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Abbildungsverzeichnis

List of Equations

Lecture 1: Introduction

Date: 03/05/2020

Lecturer: David Silver *By: Nithish Moudhgalya*

1.1. Overview

•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): $[x_i = \underline{a} + \underline{b}]_i$

1.2. Chapter 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

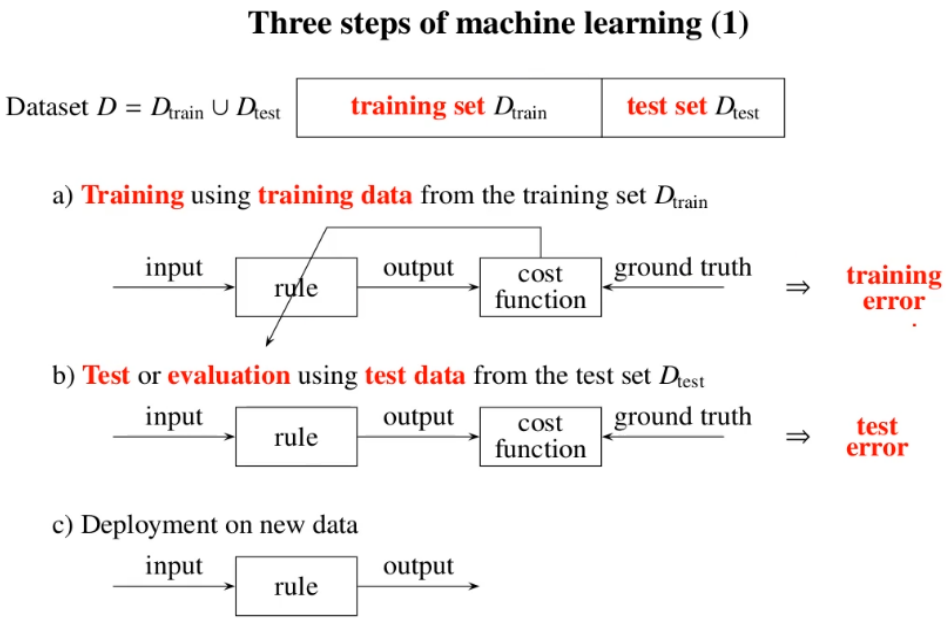

Abbildung 1.2: Three steps of machine learning

•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

1.3. Chapter 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

1.3.1. What is a neural network (NN)

•Cascaded pipeline of layers

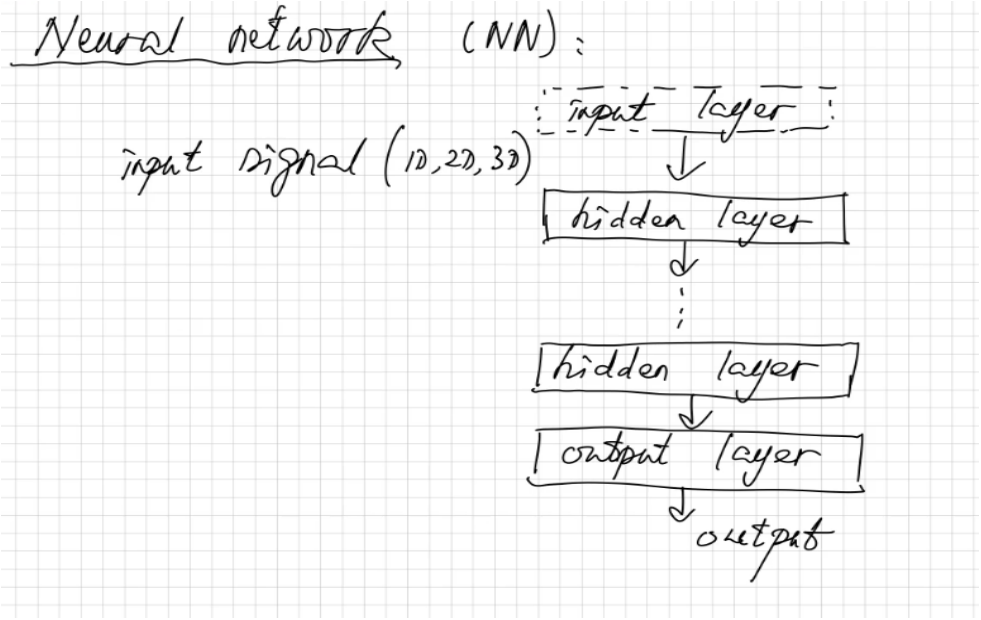

Abbildung 1.3: Neural Network

1.4. Chapter 1.3 - Examples for Deep Learning

•Semantic image segmentation is pixelwise classification

Lecture 2: Tools for Deep Learning	
Date: 02/05/2020	
Lecturer: David Silver	*By: Nithish Moudhgalya*

2.1. Datasets

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

Lecture 3: Machine learning basics	
Date: 02/05/2020	
Lecturer: David Silver	*By: Nithish Moudhgalya*

3.1. Linear Algebra

•TODO get Math nicely into the Context book

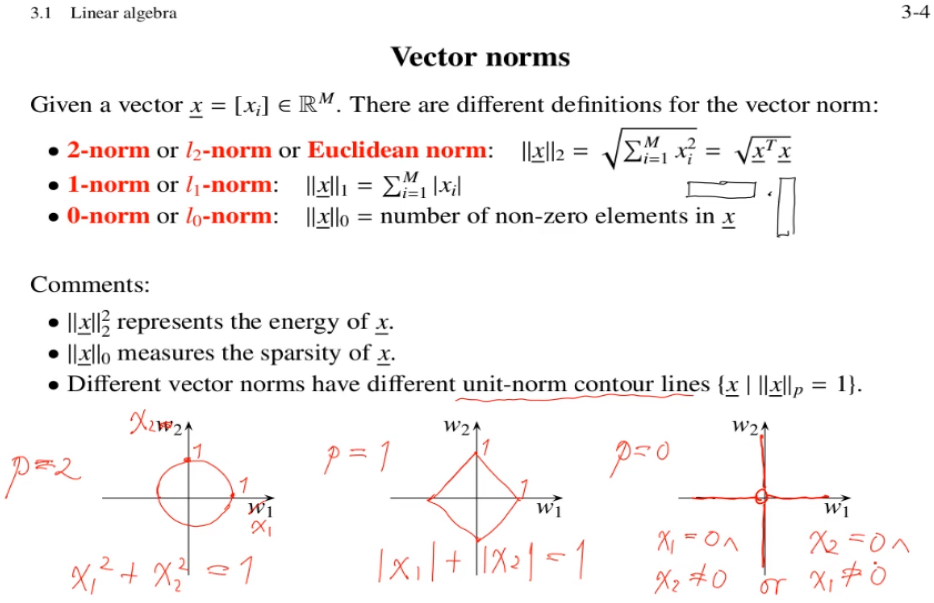

Abbildung 3.1: Vector Normes

3.2. Chapter 3.2 Random variable and probability distribution

3.2.1. 3.2.1 One random vector

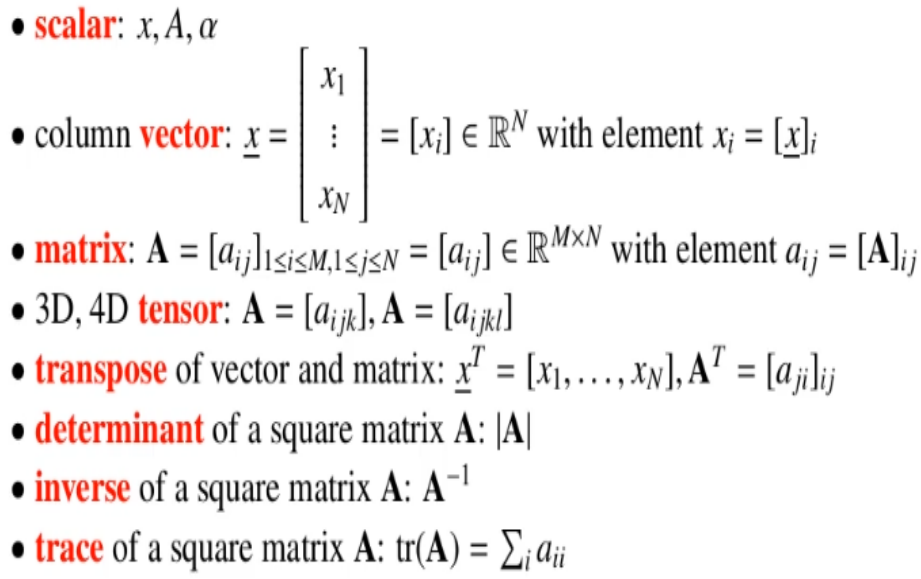

Abbildung 3.2: One random vector

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
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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

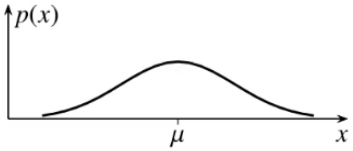
$$\underline{X} \in \mathbb{R}^d \sim N(\underline{\mu}, \mathbf{C})$$

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

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

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

1D-Visualization



Moments

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

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
Reforumulation 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

3.3. Chapter 3.3 - 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)
$P(\underline{x}_1, ..., \underline{x}_N) = \prod_{i=1}^{N} p_i(\underline{x}_i), \underline{X}_i \sim p_i(\underline{x}_i)$
$p_i(\underline{x}_i) = p(\underline{x}_i) \rightarrow p(\underline{x}_1, ..., \underline{x}_N) = \prod_{i=1}^{N} p(\underline{x}_i)$

3.3.1. Chapter 3.2.3 - Kernel basaed density estimation

PDF: $p(\underline{x})$ of $\underline{X} \in \boldsymbol{R}^d$ 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. $\int k(\underline{x}) d\underline{x} = 1$
$\hat{p}(\underline{x}) = \frac{1}{N} \sum_{n=1}^{N} k(\underline{x} - \underline{x}(n))$

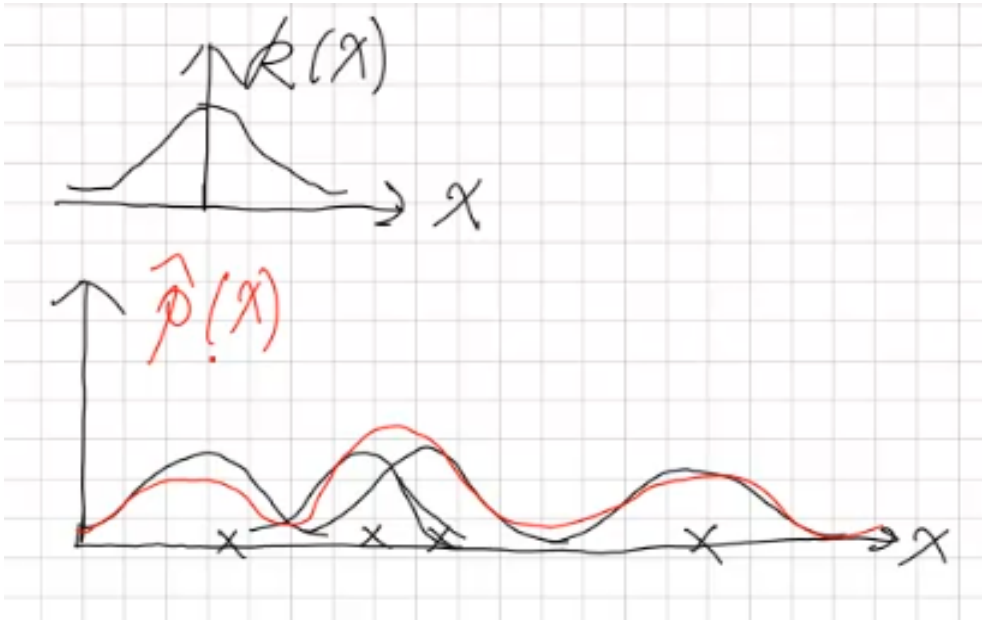


Abbildung 3.5: Kernel function

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

3.4. Chapter 3.4 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": $ln(\frac{p(\underline{x})}{q(\underline{x})}) = 0 \forall \underline{x}$

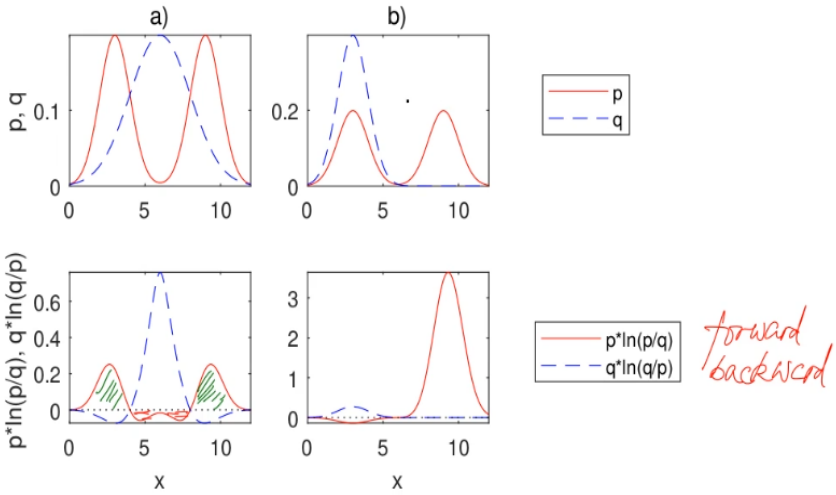
P1 and P2: $D_{KL}(p||1)$ is a suitable metric for approximation p by q

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.

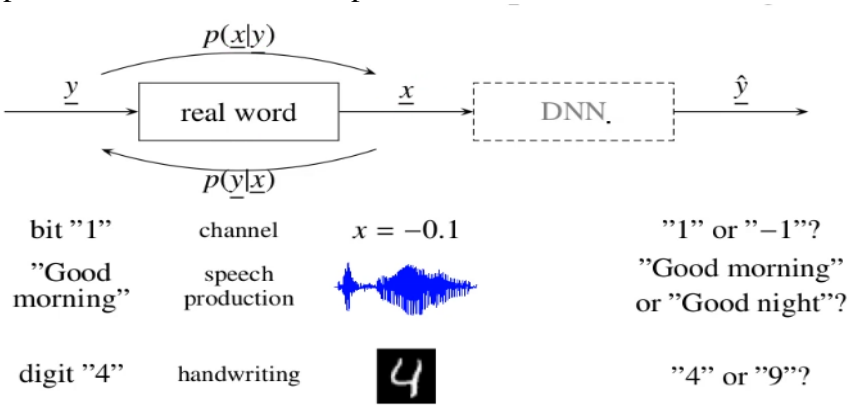
Abbildung 3.7: Forward vs. Backward KL divergence

3.4.1. 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

3.5. Chapter 3.5 Probabilistic framework

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:

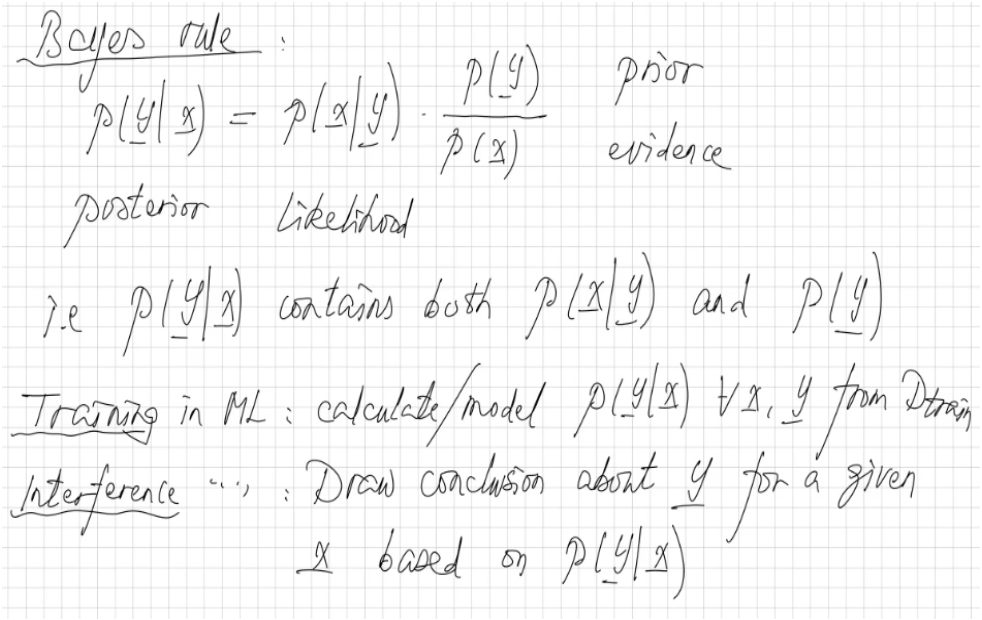


Abbildung 3.10: Bayes Rule in DL

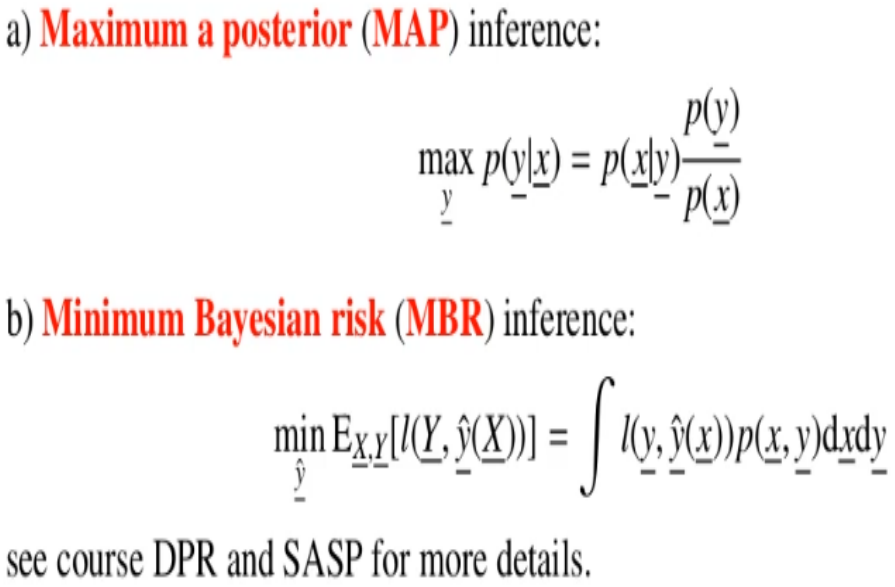


Abbildung 3.11: Bayes decision theorem

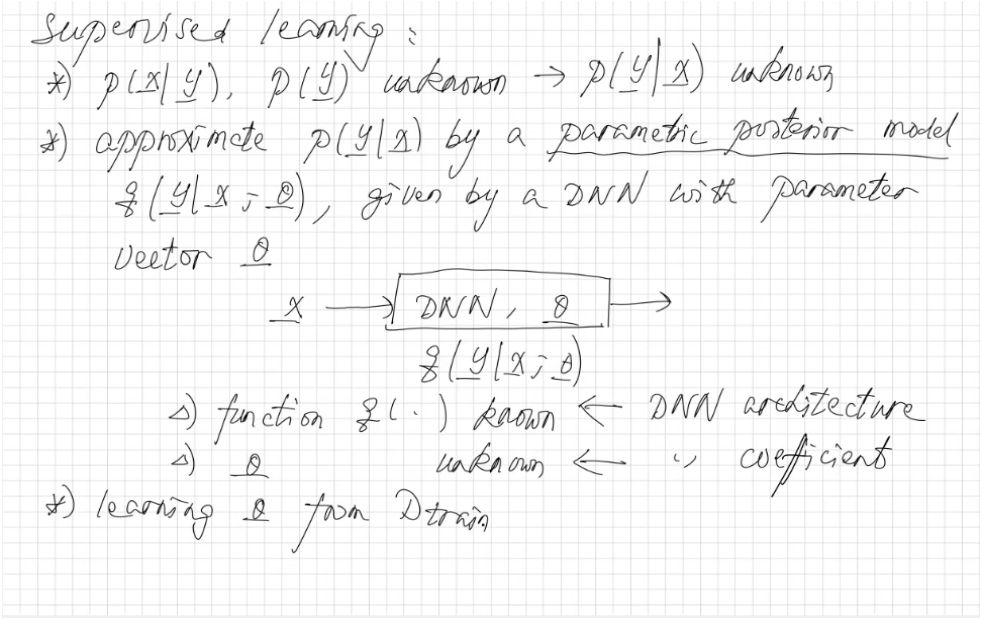


Abbildung 3.12: Supervised learning

Learning Criterion:

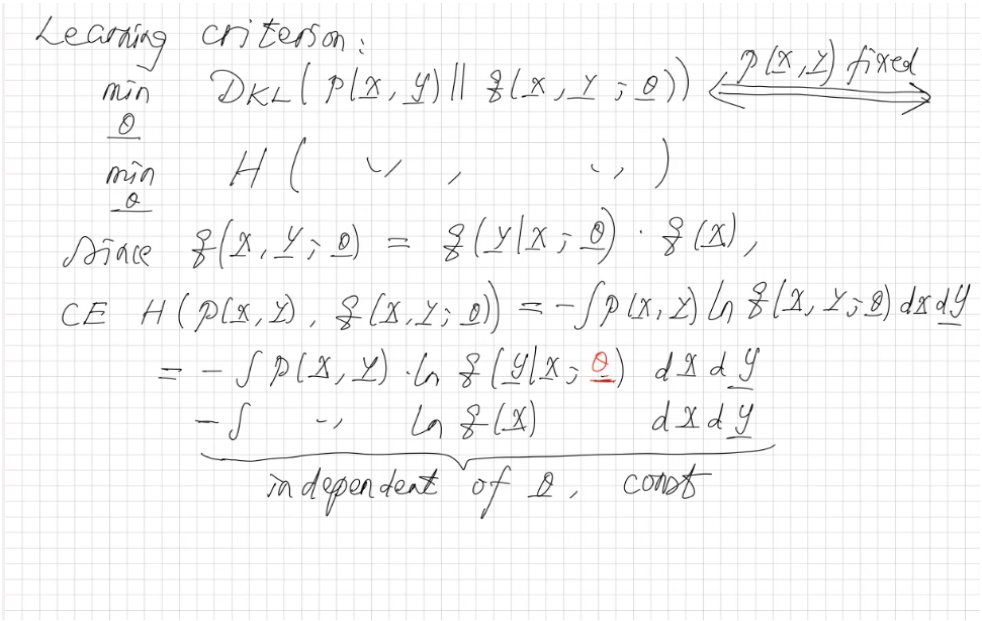


Abbildung 3.13: Calc part1

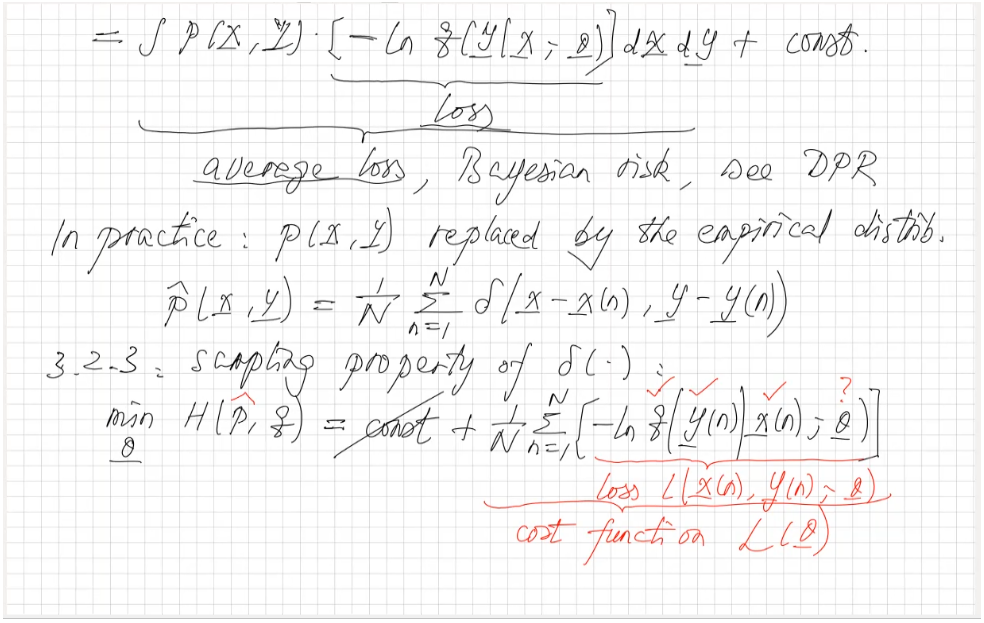


Abbildung 3.14: Calc part2

3.5.1. 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}

Lecture 4: Dense Neural Networks	
Date: 05/05/2020	
Lecturer: David Silver	*By: Nithish Moudhgalya*

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)

4.0.1. 4.1 Fully connected neural networks - Neuron

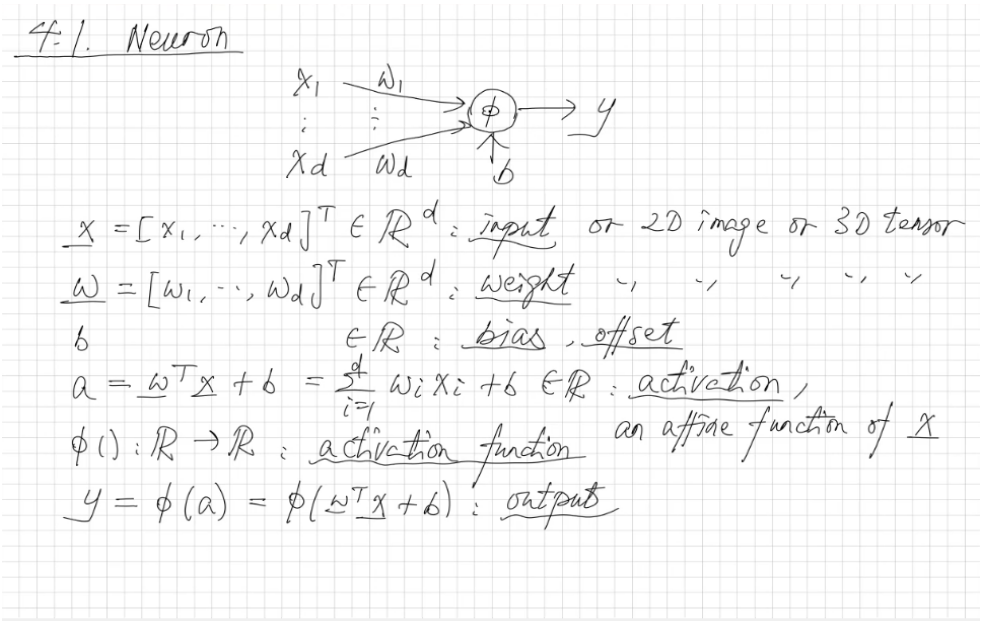


Abbildung 4.1: Neuron

4.0.2. Chapter 4.2 Layer of Nurons

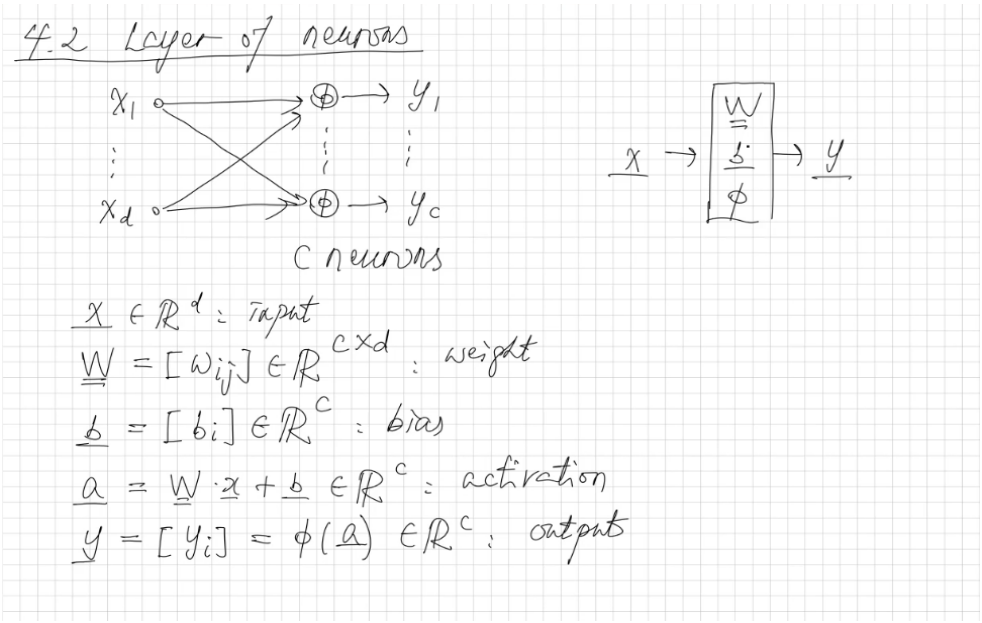


Abbildung 4.2: Layer of Neurons

2 meanings of $\phi()$:

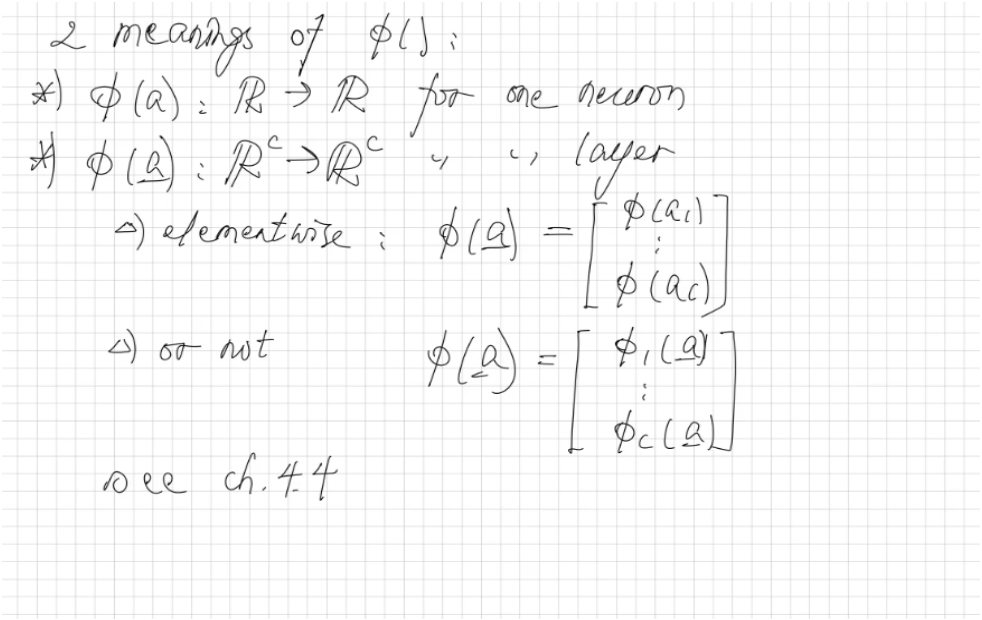


Abbildung 4.3: Meanings of phi

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

4.1. 4.3 Feedforward neural network

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

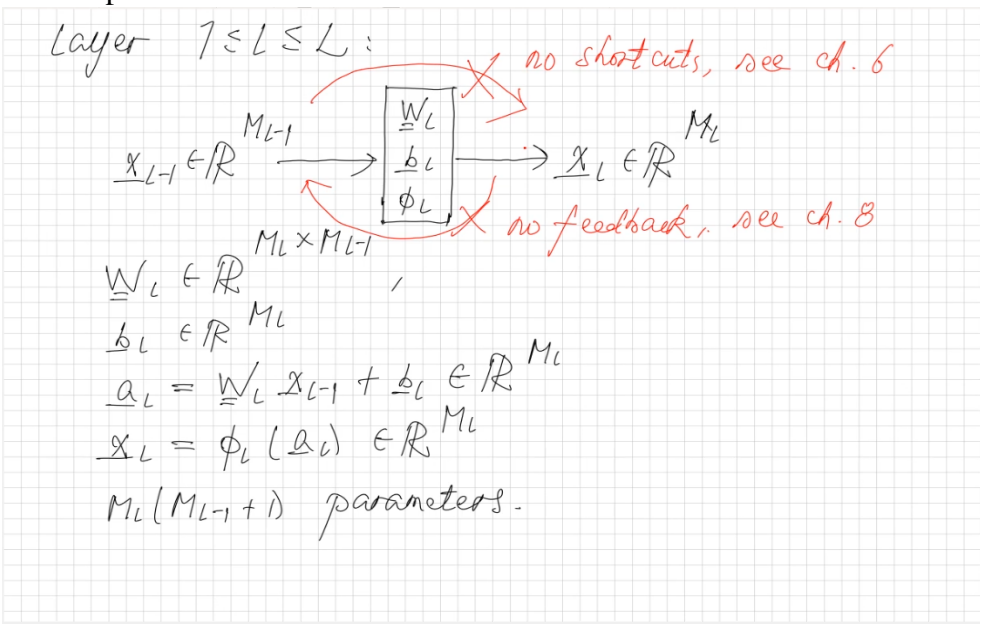


Abbildung 4.4: Feedforward multilayer neural network

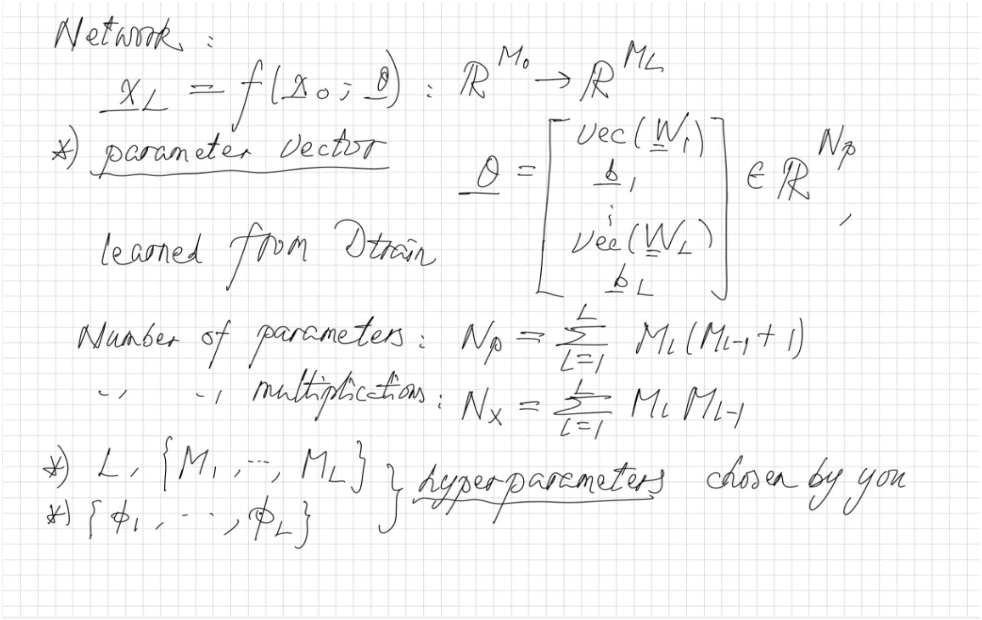


Abbildung 4.5: Network Parameters

Lecture 4: Dense Neural Networks

Date: 15/05/2020

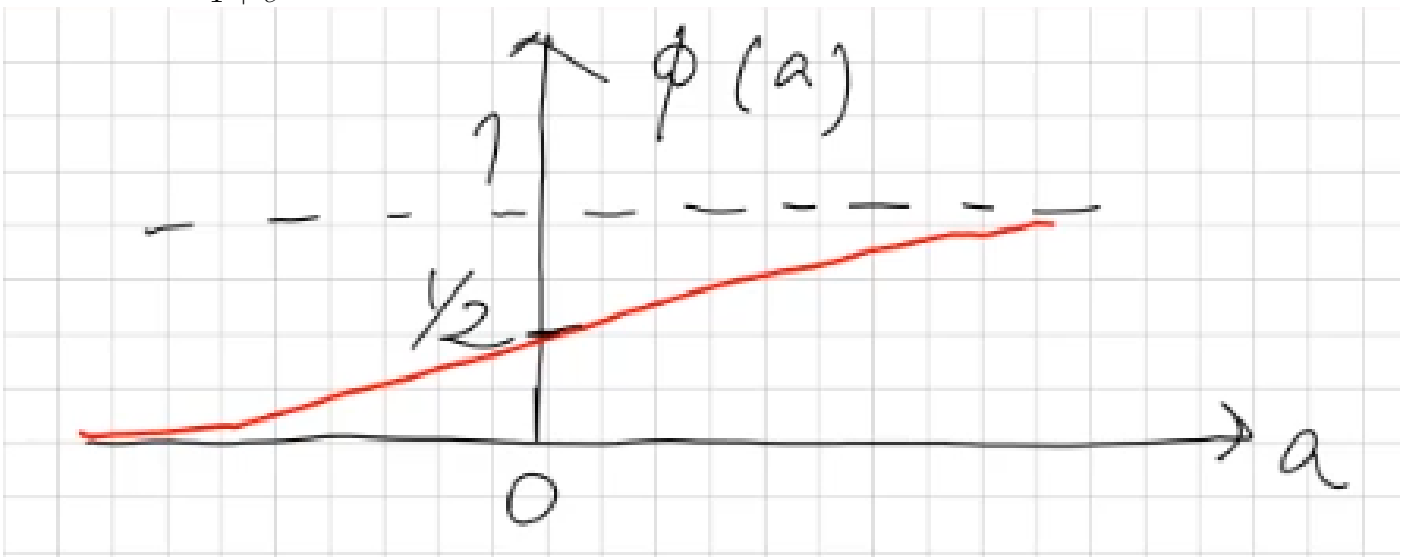
Lecturer: David Silver *By: Nithish Moudhgalya*

5.1. 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

5.1.1. Sigmoid activation function

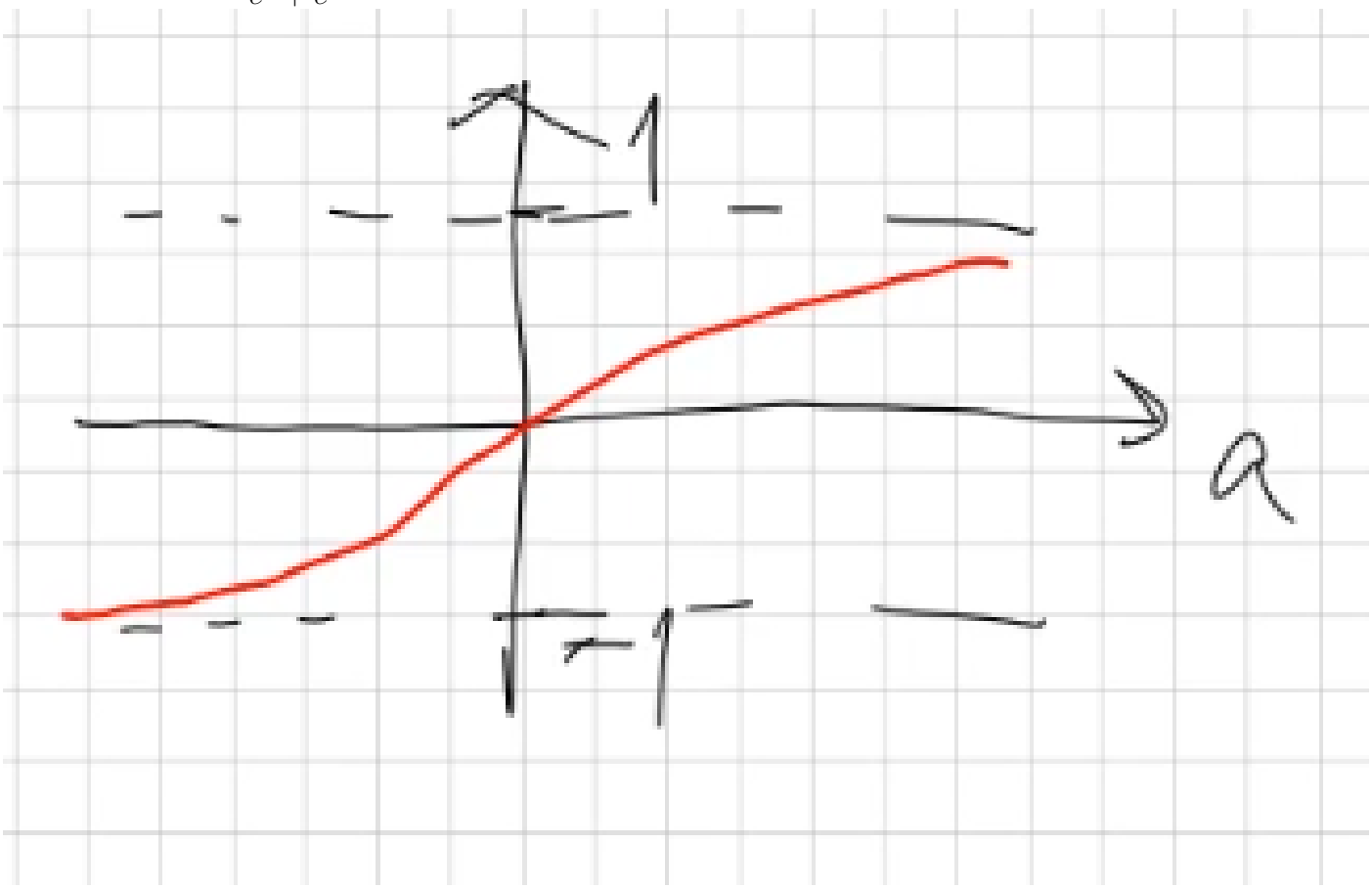
$\phi(a) = \sigma(a) = \frac{1}{1+e^{-a}}$



•$0 < \phi < 1 \hat{=}$ 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)

5.1.2. hyperbolic tangent activation function

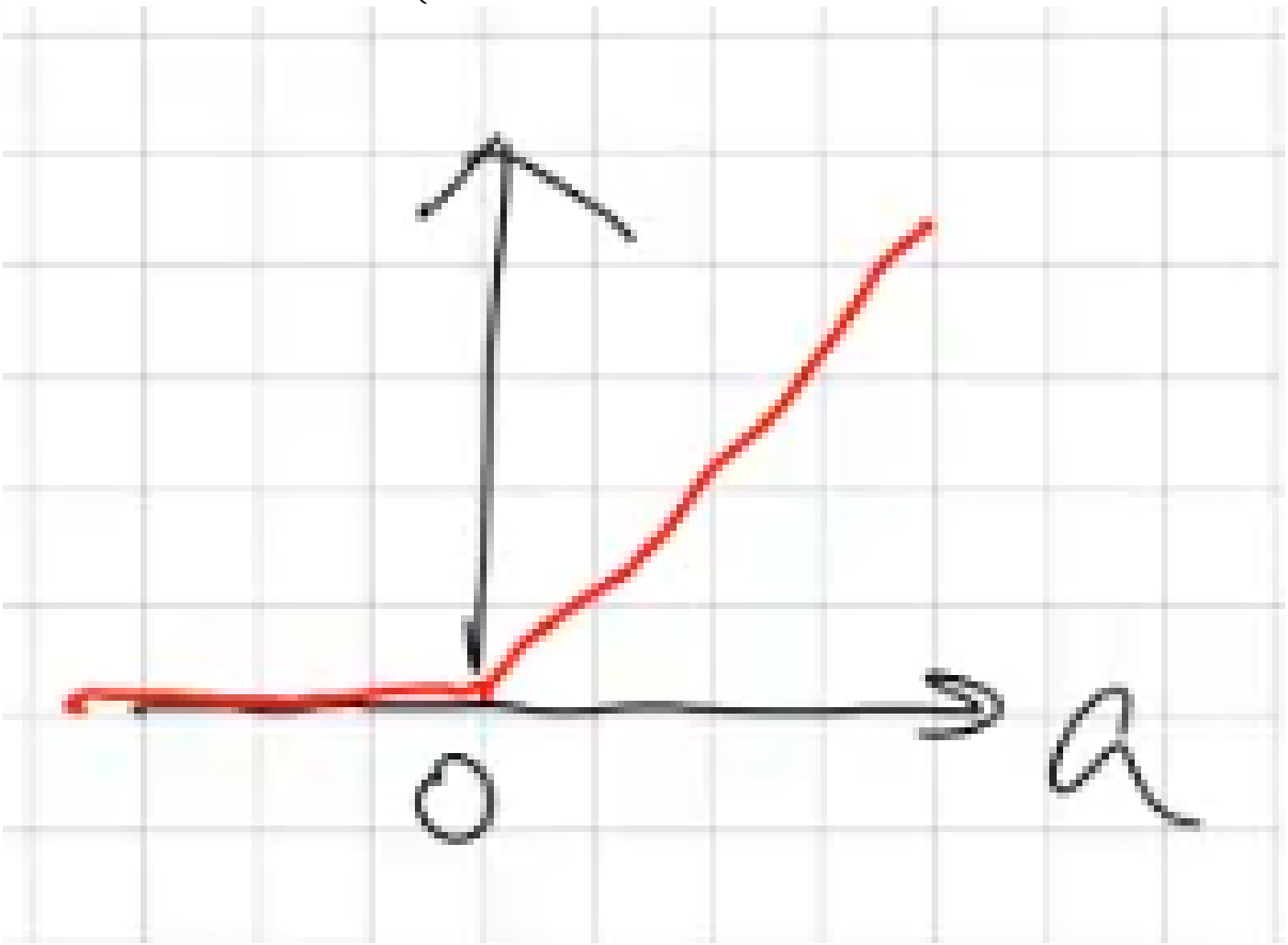
$$\phi(a) = tanh(a) = \frac{e^a - e^{-a}}{e^a + e^{-a}}$$



like sigmoid but another output range

5.1.3. rectifier linear unit(ReLU

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



•$\equiv$ 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

5.1.4. Softmax activatoin function(classification problem)

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

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

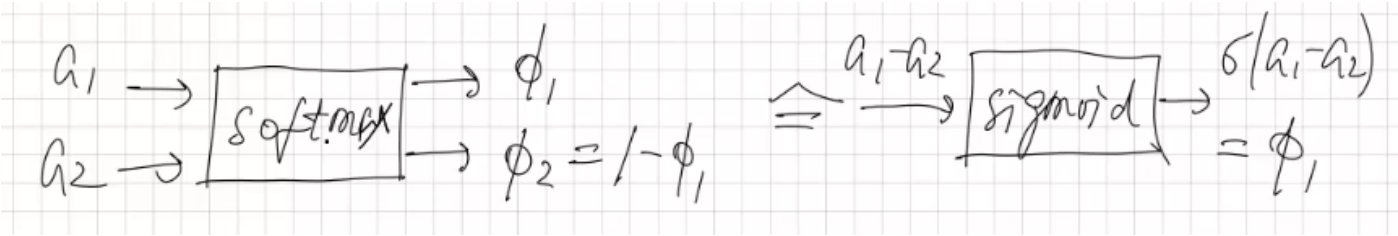
$\phi(\underline{a}) = \frac{a^{a_i}}{\sum_{j=1}^{c} e^{a_i}}, \in (0, 1), \sum_{i=1}^{c} \phi_i(\underline{a}) = 1$
•maps $\underline{a} \in \Re^c$ to a categorical PMF with c classes
•a_i large$\rightarrow$ $\phi_i(\underline{a})$ close to 1
•a_i small $\rightarrow$ $\phi_i(\underline{a})$ close to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

5.2. 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



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

5.3. Chapter 4.5 Universal approximation

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}:

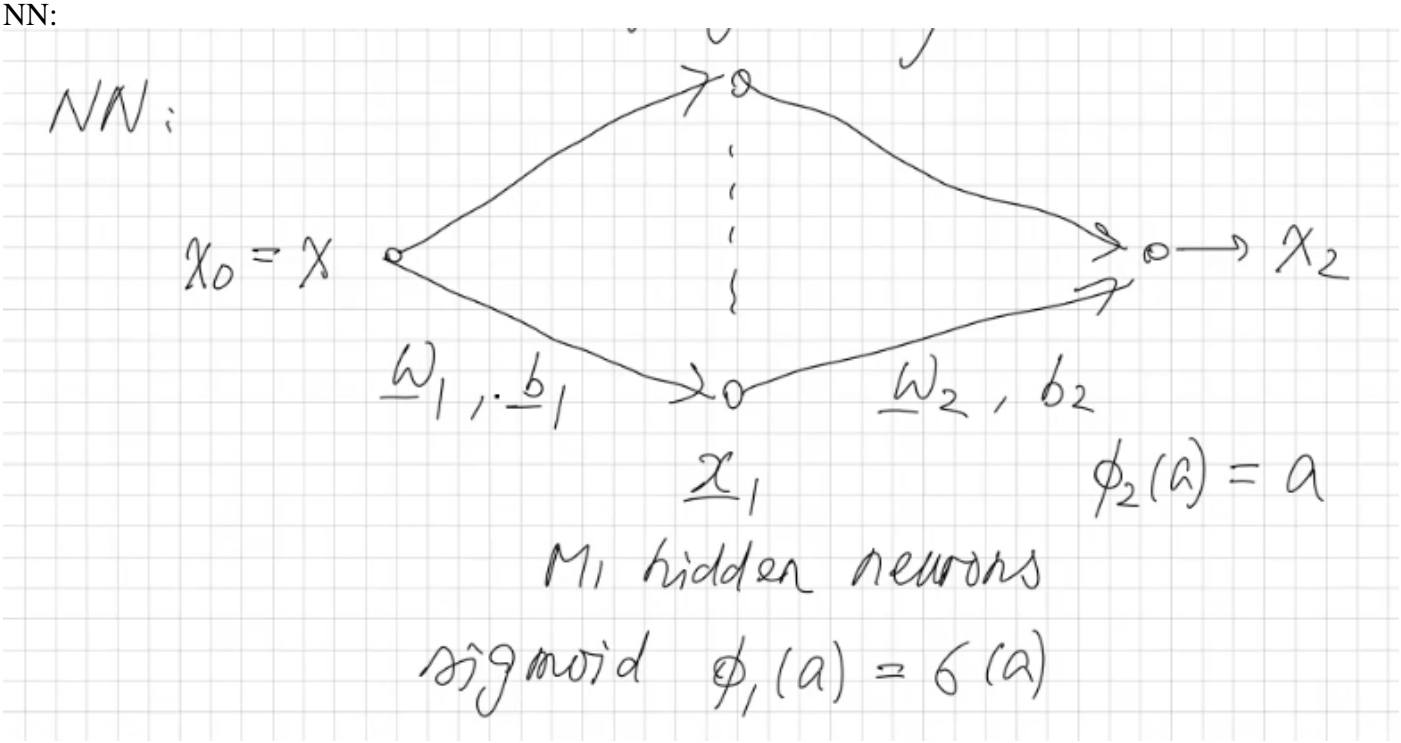
- deep networks are better than shallow ones,
- some activation functions are better than others.

≙ how to find a good solution.

+

5.3.1. 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:

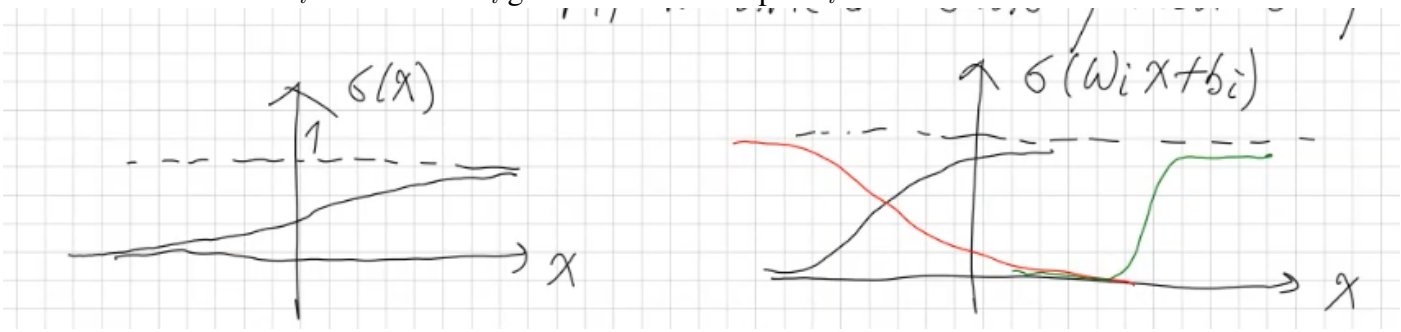


i.e. $x_2 = f(x, \underline{\theta}) = \underline{w}_2^T \sigma(\underline{w}_1 x + \underline{b}_1)$, column times row times scalar
$= \sum_{i=1}^{N_1} w_{2,i} \cdot \underbrace{\sigma(w_{1,i}x + b_{1,i})}_{M_1 \text{ nonllinear basis functions of } x} + b_2$

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

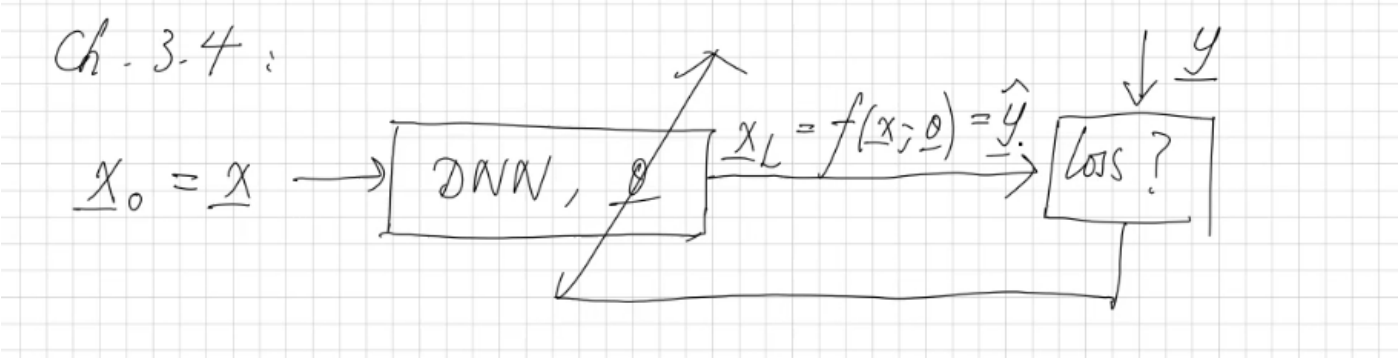
new center at $\frac{-b_i}{w_i}$ and new slope value w_i

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



5.4. Chapter 4.4 - 4.6 Loss and cost function

Review chapter 3.4



$\min_{\underline{\theta}} L(\underline{\theta}) = \frac{1}{N} = \sum_{n=1}^{N} (l(\underline{x}(n), y(n)_i \underline{\theta}$ 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: : $\underline{z} \sim N(\underline{0}, \sigma^2 \underline{\underline{I}})$, white Gaussian noise
$\underline{y} \sim N(f(\underline{x}, \underline{\theta}), \sigma^2 \underline{\underline{I}})$
$q(\underline{y}|\underline{x}, \underline{\theta}) = \frac{1}{(2\pi\sigma^2)^{c/2}} exp(\frac{-1}{2\sigma^2} ||\underline{y} - f(\underline{x}, \underline{\theta})||^2)$
$l(\underline{x}, \underline{y}, \underline{\theta}) = -ln(q(\underline{y}|\underline{x}, \underline{\theta})) = const. + \frac{1}{\sigma^2} ||\underline{y} - f(\underline{x}, \underline{\theta})||^2$
$L(\underline{\theta}) = \frac{1}{N} \sum_{n=1}^{N} ||\underline{y}(n) - f(\underline{x}, \underline{\theta})||^2$
$\rightarrow l_2 - loss$, 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

5.4.1. 4.6.3 Semantic segmentation

pixelwise classification
categorical cross entropy loss:
$l(\underline{\underline{X}}, \underline{\underline{Y}}; \underline{\theta}) = \sum_{m=1}^{M} \sum_{n=1}^{N} [-\underline{y}_{mn} \cdot ln(\underline{\hat{y}}_{mn}(\underline{\underline{X}}, \underline{\theta}))]$ 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 $\underline{\hat{y}}$ contains real numbers $\in (0,1) \in softmax$
$\rightarrow$ 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

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

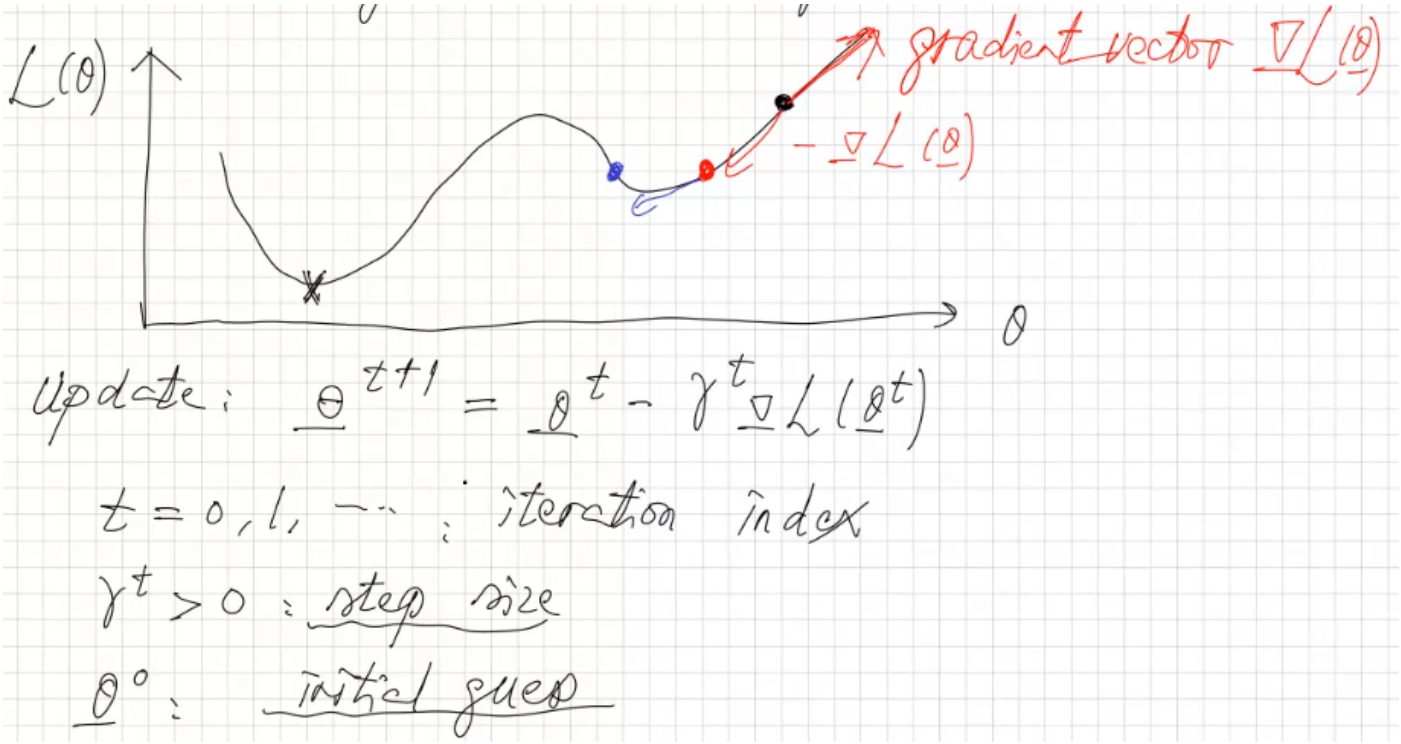
$\odot$ is the elementwise multiplication. α_i and β_i represent arithmetic calculations of $|A_i \cap B_i|$ and $|A_i| + |B_i|$ for class i, respectively. J_i is the soft Jaccard index for class i where $\epsilon > 0$ is a suitable number to avoid $0/0$ if $\alpha_i = \beta_i = 0$. $l(\mathbf{X}, \mathbf{Y};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

Very good for strongly imbalanced classes

5.5. Chapter 4.7 Training

•training set $_{train} = \{\underline{x}, \underline{y}, 1 \leq n \leq N\}$
•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 $L(\underline{\theta})$



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

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

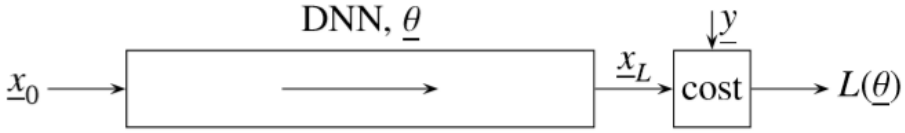
Layer $L-1$:

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

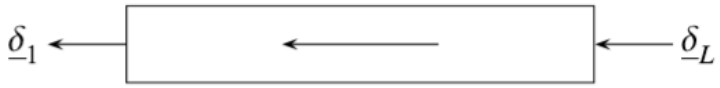
Layer 1: $\frac{\partial L(\underline{\theta})}{\partial w_{1,ij}} = \underline{\underline{J}}_L(\underline{a}_L) \cdot \underline{\underline{J}}_{\underline{a}_L}(\underline{a}_{L-1}), ..., \underline{\underline{J}}_{\underline{a}_2}(\underline{a}_1) \cdot \underline{\underline{J}}_{\underline{a}_1}(w_{1,ij})$

Forward pass vs. backward pass in DNN

Forward pass to calculate $\underline{x}_L$ from $\underline{x}_0$:



Backward pass or **backpropagation** of so called **error vectors** $\underline{\delta}_l^T := \mathbf{J}_L(\underline{a}_l) = \frac{\partial L(\underline{\theta})}{\partial \underline{a}_l} \in \mathbb{R}^{1 \times M_l}$:



For $l = L-1, \ldots, 1$

$$\underline{\delta}_l^T = \underline{\delta}_{l+1}^T \cdot \mathbf{J}_{\underline{a}_{l+1}}(\underline{x}_l)\mathbf{J}_{\underline{x}_l}(\underline{a}_l) = \square \cdot \square$$

$$\frac{\partial L(\underline{\theta})}{\partial w_{l,ij}} = \underline{\delta}_l^T \cdot \mathbf{J}_{\underline{a}_l}(w_{l,ij}) = \square \cdot \square$$

$$\frac{\partial L(\underline{\theta})}{\partial b_{l,i}} = \underline{\delta}_l^T \cdot \mathbf{J}_{\underline{a}_l}(b_{l,i}) = \square \cdot \square$$

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