Inhaltsverzeichnis

Chapter 1: Introduction

Date: 03/05/2020

Lecturer:Bin Yang *By: Nicolas Hornek*

•p.4 expert talks are not relevant for the exam

- **scalar**: x, A, α
- column **vector**: $\underline{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix} = [x_i] \in \mathbb{R}^N$ with element $x_i = [\underline{x}]_i$
- **matrix**: $\mathbf{A} = [a_{ij}]_{1 \le i \le M, 1 \le j \le N} = [a_{ij}] \in \mathbb{R}^{M \times N}$ with element $a_{ij} = [\mathbf{A}]_{ij}$
- 3D, 4D **tensor**: $\mathbf{A} = [a_{ijk}], \mathbf{A} = [a_{ijkl}]$
- **transpose** of vector and matrix: $\underline{x}^T = [x_1, \ldots, x_N], \mathbf{A}^T = [a_{ji}]_{ij}$
- **determinant** of a square matrix $\mathbf{A}$: $|\mathbf{A}|$
- **inverse** of a square matrix $\mathbf{A}$: $\mathbf{A}^{-1}$
- **trace** of a square matrix $\mathbf{A}$: $\mathrm{tr}(\mathbf{A}) = \sum_i a_{ii}$

Abbildung 1.1: Mathematical notations

•Element notation (element of vector): $[x_i = \underline{a} + \underline{b}]_i$

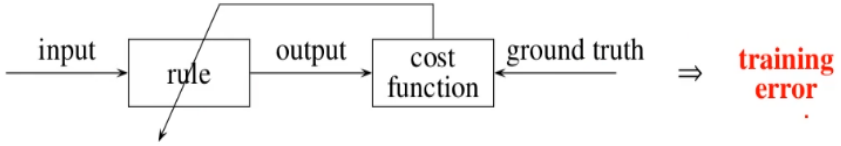
1.1. What is machine learning

•Signal processing is not a subset of ML or the other way around, they are identical in the task
•Basic difference is in how to design the processing rule
•Regression means to calculate (SP,ML) a continuous-valued output in the real numbers from a signal, can be one-dimensional
•Classification means to calculate (SP,ML) a discrete-valued output from the natural numbers
•p. 1-5 filter in the middle is the view of a pixel and its 8 neighbours

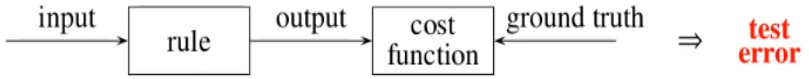
Three steps of machine learning (1)

Dataset $D = D_{\text{train}} \cup D_{\text{test}}$ | **training set** D_{train} | **test set** D_{test}

a) **Training** using **training data** from the training set D_{train}



b) **Test** or **evaluation** using **test data** from the test set D_{test}



c) Deployment on new data

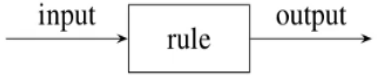


Abbildung 1.2: Three steps of machine learning

•over-fitting just memorizes the training set so test set is needed
•testerrorrate is similar to training error rate → no over-fitting
•Test set and training set need to be disjuct concatenated
•TODO: Summary supervised learning and unsupervised learning

1.2. What is deep learning?

•feature extraction: a feature is a clustered subset of information for recognition
•fish example: fish length, color etc.
•Needs human experience, can't be calculated
•DNN solves the problem without feature extraction

1.2.1. What is a neural network (NN)

•Cascaded pipeline of layers

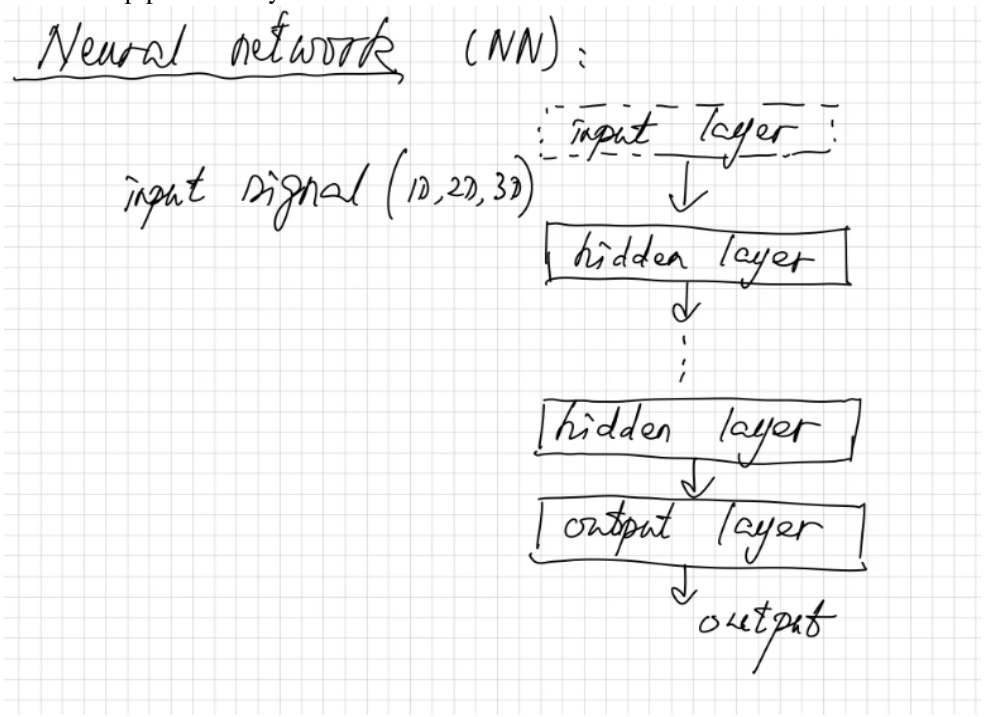


Abbildung 1.3: Neural Network

1.3. Examples for Deep Learning

•Semantic image segmentation is pixelwise classification

Chapter 2: Tools for Deep Learning

Date: 02/05/2020

Lecturer:Bin Yang *By: Nicolas Hornek*

2.1. Software

2.2. Hardware

2.3. Datasets

•Overview for Training Datasets up to ImageNet they are for teaching

Chapter 3: Machine learning basics

Date: 02/05/2020

Lecturer:Bin Yang *By: Nicolas Hornek*

3.1. Linear Algebra

•TODO get Math nicely into the Context book

Vector norms

Given a vector $\underline{x} = [x_i] \in \mathbb{R}^M$. There are different definitions for the vector norm:

- **2-norm** or l_2**-norm** or **Euclidean norm**: $\|\underline{x}\|_2 = \sqrt{\sum_{i=1}^{M} x_i^2} = \sqrt{\underline{x}^T \underline{x}}$
- **1-norm** or l_1**-norm**: $\|\underline{x}\|_1 = \sum_{i=1}^{M} |x_i|$
- **0-norm** or l_0**-norm**: $\|\underline{x}\|_0 =$ number of non-zero elements in $\underline{x}$

Comments:

- $\|\underline{x}\|_2^2$ represents the energy of $\underline{x}$.
- $\|\underline{x}\|_0$ measures the sparsity of $\underline{x}$.
- Different vector norms have different unit-norm contour lines $\{\underline{x} \mid \|\underline{x}\|_p = 1\}$.

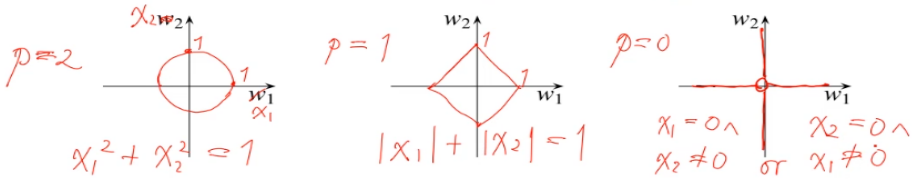


Abbildung 3.1: Vector Normes

3.2. Random variable and probability distribution

3.2.1. One random vector

- **scalar**: x, A, α
- column **vector**: $\underline{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix} = [x_i] \in \mathbb{R}^N$ with element $x_i = [\underline{x}]_i$
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Abbildung 3.2: One random vector

PDF for a discrete-valued RV:
$p(\underline{x}) = \sum_i p_i \delta(\underline{x} - \underline{x}_i,)$ $\delta(\underline{x} :)$ Dirac function
cumulative distribution function CCDF
$F(\underline{x}) = \int_{-\infty}^{\infty} p(\underline{z}) d\underline{z}, \quad p(\underline{x}) = \frac{\partial^d F(\underline{x})}{\partial x_i \ldots \partial x_d}$

- **scalar**: x, A, α
- column **vector**: $\underline{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix} = [x_i] \in \mathbb{R}^N$ with element $x_i = [\underline{x}]_i$
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Abbildung 3.3: Moments of a vector

special case d = 1: $\underline{X} \to X \in \mathbb{R}$
$\mu \to \mu \in \mathbb{R}$
$\underline{\underline{C}} \to$ variance of $X = Var(X) = \delta^2 = E[(X - \mu)^2] = ... = E(X^2) - \mu^2$
$\delta = \sqrt{Var(X)}$: standard deviation
For any function $g(\underline{X})$ of $\underline{X}$: $E[g(\underline{x})] = \int g(x) \cdot p(\underline{x}) d\underline{x} = (d.v.) \sum_i g(\underline{x}_i \cdot P(\underline{x}_i))$

Multivariate normal (Gaussian) distribution

PDF

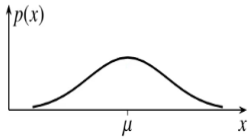
$$\underline{X} \in \mathbb{R}^d \sim N(\underline{\mu}, \mathbf{C})$$

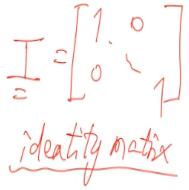
$$p(\underline{x}) = \frac{1}{(2\pi)^{d/2}|\mathbf{C}|^{1/2}} e^{-\frac{1}{2}(\underline{x}-\underline{\mu})^T \mathbf{C}^{-1}(\underline{x}-\underline{\mu})}$$

$$\ln(p(\underline{x})) = -\frac{d}{2}\ln(2\pi) - \frac{1}{2}\ln(|\mathbf{C}|) - \frac{1}{2}(\underline{x}-\underline{\mu})^T \mathbf{C}^{-1}(\underline{x}-\underline{\mu})$$

$N(\underline{0}, \mathbf{I})$ is called the **standard normal distribution**.

1D-Visualization





Moments

$$E(\underline{X}) = \underline{\mu}, \quad Cov(\underline{X}) = \mathbf{C}$$

Abbildung 3.4: Multivariate normal (Gaussian) distribution

one-hot coding : Only one bit is 1 e.g. 0100 one cold coding is the inverse
Coding for class label, random vector y of length c so the identity matrix with dimension c is used for class labels
Reformulation of the PMF (categorical distribution) by one-hot coding of the classes $\underline{x} = [x_i] \in \{\underline{e}_1, \underline{e}_2, .., \underline{e}_c\}$, i.e. all $x_i = 0$ except for one single element equal to 1

PMF: $P(\underline{X} = \underline{x}) = P(\underline{x}) = \begin{cases} P_i \text{ if } \underline{x} = \underline{e}_1 \text{ or } x_1 = 1 \\ \ldots \\ P_c \text{ if } \underline{x} = \underline{e}_c \text{ or } x_c = 1 \end{cases} = {p_1}^{x_1} \cdot {p_2}^{x_2} \cdot, \ldots \cdot {p_c}^{x_c} = \prod_{i=1}^{c} p_i^{x_i}$

$$ln(P(\underline{x}) = sum_{i=1}^{c} x_i \cdot ln(p_i) = [x_i, ..., x_c] \cdot \begin{bmatrix} ln(P_i) \\ ... \\ ln(P_c) \end{bmatrix} = \underline{x}^T \cdot ln(\underline{P})$$

ln function applied element wise

3.2.2. Multiple random vectors

•3-16 Table for distributions
•product rule for probability $p(\underline{x}, \underline{y}) = p(\underline{x}) \cdot p(\underline{y})$
•Bayes rule $p(\underline{y}|\underline{x}) = p(\underline{y}|\underline{x}) \cdot) \frac{p(\underline{x}}{p(\underline{y}}$
•Independent and identically distributed
$\underline{x}$ and $\underline{y}$ are independent if:
$p(\underline{x}, \underline{y}) = p(\underline{x}) \cdot p(\underline{y}) \leftrightarrow p(\underline{x}|\underline{y})$ or $p(\underline{x}|\underline{y}) = p(\underline{y})$

$\underline{x}_1, ..., \underline{x}_N$ are independent and identically distributed (i.i.d)
$P(\underline{x}_1, ..., \underline{x}_N) = \prod_{i=1}^{N} p_i(\underline{x}_i), \underline{X}_i \sim p_i(\underline{x}_i)$
$p_i(\underline{x}_i) = p(\underline{x}_i) \rightarrow p(\underline{x}_1, ..., \underline{x}_N) = \prod_{i=1}^{N} p(\underline{x}_i)$

3.2.3. Kernel based density estimation

PDF: $p(\underline{x})$ of $\underline{X} \in \mathbb{R}^d$ unknown , only i.i.d samples $\underline{x}(n), 1 \leq n \leq N$
kernel-based estimate $\hat{p}(\underline{x}) of p(\underline{x})$ from $\underline{x}(n)$
kernel function $k(\underline{x})$, like a PDF
1. $k(\underline{x}) \geq 0 \forall \underline{x}$
2. $\int k(\underline{x}) d\underline{x} = 1$
$\hat{p}(\underline{x}) = \frac{1}{N} \sum_{n=1}^{N} k(\underline{x} - \underline{x}(n))$

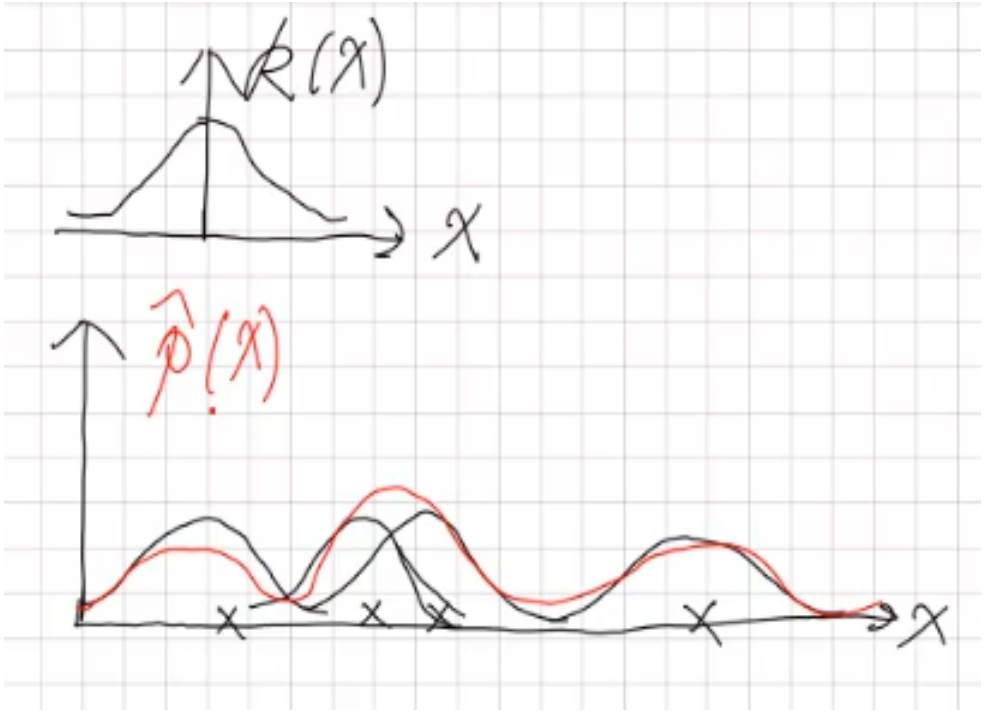


Abbildung 3.5: Kernel function

Smooth Gaussian Kernel:
$N(\underline{0}, \underline{I}) : k(\underline{x}) = \frac{1}{2\pi^{\frac{d}{2}}} \cdot e^{-\frac{1}{2}||\underline{x}||^2}$

Dirac Kernel
$k(\underline{x}) = \delta(\underline{x})$: Dirac function
$\delta(\underline{x}) = \begin{cases} \infty, \underline{x} = \underline{0} \\ 0, \underline{x} \neq \underline{0} \end{cases}$
$\int \delta(\underline{x}) d\underline{x} = 1$
sampling property : $\int \delta(\underline{x} - \underline{x}_0 f(\underline{x}) d\underline{x}) = f(\underline{x}_0)$
empirical distribution
$\hat{p}(\underline{x}) \cdot \frac{1}{N} \sum_{n=1}^{N} \delta(\underline{x} - \underline{x}(n))$

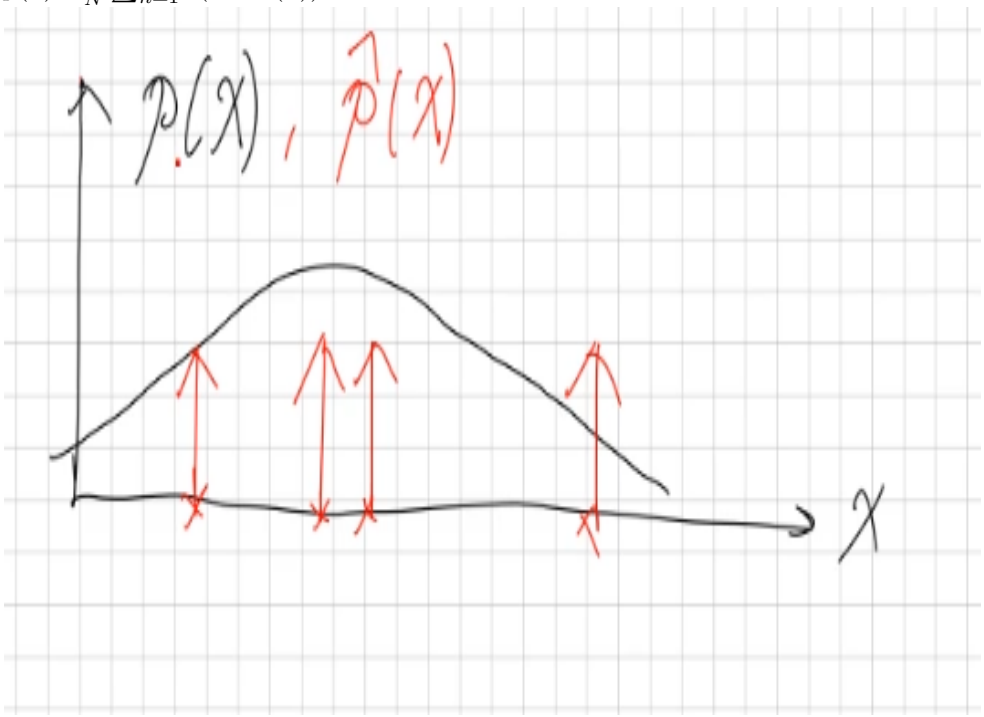
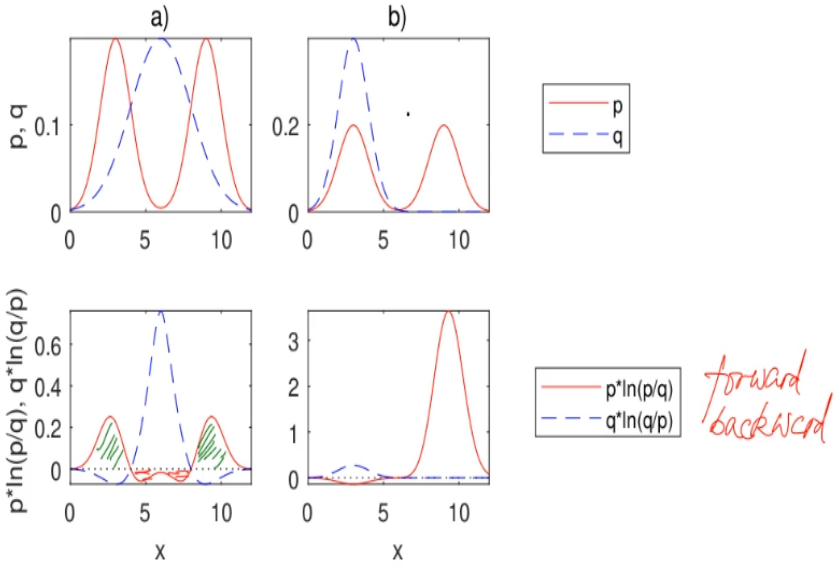


Abbildung 3.6: Estimated PDF function

3.3. Kullback-Leibler divergence and cross entropy

Dissimilarity measure between 2 distributions:
Case A: continuous-valued random variables: PDF
$\underline{X} \sim p(\underline{x})$: true statistical distribution of $\underline{X}$
$q(\underline{x})$: approximation for $p(\underline{x})$, e.g. by DNN
KL divergence (KLD) between p and q:
$D_{KL}(p||q) = \int p(\underline{x}) \cdot ln(\frac{p(\underline{x})}{q(\underline{x})}) d\underline{x}$

$= E_{\underline{X}\sim p}[ln(\frac{p(\underline{X})}{q(\underline{X})})]$
expectation over $p(\underline{x})$
DKL is real valued scalar positive or negative or 0
Case B: discrete-valued random vector: PMF
$\underline{X} \in \{\underline{x}_1, ...\underline{x}_c\}$ $\sim$: true PMF of $\underline{X} \sim Q(\underline{x})$: approximation for $P(\underline{x})$
$D_{KL}(P||Q) = \sum_{i=1}^{c} P(\underline{x}_i) \cdot ln(\frac{P(\underline{x})}{Q(\underline{x})}) = E_{\underline{X}\sim P}[ln(\frac{P(\underline{x})}{Q(\underline{x})})]$
Properties of the KL divergence: P1) Nonnegative $D_{KL}(P||Q) \geq 0 \forall p, q$
P2) Eguality $D_{KL}(P||Q) = 0$ iff(if and only if) $p(\underline{x}) = q(\underline{x})$
proof for ßufficient": $ln(\frac{p(\underline{x})}{q(\underline{x})}) = 0 \forall \underline{x}$
P1 and P2: $D_{KL}(p||1)$ is a suitable metric for approximation p by q
P3 Asymmetry
$D_{KL}(p||q) = E_{\underline{X}\sim p} = ln(\frac{p(\underline{x})}{q(\underline{x})}) \neq D_{KL}(q||p) = E_{\underline{X}\sim q} = ln(\frac{q(\underline{x})}{p(\underline{x})})$
forward KLD backward KLD
D_{KL} is not a true distance measure with $D(\underline{x}, \underline{y}) = D(\underline{y}, \underline{x})$



- When minimizing $D_{\mathrm{KL}}(p\|q)$, a) is better than b) because $q(x)$ is broad.
- When minimizing $D_{\mathrm{KL}}(q\|p)$, b) is better than a) because $q(x)$ is narrow.

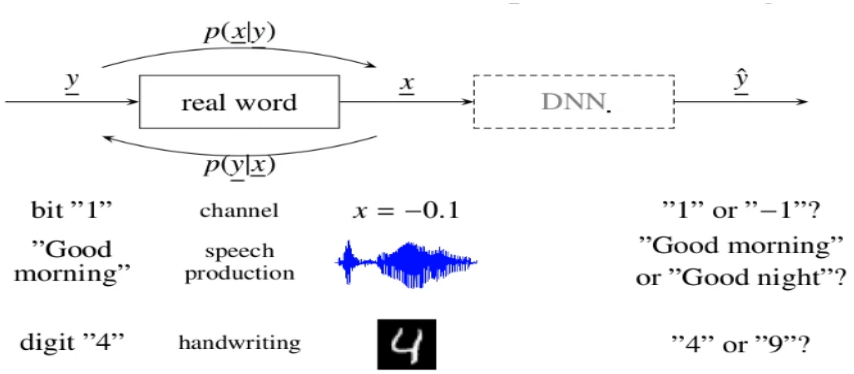
Abbildung 3.7: Forward vs. Backward KL divergence

3.3.1. E3.5 KLD between normal and Laplace distribution

$p(x) =\sim N(0, \sigma^2), p(x) = \frac{1}{\sqrt{2\pi}\sigma} \cdot e^{-\frac{x^2}{2\sigma^2}}$
$q(x) \sim$ Laplace: $(0, b) q(x) = \frac{1}{2b} e^{-\frac{|x|}{b}}$
Task: choose b to best approximate p by q.
$\frac{p(x)}{q(x)} = \sqrt{\frac{2}{\pi}} \cdot \frac{b}{\sigma} cdotexp(-\frac{x^2}{2\sigma^2} + \frac{|x|}{b})$
$D_{KL}(p||q) = E_{\underline{X}\ simp} = ln(\frac{p(\underline{x})}{q(\underline{x})}) = ln(\sqrt{\frac{2}{\pi}} \cdot \frac{b}{\sigma}) + E_{X\sim p}((-\frac{x^2}{2\sigma^2} + \frac{|x|}{b}))$
$E_{\underline{X}\ simp} = \sigma^2$
$E_{\underline{X}\ simp}(|x|) = \int_{-\infty}^{\infty} |x| \cdot \frac{1}{\sqrt{2\pi}\sigma} exp(-\frac{x^2}{2\sigma^2}) dx = 2 \int_0^{\infty} | \cdot \frac{1}{\sqrt{2\pi}\sigma} exp(-\frac{x^2}{2\sigma^2}) dx = \sqrt{\frac{2}{\pi}} \cdot \sigma$
Let $\alpha = \frac{\sigma}{b}, D_{KL}(p||q) = ... = \sqrt{\frac{2}{\pi}} \cdot \alpha - ln(\alpha) + ln(\sqrt{\frac{2}{\pi}}) - \frac{1}{2} \frac{dD_{KL}(p||q)}{d\alpha} = \sqrt{\frac{2}{\pi}} - \frac{1}{\alpha} =$
$0 \rightarrow \alpha = \sqrt{\frac{2}{\pi}}$, i.e. $b \approx 0,86$
$D_{KL,min}(p||q) = D_{KL}(p||q)|\alpha = \sqrt{\frac{2}{\pi}} = .. = \frac{1}{2} - ln(\frac{\pi}{2}) \approx 0,048$
•Probable exam question calculate this for 2 distributions
P4) Additive :
$\underline{X}) = (\underline{x}_1, \underline{x}_2), \underline{x}_1$ and $\underline{x}_2$ are independent, $i.e.$
$p(\underline{x})?p_1(\underline{x}_1) \cdot p_2(\underline{x}_2), q(\underline{x})?q_1(\underline{x}_1) \cdot q_2(\underline{x}_2)$
Then: $D_{KL}(p||q) = D_{KL}(p_1||q_1) + D_{KL}(p_2||q_2)$
P5) Relation to cross entropy :
Definiton of entropy 3-24 probability always greater than 0 but smaller than 1
$D_{KL}(p||q) = \int pln(\frac{p}{q}) d\underline{x} = \int pln(p) dx - \int pln(q) dx = -H(p) + H(p, q)$ or
cross entropy: $H(p, q) = D_{KL}(p||q) + H(p) \geq H(p) \geq 0$
For a given (fixed) $p(\underline{x})$: $H(p)$ fixed
Hence: min $D_{KL}(p||q) \leftrightarrow minH(p, q)$
Not the case for backward KLD $D_{KL}(q||p)$!
Minimizing is not the same anymore because then it is $H(q)$ and thats what we are trying to optimize

3.4. Probabilistic framework for machine learning

valid for both SP and ML
valid for both regression problem and classicication problem



- $\underline{y}$: **latent variable**, hidden, not directly measurable, quantity of interest
- $\underline{x}$: **observed variable**, measurement, input for DNN
- $\hat{\underline{y}}$: output of DNN as estimate for $\underline{y}$
- real world: describes how is $\underline{x}$ generated from $\underline{y}$
- DNN: describes how to estimate $\underline{y}$ from $\underline{x}$

Abbildung 3.8: Probabilistic framework of supervised learning

Both $\underline{y}$ and $\underline{x}$ are modeled as random variables. They are described by the joint **data generating distribution**

$$p(\underline{x}, \underline{y}) = p(\underline{x}|\underline{y})p(\underline{y}) = p(\underline{y}|\underline{x})p(\underline{x}).$$

$p(\underline{y})$ prior PDF of $\underline{y}$ or **prior**, available before any measurement of $\underline{x}$

$p(\underline{x}|\underline{y})$ **likelihood**. It describes the real word, the generation of $\underline{x}$ from $\underline{y}$. It is a kind of channel-sensor model, e.g.

- bit: communication channel + receiver
- speech: speech production system + microphone
- digit: handwriting + camera

$p(\underline{x})$ prior PDF of $\underline{x}$, also called **evidence**

$p(\underline{y}|\underline{x})$ posterior PDF of $\underline{y}$ after a measurement $\underline{x}$ or **posterior**

Abbildung 3.9: The data generating distribution

Bayes Rule:

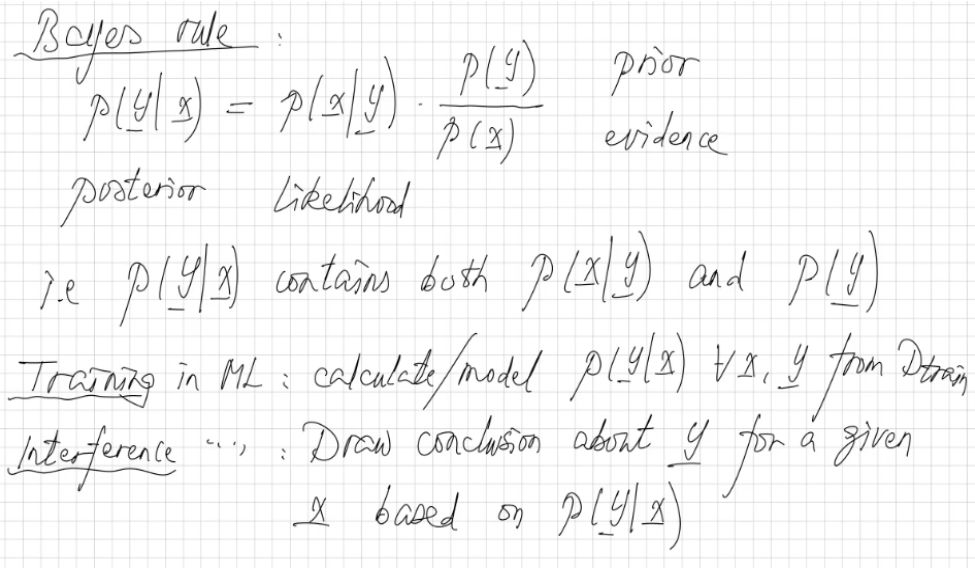


Abbildung 3.10: Bayes Rule in DL

a) **Maximum a posterior (MAP)** inference:

$$\max_{\underline{y}} p(\underline{y}|\underline{x}) = p(\underline{x}|\underline{y})\frac{p(\underline{y})}{p(\underline{x})}$$

b) **Minimum Bayesian risk (MBR)** inference:

$$\min_{\hat{\underline{y}}} \mathrm{E}_{\underline{X},\underline{Y}}[l(\underline{Y}, \hat{\underline{y}}(\underline{X}))] = \int l(\underline{y}, \hat{\underline{y}}(\underline{x}))p(\underline{x}, \underline{y})\mathrm{d}\underline{x}\mathrm{d}\underline{y}$$

see course DPR and SASP for more details.

Abbildung 3.11: Bayes decision theorem

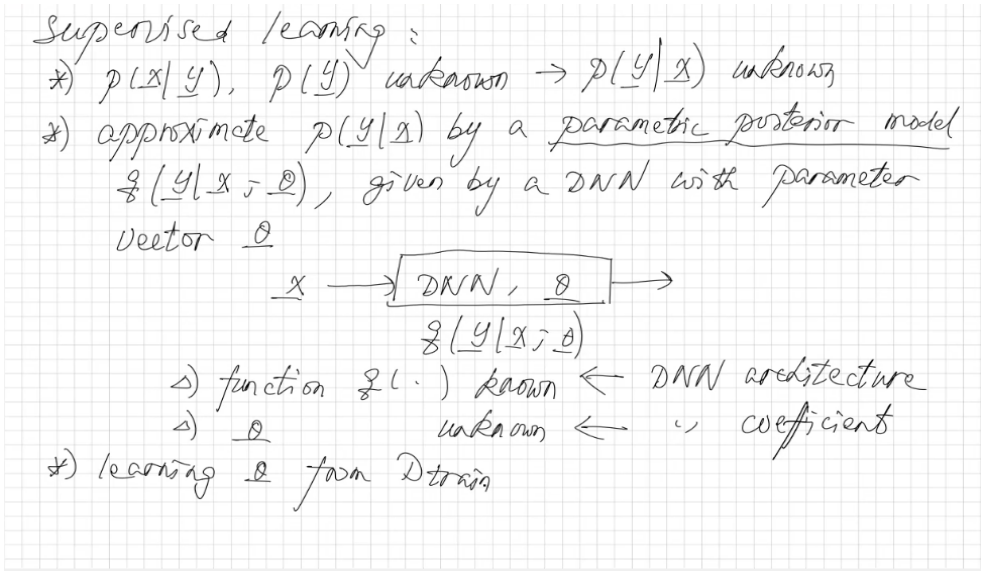


Abbildung 3.12: Supervised learning

Learning Criterion:

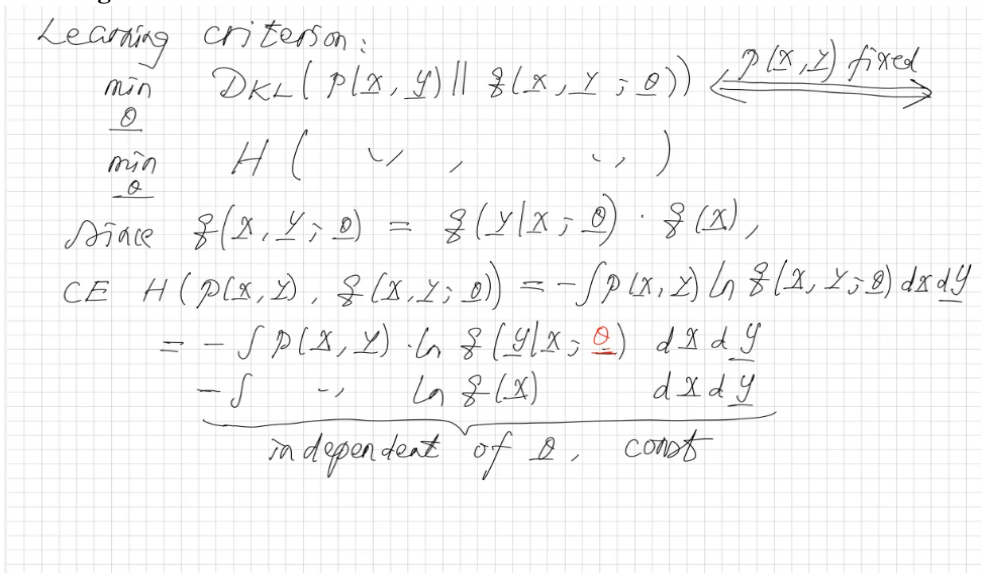


Abbildung 3.13: Calc part1

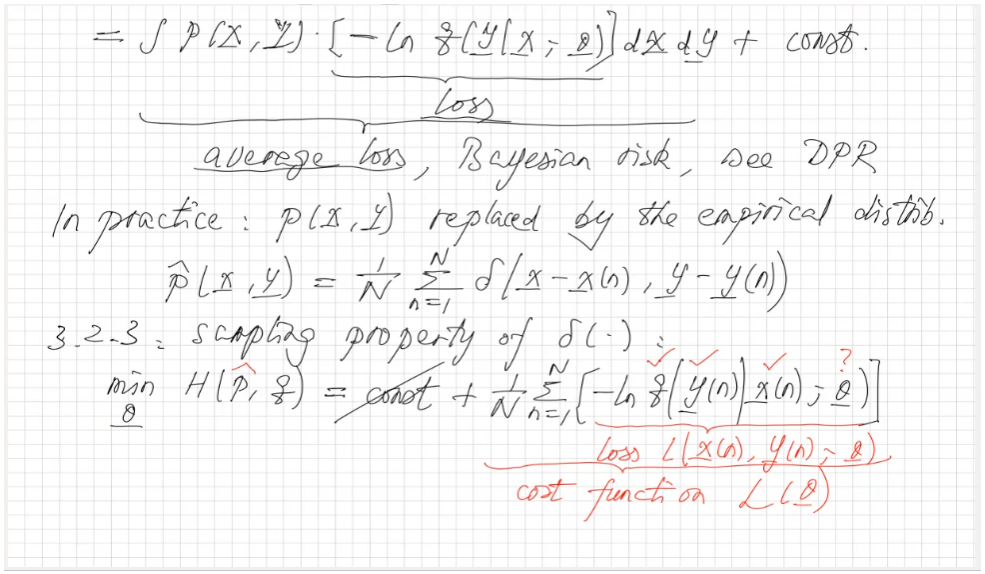


Abbildung 3.14: Calc part2

3.4.1. Role of a NN

1. approximate true posterior $p(\underline{y}|\underline{x})$ by $q(\underline{y}|\underline{x};\Theta)$
2. learn $\underline{\Theta}$ from D_{train}

Chapter 4: Dense Neural Networks

Date: 05/05/2020

Lecturer:Bin Yang *By: Nicolas Hornek*

A general model for $q(\underline{y}|\underline{x};\Theta)$
*) can learn any linear or nonlinear mapping
*) suitable for both regression and classification problems
artificial NN: mimic biological NN (brain)

4.1. Fully connected neural networks - Neuron

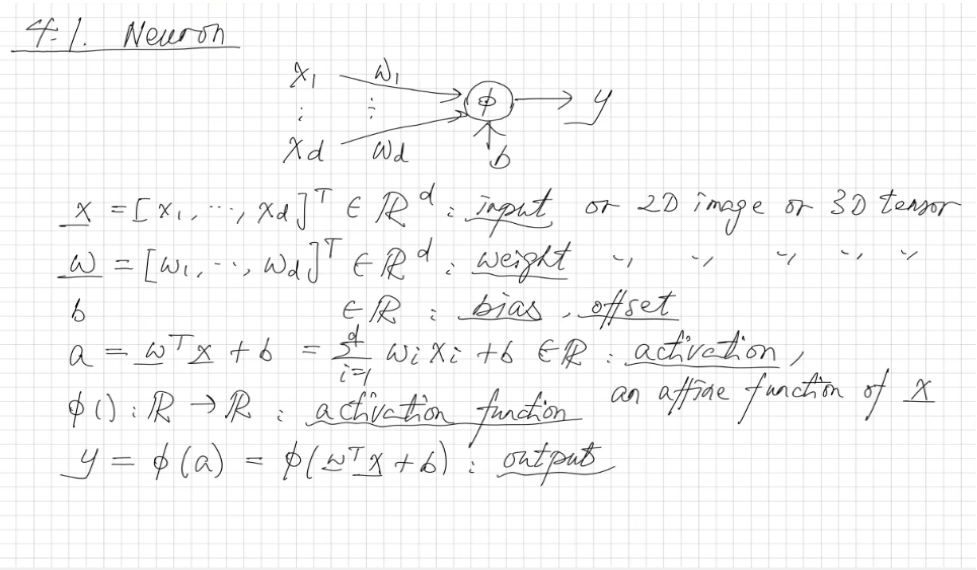


Abbildung 4.1: Neuron

4.2. Chapter 4.2 Layer of Nurons

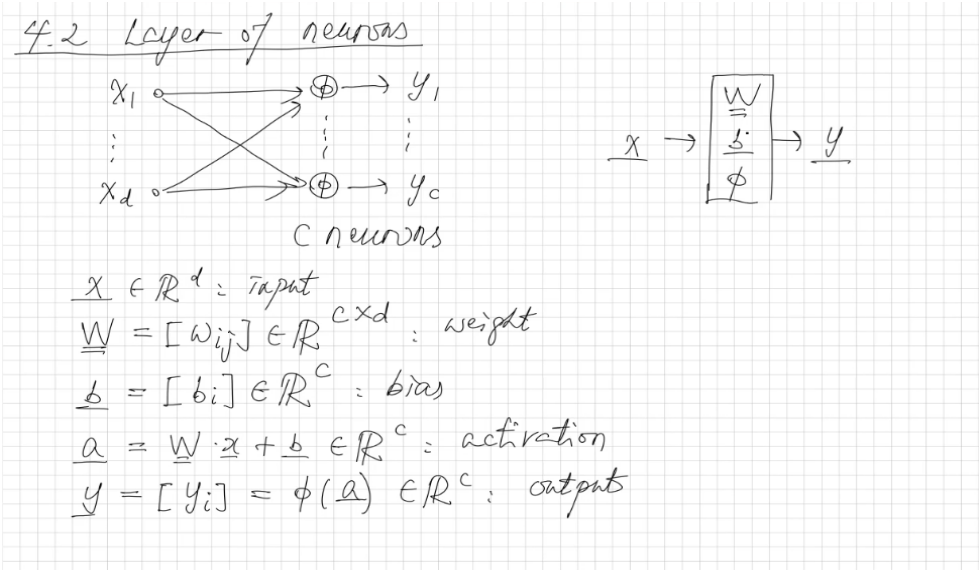


Abbildung 4.2: Layer of Neurons

2 meanings of $\phi()$:

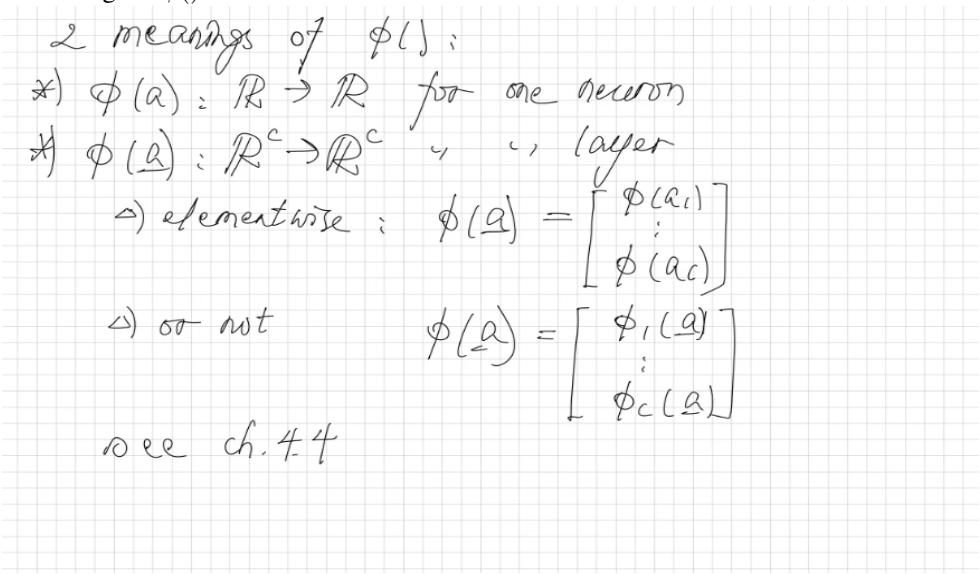


Abbildung 4.3: Meanings of phi

Comments :
•no interconnections between neurons in the same layer
•dense layer, fully connected layer: •each input x_j connected to each neuron i
$\rightarrow c \cdot d$ weights and w_{ij} an c biases b_i , $1 \leq i \leq c, 1 \leq j \leq d$,
$\rightarrow c \cdot (d+1)$ parameters

4.3. Feedforward neural network

A cascade of dense layers
Layer $1 \leq l \leq L$:
$M_l - 1$ number of the input neurons

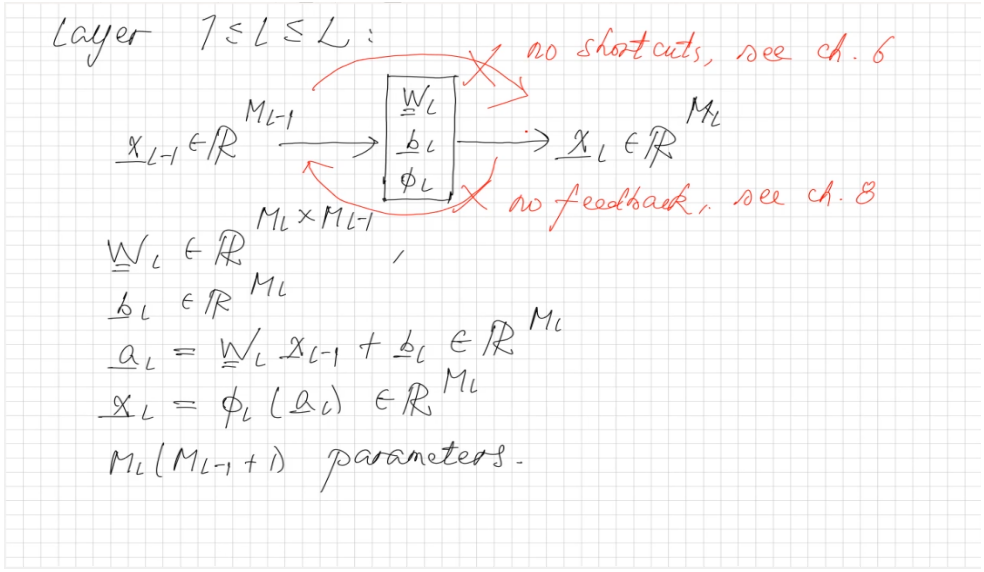


Abbildung 4.4: Feedforward multilayer neural network

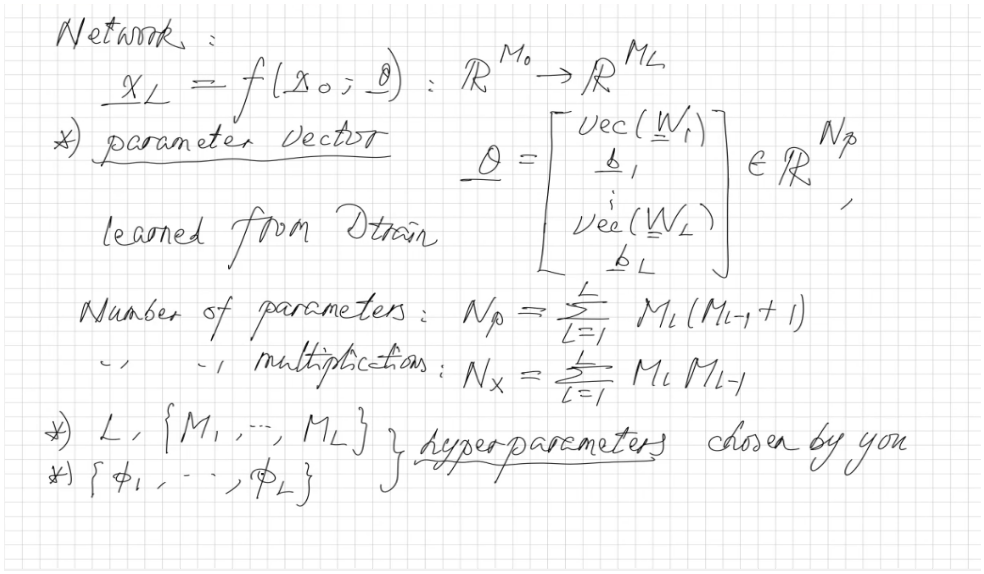


Abbildung 4.5: Network Parameters

4.4. Activation function

Mild requirements on $\phi()$:
•nonlinear in general $\rightarrow$ fundamental
•smooth, differentiable $\rightarrow$ for training
•simple calculation $\rightarrow$ low complexity
•Slides 4-6; 4-7 activation function types

4.4.1. Sigmoid activation function

$$\phi(a) = \sigma(a) = \frac{1}{1 + e^{-a}}$$

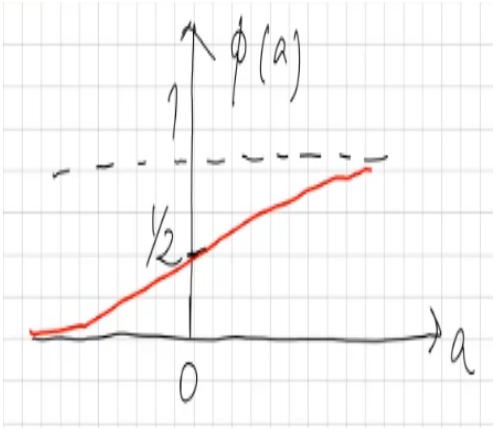


Abbildung 4.6: Sigmoid function

•$0 < \phi < 1 \hat{=}$ prob.
•symmetry: $\phi(-a) = 1 - \phi(a)$
•derivative: $\frac{d\phi(a)}{da} = ... = \frac{e^{-a}}{(1 + e^{-a})^2} = \phi(a) \cdot \phi(-a) = \phi(a)(1 - \phi(a)), \in (0, 1)$
easy calculative
•widely used in conventional NN (shallow)

4.4.2. hyperbolic tangent activation function

$$\phi(a) = tanh(a) = \frac{e^{a} - e^{-a}}{e^{a} + e^{-a}}$$

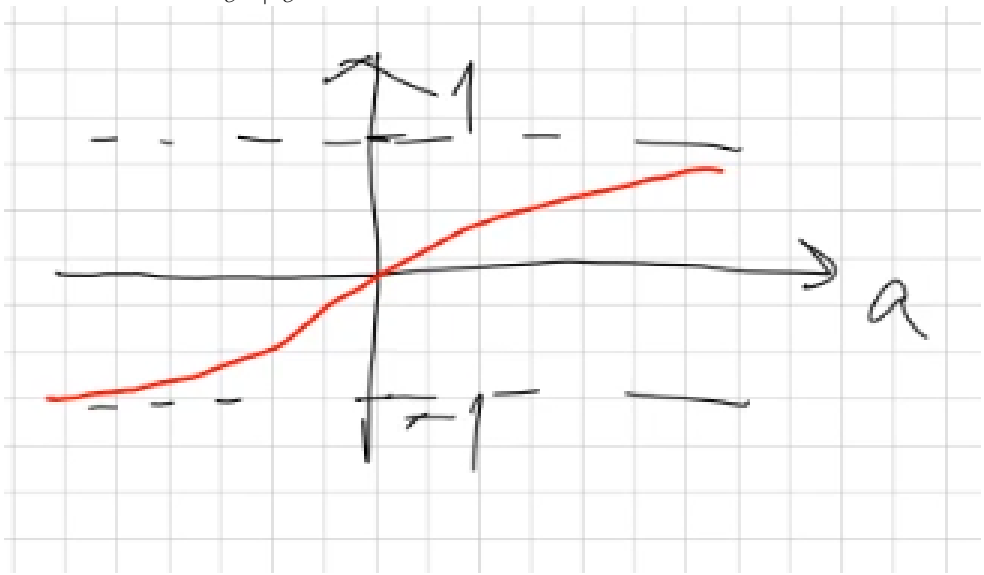


Abbildung 4.7: HyperbolicTangentActivation
like sigmoid but another output range

4.4.3. rectifier linear unit(ReLU

$$\phi(a) = ReLU(a) = max(a, 0) = \begin{cases} a & a \geq 0 \\ 0 & a < 0 \end{cases}$$

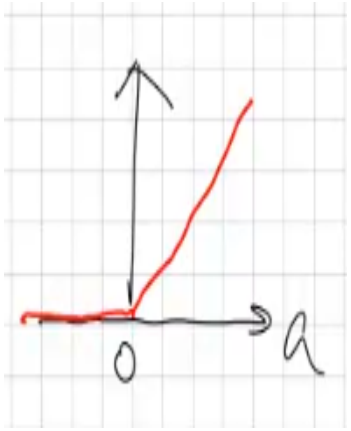


Abbildung 4.8: ReLuA ctivation Function

•≡ diode
simple calculation
•$\frac{d\phi}{da} = \begin{cases} 1 & a > 0 \\ 0 & a < 0 \end{cases} = u(a), u(0) = 0$ typically used
•most popular in DNN
•Details on 4-7

4.4.4. Softmax activatoin function(classification problem)

$\phi(\underline{a} : \underline{a} = [a_i] \in \Re^c \rightarrow \Re^c$

$$\phi(\underline{a}) = softmax(\underline{a}) = \begin{bmatrix} \phi_1(\underline{a}) \\ \vdots \\ \phi_c(\underline{a}) \end{bmatrix}$$

$\phi(\underline{a}) = \frac{a^{a_i}}{\sum_{j=1}^{c} e^{a_i}}, \in (0, 1), \sum_{i=1}^{c} \phi_i(\underline{a}) = 1$
•maps $\underline{a} \in \Re^c$ to a categorical PMF with c classes
•a_i large$\rightarrow$ $\phi_i(\underline{a})$ close to 1
•a_i small $\rightarrow$ $\phi_i(\underline{a})$ close to 0
•used in the output layer for classification problems

4.4.5. Special case c=2, binary classification problem

$: \phi_1(\underline{a}) = \frac{e^{a_i}}{e^{a_1} + e^{a_2}} = \frac{1}{1 + e^{-(a_1 - a_2)}} = \sigma(a_1 - a_2)$
$\phi_2(\underline{a} = \frac{e^{a_2}}{e^{a_1} + e^{a_2}} = 1 - \phi_1(\underline{a}) = \sigma(a_2 - a_1)$
i.e. softmax

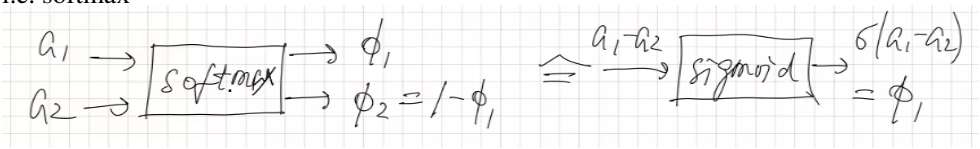


Abbildung 4.9: Outputlayer Softmax
one sigmoid output is sufficient for binary classification instead of 2 output softmax!
Derivative of softmax:
$\frac{\partial \phi_i(\underline{a})}{\partial a_j} = ... = \begin{cases} \phi : i(\underline{a}) \cdot (1 - \phi_i(\underline{a}) & i = j \\ -phi_i(\underline{a}) \cdot \phi_j(\underline{a}) & i \neq j \end{cases}$ •4-9 for details on usage

4.5. Universal approximation

4.5 Universal approximation 4-10

Universal approximation theorem ⇐ existence of a solution

The **universal approximation theorem** states that a feedforward neural network with a linear output layer ($\phi_L(a) = a$) and

- *at least one hidden layer* with
- a *nonlinear* activation function

can approximate any continuous (nonlinear) function $\underline{y}(\underline{x}_0)$ (on compact input sets) to arbitrary accuracy.

Comments:

- arbitrary accuracy: with an increasing number of hidden neurons.
- valid for a wide range of nonlinear activation functions, but excluding polynomials.
- minimum requirement for universal approximation: $\mathbf{W}_2\phi_1(\mathbf{W}_1\underline{x}_0 + \underline{b}_1) + \underline{b}_2$.

For learning $\mathbf{W}_l$ and $\underline{b}_l$ from D_{train}:

- deep networks are better than shallow ones,
- some activation functions are better than others.

⇐ how to find a good solution.

+

4.5.1. E4.3 Regression with 1 hidden layer

True function: $f_0(x)$
Given: $x(n)$ and noisy function $y(n) = f_(x(n)) + z(n), 1 \leq n \leq N, z(n)$ is the noise
NN:

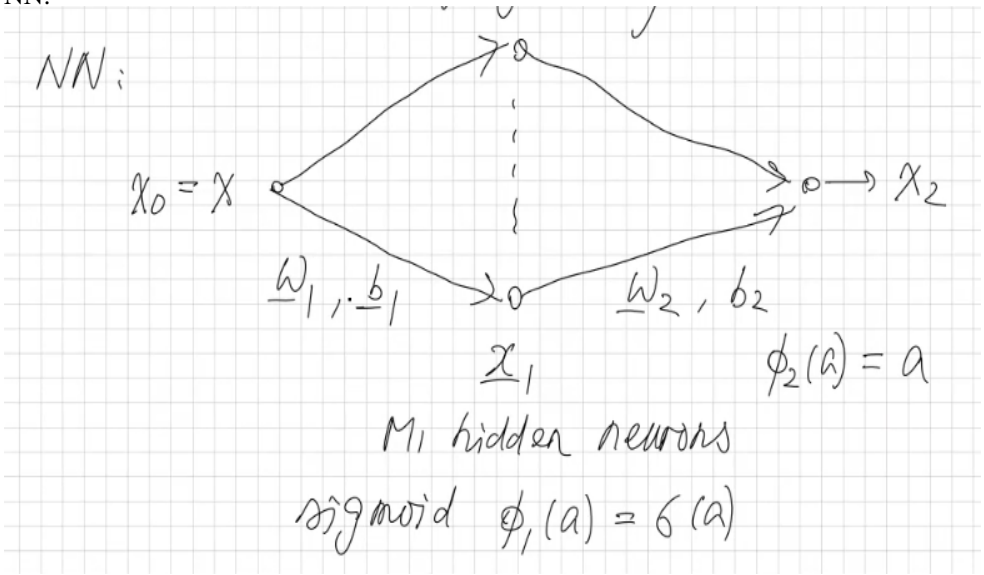


Abbildung 4.10: Example 4.3 Architecture

i.e. $x_2 = f(x, \underline{\theta}) = \underline{w}_2^T \sigma(\underline{w}_1 x + \underline{b}_1)$, column times row times scalar
$= \sum_{i=1}^{N_1} w_{2,i} \cdot \underbrace{\sigma(w_{1,i}x + b_{1,i})}_{M_1 \text{ nonllinear basis functions of } x} + b_2$

$\sigma(w_i x + b_i)\sigma(w_i(x + \frac{b_i}{w_i}))$

new center at $\frac{-b_i}{w_i}$ and new slope value w_i

Picture is for black 1 w_i red another w_i green another example w_i

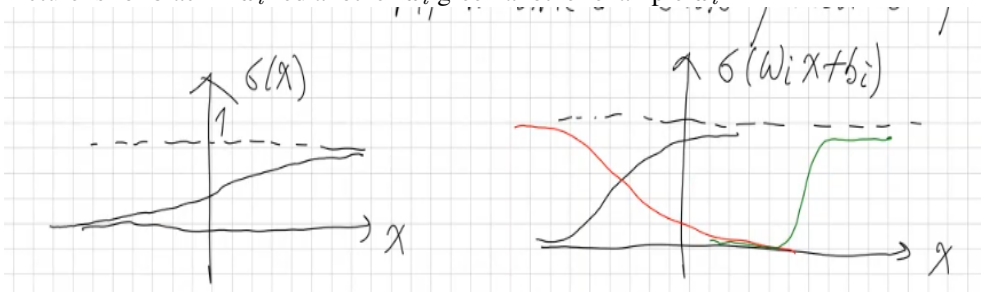


Abbildung 4.11: Sketch for sigmoid

4.6. Loss and cost function

Review chapter 3.4

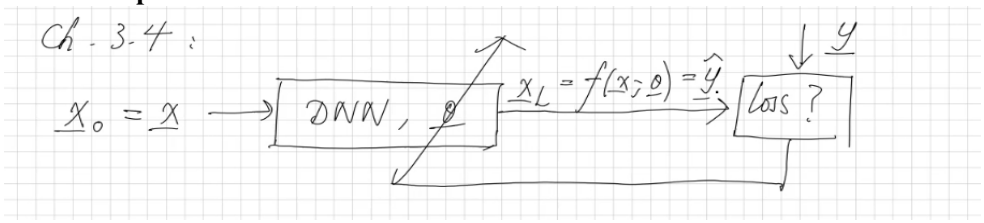


Abbildung 4.12: Probabalisitc Framework supervised learning

$\min_{\underline{\theta}} L(\underline{\theta}) = \frac{1}{N} = \sum_{n=1}^{N} (l(\underline{x}(n), y(n)_i \underline{\theta}$ cost function for d_{train}
$l(\underline{x}, \underline{y}_j \underline{\theta}) = -ln(q(\underline{y}|\underline{x}_j \underline{\theta})$ loss for one pair $(\underline{x}, \underline{y})$
$q() \leftrightarrow$ DNN ???

4.6.1. Regression Problem

$\underline{x} \in \Re^d$: random input
$\underline{y} \in \Re^c$ desired random output
Assumption: DNN estimates the mean of $\underline{y}$, i.e.
$\underline{y} = f(\underline{x}, \underline{\theta}) + \underline{z}, \underline{z}$: noise
f is calculated by DNN
case A: : $\underline{z} \sim N(\underline{0}, \sigma^2 \underline{I})$, white Gaussian noise
$\underline{y} \sim N(f(\underline{x}, \underline{\theta}), \sigma^2 \underline{I})$
$q(\underline{y}|\underline{x}, \underline{\theta}) = \frac{1}{(2\pi\sigma^2)^{c/2}} exp(\frac{-1}{2\sigma^2} ||\underline{y} - f(\underline{x}, \underline{\theta})||^2)$
$l(\underline{x}, \underline{y}, \underline{\theta}) = -ln(q(\underline{y}|\underline{x}, \underline{\theta})) = const. + \frac{1}{\sigma^2} ||\underline{y} - f(\underline{x}, \underline{\theta})||^2$
$L(\underline{\theta}) = \frac{1}{N} \sum_{n=1}^{N} ||\underline{y}(n) - f(\underline{x}, \underline{\theta})||^2$
$\rightarrow l_2 - loss$, mean square error (MSE) loss , least squares (LS) method
min $L(\underline{\theta})$ is a parameter estimation problem
case B:
$\underline{z} \sim N(\underline{0}, \underline{\underline{C}})$, colored Gaussian noise
$L(\underline{\theta}) = \frac{1}{N} \sum_{n=1}^{N} [\underline{y} - (f(\underline{x}(n), \underline{\theta})]^T \cdot \underline{\underline{C}}^{-1} \cdot [\underline{y} - (f(\underline{x}), \underline{\theta})]$, **weighted MSE loss**
Rarely used in real life applications:
•how to know $\underline{\underline{c}}$
•$\underline{\underline{C}}^{-1}$ expensive for large $\underline{\underline{C}}$

4.6.2. Classification

$\underline{x}\ in\Re^d$: input
$\underline{y} \in \{\underline{e}_1, \underline{e}_2, .., \underline{e}_c\}$
: class label for $\underline{x}$ in one-hot coding
Let $p_i = P(\underline{y} = \underline{e}i|\underline{x})$: true posterior probability
ch: 3.2 : $P(\underline{y}|\underline{x}) = \prod_{i=1}^{c} p_i^{y_i}$ true PMF
But p_i unknown
DNN: •output $f(\underline{y}, \underline{\theta}) = [f_i(\underline{x}; \underline{\theta})] \in \Re^c$ an estimate for $[p_i]$
•i. e. $P(\underline{y}|\underline{x})$ approximated $Q(\underline{y}|\underline{x}; \underline{\theta}) = \prod_{i=1}^{c} f_i(\underline{x}; \underline{\theta})^{y_i}$
in order to ensure :
•$0 < f_i(\underline{y}; \underline{\theta}) < 1$

•$\sum_{i=1}^{c} f_i(\underline{x}; \underline{\theta}) = 1$,
softmax is used in the output layer :
$\underline{x}_L = f(\underline{x}; \underline{\theta}) = \phi_L(\underline{a}_l L) = softmax(\underline{a}_L)$, see ch.4.4
$\rightarrow$ Loss $l(\underline{x}, \underline{y}; \underline{\theta}) = -ln(Q(\underline{y}|\underline{x}; \underline{\theta})) = \sum_{i=1}^{c} y_i ln(f_i(\underline{y}; \underline{\theta})) = -\underline{y}^T ln(f(\underline{x}; \underline{\theta})) \geq 0$
categorical cross entropy(CE) loss
Special case : Binary classification , c = 2
ch.4.4: $softmax, c = 2 \leftrightarrows sigmoid$
i.e. one output neuron with sigmoid activation function $f(\underline{x}; \underline{\theta}) = \sigma(a_L)$ is sufficient
Let $y_1 = y, y_2 = 1 - y; f_1 = f; f_2 = 1 - f$
$\rightarrow l(\underline{x}, \underline{y}; \underline{\theta}) = -yln(f(\underline{x}; \underline{\theta}) + (1 - y)) \cdot ln(1 - f(\underline{x}; \underline{\theta}))$, binary CE loss
True probabilistic way toward cost functions

The probabilistic way toward the cost functions

- $p(\underline{x}, \underline{y})$: true but unknown data generating distribution, application specific
- $D_{\text{train}} = \{\underline{x}(n), \underline{y}(n), 1 \leq n \leq N\}$: training set, i.i.d. samples of $p(\underline{x}, \underline{y})$
- $p(\underline{y}|\underline{x})$: true posterior describing the desired inference $\underline{x} \rightarrow \underline{y}$
- $q(\underline{y}|\underline{x}; \underline{\theta})$: a parametric model (DNN) to approximate $p(\underline{y}|\underline{x})$

min. forward KL divergence $D_{\text{KL}}(p(\underline{x}, \underline{y})||q(\underline{x}, \underline{y}; \underline{\theta}))$
$\downarrow$ ch. 3.3: p fixed
min. cross entropy $H(p, q) = -\text{E}_{\underline{X},\underline{Y} \sim p(\underline{x},\underline{y})} \ln(q(\underline{Y}|\underline{X}; \underline{\theta}))$
$\downarrow$ ch. 3.4: use empirical distribution $\hat{p}(\underline{x}, \underline{y})$
min. cross entropy $H(\hat{p}, q) = -\text{E}_{\underline{X},\underline{Y} \sim \hat{p}(\underline{x},\underline{y})} \ln(q(\underline{Y}|\underline{X}; \underline{\theta}))$
$\downarrow$ ignore constant term
min. cost function $L(\underline{\theta}) = \frac{1}{N} \sum_{n=1}^{N} [-\ln(q(\underline{y}(n)|\underline{x}(n); \underline{\theta}))]$
$\downarrow$ ch. 4.6: $q(\underline{y}|\underline{x}; \underline{\theta})$ for regression and classification?
l_2-loss or l_1-loss or categorical loss

4.6.3. Semantic segmentation

pixelwise classification
categorical cross entropy loss:
$l(\underline{\underline{X}}, \underline{\underline{Y}}; \underline{\theta}) = \sum_{m=1}^{M} \sum_{n=1}^{N} [-\underline{y}_{mn} \cdot ln(\hat{\underline{y}}_{mn}(\underline{\underline{X}}, \underline{\theta}))]$ sum over all pixels
Problem: imbalanced classes
e.g (c=2) background and foreground with 90 % background and 10 % foreground pixels , 90 % loss function for the foreground
$\rightarrow$ $l(\cdot)$ cares more about the major class and less about the minor class but the minor class(foreground) is object of interest. $\rightarrow$ reduced segmentation accuracy for the minor class
Solutions:
•Weighted categorical CE loss
•region-based loss **Jaccard index only used for result evaluation not suitable as loss function for training**
•minimize loss, not max J or D for those indexes
•$|A| \in \mathbb{N}$, not differential with respect to $\underline{\theta}$
•$\underline{y}_{mn}$ contains 0 or 1 as desired, but $\hat{\underline{y}}$ contains real numbers $\in (0, 1) \in softmax$

→ adapted definition of J and D are necessary

4.6 Lost and cost function 4-21

Soft Jaccard and Dice loss

Let again $\mathbf{Y} = [\underline{y}_{mn}]_{mn}$ and $\hat{\mathbf{Y}} = [\underline{\hat{y}}_{mn}]_{mn}$. $\underline{y}_{mn} \in \{\underline{e}_1, \ldots, \underline{e}_c\}$ is the one-hot coding and $\underline{\hat{y}}_{mn} \in \mathbb{R}^c$ is the c-class softmax output for the pixel (m, n). The **soft Jaccard loss** to be minimized in training for image segmentation is

$$\begin{aligned} \underline{\alpha} &= \textstyle\sum_{m=1}^{M} \sum_{n=1}^{N} \underline{y}_{mn} \odot \underline{\hat{y}}_{mn} = [\alpha_i] \in \mathbb{R}^c, \\ \underline{\beta} &= \textstyle\sum_{m=1}^{M} \sum_{n=1}^{N} (\underline{y}_{mn} + \underline{\hat{y}}_{mn}) = [\beta_i] \in \mathbb{R}^c, \\ J_i &= \frac{\alpha_i + \epsilon}{\beta_i - \alpha_i + \epsilon}, \\ l(\mathbf{X}, \mathbf{Y}; \underline{\theta}) &= 1 - \frac{1}{c} \textstyle\sum_{i=1}^{c} J_i \end{aligned}$$

$\odot$ is the elementwise multiplication. α_i and β_i represent arithmetic calculations of $|A_i \cap B_i|$ and $|A_i| + |B_i|$ for class i, respectively. J_i is the soft Jaccard index for class i where $\epsilon > 0$ is a suitable number to avoid $0/0$ if $\alpha_i = \beta_i = 0$. $l(\mathbf{X}, \mathbf{Y}; \underline{\theta})$ is the soft Jaccard loss differentiable w.r.t. $\underline{\theta}$. The **soft Dice loss** is defined in a similar way.

For 3D segmentation, $\underline{\alpha}$ and $\underline{\beta}$ are calculated by three-dimensional sums over all pixels.

Abbildung 4.13: Soft Jaccard / Dice loss

Very good for strongly imbalanced classes

4.7. Training

•training set $D_{train} = \{\underline{x}, \underline{y}, 1 \leq n \leq N\}$

•cost function $L(\underline{\theta}) = \frac{1}{N} \sum_{n=1}^{N} l(\underline{x}(n), \underline{y}; \underline{\theta})$

•task: $minL(\underline{\theta})$

•optimizer: optimization algorithm to solve the minimization task $L(\underline{\theta})$

No closed-form solution! Numerical minimization necessary, see AM (last part)

in DL: gradient decent approach and variants(like hiking)

need only 1. order derivative of $L(\underline{\theta})$

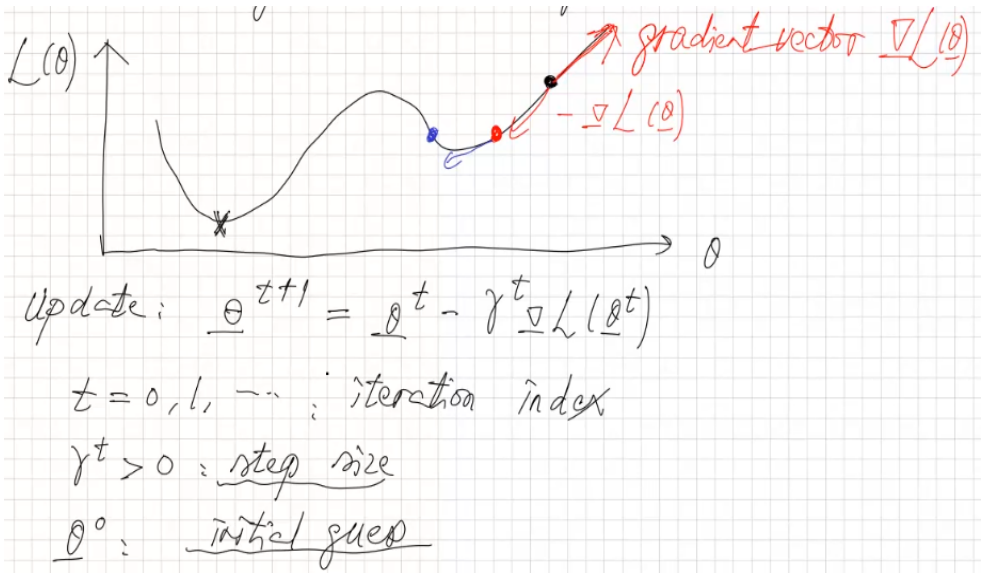


Abbildung 4.14: Gradient descent

calculation of the gradient vector $\nabla L(\underline{\theta})$ is non trivial

4.7.1. Chainrule of derivative (back propagation)

$$\frac{f(g(\theta))}{d\theta} = \frac{df}{dg} \cdot \frac{dg}{d\theta}$$

Layerindex L: $\frac{\partial L_{cost}(\underline{\theta})}{\partial w_{L,ij}} = \frac{\partial L_{cost}}{\partial \underline{x}_L} \cdot \frac{\partial \underline{x}_K}{\partial \underline{a}_L} \cdot \frac{\partial \underline{a}_L}{\partial w_{L,ij}} = \underbrace{\underline{\underline{J}}_L(\underline{x}_L) \cdot \underline{\underline{J}}_{\underline{x}_L}(\underline{a}_L)}_{\underline{\underline{J}}_L(\underline{a}_L)} \cdot \underline{\underline{J}}_{\underline{a}_L}(w_{L,ij}),$

Jacobi matrices see ch. 3.1

Notation: $\underline{\underline{J}}_y(x) = \frac{\partial y}{\partial x}$

Layer $L-1$:

$$\frac{\partial L(\underline{\theta})}{\partial w_{L-1,ij}} = \frac{\partial L}{\partial \underline{a}_L} \cdot \frac{\partial \underline{a}_L}{\partial \underline{a}_{L-1}} \cdot \frac{\partial \underline{a}_{L-1}}{\partial w_{L-1,ij}} = \underbrace{\underline{\underline{J}}_L(\underline{a}_L) \cdot \underline{\underline{J}}_{\underline{a}_L}(\underline{a}_{L-1})}_{\underline{\underline{J}}_L(\underline{a}_{L-1})} \cdot \underline{\underline{J}}_{\underline{a}_{L-1}}(w_{L-1,ij})$$

Layer 1: $\frac{\partial L(\underline{\theta})}{\partial w_{1,ij}} = \underline{\underline{J}}_L(\underline{a}_L) \cdot \underline{\underline{J}}_{\underline{a}_L}(\underline{a}_{L-1}), \ldots, \underline{\underline{J}}_{\underline{a}_2}(\underline{a}_1) \cdot \underline{\underline{J}}_{\underline{a}_1}(w_{1,ij})$

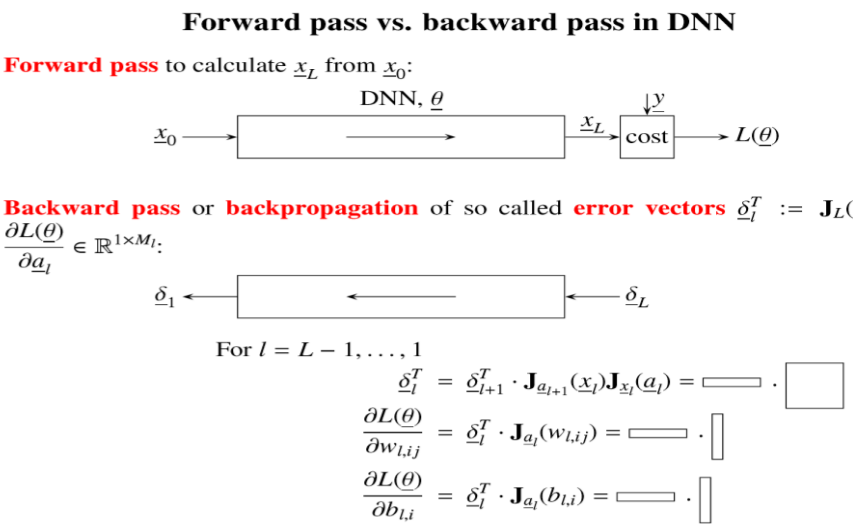


Abbildung 4.15: Forward pass vs. backward pass

Calculations for backpropagation on Slide 4-24 to 4-27

more about omptimizer in ch.5

more about model in ch. 6-8

Batch gradient descent

calculate $\nabla L(\underline{\theta}) = \frac{1}{N} \sum_{n=1}^{N} \nabla l(\underline{x}(n), \underline{y}(n); \underline{\theta})$

for the whole training set D_{train}

Difficult for too large N!

e.g. MNIST: 60.000 training smaples

ILSVRC: 1.2M training samples

$\rightarrow$ not enough ram to keep D_{train} in memory

Solution: stochastic gradient descent (SGD), i.e. calculate ∇L and update $\underline{\theta}$ for each minibatch, a block of B samples from d_{train}:

$\underline{\theta}^{t+1} = \underline{\theta}^t - \nabla L((t); \underline{\theta})|_{\underline{\theta}=\underline{\theta}_t}$

$L(t; \underline{\theta}) = \frac{1}{B} \sum_{n=t'B+1}^{(t'+1)\cdot B} l(\underline{x}(n), \underline{y}; \underline{\theta})$

$B \in \mathbb{N}$: minibatch size, small enough to fit in RAM

$N/B \; in \mathbb{N}$: number of minibatches in d_{train}

$t = 0, 1, ..,$: iteration index

$t' = mod(t, \frac{N}{B}) \in \{0, 1, .., \frac{N}{B-1}$: minibatch index

$\nabla L(t; \underline{\theta})$ more noisy than $\nabla L(\underline{\theta})$

$\rightarrow$ stochastic gradient descents

Evaluation during training:

$\hat{\underline{\theta}}_k$ after k-th epoch: $k = 1, 2, ..$

Technical performance metrics: •training loss: $L(\hat{\underline{\theta}}_k)$ calculated form training set D_{train}
•test loss::$L(\hat{\underline{\theta}}_k)$ calculated form test set D_{test}
and objective performance metrics for classification
•**training error rate :** Error rate of $DNN(\hat{\underline{\theta}}_k)$ for D_{train}
•**test error rate :** Error rate of $DNN(\hat{\underline{\theta}}_k)$ for D_{test}
or: •training/test accuracy = 1- training/test error rate

4.8. 4.8 Implementation of DNN's in Python

•$60000/128) 468, 795 \approx 469$ mini-batches (slide 4-33)
•see python script KerasDemo

Chapter 5: Advanced optimization techniques

Date: 15/05/2020

Lecturer:Bin Yang *By: Nicolas Hornek*

5.1. Difficulties in optimization

2 Questions: •universal approximation: Existence of a NN for each task
Will you find it?
•Why was the conventional NN not successful?

1D visualization

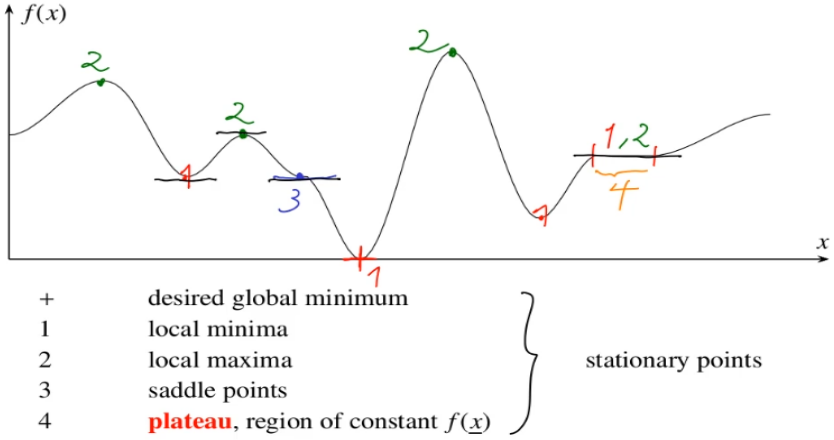


Abbildung 5.1: 1D Visualization Gradient Descent

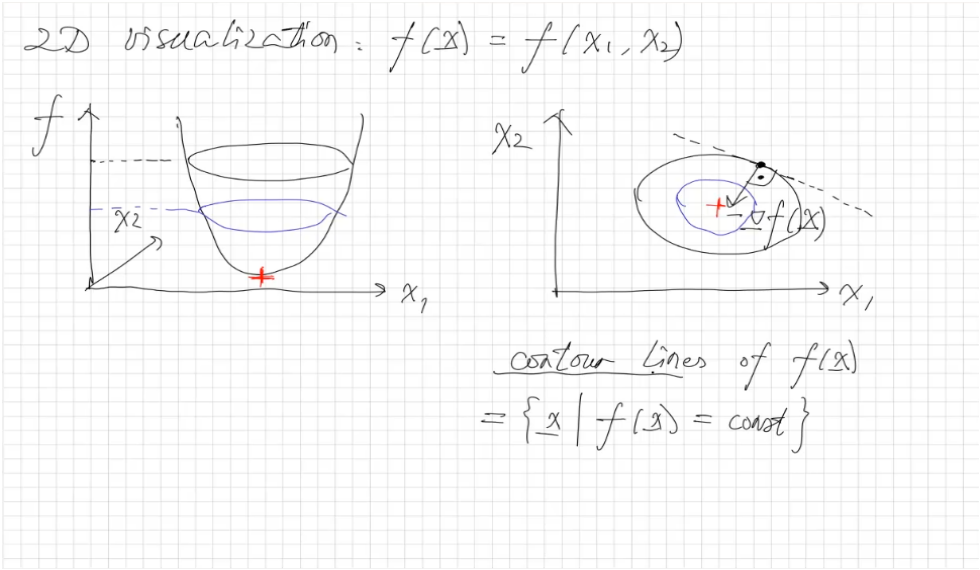


Abbildung 5.2: 2D Contour lines

D2) Ill conditioning

well conditioned (circular) contour lines
equal curvatures
$-\nabla L(t;\theta)$ points to local minimum
fast convergence

ill conditioned (narrow) contour lines
strongly different curvatures
$-\nabla L(t;\theta)$ mostly points to wrong directions
slow convergence (oscillation)

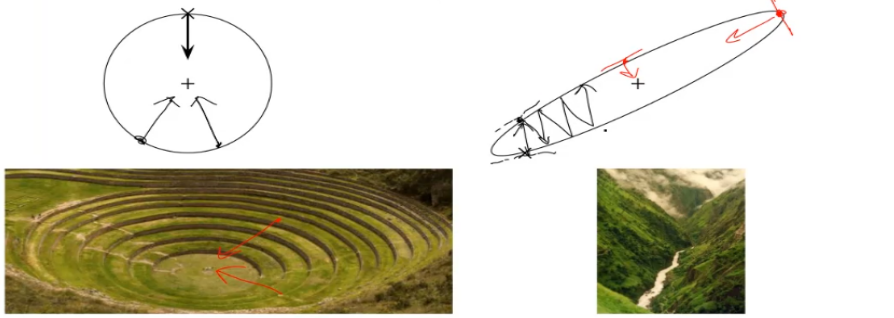
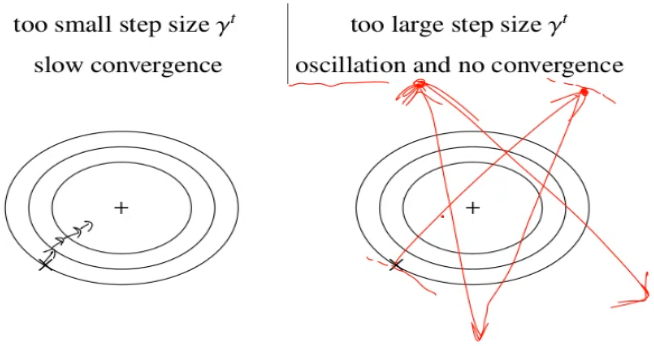


Abbildung 5.3: Ill conditioning

D3) Saddlepoint and plateau $\nabla L = 0$ no update of x^t because correction term is 0
in practice: $\nabla L \approx 0 \rightarrow$ very slow convergence

D4) Sensitive to the choice of the step size



- The optimum step size γ^t depends on the cost function $L(t;\underline{\theta})$ and the current position $\underline{\theta}^t$ and is unknown in advance.

Abbildung 5.4: Sensitive Choice for step size

Vanishing Gradient:
Backpropagation of the error vector
$\Theta = \frac{\partial L(\underline{\theta}}{\partial \underline{a}_L} \in \Re^{1\times M_L}$ in 4.7:
$\underline{\delta}_1^T = \underline{\delta}_L^T \cdot \underline{\underline{j}}_{\underline{a}_L}(\underline{a}_{L-1}), .., \underline{\underline{J}}_{\underline{a}_2}(\underline{a}_1)$, L Layers
$\underline{\underline{J}}_{\underline{a}_{L+1}}(\underline{a}_L) = \underline{\underline{J}}_{\underline{a}_{L+1}}(\underline{x}_l) \cdot \underline{\underline{J}}_{\underline{x}_L}(\underline{a}_L) = \underline{\underline{W}}_{l+1} \cdot diag(\phi_L'(\underline{a}_L))$
if $||\underline{\underline{J}}_{\underline{a}_{L+1}}(\underline{a}_L)|| < 1, \forall l$ matrix norm , then $||\underline{\delta}_L|| \to 0$
vanishing gradient $\to$ no update of $\underline{\theta}^T$ stop learning. With the multiplication of a lot of terms smaller than 1 the gradient turns to a very small number close to zero
•if $||\underline{\underline{J}}_{\underline{a}_{l+1}}(\underline{a}_l)|| > 1, \forall l$, then $||\underline{\delta}_l|| \to \infty$
exploding gradient $\to$ divergence
no problem for shallow NN's because only small number of layers
bo problem for deep NN's because of large number of layers
•vanishing gradient less serious for the last layers ($l \uparrow$)
•more serious for first layers ($l \downarrow$)

5.1.1. E5.1: sigmoid vs. ReLU

a) sigmoid or tanh:
$\phi(a) = \sigma(a) = \frac{1}{1+e^{-a}} \in (0,1)$

if $|a| >> 1 : \phi'(a) \approx 0$ due to saturation (shape of function)
$\to$ sigmoid bad for DNN die to vanishing gradient
b) ReLU
$\phi(a) = max(0,a)$
$\phi'(a) = \begin{cases} 1 & a > 0 \\ 0 & a < 0 \end{cases} = u(a)$
$\to$ ReLu less serious for vanishing gradient

5.2. Momentum method

an improvement of SGD
•change from $\underline{\theta}^t$ to $\underline{\theta}^{t+1} : \Delta\underline{\theta}^t = \beta \cdot \Delta\underline{\theta}^{t-1} \underbrace{-\gamma^t \underline{\nabla} L(t;\underline{\theta})|_{\underline{\theta}=\underline{\theta}^t}}_{\text{gradient part}}$
•update: $\underline{\theta}^{t+1} = \underline{\theta}^t + \delta\underline{\theta}^t$
$0 \le \beta \le 1$: **momentum factor**
$\beta = 0$: SGD
$\beta > 0$: recursive smoothing of $\Delta\underline{\theta}^t$
Effect of the momentum:
•reduce noise in stochastic gradient (D1)
•reduce oscillation and accelerate the convergence of the gradient method for ill conditioned contour lines(D2)

5.2.1. Nesterov Momentum

a variant of momentum method
$\Delta\underline{\theta}^t = \beta\Delta\underline{\theta}^{t-1} + \underbrace{(-\gamma^t \underline{\nabla} L(t;\underline{\theta})|_{\underline{\theta}=\underline{\theta}^t+\beta\Delta\underline{\theta}^t)}}_{\text{lookahead gradient at the predicted position } \underline{\theta}^{t-1}+\beta\Delta\underline{\theta}}$

5.3. 5.3 Learning rate schedule

How to choose the step size /learning rate γ^t?
Many possible schedules
S1 constant learning rate:
$\gamma^t = \gamma = const., \forall t$
But difficulty D4:
•γ too small: slow convergence

•γ too large: no convergence / oscillation around local minimum
$\rightarrow$ Need a trade-off between
•fast convergence at the beginning: $\gamma \uparrow$ (large step size)
•less oscillation afterwards : $\gamma \downarrow$ reduce stepsize with growing number of iterations: **learning rate decay**
Weakness:
•manual choice of γ_0, t_0, c
•same schedule for all parameters in $\underline{\theta}$
Adaptive schedules: •different schedules for different parameters in $\underline{\theta}$
•γ^t calculated dynamically depending on $\underline{\theta}^t$
Slide 5-16 Adam very popular

5.4. Input and batch normalization

5.4.1. E5.3 A Perceptron

a) large offset : $\underline{x}(n) = \underset{offset}{\underline{x}_0} + \tilde{\underline{x}}(n), ||\underline{x}_0|| >> \tilde{\underline{x}}(n), \forall n$
$\rightarrow \underline{\underline{R}} \approx \underline{x}_0 \underline{x}_0^T$, rank one

b) strongly different variances: e.g $\underline{x}(n) = \begin{bmatrix} large \\ small \\ \vdots \\ small \end{bmatrix} \sim \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \underline{e}_1, \forall n$

$\rightarrow \underline{\underline{R}} \sim \underline{e}, \underline{e}^T$, rank one
AM: $\underline{\underline{R}}$ has approximately rank one
$\rightarrow \underline{\underline{R}}$ has one large eigenvalue λ_1 with eigenvector $\underline{v}_1 = \underline{x}_0$ or $\underline{v}_1 \sim \underline{e}_1$ and d-1 small eigenvalues
$\rightarrow$ very narrow contour lines
$\rightarrow$ slow convergence (D2)
Need input normalization, e.g.: zero-mean unit-variance normalization
For each $x_i(n) = [\underline{x}_0(n)]_i, 1 \leq n \leq N$
$x_i(n) \leftarrow \dfrac{x_i(n) - \mu_i}{\sigma_i}$ with estimated mean $\mu_i = \dfrac{1}{N} \sum_{n=1}^{N} x_i(n)$
variance $\sigma_i^2 = \dfrac{1}{N-1} \sum_{n=1}^{N} (x_i(n) - \mu_i)^2$ (N-1 because unbiased mean wanted) •normalization for the whole training set D
•equally for all channels x_i
Advantage:
•no ill conditioning (D2)

•faster convergence

5.4.2. Batch normalization

Input normalization: done once for the data set
Hidden layers: data distribution changes
•over layers
•over time during training those to points are called internal covariate shift
$\rightarrow$ slower convergence
Batch normalization(BN): : like input normalization
•for any hidden layer
•for each mini batch of length B

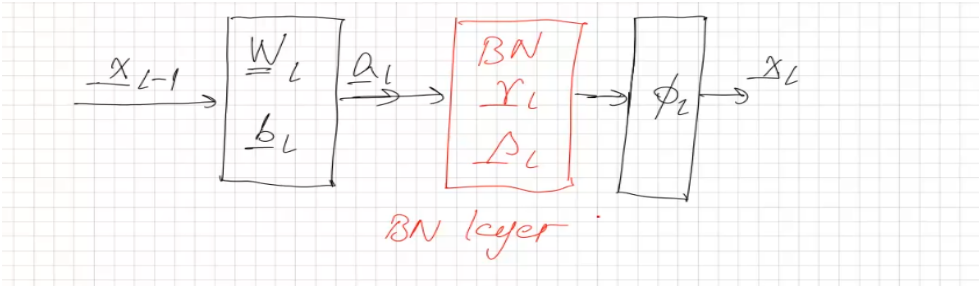


Abbildung 5.5: Sketch for mini batch normalization

5.4 Input and batch normalization 5-19

Batch normalization (1)

The **batch normalization** (**BN**) of the activation $\underline{a}_l(n)$ at layer l for one minibatch $1 \le n \le B$ is defined as

$$\left[\underline{a}_l(n)\right]_i \leftarrow \gamma_{l,i}\frac{\left[\underline{a}_l(n)\right]_i - \mu_{l,i}}{\sqrt{\sigma_{l,i}^2 + \epsilon}} + \beta_{l,i}, \quad 1 \le n \le B,\ 1 \le i \le M_l.$$

It consists of two steps for each element $\left[\underline{a}_l(n)\right]_i$ of $\underline{a}_l(n)$:

- A zero-mean unit-variance normalization like input normalization.

$$\mu_{l,i} = \frac{1}{B}\sum_{n=1}^{B}\left[\underline{a}_l(n)\right]_i \quad \text{and} \quad \sigma_{l,i}^2 = \frac{1}{B-1}\sum_{n=1}^{B}\left(\left[\underline{a}_l(n)\right]_i - \mu_{l,i}\right)^2$$

  are the sample mean and variance of $\left[\underline{a}_l(n)\right]_i$ of this minibatch. ϵ is a small positive number (e.g. 10^{-5}) to avoid division-by-zero. In contrast to the complete data set, $\sigma_{l,i}^2 \approx 0$ is likely for a short minibatch.

- Scale-and-offset $\gamma_{l,i}\square + \beta_{l,i}$ with two learnable parameters $\gamma_{l,i}$ and $\beta_{l,i}$ per neuron

Abbildung 5.6: Summary BN

5.4 Input and batch normalization 5-20

Batch normalization (2)

Why the second step $\gamma_{l,i}\square + \beta_{l,i}$?

- Allow a flexible data dynamic range for each neuron and does not change the expressiveness of the network.
  - If $\underline{\gamma}_l = \underline{\sigma}_l$ and $\underline{\beta}_l = \underline{\mu}_l$, batch normalization simplifies to the special case of no batch normalization. Normally, $\underline{\gamma}_l \neq \underline{\sigma}_l$ and $\underline{\beta}_l \neq \underline{\mu}_l$.
  - $\underline{b}_l$ is redundant due to $\underline{\beta}_l$ and can be omitted, i.e. $\underline{a}_l(n) = \mathbf{W}_l\underline{x}_{l-1}(n)$.
  - $\underline{\gamma}_l$ and $\underline{\beta}_l$ are learned from data like $\mathbf{W}_l$. Hence each neuron adjusts the individually optimum dynamic range of $\left[\underline{a}_l(n)\right]_i$ for the next nonlinear activation function $\phi_l(\cdot)$.
- Decouple the layers.
  - Batch normalization makes the dynamic range of one layer (partially) independent of the previous layers. This decouples the joint training of different layers to individual layers. It simplifies the learning, in particular for deep networks.
  - Batch normalization makes the surface of the cost function smoother.

Abbildung 5.7: Summary BN 2

5.5. Parameter initialization

SGD does a local search: The solution depends on the initial value θ^0
$\Theta^0 =??$ **2 Random onotialization of** $\underline{\underline{W}}_L$, e.g. •normal or Gaussian distribution $N()$
$[\underline{\underline{W}}_L]_{ij} \sim$ i.i.d (independent identically distributed) $\sigma \cdot N(0,1) = N(0,\sigma^2)$
•uniform distribution $U(\cdot)$
$[\underline{\underline{W}}_L]_{ij} \sim$ i.i.dl $\sigma U(-1,1) = U(\sigma,\sigma), \sigma = const, \forall l,i,j$
$\rightarrow$ not optimal
3) He initialization
as 2) , but $\delta_l \sim \frac{1}{\sqrt{M_{L-1}}} \rightarrow$ constant activation flow after initialization
layer l : $\underline{a}_l = \underline{\underline{W}}_l \cdot \underline{x}_{l-1} + \underline{b}_l \overset{b=0}{=} \underline{\underline{W}}_l \cdot \underline{x}_{l-1}$ or
$\underline{a} = \underline{\underline{W}} \cdot \underline{x}$,
$\underline{a} = [a_i] \in \mathbb{R}^{M_l}$
$\underline{\underline{W}} = [w_{ij}] \in \mathbb{R}^{M_l \times M_{l-1}}$
$\underline{x} = [x_i] \in \mathbb{R}^{M_{l-1}}$
$\rightarrow a_i = \sum_{j=1}^{M_{l-1}} w_{ij} \cdot x_j$
Assumptions:
•x_i i.i.d zero mean , variance σ_x^2
•w_{ij} i.i.d zero mean , variance σ_w^2
•x_i and w_{ij} independent
$\rightarrow$ •$E(a_i) = \sum_j E(w_{ij}) \cdot E(x_{ij}) = 0$
•$Var(a_i) = E(a_i^2) = E(\sum_j w_{ij} \cdot x_j)^2 = E(\sum_j \sum_k w_{ij} w_{ik} x_j x_k) = \sum_j \sum_k E(w_{ij} w_{ik} \cdot E(x_j x_k)) = \sum_{j=1}^{M_{l-1}} \sigma_w^2 \cdot \sigma_x^2 = M_{l-1} \cdot \sigma_w^2 \cdot \sigma_x^2$
constant activation flow $\equiv$ smooth information flow in the forward pass
$Var(a_i) = const., \forall i,l$
$\rightarrow \sigma_{w,l} \sim \frac{1}{\sqrt{M_{l-1}}}$, M_{l-1} : fan-in
4) Glorot initialization
const. gradient flow in backward pass
$||\frac{\partial L}{\partial \underline{a}_l}|| = const, \forall l \rightarrow \sigma_{w,l} \sim \frac{1}{\sqrt{M_l}}$, M_l : fan-out
compromise: $\sigma_{w,l} \sim \frac{1}{\sqrt{M_{l-1} + M_l}}$

5.6. Improved (network)-model

A) Better activation functions $\phi(\cdot)$, e.g.
•ReLU instead of sigmoid
•leaky reLu instead of ReLU
B) skip connections, shortcuts , residual network (ResNet)

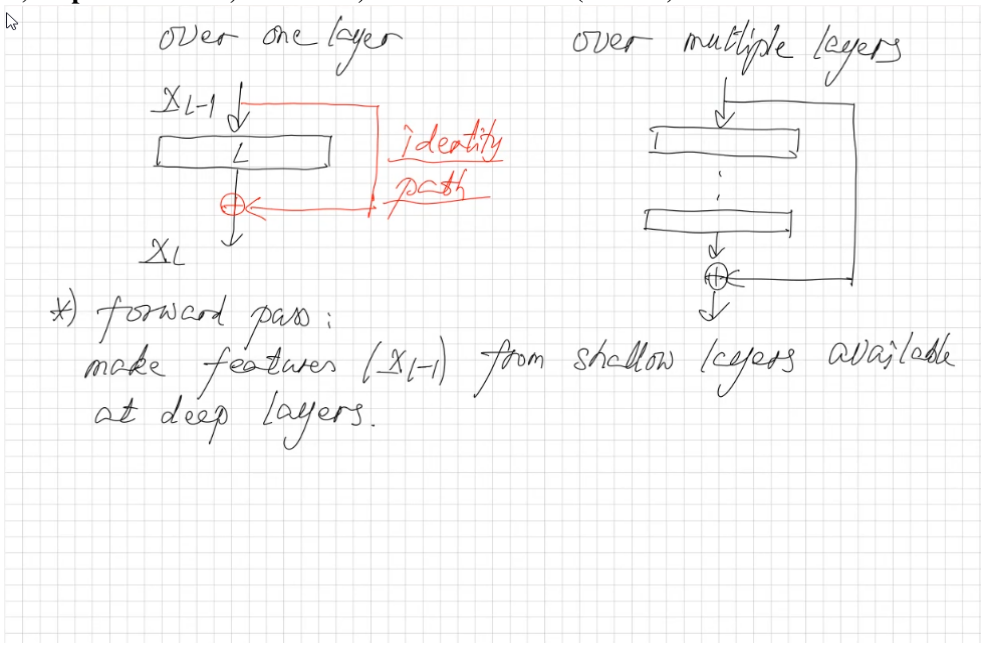


Abbildung 5.8: Layerskip / shortcuts

•backward pass<. no vanishing gradient over identity path.

$$\underline{x}_l = \phi_l(\underline{\underline{W}}\underline{x}_{l-1} + \underline{b}_l) + \underline{x}_{l-1}$$

$$\frac{\partial \underline{x}_l}{\partial \underline{x}_{l-1}} = \frac{\partial \phi_l(\cdots)}{\partial \underline{x}_{l-1}} + \underline{\underline{I}}$$

c) Many other architecture improvements see ch.10

Chapter 6: Overfitting and regularization

Date: 25/05/2020

Lecturer:Bin Yang *By: Nicolas Hornek*

6.1. Model capacity and overfitting / underfitting

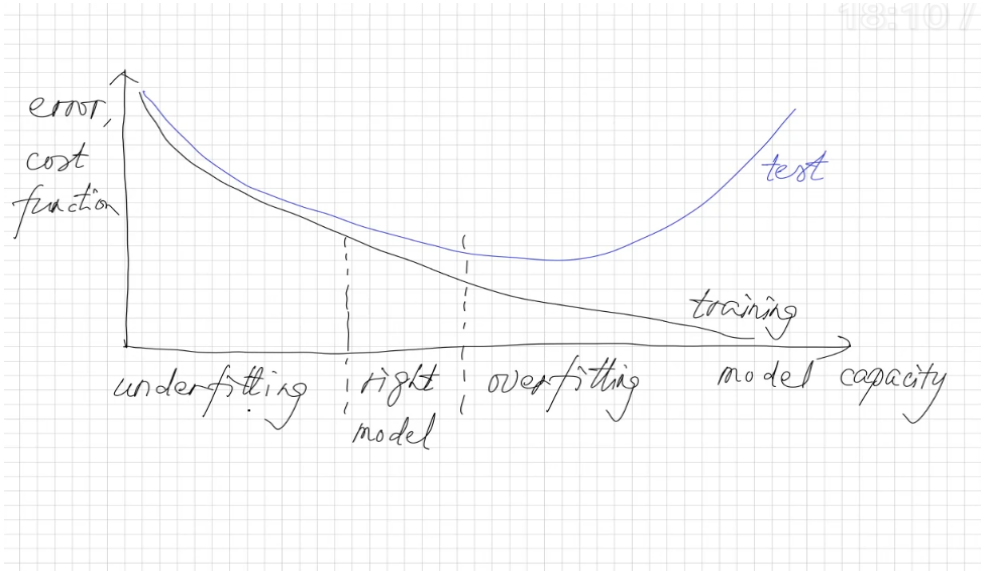


Abbildung 6.1: Model fitting curve

6.2. Weight norm penalty

change on cost function:
•old cost function: $L(\underline{\theta})$
•New regularized cost function: $L_r(\underline{\theta}) = L/\underline{\theta} + \sum_{l=1}^{L} \lambda_i P(\underline{\underline{W}}_L)$
$\lambda \geq 0$: regularized parameters
$P(\underline{\underline{W}}_L) \geq 0$: penalty terms, penalize $\underline{\theta}$ with large $P(\underline{\underline{W}}_L)$
$\rightarrow$ A compromise between $\min_{\underline{\theta}} L(\underline{\theta})$ and the min $\min_{\underline{\theta}} P(\underline{\underline{W}}_L)$
λ_L determine the relative contributions of $L(\underline{\theta}), P(\underline{\underline{W}}_L)$.

$\lambda_L = 0, \forall L$: no regularization
common choice of $P(\underline{\underline{W}}_L)$:
•a) l2-regularization: we use $l_2 - norm$ of $vec(\underline{\underline{W}}_L)$
$P(\underline{\underline{W}}_L) = ||vec(\underline{\underline{W}}_L)||_2^2 = \sum_i \sum_j W_{L,ij}^2 \rightarrow$ prefer $\underline{\theta}$ with small weight energy
$\rightarrow$ better generalization, see E6.1
Bias vector $\underline{b}_l$: no amplification effext of $\underline{x}_{l-1} \rightarrow$ no need for regularization
Mathematical analysis:
$L_r(\underline{\theta}) = L(\underline{\theta}) + \lambda ||\underline{\theta}||^2$ for simplicity
$\underline{\nabla} L_r(\underline{\theta}) = \underline{\nabla} L(\underline{\theta}) + 2 \cdot \lambda \underline{\theta}$
$\underline{\theta}^{t+1} = \underline{\theta}^t - \gamma^t \underline{\nabla} L_r(\underline{\theta}^t)$
$\underbrace{(1 - 2\lambda\gamma^t)}_{0<<factor<1} \underline{\theta}^t - \gamma^t \underline{\nabla} L(\underline{\theta}^t)$
l2-regularization leads to **weight decay**
b) l1-regularization: use l1-norm of $vec(\underline{\underline{W}}_L)$
$P(\underline{\underline{W}}_L) = ||vec(\underline{\underline{W}}_L)||_1 = \sum_i \sum_j |W_{L,ij}|$
$\rightarrow$ prefer sparse $\underline{\underline{W}}_L$ with many zero elements

6.3. Early stopping

change on optimizer:

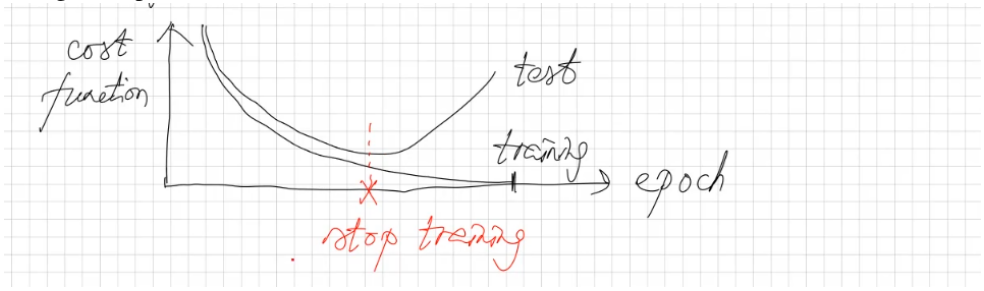


Abbildung 6.2: Early stopping

6.4. Data augmentation

change on dataset, training with ∞ many training data $\rightarrow$ no over fitting, in practice, training set is limited in size

data augmentation: Generation of artificial realistic training samples:

6.5. Ensamble learning

change dataset / model / cost function / optimizer

Ensemble learning

Ensemble learning is a model averaging method to reduce the test error by combining an ensemble of models:

- train different (independent) models for the same task
- combine these models to reduce the test error
  - regression: average of the model outputs
  - classification: voting of the model outputs, e.g. 3× cat and 1× dog

It is unlikely that all models will make the same errors on the test set. Hence the averaged model is more robust.

The different models can be trained by using

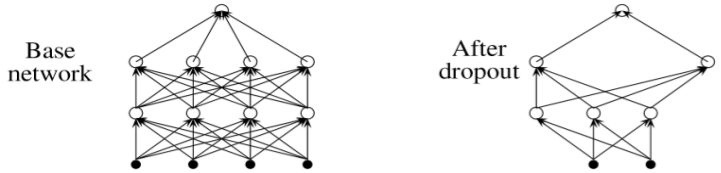
- different subsets of the training set or
- different model architectures or
- different cost functions or
- different optimizers or
- combinations of them.

Abbildung 6.3: Ensamble learning explained

6.6. Dropout

change on model
An implicit ensemble method

Dropout (1)



Training

- For each minibatch, **dropout** randomly removes some neurons in layer l of a base network with a probability d_l, the **dropout rate**.
- This results for each minibatch in a random subnetwork for solving the same task.[2]

Inference

- No dropout.
- All outgoing weights of neurons in layer l are weighted by $1-d_l$ to correct the large fan-in to the neurons (number of inputs) of the next layer.

Abbildung 6.4: Dropout explained

6.7. Hyperparameter optimization

Hyperparameters

What are they?

- In contrast to the model parameters $\underline{\theta}$ (weights and biases) to be learned from training data, **hyperparameters** $\underline{\eta}$ are configuration parameters of a machine learning algorithm which are not adapted during training.
- $\underline{\eta}$ is chosen before learning and remains fixed. It controls, together with $\underline{\theta}$, the behavior of the model $f(\underline{x};\underline{\theta},\underline{\eta})$, see next slide. Hence, they need an optimization.

Why are they not adapted?

a) Hyperparameters are often discrete valued (e.g. number of layers/neurons, type of activation function). Gradient descent is not suitable for this kind of integer optimization.

b) The training error is a monoton function of some hyperparameters, in particular those controlling the model capacity. An optimization of these hyperparameters would always maximize the model capacity (e.g. more layers, more neurons) resulting in overfitting. The training set alone is not suitable for hyperparameter optimization.

Abbildung 6.5: Hyperparameters explained

Solution for b): Use validation data set D
up to now separating dataset in 2 for training and test, but now split in three parts training set D_{train} (large). test set D_{test}(small) and validation set D_{val} (small, same size as test)

Training set, validation set and test set

Training set D_{train}: It is used for training the model, i.e. learning the model parameters $\underline{\theta}$ (weights and biases) for a fixed hyperparameter vector $\underline{\eta}$.

Validation set D_{val}: It is never used in training. It is reserved for optimizing the hyperparameter parameters $\underline{\eta}$.

Test set D_{test}: It is never used in training and hyperparameter optimization. It is used to calculate the test error of the trained ($\underline{\theta}$) and tuned ($\underline{\eta}$) model $f(\underline{x}; \underline{\theta}, \underline{\eta})$ to exam its generalization capability. The motivations of using the test set are

- to avoid overfitting of $\underline{\theta}$ to the training set and
- to avoid overfitting of $\underline{\eta}$ to the validation set.

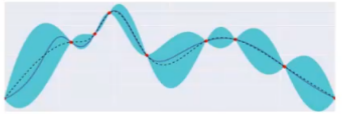
E6.4: Early stopping
Early stopping from ch. 6.3 is a hyperparameter optimization to determine the optimum value of the hyperparameter, the number of epochs. This is only possible by using a validation set because the training error often decreases continuously as the number of epochs increases.

Abbildung 6.6: Summary of data sets

Training: $\underline{\theta}$ and hyperparameter and $\underline{\eta}$
for $\underline{\eta} =$ ..... learn $\underline{\theta}$ of $f(\underline{x}; \underline{\theta}; \underline{\eta})$ frpm D_{train}
calculate validation error $(\underline{\eta})$ on D_{val}
min validation error $(\underline{\eta})$
calculate test error of $f(\underline{x}; \underline{\theta}; \underline{\eta})$ on D_{test}

Hyperparameter optimization approaches

- **Grid search** A blind exhaustive search on a grid in the hyperparameter space, e.g. $M_1 \in \{100, 150, 200\}$, $\phi_l \in \{\text{sigmoid, ReLU}\}$, . . .
  +) simple,
  −) time-consuming, especially for many hyperparameters and a fine grid
- **Bayesian optimization** Treat hyperparameter tuning as an optimization problem
  – probabilistic model for the posterior of the cost function based on Bayes rule (and Gaussian distribution)
  – samples of hyperparameters and cost function: iteratively refine the model
  – posterior: which regions of the hyperparameter space are worth exploring
  – choose next hyperparameter value based on posterior



— target function, - - - predicted function,
• samples, ▬ confidence interval

https://github.com/fmfn/BayesianOptimization:
A Python package ready for use

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Abbildung 6.7: Approaches to optimize hyperparameters