Seminar Series Neural Networks for Finance

Lecture 1

Aim

From linear to non-linear theory: towards an understanding of supervised learning

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Agenda

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Seminar Series Neural Networks for Finance

General introduction to machine learning

Machine learning - General

Machine learning is a collection of techniques to "learn" a relationship between an *input space* A and an *output space* B. Often highly automated and with a statistical approach.

Example 1: (binary classification)
We want to classify images of cats and dogs. Assuming equal format of each image A can be a space of $X \times Y-$matrices representing pixels of images and $B = \{\text{"cat"}, \text{"dog"}\}$.

Example 2: (function approximation)
We want to approximate $\mathbb{R} \ni x \mapsto f(x) \in [0, 1]$. Then, clearly $A = \mathbb{R}$ and $B = [0, 1]$.

Machine learning - General

Denote by H the true relation we want to learn, for $x \in A$, $H(x) \in B$ is the "truth". The aim for a machine learning algorithm is to achieve an accurate representation $\Phi \approx H$ in some sense. What do we need?

- A measure to define accuracy of our approximation $L(\Phi) = \mathrm{d}(H, \Phi)$, referred to as the *loss function* (d refers to a non-specified metric).
- A collection of samples, or *features* $\mathbf{x}_M = (x_1, x_2, \ldots, x_M)$ from A, *i.e.*, $x_i \in A$.
- An empirical error measure, denoted $\overline{L}(\Phi|\mathbf{x}_M)$, satisfying $\lim_{M\to\infty} \overline{L}(\Phi|\mathbf{x}_M) = L(\Phi)$. Typically referred to as the *empirical loss function*
- An optimization algorithm to approximately solve $\inf_{\Phi\in\mathcal{H}} \overline{L}(\Phi)$ in a pre-specified space $\mathcal{H}$. Typically referred to as *training*.

Machine learning - General scheme

Schematic scheme (some repetition of previous slide)
Given data: $\mathbf{x}_M$ of size M (could also have labels in supervised learning, more on this later). Evaluation data $\bar{\mathbf{x}}_M$ of size $\bar{M}$.

1. **Training:**
   Find an approximate minimizer of the loss function Φ^*, *i.e.*, $\widehat{\Phi} \approx \operatorname{argmin}_{\Phi \in \mathcal{H}} \overline{L}(\Phi|\mathbf{x}_M)$. Training or optimization is performed in a different way for each machine learning algorithm.
2. **Evaluation:**
   This step is to verify that the algorithm is able to generalize, *i.e.*, perform well beyond the training data. This is done by comparing $\overline{L}(\Phi|\mathbf{x}_M)$ and $\overline{L}(\Phi|\bar{\mathbf{x}}_M)$. If $\overline{L}(\Phi|\mathbf{x}_M) << \overline{L}(\Phi|\bar{\mathbf{x}}_M)$, then the problem might be *overfitting*, *i.e.*, the algorithm is fitted well against the training data but performs poorly on unseen data.

Machine learning - Different types of problems

Two main categories:

Supervised learning:
Each input element $x_i \in A$ comes with a corresponding output element $y_i \in B$. Implies that $H(x_i) = y_i$.

Unsupervised learning:
Only input elements are available during training. Need to rely on specific structure of the problem at hand to construct a loss function.

Machine learning - Supervised learning

Supervised learning:

- Training data comes in pairs (x_i, y_i) such that $H(x_i) = y_i$, for $i = 1, 2, \ldots, M$, where $y_1, y_2, \ldots, y_M$ are referred to as *labels*.
- As empirical loss function $L(\Phi|\mathbf{x}) = \frac{1}{M} \sum_{m=1}^{M} \mathrm{d}\big(\Phi(x_m), y_m\big)$ can be used.

Example: (Binary classification - American options)
At a certain point in time, given the price of the underlying, should the option be held or exercised? Optimal stopping policy.

Machine learning - Supervised learning Example

Input data: $x_1, \ldots, x_M$ representing M states of the underlying asset.
Labels: $y_1, \ldots, y_M$ taking on values in $\{0, 1\}$ where "0" means sub-optimal to exercise option and "1" means it is optimal to exercise option.

The aim is to approximate $H : \mathbb{R}_+ \to \{0, 1\}$ with Φ.

Loss function: $L(\Phi|\mathbf{x}) = \frac{1}{M} \sum_{m=1}^{M} \mathrm{d}\big(\Phi(x_m), y_m\big)$, where $\mathrm{d}(a, b)$ could be $|a - b|$ but usually more sophisticated to have a smoother loss function.

Machine learning - Unsupervised learning

Unsupervised learning:

- Training data consists of only input data $x_1, \ldots, x_M$ and the aim is to approximate H by Φ without being able to observe $H(x_i)$.
- We need to come up with an empirical loss function
- As empirical loss function $L(\Phi|\mathbf{x}) = \frac{1}{M}\sum_{m=1}^{M} F\big(\Phi(x_m)\big)$, where F is a certain *functional* such that if $L(\Phi|\mathbf{x})$ is minimized (or maximized), then Φ is a good approximator of H (at least for states around $x_1, \ldots, x_M$).

Example: (Option valuation - European options)
At a certain point in time, given the price of the underlying, what is the value of a European option? Solving the pricing PDE.

Machine learning - Unsupervised learning Example

Pricing PDE:

$$\begin{cases} \frac{\partial V}{\partial t} = f\left(t, x, V, \frac{\partial V}{\partial x}, \frac{\partial^2 V}{\partial x^2}\right) & (t,x) \in [0,T] \times \Omega = (x_{\min}, x_{\max}), \\ V(t,x) = f(t,x), & (t,x) \in [0,T] \times \overline{\Omega}, \\ V(T,x) = g(x), & x \in \Omega = \{x_{\min}, x_{\max}\}. \end{cases}$$

Here f is determined by the dynamics of the underlying asset, g is the pay-off function and the boundary conditions are set up to be "asymptotically reasonable".

For instance, the Black–Scholes model gives f linear in $V, \frac{\partial V}{\partial x}, \frac{\partial^2 V}{\partial x^2}$ making the PDE linear. Other models may yield a semi-linear or even a fully non-linear PDE.

Machine learning - Unsupervised learning Example

We do not know the PDE solution apriori and therefore, have no acccess to labels as in supervised learning. Need to create a loss function which uses the structure from the PDE.

$$L(\Phi) = \text{MSE}_{\text{inner}} + \text{MSE}_{\text{TC}} + \text{MSE}_{\text{BC}},$$

where

$$\begin{cases} \text{MSE}_{\text{inner}} = \frac{1}{M_{\text{inner}}} \sum_{m=1}^{M_{\text{inner}}} \left| \frac{\partial \Phi(t_m, x_m)}{\partial t} - f\left(t_m, x_m, \Phi, \frac{\partial \Phi}{\partial x}, \frac{\partial^2 \Phi}{\partial x^2}\right) \right|^2 \\ \text{MSE}_{\text{TC}} = \frac{1}{M_{\text{TC}}} \sum_{m=1}^{M_{\text{IC}}} |g(x_m) - \Phi(T, x_m)|^2, \\ \text{MSE}_{\text{BC}} = \frac{1}{M_{\text{BC}}} \sum_{m=1}^{M_{\text{BC}}} |f(t_m, x_m) - \Phi(t_m, x_m)|^2. \end{cases}$$

Machine learning – Other categories of tasks

- Anomaly detection
- Synthesis and sampling
- Denoising
- Density estimations
- ...

From statistics to machine learning: classical statistical inference

From statistics to machine learning: classical statistical inference

"Machine learning is essentially a form of applied statistics with increased emphasis on the use of computers to statistically estimate complicated functions and a decreased emphasis on proving confidence intervals around these functions[...]"

Goodfellow et al.: Deep Learning (2016), MIT Press

Statistical Estimates

- Statistics is about extracting as much information as possible from measurement data, e.g. *fitting functions, estimating finite/infinite parameters, distributions, assessing confidence intervals around estimates*
- In the most general, measure theoretic statement: a statistical model is a family of probability measures $\{\mathbb{P}_\theta, \theta \in \Omega\}$ on a measurable space $(\mathcal{X}, \mathcal{B})$ acting on the distribution of data X
  - Ω **finite dimensional: parametric models**
  - Ω infinite dimensional: non-parametric models
- In this course we will focus on **parametric models**

Statistical Point Estimates

- Two main schools of statistical inference:
  1. Classical/Frequentist: the true value of a parameter θ is fixed but not known; the *point estimate* $\widehat{\theta}$ is a random variable as a function of the randomly generated data
  2. Bayesian: data is directly observed thus cannot be random; the true value of the parameter θ is unknown therefore uncertain and thus can modeled as a random variable
- Frequentist: summarizes data into a single value of the parameter set $\widehat{\theta}$ and then makes predictions
- Bayesian: encompasses prior knowledge into a **prior** probability distribution $p(\theta)$ which is then used to make predictions through the Bayes theorem $p(\theta|x) = \frac{p(x|\theta)p(\theta)}{p(x)}$
- Through most of the course we will take the frequentists' perspective, however when studying **General Adversarial Networks** (GANs) we will rely on the **Bayesian approach**

Estimators, bias, variance

- Given data $\{x_1, \ldots, x_m\}$, a point estimator is a function which maps the data to an element of the parameter space $\widehat{\theta}_m := g(x_1, \ldots, x_m)$
  - Example: $x_i \in \mathbb{R}$, the statistical model consists of fitting a line on the data points
- **Bias**: $\text{bias}(\widehat{\theta}) := \mathbb{E}\left[\widehat{\theta}\right] - \theta$, where the expectation is taken over the data-generating distribution, $\text{bias}(\widehat{\theta}_m) = 0 \implies$ **unbiased** estimator
- **Variance**: $\text{Var}\left[\widehat{\theta}_m\right]$
- The **mean-squared error (MSE)** defines a trade-off between the minimization of the two

$$\text{MSE}(\widehat{\theta}_m) = \mathbb{E}\left[(\widehat{\theta}_m - \theta)^2\right] = \text{bias}^2(\widehat{\theta}_m) + \text{Var}\left[\widehat{\theta}_m\right]$$

Notions of generalization

$$\text{MSE}(\widehat{\theta}_m) = \mathbb{E}\left[(\widehat{\theta}_m - \theta)^2\right] = \text{bias}^2(\widehat{\theta}_m) + \text{Var}\left[\widehat{\theta}_m\right]$$

- Notions of generalization: capacity, underfitting, overfitting
  1. underfitting: small capacity leads to low variance, large bias
  2. overfitting: increased capacity, decreases bias but increases variance

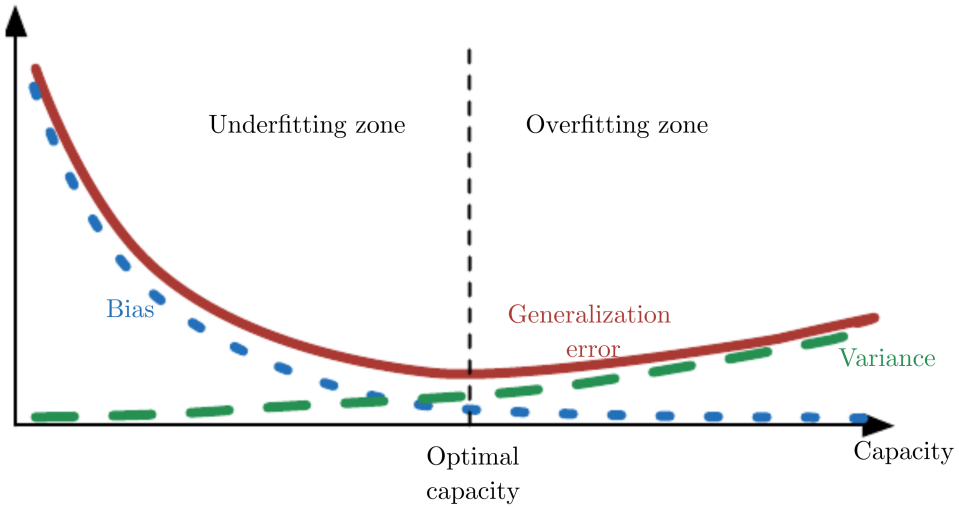


Figure: Goodfellow et al.: Deep Learning (2016), MIT Press [Figure 5.6, pg. 128]

Maximum Likelihood Principle

- **Maximum Likelihood Estimator (MLE)** principle: given a data generating distribution $\mathbb{P}_{\text{data}}(x)$ and a statistical model $\mathbb{P}_{\text{model}}(x|\theta)$

$$\widehat{\theta}_{\text{ML}} := \arg\max_{\theta} \mathbb{P}_{\text{model}}(X|\theta) \tag{1}$$

- Under the assumption of **independent, identically distributed (iid)** data samples $X = \{x_1, \ldots, x_M\}$, this can be written $\widehat{\theta}_{\text{ML}} := \arg\max_{\theta} \prod_{m=1}^{M} \mathbb{P}_{\text{model}}(x_m|\theta)$

From linear to non-linear theory: regression

Ordinary Least-Squares Regression

- We are given a data set $\{x_{m1}, \ldots, x_{md}; y_m\}_{m=1}^{M}$ of M measurements drawn from the same distribution
- The elements of the vector $\mathbf{x}_m := (x_{m1}, \ldots, x_{md}) \in \mathbb{R}^d$ are called the *explanatory/independent* variables; $y_m \in \mathbb{R}$ is the response/dependent variable
- We assume a *linear* relation *with noise* between the *fixed* measurements of independent variables and the response variable

$$y = \mathbf{x}^T \boldsymbol{\beta} + \epsilon \tag{2}$$

  with some **parameter** vector $\boldsymbol{\beta} \in \mathbb{R}^d$
- the *noise term* ϵ incorporates the residual influence on y not captured by the regressors (measurement errors in y, missing regressors, etc.)

Ordinary Least-Squares Regression

Goal

The goal of Ordinary Least-Squares (OLS) regression is to find a(/the?) set of regression coefficients $\beta = (\beta_1, \ldots, \beta_d)$ such that the Euclidean norm of the noise term is minimized

$$\widehat{\beta} := \arg\min_{\beta} \|\epsilon\|_2^2 = \arg\min_{\beta} \|\mathbf{y} - \mathbf{X}\beta\|_2^2 = \sum_{m=1}^{M} \left| y_m - \mathbf{x}_m^T \beta \right|^2, \quad (3)$$

where $\mathbf{X} = \begin{pmatrix} x_{11} & \ldots & x_{1d} \\ \ldots & \ldots & \ldots \\ x_{m1} & \ldots & x_{md} \end{pmatrix}$, $\mathbf{y} = (y_1, \ldots, y_m), \epsilon = (\epsilon_1, \ldots, \epsilon_m)$

Ordinary Least-Squares Regression

- Denote mean-squared *loss*, subject to the measurements $\mathbf{D} := (\mathbf{X}, \mathbf{y})$ by $L(\beta|\mathbf{D}) = \|\mathbf{y} - \mathbf{X}\beta\|_2^2$ which is equal to

$$L(\beta|\mathbf{D}) = \mathbf{y}\mathbf{y}^T - \mathbf{y}^T\mathbf{X}\beta - \beta^T\mathbf{X}^T y + \beta^T\mathbf{X}^T\mathbf{X}\beta$$

- Due to the **convexity** of $\beta \mapsto L(\beta|\mathbf{D})$ the unique global minimum is found where the gradient vanishes

$$\mathbf{0} = \nabla_\beta L(\widehat{\beta}|\mathbf{D}) = -2\mathbf{y}^T\mathbf{X} + 2\widehat{\beta}^T\mathbf{X}^T\mathbf{X}$$

Unique Solution

The unique minimizer of (3) is given by

$$\widehat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}, \tag{4}$$

and the corresponding approximations

$$\widehat{\mathbf{y}} := \mathbf{X}\widehat{\beta} \tag{5}$$

Key Remarks

- Under standard assumptions (linearity, independence of ϵ_m's, homoscedasticity – the variance of ϵ_m does not depend on the values $\mathbf{x}_m$, lack of *perfect multicollinearity* – $\mathbf{X}$ has full column rank d) the OLS problem admits to a **unique, closed-form solution**
- The intercept (constant) can be incorporated into the model as a zero'th dimension
- The distribution of $\mathbf{X}$ has a great impact on the accuracy of $\widehat{\boldsymbol{\beta}}$ – assumes high-quality sampling methods
- The OLS estimate coincides with the Maximum Likelihood Estimate (MLE)

Non-linear regression

- Same setting
  - data coming from a fixed *data generating* distribution: $\{x_{m1}, \ldots, x_{md}; y_m\}_{m=1}^{M}$ of M measurements drawn from the same distribution
  - explanatory and response variables $\mathbf{x}_m := (x_{m1}, \ldots, x_{md}) \in \mathbb{R}^d$, $y_m \in \mathbb{R}$
- However, the assumptions of linearity established by (2) **no longer holds**
- Instead, we consider the following **non-linear extension** of the model

$$y = H(\mathbf{x}) + \epsilon \tag{6}$$

where $H : \mathbb{R}^d \to \mathbb{R}$ is a deterministic mapping

Non-linear regression

Question?

What could be an appropriate family of statistical models $\{\phi(x|\theta) : \mathbb{R}^d \to \mathbb{R} : \theta \in \mathbb{R}^p\}$ which spans a *"large enough"* space for all potential *H*s?

- In what follows we will study classes of statistical models which are suitable for specific tasks
- For now, let us briefly assume we have a family of **"black box"** statistical models of the form $\{\phi(x|\theta) : p \in \mathbb{N}, \theta \in \mathbb{R}^p\}$ which possess this quality
- Within such a family of statistical models, the question still remains: *how do we choose the "right" number of p parameters?*

Generalization Properties

- Here p is called a **hyperparameter** of the model which needs to be chosen carefully
- The ultimate goal of the regression problem is not to fit the *training data* $\{x_{m1}, \ldots, x_{md}; y_m\}_{m=1}^{M}$ with arbitrary accuracy but rather to **approximate the relation** (6)
- In fact, we seek to find a set of parameters $\{\widehat{\theta} \in \mathbb{R}^p : p \in \mathbb{N}\}$ such that $\phi(x|\widehat{\theta}) \approx H(x)$ for any x **drawn from the data generating distribution** – regardless whether it is in the training data or not
- trade-off: representational capacity naturally grows with p, however generalization capibility decreases – recall Figure 1

Hyperparameter Selection: Under- and Overfitting

In some applications one has direct access to the data generating distribution (e.g.: Monte Carlo option pricing), in most cases however we are only provided with a finite sample $\mathbf{D} = \{(\mathbf{x}_m, y_m)\}_{m=1}^{M}$

Question

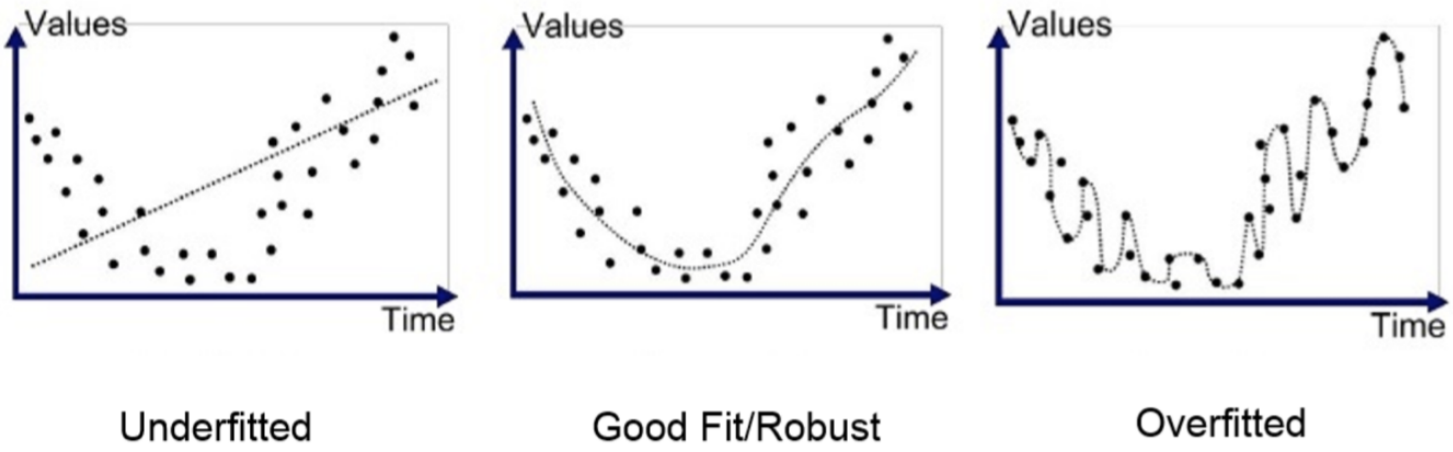
Question: in case of the latter, how does one ensure *unbiased* estimates, with good generalization properties?

- Idea: split the data set $\mathbf{D}$ into a partition, a subset for training $\mathbf{D}_{train} \subset \mathbf{D}$ and one for testing $\mathbf{D}_{test} \subset \mathbf{D}$, such that $\mathbf{D}_{train} \cap \mathbf{D}_{test} = \emptyset$ and $\mathbf{D}_{train} \cup \mathbf{D}_{test} = \mathbf{D}$.
- We choose multiple p:s and *optimize* their corresponding statistical models with a black box optimization method (soon explained) according to an appropriately selected *loss function* (e.g. MSE)

Hyperparameter Selection: Under- and Overfitting

- Out of the optimal parameter sets, the one with lowest loss generalizes best. However, the error measure remains inaccurate to future predictions due to overfitting on the test set.
- Partitioning into three subsets: training data $\mathbf{D}_{train} \subset \mathbf{D}$, validation data $\mathbf{D}_{val} \subset \mathbf{D}$ and test data $\mathbf{D}_{test} \subset \mathbf{D}$, such that $\mathbf{D}_{train} \cup \mathbf{D}_{val} \cup \mathbf{D}_{test} = \mathbf{D}$ and $\mathbf{D}_{train} \cap \mathbf{D}_{val} \cap \mathbf{D}_{test} = \emptyset$ resolves this problem
- First, multiple parameter sets are trained on the training set.
- Second, the best performing set of parameters is chosen from the validation set.
- At last, the error measure is calculated on the test set.
- This method gives an unbiased estimate of the error measure on future data.
- Similarly to **cross validation**

Summary: Under- and Overfitting

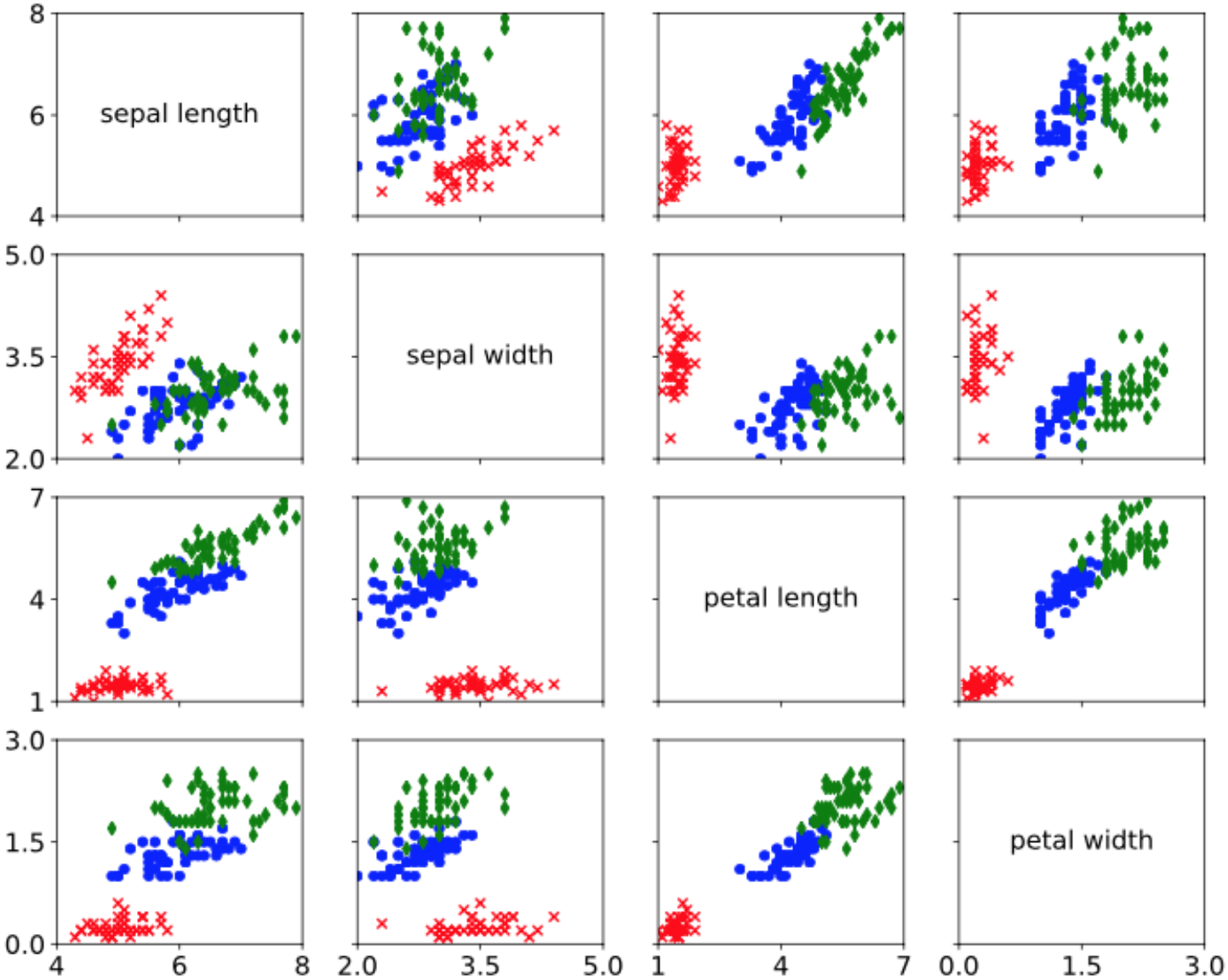


From linear to non-linear theory: classification

Motivating Example: Iris data set

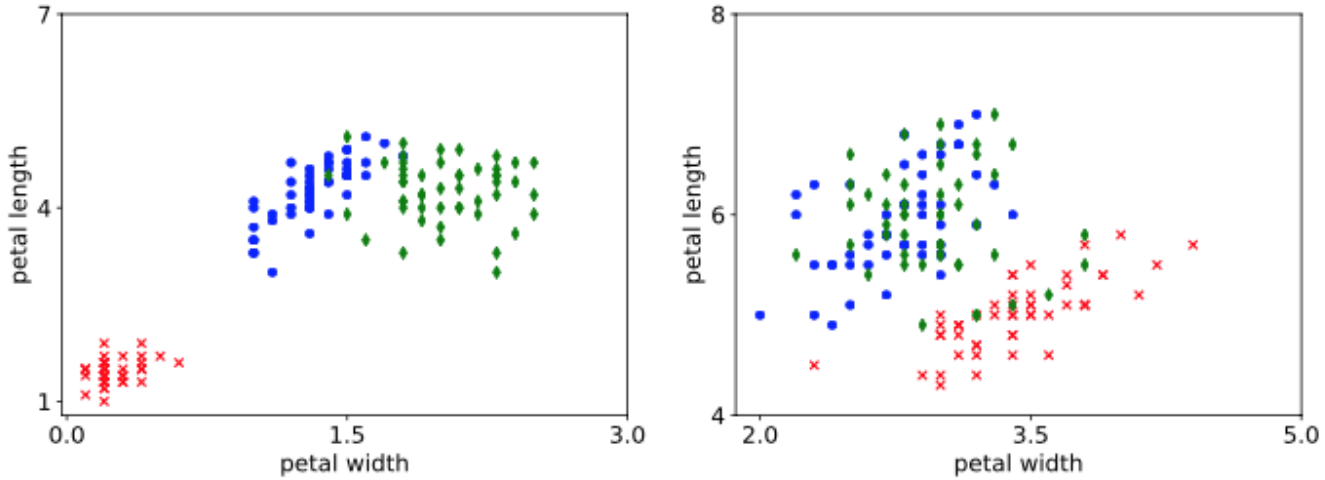
- The Iris data set is a multivariate set with 50 entries for each species. There are three species, consisting of four features: sepal length, sepal width, petal length and petal width.
- The four features can be displayed in a scatter plot
- Determining categories by using their features is called **classification**
- Setosa is blue, Versicolor is red, and Virginica is green colored

Motivating Example: Iris data set



Motivating Example: Iris data set

- See, left figure below, the Setosa species can be distinguished from the others, by using the petal length.



(a) Zoom 1 **(b)** Zoom 2

- In mathematical terms, it can be stated that the Setosa is **linearly separable**.
- Two sets $X_1 \subset X$ and $X_2 \subset X$ are called **linearly separable** if their convex hulls are disjoint.

Motivating Example: Iris data set

- Consider the set X_1, the petal lengths of the Versicolor and the Virginica species and the set X_2, the petal lengths of the Setosa species. In this case

$$convhull(X_1) = \{x | x \in [\min(X_1), \max(X_1)]\} = [3.0, 6.9]$$

and

$$convhull(X_2) = \{x | x \in [\min(X_2), \max(X_2)]\} = [1.0, 1.9]$$

- Clearly, $convhull(X_1) \cap convhull(X_2) = \emptyset$, therefore X_1 and X_2 are linearly separable, and thus it is possible to classify the Setosa species in the Iris data set

Motivating Example: Iris data set

- From the scatter plot at the right side of the last figure, the species are not easily distinguishable
- By creating convex hulls of the individual features, the two species are not linearly separable for the individual features
- It is impossible to classify the species using linear classifiers deterministically. We could create (hyper-)planes such that a minimal number of data entries is incorrectly separated
- This gives a statistically optimal result for the data set on which the classifier is trained
- **Support Vector Machines (SVM)** designed to find such optimal hyperplanes

Standard models of classification

Standard Models of Classification

- We are given a **binary** *response variable* $Y \in \{0, 1\}$; and a vector of real-valued regressors $\mathbf{x}$ which are assumed to influence Y – *multinomial extensions are straightforward*
- We obtained a data set of measurements $\{\mathbf{x} = (x_{m1}, \ldots, x_{md}), y_m\}_{m=1}^{M}$
- Formally we describe the outcome of each measurement with a Bernoulli distribution with *unobserved* probability p_m

$$Y_m | x_{m1}, \ldots x_{md} \sim \text{Bernoulli}(p_m)$$

- Define the linear *latent variable model* with an *auxiliary random variable* $\widetilde{Y}$ such that

$$\widetilde{Y} = \mathbf{x}^T \boldsymbol{\beta} + \epsilon, \tag{7}$$

where ϵ follows a given **symmetric, centered** distribution

Standard Models of Classification

- Thereby Y can be interpreted as the indicator function

$$Y = \begin{cases} 1, & \widetilde{Y} > 0 \\ 0, & \widetilde{Y} \leq 0 \end{cases}$$

- By the symmetricity of the distribution of the noise term we have

$$\mathbb{P}\left[Y = 1|\mathbf{x}\right] = \mathbb{P}\left[\widetilde{Y} > 0|\mathbf{x}\right] = \mathbb{P}\left[\epsilon > -\mathbf{x}^T\boldsymbol{\beta}\right] = \text{CDF}(\mathbf{x}^T\boldsymbol{\beta})$$

- The corresponding estimates are then defined by setting the distribution of the noise term, two classical choices
  1. **Probit regression**: $\epsilon \sim \mathcal{N}(0,1)$ which implies
  $$\mathbb{P}\left[Y = 1|\mathbf{x}\right] = \Phi(\mathbf{x}^T\boldsymbol{\beta})$$
  2. **Logistic regression**: ϵ follows a *standard logistic distribution* whose CDF is given by $\frac{1}{1+e^{-x}}$
  $$\mathbb{P}\left[Y = 1|\mathbf{x}\right] = \frac{1}{1 + e^{-\mathbf{x}^T\boldsymbol{\beta}}}$$

Logistic Regression

- Logistic regression is more common in machine learning practices due to the convenience of a closed form CDF
- So far we have a prediction for the probability of the m'th measurement taking the value 1

$$\mathbb{P}\left[Y_m = 1 | \mathbf{x}_m, \boldsymbol{\beta}\right] = p(\mathbf{x}_m | \boldsymbol{\beta}) = \frac{1}{1 + e^{-\mathbf{x}_m^T \boldsymbol{\beta}}}$$

- Notice that the prediction of each class is no longer a linear mapping of X; only in case of the latent variable
- In fact, the model is not linear in the predicted probabilities but rather in the so called log-**odds**'es

$$\text{odds}(\mathbf{x}) := \frac{p(\mathbf{x}|\boldsymbol{\beta})}{1 - p(\mathbf{x}|\boldsymbol{\beta})} = e^{-\mathbf{x}^T \boldsymbol{\beta}}$$

- This establishes the direct relation between standard linear and logistic regressions

Logistic Regression

- Due to the Bernoulli condition, under the assumption of independent samples the corresponding likelihood function is of the form

$$\mathcal{L}(\beta|\mathbf{X},\mathbf{y}) = \prod_{m=1}^{M} \mathbb{P}\left[y_m|\mathbf{x}_m,\beta\right] = \prod_{m=1}^{M} p(\mathbf{x}_m|\beta)^{y_m}(1-p(\mathbf{x}_m|\beta))^{1-y_m}$$

- Unlike in OLS regression the model **does not have a closed-form** (maximum likelihood) solution
- To formulate an equivalent loss minimization problem we define $L(\beta|\mathbf{X},\mathbf{y}) := -\log \mathcal{L}(\beta|\mathbf{X},\mathbf{y})$ leading to the **cross-entropy loss**

$$L(\beta|\mathbf{X},\mathbf{y}) = -\sum_{m=1}^{M} y_m \log(p(\mathbf{x}_m|\beta)) + (1-y_m)(1-p(\mathbf{x}_m|\beta)) \tag{8}$$

Logistic Regression

$$L(\beta|\mathbf{X},\mathbf{y}) = -\sum_{m=1}^{M} y_m \log(p(\mathbf{x}_m|\beta)) + (1-y_m)(1-p(\mathbf{x}_m|\beta)) \quad (9)$$

- There is **no closed-form** solution for the minimizer
- Iterative root searching methods can be applied to gather an estimate for the minimizer

$$\widehat{\beta} := \arg\min_{\beta} L(\beta|\mathbf{X},\mathbf{y})$$

- For instance: Newton's method, *(stochastic) gradient descent coming soon...*
- The gradient of the cross-entropy loss is equal to that of MSE

$$\nabla_{\beta} L(\beta|\mathbf{X},\mathbf{y}) = \mathbf{X}(\widehat{y} - y)$$

Other classification approaches

- clustering
- k-nearest neighbours
- isolation forests
- decision trees
- support vector machines (SVM)
- naive Bayes classifier
- ...

Non-linear theory: Artifical Neural Networks and Deep Neural Networks

From linear to non-linear mappings

- Linear models have the obvious defect of model capacity only spanning the space of linear mappings
- We wish to extend and represent non-linear functions of some vector input $\mathbf{x} \mapsto H(\mathbf{x})$
- Idea: apply a linear model to not $\mathbf{x}$ itself but rather to a non-linear, vector-valued transformation of it $\phi(\mathbf{x}|\theta) : \mathbb{R}^d \to \mathbb{R}^p$
- The resulting approximations of $H(\mathbf{x})$ read as

$$\Phi(\mathbf{x}|\Theta := (\theta, \mathbf{w})) = \varphi^T(\mathbf{x}|\theta)\mathbf{w},$$

with $\mathbf{w} \in \mathbb{R}^p$

Question

How do we choose the family of $\Phi(\mathbf{x}|\Theta)$?

The Single Layer Perceptron Model

- **Single Layer Perceptron (SLP)** is the simplest neural network model originally designed to solve the binary classification problem

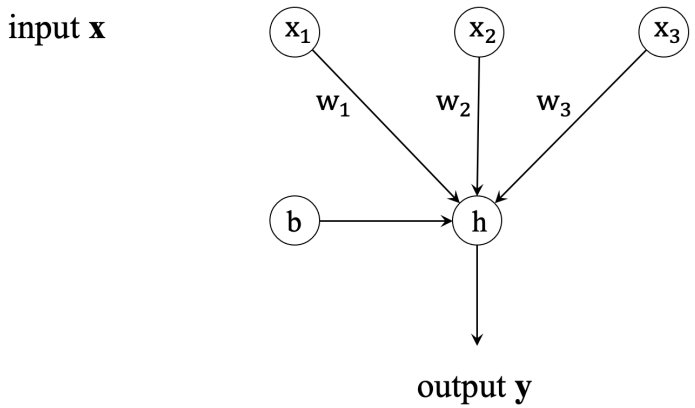


Figure: Illustration of an SLP

- Inputs (written as **x**) are passed through a weighted, directed graph.
- A function h corresponds to the non-linear mapping $\phi(\mathbf{x}|\theta)$ from above

The Single Layer Perceptron Model

- SLP has $d+1$ parameters: a d-dimensional vector of *weights* $\mathbf{w} \in \mathbb{R}^d$ connecting the node of h to each input feature; and a *bias* denoted by $b \in \mathbb{R}$
- The non-linearity $h_b : \mathbb{R} \to \{-1, 1\}$ is defined by the following step function with threshold b

$$h_b(z) := \begin{cases} 1, & z > b, \\ -1, & z \leq b, \end{cases} \tag{10}$$

  which can be interpreted as **true** or **false**
- The input of the non-linearity is a scalar defined by the inner product of the input vector $\mathbf{x} \in \mathbb{R}^d$ and the weights: $\mathbf{w}^T\mathbf{x}$
- Thus the mapping of SLP is given by the following *sequence of compositions*

$$\text{SLP}(\mathbf{x}|\boldsymbol{\theta} := (\mathbf{w}, b)) = \begin{cases} 1, & \mathbf{w}^T\mathbf{x} > b, \\ -1, & \mathbf{w}^T\mathbf{x} \leq b. \end{cases} \tag{11}$$

Training: Optimization Analytically

Question

How to find an **optimal** set of parameters properly assigning a binary classification label?

- For linearly separable data, an algorithm optimizes/trains the parameter vector $\boldsymbol{\theta} = (-b, \mathbf{w})$ such that the output of the perceptron corresponds to the correct class for all data entries in X.
- The algorithm starts by initializing a random parameter vector and a convergence test variable. It then picks a random sample from the data set and tests whether the sign of the weight vector assigns the correct label to the random sample.
- If an incorrect label is assigned, it updates the weight such that the argument of the sign function moves to the correct label.

Training: Optimization Analytically

- For notational convenience we attach the bias node to the input as a 0'th (constant) dimension $\mathbf{x}' = (1, \mathbf{x}) \in \mathbb{R}^{d+1}$, and assign it $w_0 = -b$ weight. These thresholds are equivalent

$$\boldsymbol{\theta}^T \mathbf{x}' \geq 0 \iff \mathbf{w}^T \mathbf{x} \geq b \implies h_0(\boldsymbol{\theta}^T \mathbf{x}') \equiv h_b(\mathbf{w}^T \mathbf{x}).$$

- Consider the case of a positive label in y and a negative prediction label, the weight is updated by adding the data $\mathbf{x}'$. To see why this works, consider:

$$h_0\left(\boldsymbol{\theta}^T \mathbf{x}'\right) = -1. \tag{12}$$

  Add $\mathbf{x}'$ to $\boldsymbol{\theta}$ and use the linearity of the inner product:

$$h_0\left((\boldsymbol{\theta} + \mathbf{x}')^T \mathbf{x}'\right) = h_0\left(\boldsymbol{\theta}^T \mathbf{x}' + \mathbf{x}'^T \mathbf{x}'\right) \tag{13}$$

- By definition, for the inner product we have $\mathbf{x}'^T \mathbf{x}' \geq 0$. Since $\mathbf{x}' \neq 0$ from (12), $\mathbf{x}'^T \mathbf{x} > 0$.
- Therefore the weight update improves the prediction

Perceptron Learning Algorithm for linearly separable data

- Let X be an $M \times (d+1)$ matrix with M measurements, d features and a column for the bias (all values equal 1), such that two classes in the set are linearly separable; let length M vector $\mathbf{y} \in \{-1, 1\}^M$ indicate the class of a data entry of X.
- Choose a random $\boldsymbol{\theta} \in \mathbb{R}^{d+1}$. Set $conv = 1$
- while $conv$ do
  Choose a random $r \in U(0, M)$
  Set $\mathbf{x}' = X(r, \cdot)$
  Set $y = \mathbf{y}(r)$
  Compute $\hat{y} = sign(\boldsymbol{\theta}^T \mathbf{x}')$
- if $y = 1$ and $\hat{y} = -1$ then
  Update $\boldsymbol{\theta} := \boldsymbol{\theta} + \mathbf{x}'$, endif
- if $y = -1$ and $\hat{y} = 1$ then
  Update $\boldsymbol{\theta} := \boldsymbol{\theta} - \mathbf{x}'$, endif
- Convergence test: $conv := 0$ if $h_0(X^T \mathbf{w}) = \mathbf{y}$
- end while

Summary

- After each random sample, a convergence test is done by comparing all the signs of the samples in the data set with their corresponding labels.
- If not all data entries are classified correctly, the algorithm starts over by picking a new random sample, otherwise the algorithm has successfully found a set of weights which classifies the data, and terminates.
- To speed up the training time, one might consider using different algorithms (training of perceptrons can be translated to solving an interior point problem).

Logistic regression as an SLP

- In the previous SLP example we specified a step function to model non-linear behavior
- If one replaces $h : \mathbb{R} \to \mathbb{R}$ with the CDF of the standard logistic distribution

$$\text{CDF}(\boldsymbol{\theta}^T \mathbf{x}') = \frac{1}{1 + e^{-\boldsymbol{\theta}^T \mathbf{x}'}},$$

  the resulting SLP scheme is equivalent to the logistic regression model
- The resulting equivalent SLP model can then be optimized in an identical fashion as in case of logistic regression: minimizing the cross-entropy loss with an iterative root searching algorithm

Multinomial Logistic regression

- One can easily extend the binary logistic regression to multinomial models of K outcomes $\{0, \ldots, K-1\}$
- This is done by running $K-1$ many binary classifications with a fixed outcome as pivot

$$\frac{\mathbb{P}\left[Y_m = 0\right]}{\mathbb{P}\left[Y_m = K-1\right]} = e^{-\boldsymbol{\beta}_1^T \mathbf{x}_m}, \quad \cdots \quad , \frac{\mathbb{P}\left[Y_m = K-2\right]}{\mathbb{P}\left[Y_m = K-1\right]} = e^{-\boldsymbol{\beta}_{K-1}^T \mathbf{x}_m},$$

  where $\boldsymbol{\beta}_k \in \mathbb{R}^d$
- The probabilities assigned to each class must sum up to 1:

$$\mathbb{P}\left[Y_m = K-1\right] = 1 - \sum_{k=0}^{K-2} \mathbb{P}\left[Y_m = k\right]$$

$$\implies \mathbb{P}\left[Y_m = K-1\right] = \frac{1}{1 + \sum_{k=0}^{K-2} e^{-\boldsymbol{\beta}_k^T \mathbf{x}_m}},$$

  where $\boldsymbol{\beta}_k \in \mathbb{R}^{d+1}$ is the coefficients corresponding to the k'th class

Multinomial Logistic regression

- The resulting multinomial logistic regression scheme assigns the following probabilities to class $k \leq K-2$

$$\mathbb{P}\left[Y_m = k|\boldsymbol{\theta}, \mathbf{x_m}\right] = \frac{e^{-\boldsymbol{\beta}_k^T \mathbf{x}_m}}{1 + \sum_{k=0}^{K-2} e^{-\boldsymbol{\beta}_k^T \mathbf{x}_m}} \tag{14}$$

- The set of parameters $\boldsymbol{\theta} \in \mathbb{R}^{K-1 \times d+1}$ becomes a matrix of *weights* defining the mapping to each outcome class
- For the Iris classification problem, the vector consists of three elements, where vector $(1, 0, 0)$ is assigned to Setosa, $(0, 1, 0)$ is assigned to the class Versicolor and $(0, 0, 1)$ to Virginica

Example: XOR problem

- Example that shows why an SLP may be insufficient for simple classification and gives rise more refined non-linear models
- Consider the XOR-problem (exclusive OR relation)
- In this problem the data is not linearly separable. We have input $\mathbf{x} \in \mathbb{R}^2$ and a class $y \in \{-1, 1\}$ as shown below.

x_1	x_2	y
-1	-1	1
-1	1	-1
1	-1	-1
1	1	1

- **Impossible to classify this using a Single Layer Perceptron**

Building blocks of neural networks

Composition of simple functions

- SLP is only capable of computing binary functions
- It nevertheless acts as a motivating *structure* for non-linear parametrizations
- Linear combinations of the input are passed to a non-linear function

Idea

Generalize this structure: build non-linear parametrizations as **hierarchical compositions** of non-linear and linear transformations $\rightarrow$ neural networks

Building blocks of composition: affine transformations

- *Recall: in OLS* $\widehat{y} = \boldsymbol{\beta}^T \mathbf{x}$ *where* $\boldsymbol{\beta} \in \mathbb{R}^{d+1}$ *is the parameter vector*
- In the context of neural networks, affine mappings of the form

$$\mathbb{R}^d \ni \mathbf{x} \mapsto \mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)} =: \mathbf{z}^{(1)} \in \mathbb{R}^{p_1} \tag{15}$$

  are called the **linear layers**, which map their input x to an affine combination with **weights** $\mathbf{W}^{(1)} \in \mathbb{R}^{p_1 \times d}$ and **biases** $\mathbf{b}^{(1)} \in \mathbb{R}^{p_1}$
- The total number of parameters is $\boldsymbol{\theta}^{(1)} = (\mathbf{W}^{(1)}, \mathbf{b}^{(1)}) \in \mathbb{R}^{p_1 \times (d+1)}$
- The length of $\mathbf{z}^{(1)}$ is called the **width** of the layer
- The components of $\mathbf{z}^{(1)}$ are called **neurons**
- The number of neurons in a hidden layer is a *hyperparameter*, the wider it is set, the more parameters there are

Building blocks of composition: hidden layers

- The machine learning community often confuses the terms *linear* and *affine*. This is due to the fact that the constant bias (similar as in OLS or SLP) can be viewed as an additional constant dimension with weight vector $\mathbf{b}$.
- So far this is identical to the model of (vector-valued) OLS with *cast*: $\widehat{y} \leftarrow \mathbf{z}^{(1)}$ and $\boldsymbol{\beta} \leftarrow \boldsymbol{\theta}^{(1)}$
- *Recall idea: apply a (non-)linear vector-valued mapping to the affine combinations of the input* $\mathbf{w}^T \boldsymbol{\phi}(\mathbf{z}^{(1)}|\boldsymbol{\theta}^{(1)})$

$$\mathbb{R}^{p_1} \ni \mathbf{z}^{(1)} \mapsto \left(\varphi_1^{(1)}(z_1^{(1)}), \ldots, \varphi_{p_1}^{(1)}(z_{p_1}^{(1)})\right) =: \mathbf{a}^{(1)} \in \mathbb{R}^{p_1},$$

  where $\varphi_i^{(1)} : \mathbb{R} \to \mathbb{R}$ are non-linear **activations**
- The composition of these transformations is called a **hidden layer** of a neural network

$$\mathbf{x} \mapsto \varphi_i^{(1)} \left(\sum_{j=1}^{d} W_{ij}^{(1)} x_j + b_i^{(1)}\right) =: a_i^{(1)}, \forall i = 1, \ldots, p_1 \quad (16)$$

Building blocks of composition: output layer

- In above, p is a *hyperparameter* which, similarly to OLS, can be interpreted as the number of *basis functions* $\{x_1, \ldots, x_d\}$ in a regression
- In order to approximate vector valued functions $H : \mathbb{R}^d \to \mathbb{R}^q$, one needs to transform the mapping of the hidden layer to the appropriate dimension of the *output*
- As before, we do this by an affine combination of the output with another set of *weights* and *biases*

$$\mathbb{R}^{p_1} \ni \mathbf{a}^{(1)} \mapsto \mathbf{W}^{(2)}\mathbf{a}^{(1)} + \mathbf{b}^{(2)} =: \mathbf{z}^{(2)} \in \mathbb{R}^q \tag{17}$$

with $\mathbf{W}^{(2)} \in \mathbb{R}^{q \times p_1}, \mathbf{b}^{(2)} \in \mathbb{R}^q$,
$\boldsymbol{\theta}^{(2)} := (\mathbf{W}^{(2)}, \mathbf{b}^{(2)}) \in \mathbb{R}^{q \times (p_1+1)}$

- Finally, in order to support the most general (bounded, binary, ...) output, the **output layer** is a composition

$$\mathbb{R}^{p_1} \ni \mathbf{a}^{(1)} \mapsto \left(\varphi_1^{(2)}(z_1^{(2)}), \ldots, \varphi_q^{(2)}(z_q^{(2)})\right) =: \mathbf{a}^{(2)} \in \mathbb{R}^q$$

(Fully-Connected) Feedforward Artificial Neural Networks

- A **fully-connected, feedforward artificial neural network** is simply a **hierarchical composition** of the transformations above, mapping an input $\mathbf{x} \in \mathbb{R}^d$ to the output $\mathbf{\Phi} \in \mathbb{R}^q$ whose i'th coordinate reads as follows

$$\Phi_i(\mathbf{x}|\mathbf{\Theta}) := \varphi_i^{(2)}\left(\sum_{j=1}^{p_1} W_{ij}^{(2)} \varphi_j^{(1)}\left(\sum_{k=1}^{d} W_{jk}^{(1)} x_k + b_j^{(1)}\right) + b_i^{(2)}\right) \tag{18}$$

where $\mathbf{\Theta} := (\boldsymbol{\theta}^{(1)}, \boldsymbol{\theta}^{(2)}) := (\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \mathbf{W}^{(2)}, \mathbf{b}^{(2)}) \in \mathbb{R}^{p_1 \times (d+1) + q \times (p_1+1)}$

- The total number of parameters in the statistical model is

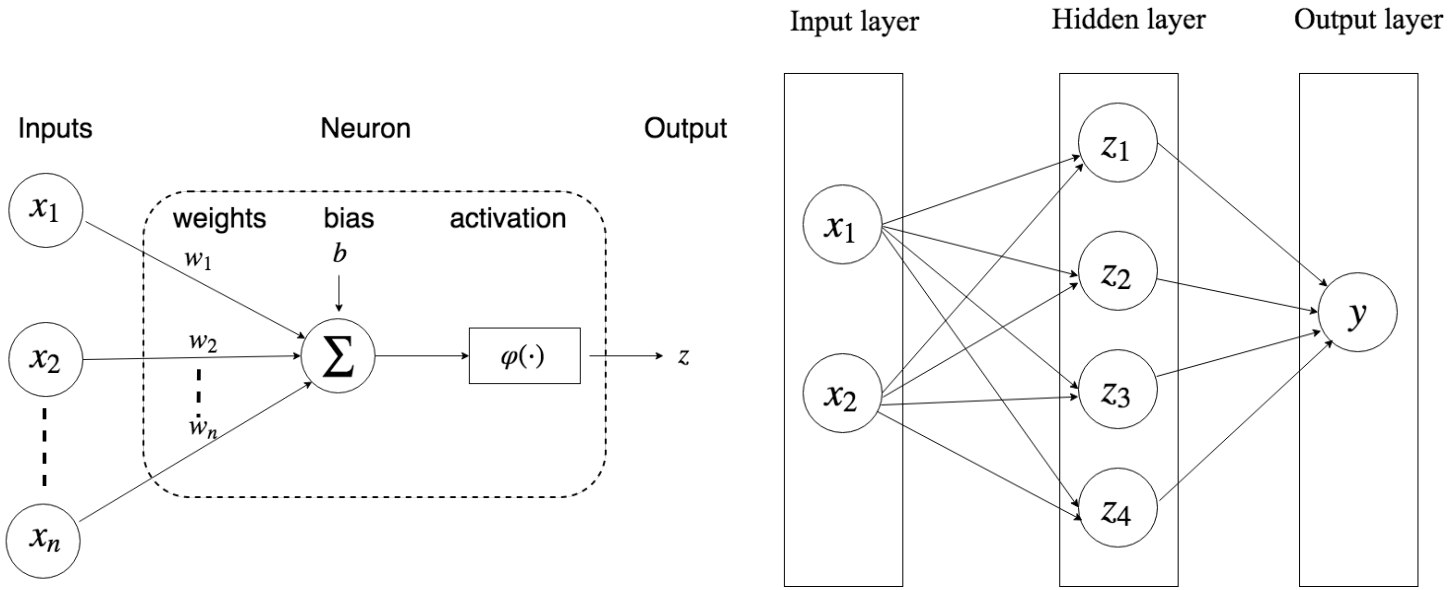
$$p = p_1 \times (d+1) + q \times (p_1 + 1) \tag{19}$$

(Fully-Connected) Feedforward Artificial Neural Networks

- Denoting the *element-wise* non-linearities by $\boldsymbol{\varphi}^{(n)}(\mathbf{z}^{(n)}) := (\varphi_1^{(n)}(z_1^{(n)}), \ldots, \varphi_{p_n}^{(n)}(z_{p_n}^{(n)})) \in \mathbb{R}^{p_n}$, in vector notation this can be written as follows

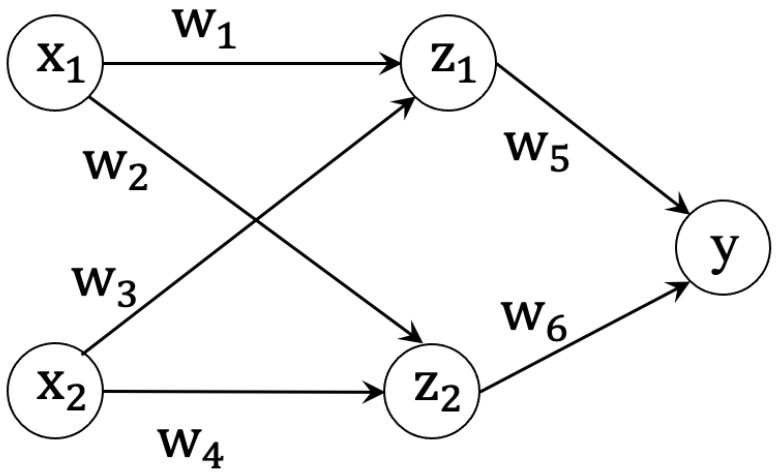
$$\Phi(\mathbf{x}|\boldsymbol{\Theta}) := \boldsymbol{\varphi}^{(2)} \circ \mathbf{z}^{(2)}(\cdot|\boldsymbol{\theta}^{(2)}) \circ \boldsymbol{\varphi}^{(1)} \circ \mathbf{z}^{(1)}(\mathbf{x}|\boldsymbol{\theta}^{(1)}) \qquad (20)$$

- FCFF ANNs can be thought of as **directed, acyclic graphs**



Example: XOR revisited

- Unlike with SLP, adding a *hidden layer*, and parametrizing with ANNs solves the problem



- x_1 and x_2 are first mapped to intermediate binary values $z_1 = h_{b_1}(w_1 x_1 + w_3 x_2)$ and $z_2 = h_{b_2}(w_2 x_1 + w_4 x_2)$

Example: XOR revisited

- Using $w_1 = -1, w_2 = 1, w_3 = 1, w_4 = -1$, the outputs are shown in columns z_1 and z_2. Passing this onto the non-linearities h_{b_1}, h_{b_2} with $b_1 = b_2 = 0$ results in activations a_1, a_2.

x_1	x_2	z_1	z_2	a_1	a_2	y
-1	-1	2	-2	1	-1	1
-1	1	0	0	-1	-1	-1
1	-1	0	0	-1	-1	-1
1	1	-2	2	-1	1	1

- It remains to compute $h_{b_3}(w_5 z_1 + w_6 z_2)$, by setting threshold $b_3 = -1$ and $w_5 = 1, w_6 = 1$ the desired output is obtained in y and the XOR-problem is solved.

Activations: the key feature of non-linearity

Activation Functions

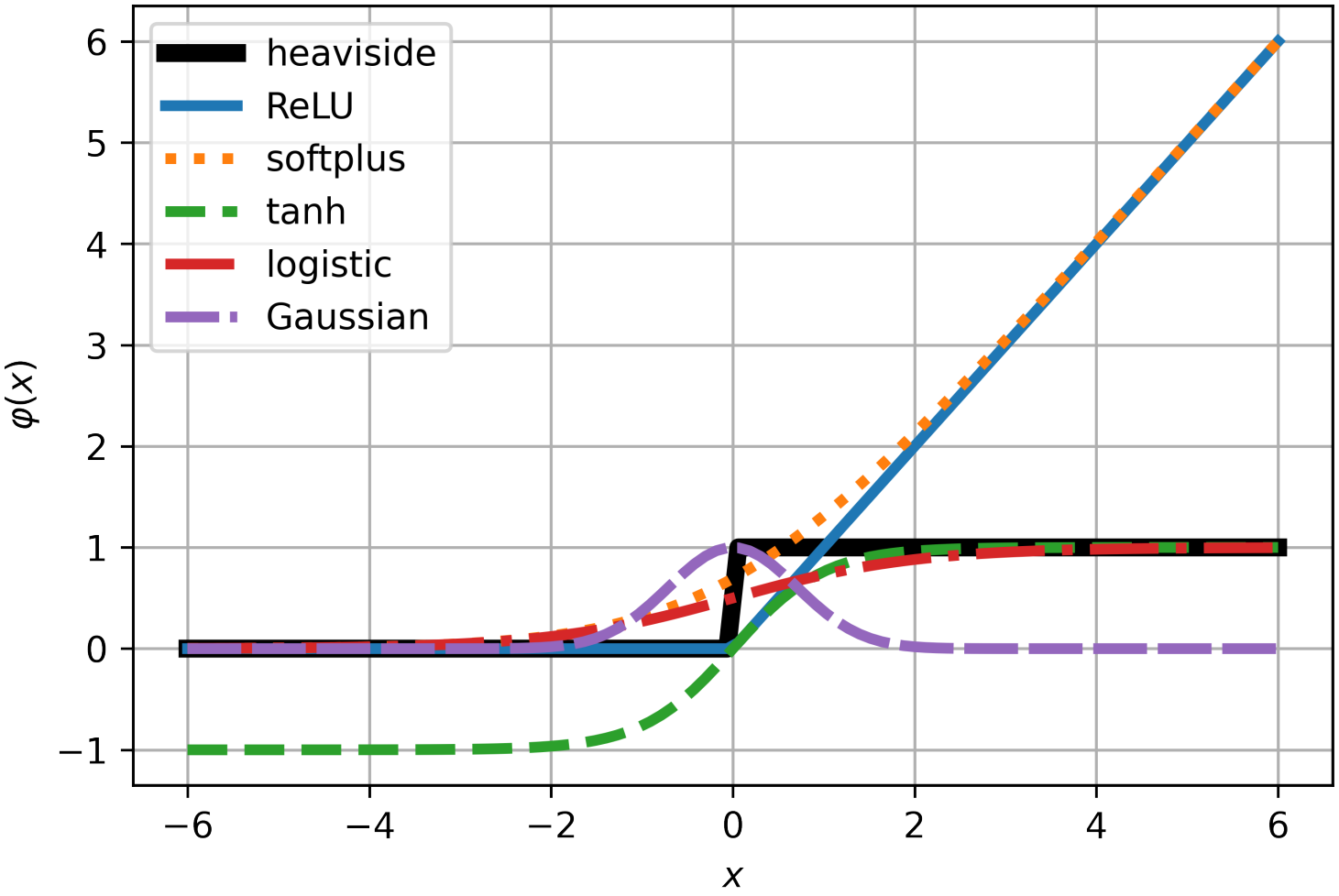
- The key component of *non-linearity* is given by the **activation functions** $\varphi_j^{(n)} : \mathbb{R} \to \mathbb{R}, j = 1, \ldots, p_n$
- For SLP we had $\varphi_1^{(1)}(x) = \text{sgn}(x)$
- Most often, application functions within the same layer are chosen the same $\varphi_1^{(n)}(x) = \cdots = \varphi_{p_n}^{(n)}(x)$
- In regression applications the output activations are usually chosen to be the identity function $\varphi^{(2)}(\mathbf{z}^{(2)}) = \mathbf{z}^{(2)}$
- The parametrization inherits **continuity** and **differentiability** properties from the chosen activations
- The non-linear activation functions are *hyperparameters* of the statistical model, appropriate choices vary depending on the problem

Activation Functions

name	$\varphi(x)$	$\varphi'(x)$	range	continuity
heaviside	$\begin{cases} 0, & x \leq 0 \\ 1, & x > 0 \end{cases}$	$\begin{cases} 0, & x \neq 0 \\ \text{undefined}, & x = 0 \end{cases}$	$\{0, 1\}$	C^{-1}
ReLU	$\begin{cases} 0, & x \leq 0 \\ x, & x > 0 \end{cases}$	$\begin{cases} 0, & x < 0 \\ x, & x > 0 \\ \text{undefined}, & x = 0 \end{cases}$	$[0, \infty)$	C^0
Gaussian	e^{-x^2}	$-2xe^{-x^2}$	$(0, 1]$	C^∞
tanh	$\frac{e^x - e^{-x}}{e^x + e^{-x}}$	$1 - \tanh^2(x)$	$(-1, 1)$	C^∞
logistic	$\frac{1}{1+e^{-x}}$	$\frac{e^{-x}}{1+e^{-x}}$	$(0, 1)$	C^∞
softplus	$\log(1 + e^x)$	$\frac{1}{1+e^{-x}}$	$(0, \infty)$	C^∞
...	...	...	...	...

See wiki

Activation Functions



Layer dependent activations

- For classification problems it is chosen such that $\sum_{k=1}^{q} \varphi_k^{(2)}(z_k^{(2)}) = 1$
- In order to ensure that output *probabilities* indeed sum to one, activations are chosen such that they are not a collection of scalar-valued mappings of neurons but vector-valued functions depending on the whole layer $\varphi^{(n)} : \mathbb{R}^{p_n} \to \mathbb{R}^{p_n}$

name	$\varphi_i(\mathbf{x})$	$\partial_j \varphi_i(\mathbf{x})$	range	cont.
softmax	$\frac{e^{x_i}}{\sum_{j=1}^{p_n} e^{x_j}}$	$\varphi_i(\mathbf{x})(\delta_{ij} - \varphi_j(\mathbf{x}))$	$(0, 1)$	C^∞
maxout	$\max_{i=1,\ldots,p_n} x_i$	$\begin{cases} 1, & j = \arg\max_i x_i \\ 0, & j \neq \arg\max_i x_i \end{cases}$	$(-\infty, \infty)$	C^0
...	...	...	...	...

Deep Neural Networks

Fully-Connected Feedforward Deep Neural Networks

- So far: neural network = input + hidden + output layer
- These are called **shallow** feedforward ANNs

$$\Phi(\mathbf{x}|\boldsymbol{\Theta}) := \boldsymbol{\varphi}^{(2)} \circ \mathbf{z}^{(2)}(\cdot|\boldsymbol{\theta}^{(2)}) \circ \boldsymbol{\varphi}^{(1)} \circ \mathbf{z}^{(1)}(\mathbf{x}|\boldsymbol{\theta}^{(1)})$$

- One can extend the model to allow for L-many hidden layers in the composition, with corresponding widths $p_l, l = 1 \ldots, L$
- The resulting, **deep neural network** mapping reads as follows

$$\Psi(\mathbf{x}|\boldsymbol{\Theta}) := \boldsymbol{\varphi}^{(L+1)} \circ \mathbf{z}^{(L+1)}(\cdot|\boldsymbol{\theta}^{(L+1)}) \circ \cdots \circ \boldsymbol{\varphi}^{(1)} \circ \mathbf{z}^{(1)}(\mathbf{x}|\boldsymbol{\theta}^{(1)}), \tag{21}$$

  where $\boldsymbol{\Theta} := (\boldsymbol{\theta}^{(1)}, \ldots, \boldsymbol{\theta}^{(L+1)}) \in \mathbb{R}^p$
- The total number of parameters in the statistical model rapidly increases

$$p = d \times (p_1 + 1) + \sum_{l=1}^{L-1} p_l \times (p_{l+1} + 1) + p_L \times (q + 1) \tag{22}$$

Fully-Connected Feedforward Deep Neural Networks

$$\Psi(\mathbf{x}|\boldsymbol{\Theta}) := \boldsymbol{\varphi}^{(L+1)} \circ \mathbf{z}^{(L+1)}(\cdot|\boldsymbol{\theta}^{(L+1)}) \circ \cdots \circ \boldsymbol{\varphi}^{(1)} \circ \mathbf{z}^{(1)}(\mathbf{x}|\boldsymbol{\theta}^{(1)}),$$

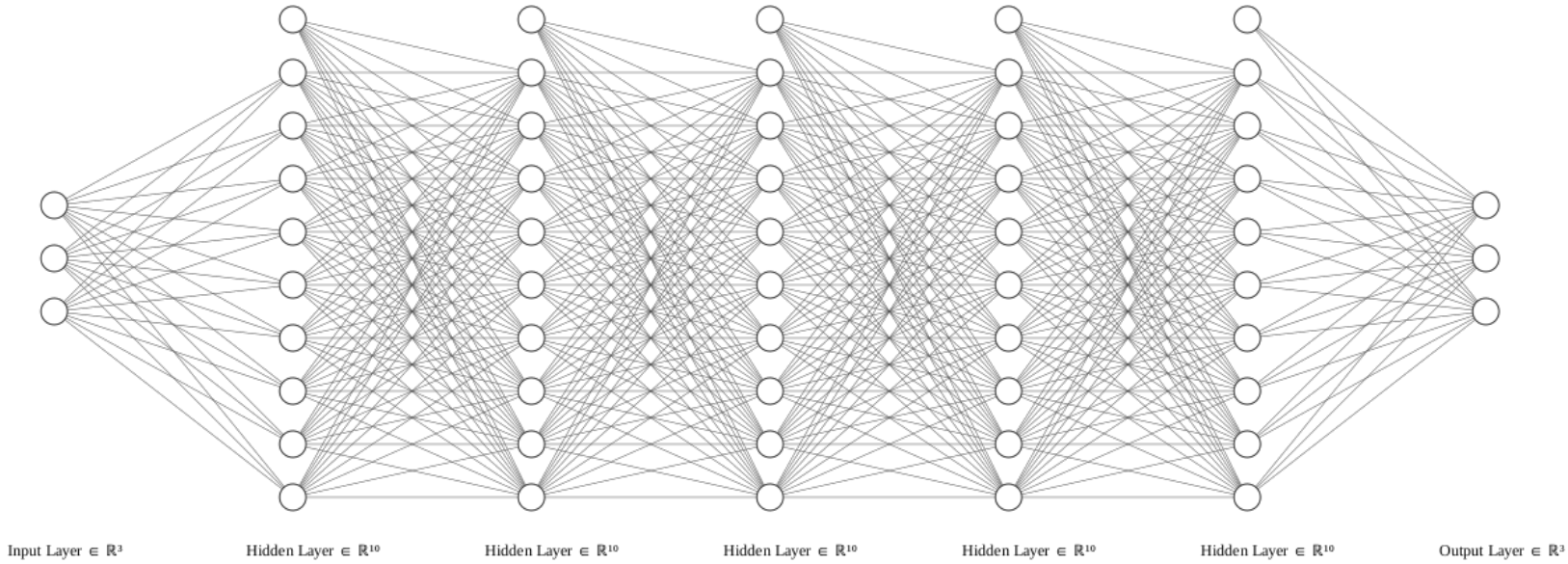


Figure: Illustration DNN, source: NN-SVG

$$p = d \times (p_1 + 1) + \sum_{l=1}^{L-1} p_l \times (p_{l+1} + 1) + p_L \times (q + 1)$$

Teaser: capacity and optimization

What we've seen so far

- We gathered **one potential** parametrization for non-linear problems via (deep) neural networks: $\mathbf{\Phi}(\mathbf{x}|\mathbf{\Theta}) : \mathbb{R}^d \to \mathbb{R}^q$
- Similarly to MSE in OLS, one can define a *performance measure* $L(\Theta|\mathbf{x})$ which quantifies the *"goodness"* of a certain parameter set, under measurements $\mathbf{x}$
- Such **losses** can be of various forms
  - $L(\Theta|\mathbf{x}) = \mathbb{E}\left[d(\mathbf{\Phi}(\mathbf{x}|\mathbf{\Theta}), H(\mathbf{x}))\right]$ (supervised learning)
  - $L(\Theta|\mathbf{x}) = \mathbb{E}\left[d(F(\mathbf{\Phi}(\mathbf{x}|\mathbf{\Theta})), 0)\right]$ (unsupervised learning)

  where d is a desired *distance function* – such as the ones induce by L^p norms $1 \leq p < \infty$

$$d(f, g) = \|f - g\|_p := \sqrt[p]{\int_{\mathbf{X}} |f(\mathbf{x}) - g(\mathbf{x})|^p \mathrm{d}\mu(\mathbf{x})}$$

Questions remaining

- DNNs provide a certain family of statistical models how do we know what problems are they also **appropriate** for?
- In order to find a *"good"* statistical model we want to minimize the loss function

$$\arg\min_{\theta} L(\theta|\mathbf{x}),$$

- Unlike in case of OLS, the MSE of supervised, neural network regression is no longer *convex* in $\mathbf{\Theta} \mapsto L(\mathbf{\Theta}|\mathbf{x}) \rightarrow$ no closed-form minimizer

Next week

1. **Universal Approximation Theorem (UAT)**: ANNs are *dense* in a very wide class of target functions $\mathcal{H}$
2. **Stochastic Gradient Descent (SGD)**: an empirically successful iterative optimization method