.

generalization Many current ML (and AI) methods are an instance of ERM: At their core, they train a model (learn a hypothesis $\hat{h} \in \mathcal{H}$) by minimizing the average loss (or empirical risk) on some data points $\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(m)}$, which serve as a training set $\mathcal{D}^{(\text{train})}$. Generalization refers to a ML method's ability to perform well outside the training set. Any mathematical theory of generalization needs some mathematical concept for the *outside the training set*. For example, statistical learning theory uses a probabilistic model such as the i.i.d. assumption for data generation: the data points in the training set are i.i.d. realizations of some underlying probability distribution $p(\mathbf{z})$. Using a probabilistic model allows to explore the *outside of the training set* by drawing additional i.i.d. realizations from $p(\mathbf{z})$. Moreover, using the i.i.d. assumption allows to define the risk of a trained model $\hat{h} \in \mathcal{H}$ as the expected loss $\bar{L}\big(\hat{h}\big)$. What is more, we can use concentration bounds or convergence results for sequences of i.i.d. RVs to bound the deviation between the empirical risk $\widehat{L}\big(\hat{h}|\mathcal{D}^{(\text{train})}\big)$ of a trained model and its risk [46]. It is possible to study generalization also without using probabilistic models. For example, we could use (deterministic) perturbations of the data points in the training set to study its *outside*. In general, we would like the trained model to be robust, i.e., its predictions should not change too much for small perturbations of a data point. Consider a trained model for detecting an object in a smartphone snapshot. The detection result should not change if we mask a small number of randomly chosen pixels in the image [47].

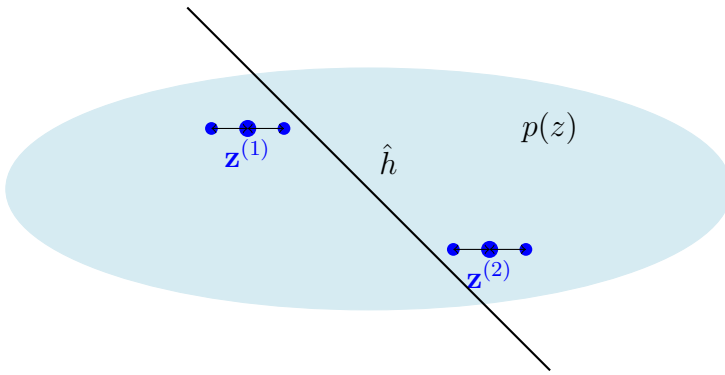


Abbildung 3: Two data points $\mathbf{z}^{(1)}, \mathbf{z}^{(2)}$ that are used as a training set to learn a hypothesis $\hat{h}$ via ERM. We can evaluate $\hat{h}$ *outside* $\mathcal{D}^{(\text{train})}$ either by an i.i.d. assumption with underlying probability distribution $p(\mathbf{z})$ or by perturbing the data points.

generalized total variation Generalized total variation measures the changes of vector-valued node attributes over a weighted undirected graph.

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

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

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

with a sufficiently small step size $\eta > 0$. Figure 4 illustrates the effect of a single GD step (2).

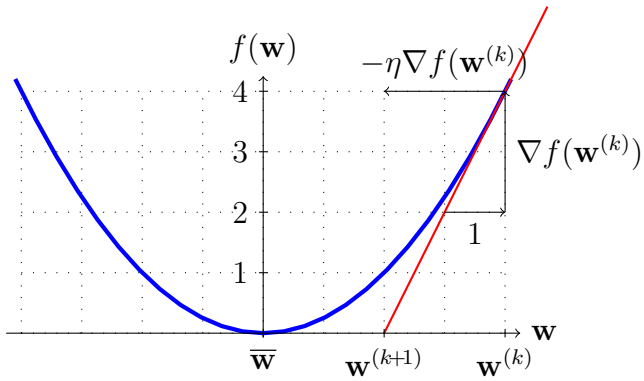


Abbildung 4: A single gradient step (2) towards the minimizer $\overline{\mathbf{w}}$ of $f(\mathbf{w})$.

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

$$\widehat{\mathbf{w}} := \mathbf{w} - \eta \nabla f(\mathbf{w}). \tag{3}$$

Mathematically, the gradient step is a (typically non-linear) operator $\mathcal{T}^{(f,\eta)}$ that is parametrized by the function f and the step size η. Note that the gradient step (3) optimizes locally - in a neighbourhood whose size is determined by the step size η - a linear approximation to the function $f(\cdot)$. A natural generalization of (3) is to locally optimize the function itself (instead of its linear approximation),

$$\widehat{\mathbf{w}} = \underset{\mathbf{w}' \in \mathbb{R}^d}{\operatorname{argmin}} f(\mathbf{w}') + (1/\eta) \left\| \mathbf{w} - \mathbf{w}' \right\|_2^2 . \tag{4}$$

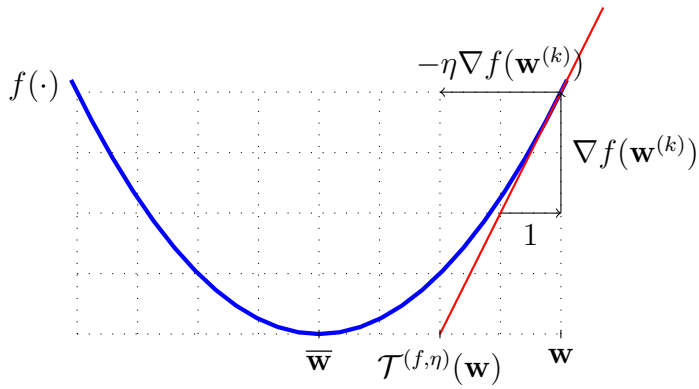


Abbildung 5: The basic gradient step (3) maps a given vector $\mathbf{w}$ to the updated vector $\mathbf{w}'$. It defines an operator $\mathcal{T}^{(f,\eta)}(\cdot) : \mathbb{R}^d \rightarrow \mathbb{R}^d : \mathbf{w} \mapsto \widehat{\mathbf{w}}$.

We intentionally use the same symbol η for the parameter in (4) as we used for the step-size in (3). The larger we choose η in (4), the more progress the update will make towards reducing the function value $f(\widehat{\mathbf{w}})$. Note that, much like the gradient step (3), also the update (4) defines a (typically non-linear) operator that is paramterized by the function $f(\cdot)$ and the parameter η. For a convex function $f(\cdot)$, this operator is known as the proximal operator of $f(\cdot)$ [48].

gradient-based method 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 for a gradient-based method is GD.

graph A graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is a pair that consists of a node set $\mathcal{V}$ and an edge set $\mathcal{E}$. In its most general form, a graph is specified by a map that assigns to each edge $e \in \mathcal{E}$ a pair of nodes [49]. One important family of graphs are 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 $e \in \mathcal{E}$.

graph clustering Graph clustering aims at clustering data points that are represented as the nodes of a graph $\mathcal{G}$. The edges of $\mathcal{G}$ represent pair-wise similarities between data points. Sometimes we can quantity the extend of these similarities by an edge weight [42, 50].

GTV minimization GTV minimization is an instance of regularized empirical risk minimization (RERM) using the generalized total variation (GTV) of local model parameters as a regularizer [51].

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

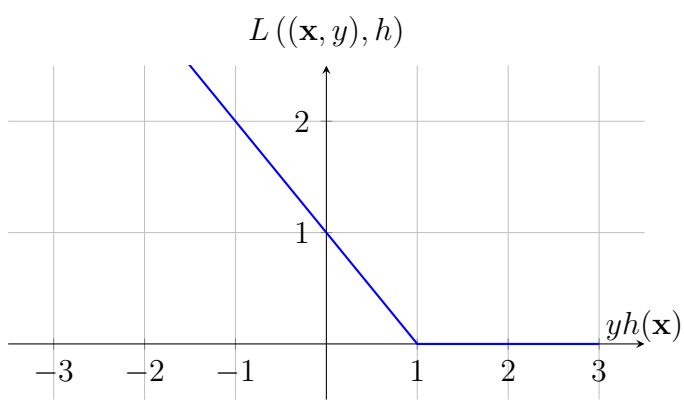
high-dimensional regime The high-dimensional regime of ERM is characterized by the effective dimension of the model being larger than the sample size, i.e., the number of (labeled) data points in the training set. For example, linear regression methods operate in the high-dimensional regime whenever the number d of features used to characterize data

points exceeds the number of data points in the training set. Another example of ML methods that operate in the high-dimensional regime are large ANNs, having far more tunable weights (and bias terms) than the number of data points in the training set. High-dimensional statistics is a recent main thread of probability theory that studies the behavior of ML methods in the high-dimensional regime [52, 53].

Hilbert space A Hilbert space is a linear vector space equipped with an inner product between pairs of vectors. One important example of a Hilbert space is the Euclidean space $\mathbb{R}^d$, for some dimension d, which consists of Euclidean vectors $\mathbf{u} = \left(u_1, \ldots, u_d\right)^T$ along with the inner product $\mathbf{u}^T\mathbf{v}$.

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

$$L\left((\mathbf{x}, y), h\right) := \max\{0, 1 - yh(\mathbf{x})\}. \tag{5}$$



A regularized variant of the hinge loss is used by the support vector

machine (SVM) [54].

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

horizontal FL Horizontal FL uses local datasets that are constituted by different data points but using the same features to characterize them [55]. For example, weather forecasting uses a network of spatially distributed weather (observation) stations. Each weather station measures the same quantities such as daily temperature, air pressure and precipitation. However, different weather stations measure the characteristics or features of different spatio-temporal regions (each such region being a separate data point).

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

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

hypothesis A map (or function) $h : \mathcal{X} \rightarrow \mathcal{Y}$ from the feature space $\mathcal{X}$ to the label space $\mathcal{Y}$. Given a data point with features $\mathbf{x}$, we use a hypothesis map h to estimate (or approximate) the label y using the prediction $\hat{y} = h(\mathbf{x})$. ML is all about learning (or finding) a hypothesis map h such that $y \approx h(\mathbf{x})$ for any data point (having features $\mathbf{x}$ and label y).

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

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

i.i.d. assumption The i.i.d. assumption interprets data points of a dataset as the realizations of i.i.d. RVs.

interpretability A ML method is interpretable for a specific user if they can well anticipate the predictions delivered by the method. The notion of interpretability can be made precise using quantitative measures of

the uncertainty about the predictions [31].

kernel Consider data points characterized by a feature vector $\mathbf{x} \in \mathcal{X}$ with a generic feature space $\mathcal{X}$. A (real-valued) kernel $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ assigns each pair of feature vectors $\mathbf{x}, \mathbf{x}' \in \mathcal{X}$ a real number $K\big(\mathbf{x}, \mathbf{x}'\big)$. The value $K\big(\mathbf{x}, \mathbf{x}'\big)$ is often interpreted as a measure for the similarity between $\mathbf{x}$ and $\mathbf{x}'$. Kernel methods us a kernel to transform the feature vector $\mathbf{x}$ to a new feature vector $\mathbf{z} = K\big(\mathbf{x}, \cdot\big)$. This new feature vector belongs to a linear feature space $\mathcal{X}'$ which is (in general) different from the original feature space $\mathcal{X}$. The feature space $\mathcal{X}'$ has a specific mathematical structure, i.e., it is a reproducing kernel Hilbert space [39, 54].

kernel method A kernel method is a ML method that uses a kernel K to map the original (raw) feature vector $\mathbf{x}$ of a data point to a new (transformed) feature vector $\mathbf{z} = K\big(\mathbf{x}, \cdot\big)$ [39, 54]. The motivation for transforming the feature vectors is that, 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 to use linear models, even if the data points are not linearly separable in the original feature space (see Figure 6).

Kullback-Leibler divergence The Kullback–Leibler divergence is a quantitative measure for how much one probability distribution is different from another probability distribution [15].

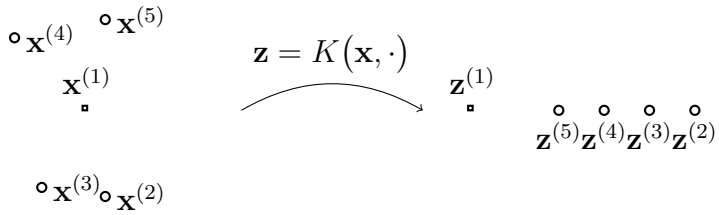
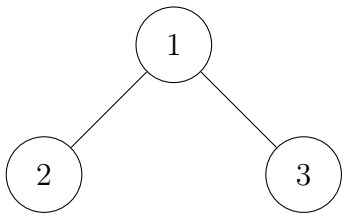


Abbildung 6: Five data points characterized by feature vectors $\mathbf{x}^{(r)}$ and labels $y^{(r)} \in \{\circ, \square\}$, for $r = 1, \ldots, 5$. With these feature vectors, there is no way to separate the two classes by a straight line (representing the decision boundary of a linear classifier). In contrast, the transformed feature vectors $\mathbf{z}^{(r)} = K\big(\mathbf{x}^{(r)}, \cdot\big)$ allow to separate the data points using a linear classifier.

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* [36–38].

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

labeled datapoint A data point whose label is known or has been determi-



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

Abbildung 7: Left: Some undirected graph $\mathcal{G}$ with three nodes $i = 1, 2, 3$. Right: Laplacian matrix $\mathbf{L}^{(\mathcal{G})} \in \mathbb{R}^{3\times 3}$ of $\mathcal{G}$.

ned by some means which might involve human experts.

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 [50, 56]. It is defined element-wise as (see Fig. 7)

$$L^{(\mathcal{G})}_{i,i'} := \begin{cases} -A_{i,i'} & \text{for } i \neq i', \{i, i'\} \in \mathcal{E} \\ \sum_{i'' \neq i} A_{i,i''} & \text{for } i = i' \\ 0 & \text{else.} \end{cases} \tag{6}$$

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

Large Language Model Large Language Models (LLMs) is an umbrella term for ML methods that process and generate human-like text. These methods typically use deep nets with billions (or even trillions) of parameters. A widely used choice for the network architecture is referred to as Transformers [57]. The training of LLMs is often based on the task of predicting a few words that are intentionally removed from a

large text corpus. Thus, we can construct labelled data points simply by selecting some words of a text as labels and the remaining words as features of data points. This construction requires very little human supervision and allows for generating sufficiently large training sets for LLMs.

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 using different notions of convergence [43].

learning rate Consider an iterative 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. A prime example of such an iterative learning method is GD and its variants such as SGD or projected GD. We refer by learning rate to a parameter of an iterative learning method that controls the extent by which the current hypothesis can be modified during a single iteration. A prime example of such a parameter is the step size used in GD [6, Ch. 5].

learning task Consider a dataset $\mathcal{D}$ constituted by several data points, each of them characterized by features $\mathbf{x}$. For example, the dataset $\mathcal{D}$ might be constituted by the images of a particular database. Sometimes it might be useful to represent a dataset $\mathcal{D}$, along with the choice of features, by a probability distribution $p(\mathbf{x})$. A learning task associated with $\mathcal{D}$ consists of a specific choice for the label of a data point and

the corresponding label space. Given a choice for the loss function and model, a learning task gives rise to an instance of ERM. Thus, we could define a learning task also via an instance of ERM, i.e., via an objective function. Note that, for the same dataset, we obtain different learning tasks by using different choices for the features and label of a data point. These learning tasks are related, as they are based on the same dataset, and solving them jointly (via multitask learning methods) is typically preferable over solving them separately [58–60].

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

least absolute shrinkage and selection operator (Lasso) The least absolute shrinkage and selection operator (Lasso) is an instance of structural risk minimization (SRM) to learn the weights $\mathbf{w}$ of a linear map $h(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$ based on a training set. The 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.

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 characterized by having decision regions separated by hyperplanes in the Euclidean space $\mathbb{R}^d$ [6, Ch. 2].

linear model Consider data points, each characterized by a numeric feature vector $\mathbf{x} \in \mathbb{R}^d$. A linear model is a hypothesis space which consists of

all linear maps,

$$\mathcal{H}^{(d)} := \left\{ h(\mathbf{x}) = \mathbf{w}^T \mathbf{x} : \mathbf{w} \in \mathbb{R}^d \right\}. \tag{7}$$

Note that (7) defines an entire family of hypothesis spaces, which is parameterized by the number d of features that are linearly combined to form the prediction $h(\mathbf{x})$. The design choice of d is guided by computational aspects (smaller d means less computation), statistical aspects (increasing d might reduce prediction error) and interpretability. A linear model using few carefully chosen features tends to be considered more interpretable [33, 40].

linear regression Linear regression aims to learn a linear hypothesis map to predict a numeric label based on 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.

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

local model Consider a collections of local datasets that are assigned to the nodes of a FL network. A local model $\mathcal{H}^{(i)}$ is a hypothesis space assigned

to a node $i \in \mathcal{V}$. Different nodes might be assigned different hypothesis spaces, i.e., in general $\mathcal{H}^{(i)} \neq \mathcal{H}^{(i')}$ for different nodes $i, i' \in \mathcal{V}$.

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

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

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

logistic regression Logistic regression learns a linear hypothesis map (classifier) $h(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$ to predict a binary label y based on 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 (the training set).

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

loss function A loss function is a map

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

which assigns a pair of a data point, with features $\mathbf{x}$ and label y, and a hypothesis $h \in \mathcal{H}$ the non-negative real number $L\left((\mathbf{x}, y), h\right)$. The

loss value $L((\mathbf{x}, y), h)$ quantifies the discrepancy between the true label y and the prediction $h(\mathbf{x})$. Lower (closer to zero) values $L((\mathbf{x}, y), h)$ indicate a smaller discrepancy between prediction $h(\mathbf{x})$ and label y. Figure 8 depicts a loss function for a given data point, with features $\mathbf{x}$ and label y, as a function of the hypothesis $h \in \mathcal{H}$.

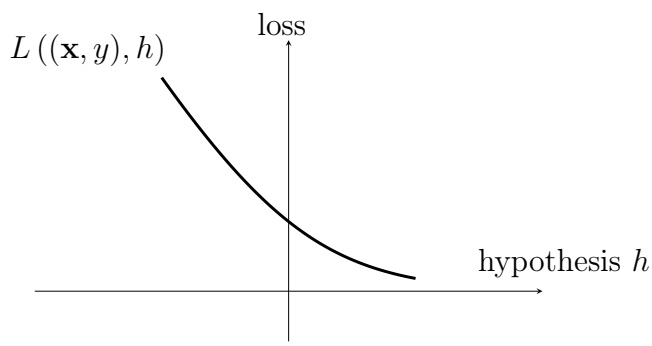


Abbildung 8: Some loss function $L((\mathbf{x}, y), h)$ for a fixed data point, with feature vector $\mathbf{x}$ and label y, and varying hypothesis h. ML methods try to find (learn) a hypothesis that incurs minimum loss.

maximum Given a set of real numbers, the maximum is the largest of those numbers.

maximum likelihood Consider data points $\mathcal{D} = \left\{\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(m)}\right\}$ that are interpreted as realizations of i.i.d. RVs with a common probability distribution $p(\mathbf{z}; \mathbf{w})$ 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) $p(\mathcal{D}; \mathbf{w}) = \prod_{r=1}^{m} p(\mathbf{z}^{(r)}; \mathbf{w})$ of observing the dataset is maximized. Thus, the maximum likelihood estimator is a solution to the optimization problem $\max_{\mathbf{w} \in \mathcal{W}} p(\mathcal{D}; \mathbf{w})$.

mean The expectation $\mathbb{E}\{\mathbf{x}\}$ of a numeric RV $\mathbf{x}$.

mean squared estimation error Consider a ML method that learns model parameters $\widehat{\mathbf{w}}$ based on some dataset $\mathcal{D}$. If we interpret the data points in $\mathcal{D}$ as i.i.d. realizations of a RV $\mathbf{z}$, we define the estimation error $\Delta\mathbf{w} := \widehat{w} - \overline{\mathbf{w}}$. Here, $\overline{\mathbf{w}}$ denotes the true model parameters of the probability distribution of $\mathbf{z}$.The mean squared estimation error is defined as the expectation $\mathbb{E}\{\|\Delta\mathbf{w}\|^2\}$ of the squared Euclidean norm of the estimation error [7, 21].

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

missing data Consider a dataset constituted by data points collected via some physical device. Due to imperfections and failures, some of the feature or label values of data points might be corrupted or simply *missing*. Data imputation aims at estimating these missing values [61]. We can interpret data imputation as a ML problem where the label of a data point is the value of the corrupted feature.

model In the context of ML methods, the term *model* typically refers to the hypothesis space used by a ML method [6, 46].

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

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 (i) training each candidate model, (ii) computing the validation error for each trained model, (iii) choosing the model with smallest validation error [6, Ch. 6].

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

multitask learning Multitask learning aims at leveraging relations between different learning tasks. Consider two learning tasks obtained from the same dataset of webcam snapshots. The first task is to predict the presence of a human, while the second is the predict the presence of a car. It might be useful to use the same deep net structure for both tasks and only allow the weights of the final output layer to be different.

multivariate normal distribution The multivariate normal distribution $\mathcal{N}(\mathbf{m}, \mathbf{C})$ is an important family of probability distributions for a continuous RV $\mathbf{x} \in \mathbb{R}^d$ [5, 8, 62]. This family is parameterized by the mean $\mathbf{m}$ and covariance matrix $\mathbf{C}$ of $\mathbf{x}$. If the covariance matrix is invertible, the probability distribution of $\mathbf{x}$ is

$$p(\mathbf{x}) \propto \exp\Big(-(1/2)\big(\mathbf{x}-\mathbf{m}\big)^T \mathbf{C}^{-1}\big(\mathbf{x}-\mathbf{m}\big)\Big).$$

mutual information The mutual information $I(\mathbf{x}; y)$ between two RVs $\mathbf{x}$,

y defined on the same probability space is given by [15]

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

It is a measure for how well we can estimate y based solely from $\mathbf{x}$. A large value of $I(\mathbf{x}; y)$ indicates that y can be well predicted solely from $\mathbf{x}$. This prediction could be obtained by a hypothesis learnt by a ERM-based ML method.

nearest neighbour Nearest neighbour methods learn a hypothesis $h : \mathcal{X} \rightarrow \mathcal{Y}$ whose function value $h(\mathbf{x})$ is solely determined by the nearest neighbours within a given dataset. Different methods use different metrics for determining the nearest neighbours. If data points are characterized by numeric feature vectors, we can use their Euclidean distances as the metric.

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

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

networked data Networked data consists of local datasets that are related by some notion of pair-wise similarity. We can represent networked data using a graph whose nodes carry local datasets and edges encode pairwise similarities. One example for networked data arises in FL applications where local datasets are generated by spatially distributed devices.

networked exponential families A collection of exponential families, each of them assigned to a node of a FL network. The model parameters are coupled via the network structure by requiring them to have a small GTV [63].

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

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

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

non-smooth We refer to a function as non-smooth if it is not smooth [64].

norm A norm is a function that maps each element (vector) of a linear vector space to a non-negative real number. This function must be homogeneous, definite and satisfy the triangle inequality [65].

objective function An objective function is a map that assigns each value of an optimization variable, such as the model parameters $\mathbf{w}$ of a hypothesis $h^{(\mathbf{w})}$, to an objective value $f(\mathbf{w})$. The objective value $f(\mathbf{w})$ could be the risk or the empirical risk of a hypothesis $h^{(\mathbf{w})}$.

online GD Consider a ML method that learns model parameters $\mathbf{w}$ from some parameter space $\mathcal{W} \subseteq \mathbb{R}^d$. The learning 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 a 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*: 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 it name suggests, online GD updates $\mathbf{w}^{(t)}$ via a (projected) gradient step

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

Note that (9) is a gradient step for the current component $L\left(\mathbf{z}^{(t)}, \cdot\right)$ of the risk. The update (9) ignores all the previous components $L\left(\mathbf{z}^{(t')}, \cdot\right)$, for $t' < t$. It might therefore happen that, compared to $\mathbf{w}^{(t)}$, the updated model parameters $\mathbf{w}^{(t+1)}$ increase the retrospective average loss $\sum_{t'=1}^{t-1} L\left(\mathbf{z}^{(t')}, \cdot\right)$. However, for a suitably chosen learning rate η_t, online GD can be shown to be optimal in practically relevant settings. By optimal, we mean that the model parameters $\mathbf{w}^{(T+1)}$ delivered by online GD after observing T data points $\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(T)}$ are at least as good as those delivered by any other learning method [28, 66].

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

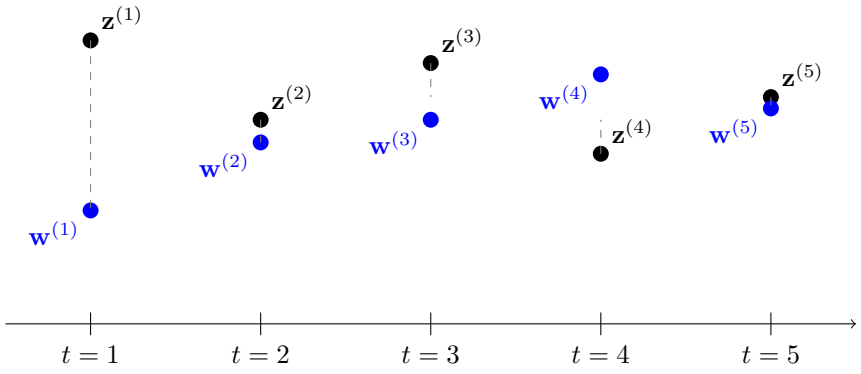


Abbildung 9: An instance of online GD that updates the model parameters $w^{(t)}$ using the data point $\mathbf{z}^{(t)} = x^{(t)}$ arriving at time t. This instance uses the squared error loss $L\left(\mathbf{z}^{(t)}, w\right) = (x^{(t)} - w)^2$.

$f(\mathbf{w})$. As a case in point, ERM-based methods use the average loss on a given dataset (the training set) as an estimate for the risk of a hypothesis. Using a probabilistic model, one can construct a confidence interval $\left[l^{(\mathbf{w})}, u^{(\mathbf{w})}\right]$ for each choice $\mathbf{w}$ for the model parameters. One simple construction is $l^{(\mathbf{w})} := f(\mathbf{w}) - \sigma/2$, $u^{(\mathbf{w})} := f(\mathbf{w}) + \sigma/2$ with σ being a measure for the (expected) deviation of $f(\mathbf{w})$ from $\bar{f}(\mathbf{w})$. We can also use other constructions for this interval as long as they ensure that $\bar{f}(\mathbf{w}) \in \left[l^{(\mathbf{w})}, u^{(\mathbf{w})}\right]$ with sufficiently high probability. As an optimist, we choose the model parameters according to the most favourable - yet still plausible - value $\tilde{f}(\mathbf{w}) := l^{(\mathbf{w})}$ of the performance criterion. Two examples of ML methods that use such an optimistic construction of an objective function are SRM [46, Ch. 11] and upper confidence bound (UCB) methods for sequential decision making [67, Sec. 2.2].

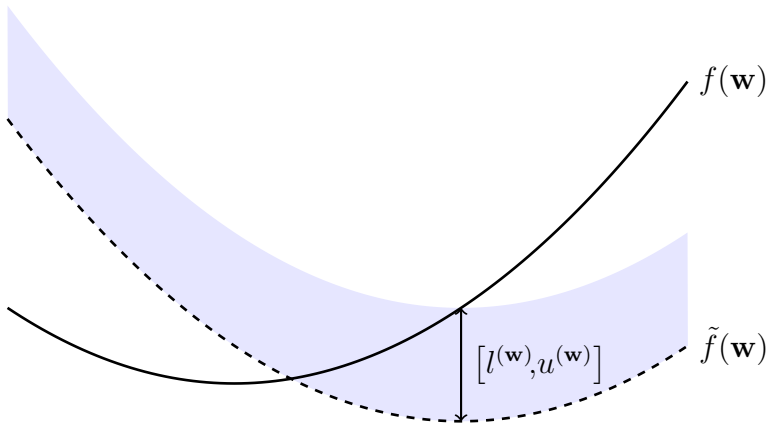


Abbildung 10: ML methods learn model parameters $\mathbf{w}$ by using some estimate $f(\mathbf{w})$ for the ultimate performance criterion $\bar{f}(\mathbf{w})$. Using a probabilistic model, one can use $f(\mathbf{w})$ to construct confidence intervals $\left[l^{(\mathbf{w})}, u^{(\mathbf{w})}\right]$ which contain $\bar{f}(\mathbf{w})$ with high probability. The best plausible performance measure for a specific choice $\mathbf{w}$ of model parameters is $\tilde{f}(\mathbf{w}) := l^{(\mathbf{w})}$.

outlier Many ML methods are motivated by the i.i.d. assumption which interprets data points as realizations of i.i.d. RVs with a common probability distribution. The i.i.d. assumption is useful for applications where the statistical properties of the data generation process are stationary (or time-invariant) [68]. However, in some applications the data consists of a majority of *regular* data points that conform with an i.i.d. assumption and a small number of data points that have fundamentally different statistical properties compared to the regular data points. We refer to a data point that substantially deviates from the statistical properties of most data points as an outlier. Different methods for outlier detection use different measures for this deviation. Stastistical learning theory studies fundamental limits on the ability to mitigate outliers reliably [69, 70].

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

parameter space The parameter space $\mathcal{W}$ of a ML model $\mathcal{H}$ is the set of all feasible choices for the model parameters (see Figure 11). Many important ML methods use a model that is parametrized by vectors of the Euclidean space $\mathbb{R}^d$. Two widely used examples of parametrized models are the linear model 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 norm smaller than

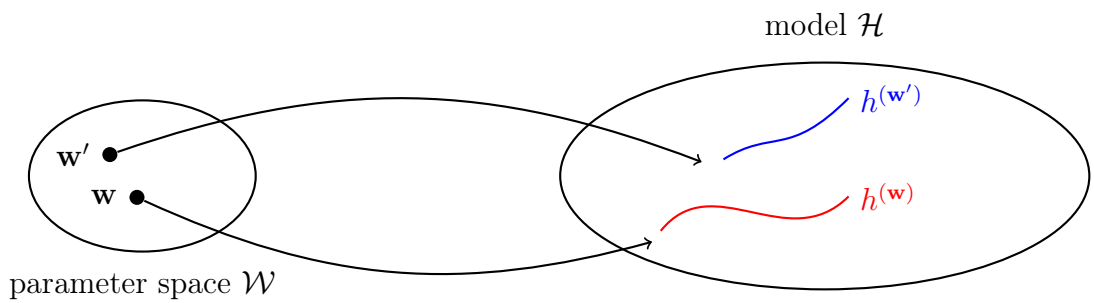


Abbildung 11: The parameter space $\mathcal{W}$ of a ML model $\mathcal{H}$ consists of all feasible choices for the model parameters. Each choice $\mathbf{w}$ for the model parameters selects a hypothesis map $h^{(\mathbf{w})} \in \mathcal{H}$.

one.

parameters The parameters of a ML model are tunable (learnable or adjustable) quantities that allow 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 parameters is the weights assigned to the connections between neurons of an ANN.

polynomial regression Polynomial regression aims at learning a polynomial hypothesis map to predict a numeric label based on 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 training set).

positive semi-definite A (real-valued) symmetric matrix $\mathbf{Q} = \mathbf{Q}^T \in \mathbb{R}^{d \times d}$ is referred to as positive semi-definite if $\mathbf{x}^T \mathbf{Q} \mathbf{x} \geq 0$ for every vector $\mathbf{x} \in \mathbb{R}^d$. The property of being psd can be extended from matrices to (real-valued) symmetric kernel maps $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ (with $K(\mathbf{x}, \mathbf{x}') = K(\mathbf{x}', \mathbf{x})$ as follows: For any finite set of feature vectors $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)}$, the resulting matrix $\mathbf{Q} \in \mathbb{R}^{m \times m}$ with entries $Q_{r,r'} = K\big(\mathbf{x}^{(r)}, \mathbf{x}^{(r')}\big)$ is psd [39].

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.

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

principal component analysis (PCA) Principal component analysis determines a linear feature map such that the new features allow to reconstruct the original features with minimum reconstruction error [6].

privacy funnel The privacy funnel is a method for learning privacy-friendly features of data points [71].

privacy leakage Consider a (ML or FL) system that processes a local dataset $\mathcal{D}^{(i)}$ and shares data, such as the predictions obtained for new data points, with other parties. Privacy leakage arises if the shared data

carries information about a private (sensitive) feature of a data point (which might be a human) of $\mathcal{D}^{(i)}$. The amount of privacy leakage can be measured via mutual information (MI) using a probabilistic model for the local dataset. Another quantitative measure for privacy leakage is differential privacy (DP).

privacy protection Consider some ML method $\mathcal{A}$ that reads in a $\mathcal{D}$ and delivers some output $\mathcal{A}(\mathcal{D})$. The output could be the learnt 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.

probabilistic model A probabilistic model interprets data points as realizations of RVs with a joint probability distribution. This joint probability distribution typically involves parameters which have to be manually chosen or learnt via statistical inference methods such as maximum likelihood [7].

probabilistic PCA Probabilistic principal component analysis (PCA) (PPCA) extends basic PCA by using a probabilistic model for data points.

The probabilistic model of PPCA reduces the task of dimensionality reduction to an estimation problem that can be solved using expectation maximization (EM) methods.

probability We assign a probability value, typically chosen in the interval $[0,1]$, to each event that might occur in a random experiment [5, 23, 24, 72].

probability density function (pdf) The probability density function (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 $p(x \in \mathcal{B}) = \int_{\mathcal{B}} p(x')dx'$ [5, Ch. 3]. The pdf of a vector-valued RV $\mathbf{x} \in \mathbb{R}^d$ (if it exists) allows to compute the probability that $\mathbf{x}$ falls into a (measurable) region $\mathcal{R}$ via $p(\mathbf{x} \in \mathcal{R}) = \int_{\mathcal{R}} p(\mathbf{x}')dx'_1 \ldots dx'_d$ [5, Ch. 3].

probability distribution To analyze ML methods it can be useful to interpret data points as i.i.d. realizations of a 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 $p(y=0)$ and $p(y=1) = 1 - p(y=0)$. The probability distribution of a real-valued RV $x \in \mathbb{R}$ might be specified by a probability density function $p(x)$ such that $p(x \in [a,b]) \approx p(a)|b-a|$. In the most general case, a probability distribution is defined by a probability measure [8, 24].

projected gradient descent (projected GD) Consider a ERM-based method, using a parametrized model with parameter space $\mathcal{W} \subseteq \mathbb{R}^d$. Even

if the objective function of ERM is smooth, we cannot use basic GD as it does not take into account contraints on the optimization variable (the model parameters). Projected GD extends basic GD to handle constraints on the optimization variable (model parameters). A single iteration of projected GD consists of first taking a gradient step and then projecting the result back into the parameter space.

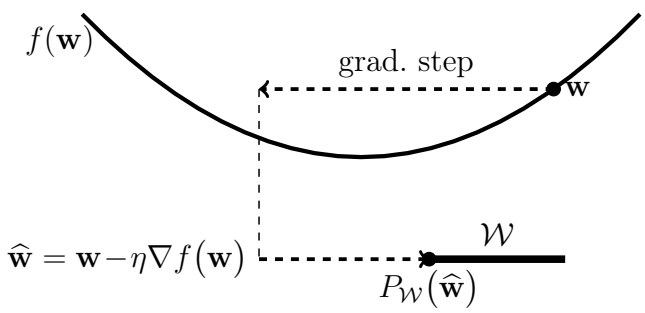


Abbildung 12: Projected GD augments a basic gradient step with a projection back onto the constraint set $\mathcal{W}$.

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

$$P_{\mathcal{W}}(\mathbf{w}) = \operatorname*{argmin}_{\mathbf{w}' \in \mathcal{W}} \|\mathbf{w} - \mathbf{w}'\|_2 . \tag{10}$$

In other words, $P_{\mathcal{W}}(\mathbf{w})$ is the vector in $\mathcal{W}$ which is closest to $\mathbf{w}$. The projection is only well-defined for subsets $\mathcal{W}$ for which the above minimum exists [10].

proximable A convex function for which the proximal operator can be computed efficiently are sometimes referred to as *proximable* or *simple* [73].

proximal operator Given a convex function $f(\mathbf{w}')$, we define its proximal operator as [48, 74]

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

As illustrated in Figure 13, 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). Convex functions for which the proximal operator can be computed efficiently are sometimes referred to as *proximable* or *simple* [73]. 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 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 $\rho = 1/\eta$.

quadratic function A quadratic function $f(\mathbf{w})$, reading in a vector $\mathbf{w} \in \mathbb{R}^d$ as its argument, is such that

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

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

Rényi divergence The Rényi divergence measures the (dis-)similarity between two probability distributions [75].

random forest A random forest is a set (ensemble) of different decision trees. Each of these decision trees is obtained by fitting a perturbed copy of the original dataset.

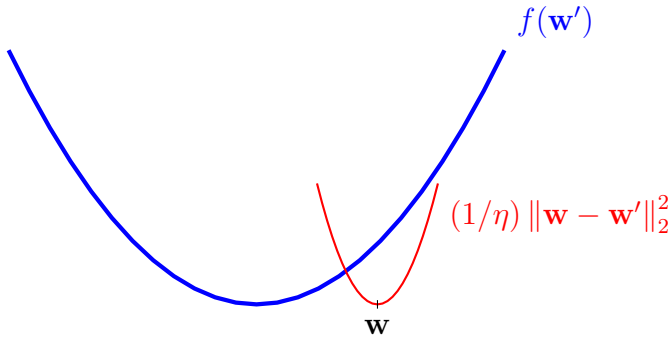


Abbildung 13: A generalized gradient step updates a vector $\mathbf{w}$ by minimizing a penalized version of the function $f(\cdot)$. The penalty term is the squared Euclidean distance between the optimization variable $\mathbf{w}'$ and the given vector $\mathbf{w}$.

random variable (RV) A random variable is a mapping from a probability space $\mathcal{P}$ to a value space [24]. The probability space, whose elements are elementary events, is equipped with a probability measure that assigns a probability to subsets of $\mathcal{P}$. A binary random variable maps elementary events to a set containing two different values, e.g., $\{-1, 1\}$ or $\{\text{cat}, \text{no cat}\}$. A real-valued random variable maps elementary events to real numbers $\mathbb{R}$. A vector-valued random variable maps elementary events to the Euclidean space $\mathbb{R}^d$. Probability theory uses the concept of measurable spaces to rigorously define and study the properties of (large) collections of random variables [8, 24].

realization Consider a RV x which maps each element (outcome, or elementary event) $\omega \in \mathcal{P}$ of a probability space $\mathcal{P}$ to an element a of a measurable space $\mathcal{N}$ [2, 23, 24]. A realization of x is any element $a' \in \mathcal{N}$

such that there is an element $\omega' \in \mathcal{P}$ with $x(\omega') = a'$.

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

regression Regression problems revolve around the problem of predicting a numeric label solely from the features of a data point [6, Ch. 2].

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

regularization A key challenge of modern ML applications is that they often use large models, having an effective dimension in the order of billions. Using basic ERM-based methods to train a high-dimensional model is prone to overfitting: the learn 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 the learnt hypothesis performs not much worse outside the training set. There are three routes for implementing regularization:

- **Model pruning.** We prune the original model $\mathcal{H}$ to obtain a smaller model $\mathcal{H}'$. For a parametrized model, the pruning can be implemented by including constraints on the model parameters (such as $w_1 \in [0.4, 0.6]$ for the weight of feature x_1 in linear

regression).

- **Loss penalization.** We modify the objective function of ERM by adding a penalty term to the training error. The penalty term estimates how much larger the expected loss (risk) is compared to the average loss on the training set.
- **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 a RV to the feature vector of a data point.

Figure 14 illustrates the above routs to regularization. These routes are often 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).

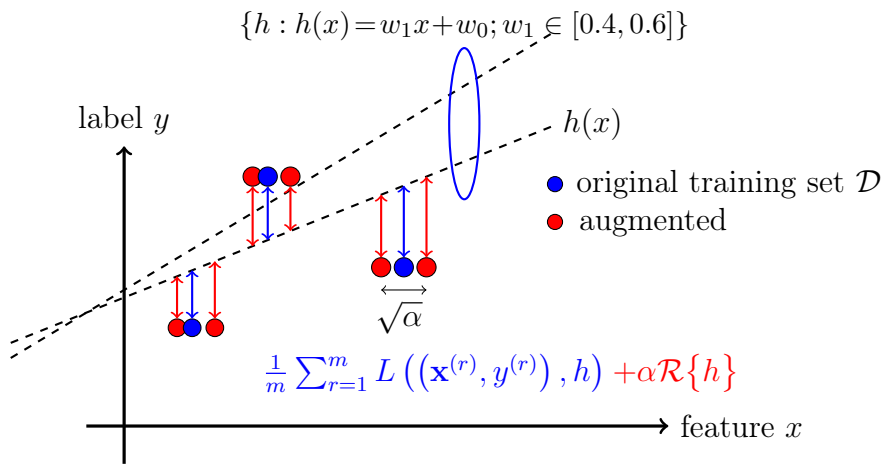


Abbildung 14: Three approaches to regularization: data augmentation, loss penalization and model pruning (via constraints on model parameters).

regularized empirical risk minimization (RERM) Synonym for SRM.

regularizer A regularizer assigns each hypothesis h from a hypothesis space $\mathcal{H}$ a quantitative measure $\mathcal{R}\{h\}$ for how much its prediction error on a training set might differ from its prediction errors on data points outside the training set. Ridge regression uses the regularizer $\mathcal{R}\{h\} := \|\mathbf{w}\|_2^2$ for linear hypothesis maps $h^{(\mathbf{w})}(\mathbf{x}) := \mathbf{w}^T\mathbf{x}$ [6, Ch. 3]. The least absolute shrinkage and selection operator (Lasso) uses the regularizer $\mathcal{R}\{h\} := \|\mathbf{w}\|_1$ for linear hypothesis maps $h^{(\mathbf{w})}(\mathbf{x}) := \mathbf{w}^T\mathbf{x}$ [6, Ch. 3].

ridge regression Ridge regression learns the weights $\mathbf{w}$ of a linear hypothesis map $h^{(\mathbf{w})}(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$. The quality of a particular choice for the parameter vector $\mathbf{w}$ is measured by the sum of two components. The first component is the average squared error loss incurred by $h^{(\mathbf{w})}$ on a set of labeled data

points (the training set). The second component is the scaled squared Euclidean norm $\alpha\|\mathbf{w}\|_2^2$ with a regularization parameter $\alpha > 0$. It can be shown that the effect of adding to $\alpha\|\mathbf{w}\|_2^2$ to the average squared error loss is equivalent to replacing the original data points by an ensemble of realizations of a RV centered around these data points.

risk Consider a hypothesis h used to predict the label y of a data point based on its features $\mathbf{x}$. We measure the quality of a particular prediction using a loss function $L\left((\mathbf{x}, y), h\right)$. If we interpret data points as the realizations of i.i.d. RVs, also the $L\left((\mathbf{x}, y), h\right)$ becomes the realization of a RV. The i.i.d. assumption allows 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.

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

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

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

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

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

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

sample size The number of individual data points contained in a dataset obtained as the realizations of i.i.d. RVs with common probability distribution.

scatterplot A visualization technique that depicts data points by markers in a two-dimensional plane.

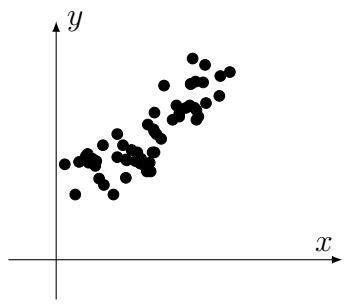


Abbildung 15: A scatterplot of data points that represent daily weather conditions in Finland. Each data point is characterized by its minimum daytime temperature x as feature and its maximum daytime temperature y as the label. The temperatures have been measured at the FMI weather station *Helsinki Kaisaniemi* during 1.9.2024 - 28.10.2024.

semi-supervised learning Semi-supervised learning methods use unlabeled data points to support the learning of a hypothesis from labeled data points [9]. This approach is particularly useful for ML applications that offer a large amount of unlabeled data points, but only a limited number of labeled data points.

sensitive attribute ML revolves around learning a hypothesis map that allows 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 to infer sensitive attributes of a data point. Which parts of a data point is considered as a sensitive attribute is a design choice that varies across different application domains.

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

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

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

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

smooth A real-valued function $f : \mathbb{R}^d \to \mathbb{R}$ is smooth if it is differentiable and its gradient $\nabla f(\mathbf{w})$ is continuous at all $\mathbf{w} \in \mathbb{R}^d$ [64, 76]. 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.,

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

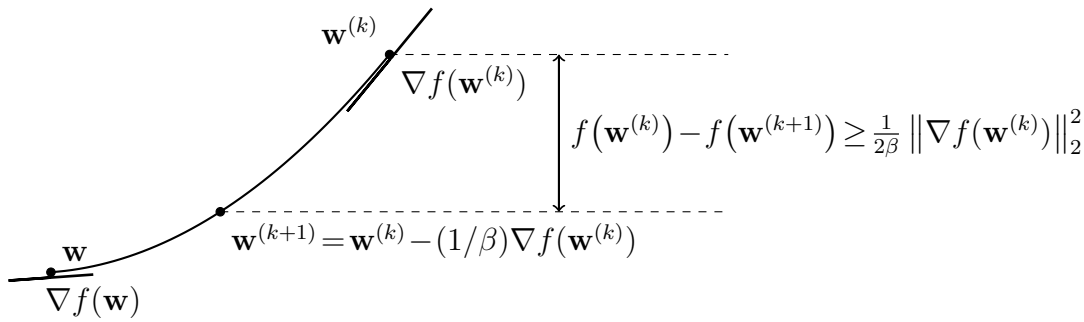


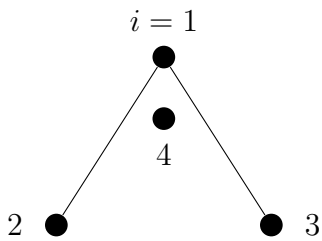
Abbildung 16: Consider an objective function $f(\mathbf{w})$ that is β-smooth. Taking a gradient step, with step size $\eta = 1/\beta$ decreases the objective by at least $\frac{1}{2\beta} \left\|\nabla f(\mathbf{w}^{(k)})\right\|_2^2$ [64,76,77]. Note that the step size $\eta = 1/\beta$ becomes larger for smaller β. Thus, for smoother objective functions (those who are β-smooth with smaller β), we can take larger steps.

The quantity β quantifies the amount of smoothness of the function f: the smaller β, the more smooth is f. Optimization problems with a smooth objective function can be solved effectively by gradient-based methods. Indeed, gradient-based methods approximate the objective function locally around a current choice $\mathbf{w}$ using its gradient. This approximation works well if the gradient does not change too rapidly. We can make this informal claim precise by studying the effect of a single gradient step with step size $\eta = 1/\beta$ (see Figure 16).

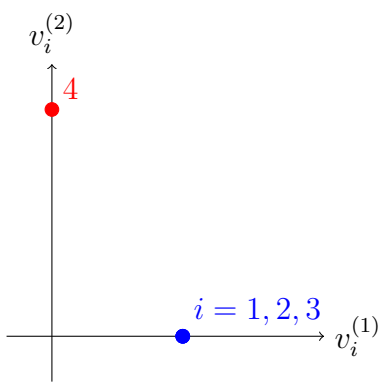
soft clustering Soft clustering refers to the task of partitioning a given set of data points into (few) overlapping clusters. Each data point is assigned to several different clusters with varying degree of belonging. Soft clustering methods determine the degree of belonging (or soft cluster

assignment) for each data point and each cluster. A principled approach to soft clustering is by interpreting data points as i.i.d. realizations of a GMM. We then obtain a natural choice for the degree of belonging as the conditional probability of a data point belonging to a specific mixture component.

spectral clustering Spectral clustering is a particular instance of graph clustering, i.e., it clusters data points represented as the nodes $i = 1, \ldots, n$ of a graph $\mathcal{G}$. Spectral clustering uses the eigenvectors of the Laplacian matrix $\mathbf{L}^{(\mathcal{G})}$ to construct feature vectors $\mathbf{x}^{(i)} \in \mathbb{R}^d$ for each node (data point) $i = 1, \ldots, n$. We can feed these feature vectors into Euclidean space-based clustering methods such as k-means or soft clustering via GMM. Roughly speaking, the feature vectors of nodes belonging to a well-connected subset (or cluster) of nodes in $\mathcal{G}$, are located nearby in the Euclidean space $\mathbb{R}^d$ (see Figure 17).



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



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

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

Abbildung 17: **Top.** Left: An undirected graph $\mathcal{G}$ with four nodes $i = 1, 2, 3, 4$, each representing a data point. Right: Laplacian matrix $\mathbf{L}^{(\mathcal{G})} \in \mathbb{R}^{4\times 4}$ and its EVD. **Bottom.** Left: Scatterplot of data points using the feature vectors $\mathbf{x}^{(i)} = \left(v_i^{(1)}, v_i^{(2)}\right)^T$. Right: Two eigenvectors $\mathbf{v}^{(1)}, \mathbf{v}^{(2)} \in \mathbb{R}^d$ of the Laplacian matrix $\mathbf{L}^{(\mathcal{G})}$ corresponding to the eigenvalue $\lambda = 0$.

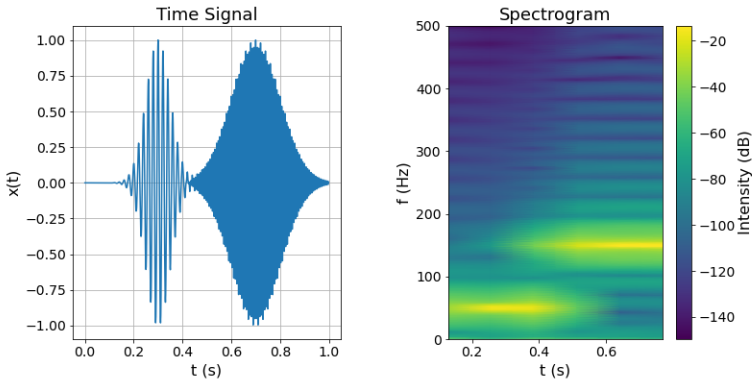


Abbildung 18: Left: A time signal consisting of two modulated Gaussian pulses. Right: Intenstity plot of the spectrogram.

spectrogram A spectrogram represents the time-frequency distribution of the energy of a time signal $x(t)$. Intuitively, it quantifies the amount of signal energy present within a specific time segment $[t_1, t_2] \subseteq \mathbb{R}$ and frequency interval $[f_1, f_2] \subseteq \mathbb{R}$. Formally, the spectrogram of a signal is defined as the squared magnitude of its short-time Fourier transform (STFT) [78]. Figure 18 depicts a time signal along with its spectrogram. The intensity plot of its spectrogram can serve as an image of a signal. A simple recipe for audio signal classification is to feed this *signal image* into deep nets originally developed for image classification and object detection [79]. It is worth noting that, beyond the spectrogram, several alternative representations exist for the time-frequency distribution of signal energy [80, 81].

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

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

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

step size See learning rate.

stochastic block model The stochastic block model (SBM) is a probabilistic generative model for an undirected graph $\mathcal{G} = \big(\mathcal{V}, \mathcal{E}\big)$ with a given set of nodes $\mathcal{V}$ [82]. 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.

stochastic gradient descent Stochastic GD is obtained from GD by replacing the gradient of the objective function with a stochastic approximation. A main application of stochastic gradient descent is to implement ERM for a parametrized model and a training set $\mathcal{D}$ is either very large or not readily available (e.g., when data points are stored in a database distributed all over the planet). To evaluate the gradient of the empirical risk (as a function of the model parameters $\mathbf{w}$), we need to compute a sum $\sum_{r=1}^{m} \nabla_{\mathbf{w}} L\left(\mathbf{z}^{(r)}, \mathbf{w}\right)$ over all data points in the training set. We obtain a stochastic approximation to the gradient by

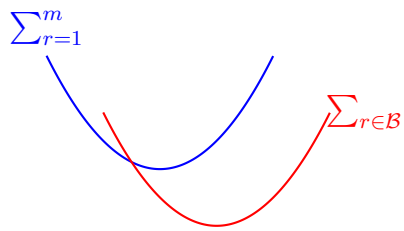


Abbildung 19: Stochastic GD for ERM approximates the gradient $\sum_{r=1}^{m} \nabla_{\mathbf{w}} L\left(\mathbf{z}^{(r)}, \mathbf{w}\right)$ by replacing the sum over all data points in the training set (indexed by $r = 1, \ldots, m$) with a sum over a randomly chosen subset $\mathcal{B} \subseteq \{1, \ldots, m\}$.

replacing the sum $\sum_{r=1}^{m} \nabla_{\mathbf{w}} L\left(\mathbf{z}^{(r)}, \mathbf{w}\right)$ with a sum $\sum_{r\in\mathcal{B}} \nabla_{\mathbf{w}} L\left(\mathbf{z}^{(r)}, \mathbf{w}\right)$ over a randomly chosen subset $\mathcal{B} \subseteq \{1, \ldots, m\}$ (see Figure 19). We often refer to these randomly chosen data points as a *batch*. The batch size $|\mathcal{B}|$ is an important parameter of stochastic GD. Stochastic GD with $|\mathcal{B}| > 1$ is referred to as mini-batch stochastic GD [83].

stopping criterion Many ML methods use iterative algorithms that construct a sequence of model parameters (such as the weights of a linear map or the weights of an ANN) that (hopefully) converge to an optimal choice for the model parameters. In practice, given finite computational resources, we need to stop iterating after a finite number of times. A stopping criterion is any well-defined condition required for stopping iterating.

strongly convex A continuously differentiable real-valued function $f(\mathbf{x})$ is strongly convex with coefficient σ if $f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^T(\mathbf{y} - \mathbf{x}) + (\sigma/2)\left\|\mathbf{y} - \mathbf{x}\right\|_2^2$ [64], [77, Sec. B.1.1.].

structural risk minimization Structural risk minimization is the problem of finding the hypothesis that optimally balances the average loss (or empirical risk) on a training set with a regularization term. The regularization term penalizes a hypothesis that is not robust against (small) perturbations of the data points in the training set.

subgradient For a real-valued function $f : \mathbb{R}^d \rightarrow \mathbb{R} : \mathbf{w} \mapsto f(\mathbf{w})$, a vector $\mathbf{a}$ such that $f(\mathbf{w}) \geq f(\mathbf{w}') + \left(\mathbf{w} - \mathbf{w}'\right)^T \mathbf{a}$ is referred to as a subgradient of f at $\mathbf{w}'$ [84, 85].

subgradient descent Subgradient descent is a generalization of GD that does not require differentiability of the function to be minimized. This generalization is obtained by replacing the concept of a gradient with that of a sub-gradient. Similar to gradients, also sub-gradients allow to construct local approximations of an objective function. The objective function might be the empirical risk $\widehat{L}\left(h^{(\mathbf{w})} \middle| \mathcal{D}\right)$ viewed as a function of the model parameters $\mathbf{w}$ that select a hypothesis $h^{(\mathbf{w})} \in \mathcal{H}$.

support vector machine The support vector machine (SVM) is a binary classification method that learns a linear hypothesis map. Thus, like linear regression and logistic regression, it is also an instance of ERM for the linear model. However, the support vector machine uses a different loss function than those methods. As illustrated in Figure 20, it aims to maximally separate data points from the two different classes in the feature space (*maximum margin principle*). Maximizing this separation is equivalent to minimizing a regularised variant of the hinge loss (5) [25, 54, 86] The above basic variant of SVM is only useful if

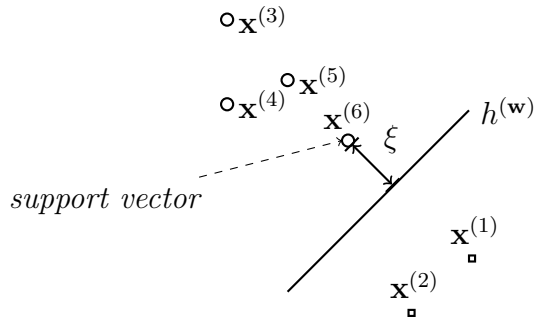


Abbildung 20: The SVM learns a hypothesis (or classifier) $h^{(\mathbf{w})}$ with minimum average soft-margin hinge loss. Minimizing this loss is equivalent to maximizing the margin ξ between the decision boundary of $h^{(\mathbf{w})}$ and each class of the training set.

the data points from different categories can be (approximately) linearly separated. For a ML application where the categories are not derived from a kernel.

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

total variation See GTV.

training error The average loss of a hypothesis when predicting the labels of data points in a training set. We sometimes refer by training error also the minimum average loss incurred on the training set by the optimal hypothesis from a hypothesis space.

training set A dataset $\mathcal{D}$, constituted by 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 to diagnose the ML method and informs how to improve them (e.g., using a different hypothesis space or collecting more data points) [6, Sec. 6.6.].

transparency Transparency is a key requirement for trustworthy AI [87]. In the context of ML methods, such as ERM-based methods, transparency is mainly used synonymously for explainability [31, 88]. However, in the wide context of AI systems, transparency also includes providing information about limitations and reliability of the AI system. As a point in case, logistic regression provides a quantitative measure for the reliability of a classification in the form of the value $|h(\mathbf{x})|$. Transparency also includes the user interface, by requiring to clearly indicate when a user is interaction with an AI system. Another component of transparency is the documentation of the system's purpose, design choices and intended use cases [89–91].

trustworthiness Beside the computational aspects and statistical aspects, a third main design aspect for ML methods is their trustworthiness [92]. The European Union has put forward seven key requirements (KRs) for trustworthy AI (that typically build on ML methods) [93]: **KR1 - Human Agency and Oversight**, **KR2 - Technical Robustness and Safety**, **KR3 - Privacy and Data Governance**, **KR4 - Transparency**, **KR5 - Diversity Non-Discrimination and Fairness**, **KR6 Societal and Environmental Well-Being**, **KR7 - Accountability**.

underfitting Consider a ML method that uses ERM to learn a hypothesis with 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 sufficiently small empirical risk on the training set. If a method is underfitting it will typically also not be able to learn a hypothesis with a small risk.

upper confidence bound Consider an ML application which requires to predict, for each new time instant, the optimal action out of a finite set of different actions. We measure the usefulness of a prediction (taking a specific action) by some numeric reward. One popular probabilistic model for such a sequential decision making problem is a multi-armed bandit .... can be modelled as a realization of a RV with some mean and variance.

validation Consider a hypothesis $\hat{h}$ that has been learnt via some ML method, e.g., by solving ERM on a training set $\mathcal{D}$. Validation refers to the practice of evaluating the loss incurred by hypothesis $\hat{h}$ on a validation set that consists of data points that are not contained in the training set $\mathcal{D}$.

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

validation set A set of data points used to estimate the risk of a hypothesis $\hat{h}$ that has been learnt 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 a ML method (see [6, Sec. 6.6.]). The comparison between training error and validation error can inform directions for improvements of the ML method (such as using a different hypothesis space).

Vapnik–Chervonenkis (VC) dimension The VC dimension of an infinite hypothesis space is a widely-used measure for its size. We refer to [46] for a precise definition of VC dimension as well as a discussion of its basic properties and use in ML.

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

vertical FL Vertical FL uses local datasets that are constituted by the same data points but characterizing them with different features [94]. For example, different healthcare providers might all contain information about the same population of patients. However, different healthcare providers collect different measurements (blood values, electrocardiography, lung X-ray) for the same patients.

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.

zero-gradient condition Consider the unconstrained optimization problem $\min_{\mathbf{w}\in\mathbb{R}^d} f(\mathbf{w})$ with a smooth and convex objective function $f(\mathbf{w})$. A necessary and sufficient condition for a vector $\widehat{\mathbf{w}} \in \mathbb{R}^d$ to solve this problem is that the gradient $\nabla f\left(\widehat{\mathbf{w}}\right)$ is the zero-vector,

$$\nabla f\left(\widehat{\mathbf{w}}\right) = \mathbf{0} \Leftrightarrow f\left(\widehat{\mathbf{w}}\right) = \min_{\mathbf{w}\in\mathbb{R}^d} f(\mathbf{w}).$$

0/1 **loss** The 0/1 loss $L\left((\mathbf{x}, y), h\right)$ measures the quality of a classifier $h(\mathbf{x})$ that delivers a prediction $\hat{y}$ (e.g., via thresholding (1)) for the label y of a data point with features $\mathbf{x}$. It is equal to 0 if the prediction is correct, i.e., $L\left((\mathbf{x}, y), h\right) = 0$ when $\hat{y} = y$. It is equal to 1 if the prediction is wrong, $L\left((\mathbf{x}, y), h\right) = 1$ when $\hat{y} \neq y$.

Index

0/1 loss, 85

k-means, 13

absolute error loss, 13

accuracy, 13

activation function, 14

application programming interface, 14

artificial intelligence, 14

artificial neural network, 14

autoencoder, 14

backdoor, 15

bagging, 15

baseline, 15

batch, 17

Bayes estimator, 17

Bayes risk, 18

bias, 18

bootstrap, 18

classification, 18

classifier, 19

cluster, 19

clustered federated learning, 19

clustering, 20

clustering assumption, 20

computational aspects, 20

condition number, 21

confusion matrix, 21

connected graph, 21

convex, 21

convex clustering, 21

covariance matrix, 22

data, 22

data augmentation, 22

data minimization principle, 23

data normalization, 24

data point, 24

data poisoning, 25

dataset, 25

DBSCAN, 26

decision boundary, 25

decision region, 25

decision tree, 26

deep net, 26

degree of belonging, 26

denial-of-service attack, 26

differentiable, 27

dimensionality reduction, 28
discrepancy, 28

edge weight, 28
effective dimension, 28
eigenvalue decomposition, 29
eigenvector, 29
empirical risk, 29
empirical risk minimization, 29
estimation error, 29
Euclidean space, 30
expectation, 30
expectation-maximization, 30
expert, 31
explainability, 31
explainable AI, 32
explainable empirical risk minimization, 31
explanation, 32

feature, 32
feature learning, 32
feature map, 33
feature matrix, 33
feature space, 33
feature vector, 34
federated averaging (FedAvg), 34
federated learning, 34
federated learning (FL) network, 34
Finnish Meteorological Institute, 34
flow-based clustering, 35

Gaussian mixture model, 35
Gaussian random variable, 35
GDPR, 36
generalization, 37
generalized total variation, 38
gradient, 38
gradient descent, 38
gradient step, 39
gradient-based methods, 40
graph, 41
graph clustering, 41

hard clustering, 41
high-dimensional regime, 41
Hilbert space, 42
hinge loss, 42
histogram, 43
horizontal FL, 43
Huber loss, 43
Huber regression, 43

hypothesis, 44
hypothesis space, 44

i.i.d., 44
interpretability, 44

k-fold cross-validation, 13
kernel, 45
kernel method, 45
KL divergence, 45

label, 46
label space, 46
labeled data, 46
Laplacian matrix, 47
Lasso, 49
law of large numbers, 48
learning rate, 48
learning task, 48
least absolute deviation regression, 49
linear classifier, 49
linear model, 49
linear regression, 50
local dataset, 50
local model, 50
logistic loss, 51
logistic regression, 51
loss, 51
loss function, 51

maximum, 52
maximum likelihood, 52
mean, 53
mean squared estimation error, 53
minimum, 53
missing data, 53
model parameters, 53
model selection, 54
multi-label classification, 54
multitask learning, 54
multivariate normal distribution, 54
mutual information, 54

nearest neighbour, 55
neighbourhood, 55
neighbours, 55
networked data, 55
networked exponential families, 56
networked federated learning, 56
networked model, 56
node degree, 56
non-smooth, 56

norm, 56

objective function, 56
online GD, 56
optimism in face of uncertainty, 57
outlier, 60
overfitting, 60

parameter space, 60
parameters, 61
polynomial regression, 61
positive semi-definite, 62
prediction, 62
predictor, 62
principal component analysis, 62
privacy leakage, 62
privacy protection, 63
probabilistic model, 63
probabilistic PCA, 63
probability, 64
probability density function, 64
probability distribution, 64
probability space, 67
projected gradient descent (projected GD), 65
projection, 65
proximable, 65
proximal operator, 66

quadratic function, 66

Rényi divergence, 66
random forest, 66
random variable (RV), 67
realization, 67
rectified linear unit (ReLU), 68
regression, 68
regret, 68
regularization, 68
regularized empirical risk minimization (RERM), 70
regularizer, 70
ridge regression, 70
risk, 71

sample, 71
sample covariance matrix, 71
sample mean, 72
sample size, 72
scatterplot, 72
semi-supervised learning, 72
sensitive attribute, 73
similarity graph, 73
singular value decomposition, 73

smooth, 73
soft clustering, 74
spectral clustering, 75
spectrogram, 77
squared error loss, 77
statistical aspects, 78
step size, 78
stochastic block model, 78
stochastic gradient descent, 78
stopping criterion, 79
strongly convex, 79
structural risk minimization, 80
subgradient, 80
subgradient descent, 80
support vector machine, 80

test set, 81
total variation minimization, 41
training error, 81
training set, 81
transparency, 82
trustworthy AI, 82

underfitting, 83
upper confidence bound, 83

validation, 83
validation error, 83
validation set, 83
variance, 84
VC dimension, 84
vertical FL, 84

weights, 84

zero-gradient condition, 85

Literatur

[1] W. Rudin, *Real and Complex Analysis*, 3rd ed. New York: McGraw-Hill, 1987.

[2] ——, *Principles of Mathematical Analysis*, 3rd ed. New York: McGraw-Hill, 1976.

[3] G. H. Golub and C. F. Van Loan, *Matrix Computations*, 4th ed. Baltimore, MD: Johns Hopkins University Press, 2013.

[4] G. Golub and C. van Loan, "An analysis of the total least squares problem," *SIAM J. Numerical Analysis*, vol. 17, no. 6, pp. 883–893, Dec. 1980.

[5] D. Bertsekas and J. Tsitsiklis, *Introduction to Probability*, 2nd ed. Athena Scientific, 2008.

[6] A. Jung, *Machine Learning: The Basics*, 1st ed. Springer Singapore, Feb. 2022.

[7] E. L. Lehmann and G. Casella, *Theory of Point Estimation*, 2nd ed. New York: Springer, 1998.

[8] R. Gray, *Probability, Random Processes, and Ergodic Properties*, 2nd ed. New York: Springer, 2009.

[9] O. Chapelle, B. Schölkopf, and A. Zien, Eds., *Semi-Supervised Learning*. Cambridge, Massachusetts: The MIT Press, 2006.

[10] S. Boyd and L. Vandenberghe, *Convex Optimization.* Cambridge, UK: Cambridge Univ. Press, 2004.

[11] D. Sun, K.-C. Toh, and Y. Yuan, "Convex clustering: Model, theoretical guarantee and efficient algorithm," *Journal of Machine Learning Research*, vol. 22, no. 9, pp. 1–32, 2021. [Online]. Available: http://jmlr.org/papers/v22/18-694.html

[12] K. Pelckmans, J. D. Brabanter, J. Suykens, and B. D. Moor, "Convex clustering shrinkage," in *PASCAL Workshop on Statistics and Optimization of Clustering Workshop*, 2005.

[13] E. Comission, "Regulation (eu) 2016/679 of the european parliament and of the council of 27 april 2016 on the protection of natural persons with regard to the processing of personal data and on the free movement of such data, and repealing directive 95/46/ec (general data protection regulation) (text with eea relevance)," no. 119, pp. 1–88, May 2016.

[14] European Union, "Regulation (eu) 2018/1725 of the european parliament and of the council of 23 october 2018 on the protection of natural persons with regard to the processing of personal data by the union institutions, bodies, offices and agencies and on the free movement of such data, and repealing regulation (ec) no 45/2001 and decision no 1247/2002/ec," nov 2018, official Journal of the European Union, L 295, 21.11.2018, pp. 39–98. [Online]. Available: https://eur-lex.europa.eu/eli/reg/2018/1725/oj

[15] T. M. Cover and J. A. Thomas, *Elements of Information Theory*, 2nd ed. New Jersey: Wiley, 2006.

[16] X. Liu, H. Li, G. Xu, Z. Chen, X. Huang, and R. Lu, "Privacy-enhanced federated learning against poisoning adversaries," *IEEE Transactions on Information Forensics and Security*, vol. 16, pp. 4574–4588, 2021.

[17] J. Zhang, B. Chen, X. Cheng, H. T. T. Binh, and S. Yu, "Poisongan: Generative poisoning attacks against federated learning in edge computing systems," *IEEE Internet of Things Journal*, vol. 8, no. 5, pp. 3310–3322, 2021.

[18] P. Halmos, *Naive set theory.* Springer-Verlag, 1974.

[19] A. Silberschatz, H. Korth, and S. Sudarshan, *Database System Concepts*, 7th ed. McGraw-Hill, 2019. [Online]. Available: https://db-book.com/

[20] I. Goodfellow, Y. Bengio, and A. Courville, *Deep Learning.* MIT Press, 2016.

[21] S. M. Kay, *Fundamentals of Statistical Signal Processing: Estimation Theory.* Englewood Cliffs, NJ: Prentice Hall, 1993.

[22] T. Hastie, R. Tibshirani, and J. Friedman, *The Elements of Statistical Learning*, ser. Springer Series in Statistics. New York, NY, USA: Springer, 2001.

[23] P. R. Halmos, *Measure Theory.* New York: Springer, 1974.

[24] P. Billingsley, *Probability and Measure*, 3rd ed. New York: Wiley, 1995.

[25] C. M. Bishop, *Pattern Recognition and Machine Learning.* Springer, 2006.

[26] M. J. Wainwright and M. I. Jordan, *Graphical Models, Exponential Families, and Variational Inference*, ser. Foundations and Trends in Machine Learning. Hanover, MA: Now Publishers, 2008, vol. 1, no. 1–2.

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

[28] E. Hazan, *Introduction to Online Convex Optimization.* Now Publishers Inc., 2016.

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

[30] L. Zhang, G. Karakasidis, A. Odnoblyudova, L. Dogruel, Y. Tian, and A. Jung, "Explainable empirical risk minimization," *Neural Computing and Applications*, vol. 36, no. 8, pp. 3983–3996, 2024. [Online]. Available: https://doi.org/10.1007/s00521-023-09269-3

[31] A. Jung and P. Nardelli, "An information-theoretic approach to personalized explainable machine learning," *IEEE Sig. Proc. Lett.*, vol. 27, pp. 825–829, 2020.

[32] J. Chen, L. Song, M. Wainwright, and M. Jordan, "Learning to explain: An information-theoretic perspective on model interpretation," in *Proc. 35th Int. Conf. on Mach. Learning*, Stockholm, Sweden, 2018.

[33] C. Rudin, "Stop explaining black box machine learning models for high-stakes decisions and use interpretable models instead," *Nature Machine Intelligence*, vol. 1, no. 5, pp. 206–215, 2019.

[34] C. Molnar, *Interpretable Machine Learning - A Guide for Making Black Box Models Explainable.* [online] Available: https://christophm.github.io/interpretable-ml-book/., 2019.

[35] R. Selvaraju, M. Cogswell, A. Das, R. Vedantam, D. Parikh, and D. Batra, "Grad-cam: Visual explanations from deep networks via gradient-based localization," in *2017 IEEE International Conference on Computer Vision (ICCV)*, 2017, pp. 618–626.

[36] D. Gujarati and D. Porter, *Basic Econometrics.* Mc-Graw Hill, 2009.

[37] Y. Dodge, *The Oxford Dictionary of Statistical Terms.* Oxford University Press, 2003.

[38] B. Everitt, *Cambridge Dictionary of Statistics.* Cambridge University Press, 2002.

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

[40] M. Ribeiro, S. Singh, and C. Guestrin, "Why Should I Trust You?: Explaining the predictions of any classifier," in *Proc. 22nd ACM SIGKDD*, Aug. 2016, pp. 1135–1144.

[41] B. McMahan, E. Moore, D. Ramage, S. Hampson, and B. A. y. Arcas, "Communication-Efficient Learning of Deep Networks from Decentralized Data," in *Proceedings of the 20th International Conference on Artificial Intelligence and Statistics*, ser. Proceedings of Machine Learning Research, A. Singh and J. Zhu, Eds., vol. 54. PMLR, 20–22 Apr 2017, pp. 1273–1282. [Online]. Available: https://proceedings.mlr.press/v54/mcmahan17a.html

[42] Y. SarcheshmehPour, Y. Tian, L. Zhang, and A. Jung, "Flow-based clustering and spectral clustering: A comparison," in *2021 55th Asilomar Conference on Signals, Systems, and Computers*, 2021, pp. 1292–1296.

[43] A. Papoulis and S. U. Pillai, *Probability, Random Variables, and Stochastic Processes*, 4th ed. New York: Mc-Graw Hill, 2002.

[44] C. Rasmussen and C. Williams, *Gaussian Processes for Machine Learning*. The MIT Press, 2006.

[45] S. M. Ross, *A First Course in Probability*, 9th ed. Boston: Pearson, 2013.

[46] S. Shalev-Shwartz and S. Ben-David, *Understanding Machine Learning – from Theory to Algorithms*. Cambridge University Press, 2014.

[47] J. Su, D. Vargas, and K. Sakurai, "One pixel attack for fooling deep neural networks," *IEEE Transactions on Evolutionary Computation*, vol. 23, no. 5, pp. 828–841, 2019.

[48] N. Parikh and S. Boyd, "Proximal algorithms," *Foundations and Trends in Optimization*, vol. 1, no. 3, pp. 123–231, 2013.

[49] R. T. Rockafellar, *Network Flows and Monotropic Optimization.* Athena Scientific, Jul. 1998.

[50] U. von Luxburg, "A tutorial on spectral clustering," *Statistics and Computing*, vol. 17, no. 4, pp. 395–416, Dec. 2007.

[51] Y. SarcheshmehPour, Y. Tian, L. Zhang, and A. Jung, "Clustered federated learning via generalized total variation minimization," *IEEE Transactions on Signal Processing*, vol. 71, pp. 4240–4256, 2023.

[52] M. Wainwright, *High-Dimensional Statistics: A Non-Asymptotic Viewpoint.* Cambridge: Cambridge University Press, 2019.

[53] P. Bühlmann and S. van de Geer, *Statistics for High-Dimensional Data.* New York: Springer, 2011.

[54] C. Lampert, "Kernel methods in computer vision," *Foundations and Trends in Computer Graphics and Vision*, 2009.

[55] Q. Yang, Y. Liu, Y. Cheng, Y. Kang, T. Chen, and H. Yu, *Horizontal Federated Learning.* Cham: Springer International Publishing, 2020, pp. 49–67. [Online]. Available: https://doi.org/10.1007/978-3-031-01585-4_4

[56] A. Y. Ng, M. I. Jordan, and Y. Weiss, "On spectral clustering: Analysis and an Algorithm," in *Adv. Neur. Inf. Proc. Syst.*, 2001.

[57] A. Vaswani, N. Shazeer, N. Parmar, J. Uszkoreit, L. Jones, A. Gomez, Ł. Kaiser, and I. Polosukhin, "Attention is all you need," in *Advances in neural information processing systems*, vol. 30, 2017, pp. 5998–6008.

[58] R. Caruana, "Multitask learning," *Machine Learning*, vol. 28, no. 1, pp. 41–75, 1997. [Online]. Available: https://doi.org/10.1023/A:1007379606734

[59] A. Jung, G. Hannak, and N. Görtz, "Graphical LASSO Based Model Selection for Time Series," *IEEE Sig. Proc. Letters*, vol. 22, no. 10, Oct. 2015.

[60] A. Jung, "Learning the conditional independence structure of stationary time series: A multitask learning approach," *IEEE Trans. Signal Processing*, vol. 63, no. 21, Nov. 2015.

[61] K. Abayomi, A. Gelman, and M. A. Levy, "Diagnostics for multivariate imputations," *Journal of The Royal Statistical Society Series C-applied Statistics*, vol. 57, pp. 273–291, 2008.

[62] A. Lapidoth, *A Foundation in Digital Communication*. New York: Cambridge University Press, 2009.

[63] A. Jung, "Networked exponential families for big data over networks," *IEEE Access*, vol. 8, pp. 202 897–202 909, 2020.

[64] Y. Nesterov, *Introductory lectures on convex optimization*, ser. Applied Optimization. Kluwer Academic Publishers, Boston, MA, 2004, vol. 87, a basic course. [Online]. Available: http://dx.doi.org/10.1007/978-1-4419-8853-9

[65] R. A. Horn and C. R. Johnson, *Matrix Analysis*, 2nd ed. Cambridge, UK: Cambridge Univ. Press, 2013.

[66] A. Rakhlin, O. Shamir, and K. Sridharan, "Making gradient descent optimal for strongly convex stochastic optimization," in *Proceedings of the 29 th International Conference on Machine Learning*, Edinburgh, Scotland, UK,, 2012.

[67] S. Bubeck and N. Cesa-Bianchi, "Regret analysis of stochastic and non-stochastic multi-armed bandit problems," *Foundations and Trends® in Machine Learning*, vol. 5, no. 1, pp. 1–122, 2012.

[68] P. J. Brockwell and R. A. Davis, *Time Series: Theory and Methods.* Springer New York, 1991.

[69] M. Kearns and M. Li, "Learning in the presence of malicious errors," *SIAM Journal on Computing*, vol. 22, no. 4, pp. 807–837, 1993. [Online]. Available: https://doi.org/10.1137/0222052

[70] G. Lugosi and S. Mendelson, "Robust multivariate mean estimation: The optimality of trimmed mean," *The Annals of Statistics*, vol. 49, no. 1, pp. 393 – 410, 2021. [Online]. Available: https://doi.org/10.1214/20-AOS1961

[71] A. Makhdoumi, S. Salamatian, N. Fawaz, and M. Médard, "From the information bottleneck to the privacy funnel," in *2014 IEEE Information Theory Workshop (ITW 2014)*, 2014, pp. 501–505.

[72] O. Kallenberg, *Foundations of modern probability.* New York: Springer, 1997.

[73] L. Condat, "A Primal–Dual Splitting Method for Convex Optimization involving Lipschitzian, Proximable and Linear Composite Terms," *Journal of Opt. Th. and App.*, vol. 158, no. 2, pp. 460–479, Aug. 2013.

[74] H. Bauschke and P. Combettes, *Convex Analysis and Monotone Operator Theory in Hilbert Spaces*, 2nd ed. New York: Springer, 2017.

[75] I. Csiszar, "Generalized cutoff rates and Renyi's information measures," *IEEE Transactions on Information Theory*, vol. 41, no. 1, pp. 26–34, 1995.

[76] S. Bubeck, "Convex optimization. algorithms and complexity." in *Foundations and Trends in Machine Learning*. Now Publishers, 2015, vol. 8.

[77] D. P. Bertsekas, *Convex Optimization Algorithms*. Athena Scientific, 2015.

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

[79] J. Li, L. Han, X. Li, J. Zhu, B. Yuan, and Z. Gou, "An evaluation of deep neural network models for music classification using spectrograms," *Multimedia Tools and Applications*, vol. 81, no. 4, pp. 4621–4647, 2022. [Online]. Available: https://doi.org/10.1007/s11042-020-10465-9

[80] B. Boashash, Ed., *Time Frequency Signal Analysis and Processing: A Comprehensive Reference*. Amsterdam, The Netherlands: Elsevier, 2003.

[81] S. G. Mallat, *A Wavelet Tour of Signal Processing – The Sparse Way*, 3rd ed. San Diego, CA: Academic Press, 2009.

[82] E. Abbe, "Community detection and stochastic block models: Recent developments," *Journal of Machine Learning Research*, vol. 18, no. 177, pp. 1–86, 2018.

[83] L. Bottou, *On-line learning and stochastic approximations.* USA: Cambridge University Press, 1999, pp. 9–42.

[84] D. Bertsekas, A. Nedic, and A. Ozdaglar, *Convex Analysis and Optimization.* Athena Scientific, 2003.

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

[86] N. Cristianini and J. Shawe-Taylor, *An Introduction to Support Vector Machines and Other Kernel-based Learning Methods.* Cambridge University Press, 2000.

[87] H.-L. E. G. on Artificial Intelligence, "Ethics guidelines for trustworthy AI," European Commission, Tech. Rep., April 2019.

[88] C. Gallese, "The ai act proposal: A new right to technical interpretability?" *SSRN Electronic Journal*, February 2023, available at SSRN: https://ssrn.com/abstract=4398206 or http://dx.doi.org/10.2139/ssrn.4398206.

[89] K. Shahriari and M. Shahriari, "IEEE Standard Review — Ethically aligned design: A vision for prioritizing human wellbeing with artificial intelligence and autonomous systems," in *2017 IEEE Canada International Humanitarian Technology Conference (IHTC)*, 2017, pp. 197–201.

[90] T. Gebru, J. Morgenstern, B. Vecchione, J. Vaughan, H. Wallach, H. Daumé, and K. Crawford, "Datasheets for datasets," *Commun. ACM*, vol. 64, no. 12, pp. 86–92, nov 2021. [Online]. Available: https://doi.org/10.1145/3458723

[91] M. M. et.al., "Model cards for model reporting," in *Proceedings of the Conference on Fairness, Accountability, and Transparency*, ser. FAT* '19. New York, NY, USA: Association for Computing Machinery, 2019, pp. 220–229. [Online]. Available: https://doi.org/10.1145/3287560.3287596

[92] D. Pfau and A. Jung, "Engineering Trustworthy AI: A Developer Guide for Empirical Risk Minimization," 2024. [Online]. Available: https://arxiv.org/abs/2410.19361

[93] E. Commission, C. Directorate-General for Communications Networks, and Technology, *The Assessment List for Trustworthy Artificial Intelligence (ALTAI) for self assessment.* Publications Office, 2020.

[94] Q. Yang, Y. Liu, Y. Cheng, Y. Kang, T. Chen, and H. Yu, *Vertical Federated Learning.* Cham: Springer International Publishing, 2020, pp. 69–81. [Online]. Available: https://doi.org/10.1007/978-3-031-01585-4_5