technische universität dortmund

Computational Intelligence

Winter Term 2022/23

Prof. Dr. Günter Rudolph

Lehrstuhl für Algorithm Engineering (LS 11)

Fakultät für Informatik

TU Dortmund

Plan for Today

- Deep Neural Networks
  - Model
  - Training
- Convolutional Neural Networks
  - Model
  - Training

Deep Neural Networks (DNN)

DNN = Neural Network with > 3 layers

we know: L = 3 layers in MLP sufficient to describe arbitrary sets

What can be achieved by more than 3 layers?

information stored in weights of edges of network

→ more layers → more neurons → more edges → more information storable

Which additional information storage is useful?

traditionally : handcrafted features fed into 3-layer perceptron

modern viewpoint : let L-k layers learn the feature map, last k layers separate!

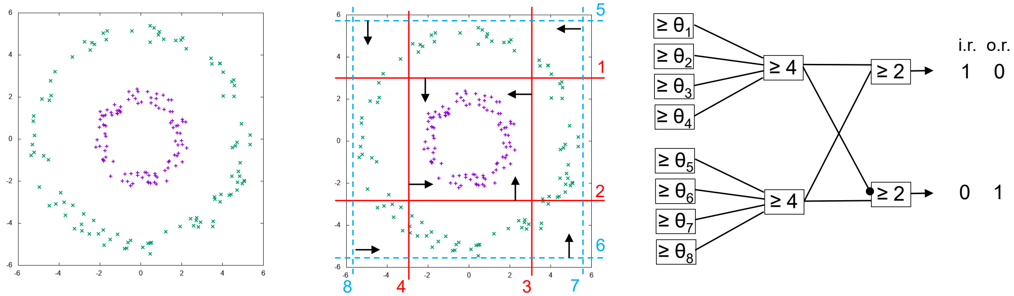
advantage:

human expert need not design features manually for each application domain

⇒ no expert needed, only observations!

Deep Neural Networks (DNN)

example: separate ‘inner ring‘ (i.r.) / ‘outer ring‘ (o.r.) / ‘outside‘



⇒ MLP with 3 layers and 12 neurons

Is there a simpler way?

observations $(x,y) \in \mathbb{R}^n \times \mathbb{B}$ feature map $F(x) = (F_1(x), \ldots, F_m(x)) \in \mathbb{R}^m$

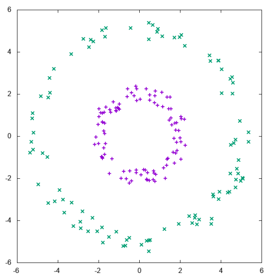
feature = measurable property of an observation or numerical transformation of observed value(s)

⇒ find MLP on transformed data points (F(x), y)

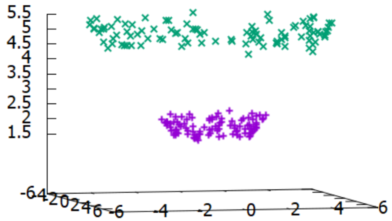
Deep Neural Networks (DNN) — Lecture 12

example: separate 'inner ring' / 'outer ring'

- feature map $F(x) = (x_1, x_2, \sqrt{x_1^2 + x_2^2}) \in \mathbb{R}^3$

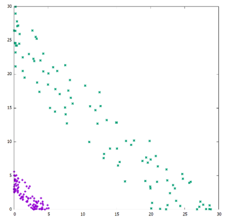


2D → 3D



- feature map $F(x) = (x_1^2, x_2^2) \in \mathbb{R}^2$

x_1^2, x_2^2 → θ ≥ 9 → { 1: outer; 0: inner }



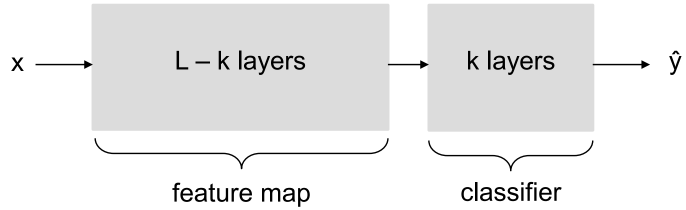
Deep Neural Networks (DNN) — Lecture 12

but: how to find useful features?

→ typically designed by experts with domain knowledge

→ traditional approach in classification:
1. design & select appropriate features
2. map data to feature space
3. apply classification method to data in feature space

modern approach via DNN: learn feature map and classification simultaneously!



proven: MLP can approximate any continuous map with aribitrary accuracy

Deep Multi-Layer Perceptrons — Lecture 12

contra:
- danger: overfitting
  → need larger training set (expensive!)
  → optimization needs more time
- response landscape changes
  → more sigmoidal activiations
  → gradient vanishes
  → small progress in learning weights

countermeasures:
- regularization / dropout
  → data augmentation
  → parallel hardware (multi-core / GPU)
- not necessarily bad
  → change activation functions
  → gradient does not vanish
  → progress in learning weights

vanishing gradient: (underlying principle)

forward pass $y = f_3(f_2(f_1(x; w_1); w_2); w_3)$ f_i ≈ activation function

backward pass $(f_3(f_2(f_1(x; w_1); w_2); w_3))' =$
$f_3'(f_2(f_1(x;w_1);w_2);w_3) \cdot f_2'(f_1(x;w_1);w_2) \cdot f_1'(x;w_1)$ ***chain rule!***

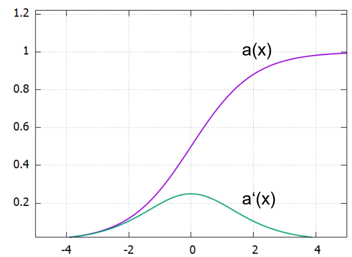
→ repeated multiplication of values in (0,1) → 0

Deep Multi-Layer Perceptrons — Lecture 12

vanishing gradient: $a(x) = \frac{e^x}{e^x+1} = \frac{1}{1+e^{-x}} \quad \to \quad a'(x) = a(x)\cdot(1-a(x))$

$\forall x \in \mathbb{R}: \quad a(x)\cdot(1-a(x)) \le \frac{1}{4} \quad \Leftrightarrow \quad \left(a(x) - \frac{1}{2}\right)^2 \ge 0$ ☑

⇒ gradient $a'(x) \in [0, \frac{1}{4}]$



principally: desired property in learning process!
if weights stabilize such that neuron almost always either fires [i.e., a(x) ≈ 1] or not fires [i.e., a(x) ≈ 0] then gradient ≈ 0 and the weights are hardly changed

⇒ leads to convergence in the learning process!

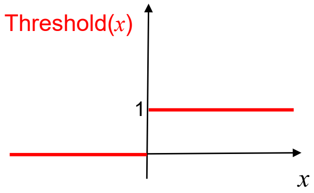
while learning, updates of weights via partial derivatives:

$$\frac{\partial f(w,u;x,z^*)}{\partial w_{ij}} = 2\sum_{k=1}^{K}[a(u_k'y) - z_k^*] \cdot \underbrace{a'(u_k'y)}_{\le \frac{1}{4}} \cdot u_{jk} \cdot \underbrace{a'(w_j'x)}_{\le \frac{1}{4}} \cdot x_i \qquad \text{(L= 2 layers)}$$

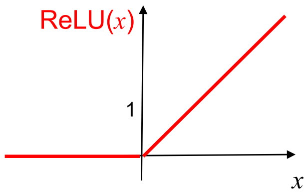
⇒ in general $f_{w_{ij}} = O(4^{-L}) \to 0$ as $L\uparrow$ $\quad L \le 3$: effect neglectable; but $L \gg 3$ ☒

non-sigmoid activation functions

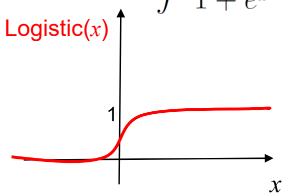
$$\int \mathbb{1}_{[x \geq 0]}(x)\, dx = \left\{ \begin{array}{ll} 0 & \text{if } x < 0 \\ x & \text{if } x \geq 0 \end{array} \right\} = \max\{0, x\} = \text{ReLU}(x)$$



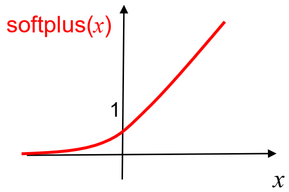
⇒



$$\int \frac{e^x}{1+e^x}\, dx = \log(1+e^x) = \text{softplus}(x)$$



⇒



dropout

- applied for regularization (against overfitting)
- can be interpreted as inexpensive approximation of **bagging**

↓

aka: bootstrap aggregating, model averaging, ensemble methods

create k training sets by drawing with replacement
train k models (with own exclusive training set)
combine k outcomes from k models (e.g. majority voting)

- parts of network is effectively switched off
  e.g. multiplication of outputs with 0,
  e.g. use inputs with prob. 0.8 and inner neurons with prob. 0.5
- gradient descent on switching parts of network
  → artificial perturbation of greediness during gradient descent
- can reduce computational complexity if implemented sophistically

data augmentation (counteracts overfitting)

→ extending training set by slightly perturbed true training examples

- best applicable if inputs are **images**: translate, rotate, add noise, resize, …


original image


rotated


resized


noisy


noisy + rotated

- if x is **real vector** then adding e.g. small gaussian noise
  → here, utility disputable (artificial sample may cross true separating line)

extra costs for acquiring additional annotated data are **inevitable**!

stochastic gradient descent

- partitioning of training set B into **(mini-) batches** of size b

<u>traditionally:</u> 2 extreme cases

update of weights
- after each training example b = 1
- after all training examples b = |B|

<u>now:</u>

update of weights
- after b training examples where 1 < b < |B|

- search in subspaces → counteracts greediness → better generalization
- accelerates optimization methods (parallelism possible)

choice of batch size b
b large ⇒ better approximation of gradient
b small ⇒ better generalization

b also depends on available hardware
b too small ⇒ multi-cores underemployed

} often b ≈ 100 (empirically)

cost functions

- *regression*

  N training samples (x_i, y_i)

  insist that $f(x_i; \theta) = y_i$ for i=1,…, N

  if $f(x; \theta)$ linear in θ then $\theta^T x_i = y_i$ for i=1,…, N or $X \theta = y$

  $\Rightarrow$ best choice for θ: least square estimator (LSE)

  $\Rightarrow (X \theta - y)^T (X \theta - y) \underset{\theta}{\rightarrow} \min!$

  in case of MLP: $f(x; \theta)$ is <u>nonlinear</u> in θ

  $\Rightarrow$ best choice for θ: (nonlinear) least square estimator; aka TSSE

  $\Rightarrow \sum_i (f(x_i; \theta) - y_i)^2 \underset{\theta}{\rightarrow} \min!$

cost functions

- *classification*

  N training samples (x_i, y_i) where $y_i \in$ { 1, …, C }, C = #classes

  → want to estimate probability of different outcomes for unknown sample

  → decision rule: choose class with highest probability (given the data)

  <u>idea</u>: use maximum likelihood estimator (MLE)

  = estimate unknown parameter θ such that likelihood of sample $x_1, \ldots, x_N$ gets maximal as a function of θ

  <u>likelihood function</u>

  $$L(\theta; x_1, \ldots, x_N) := f_{X_1,\ldots,X_N}(x_1, \ldots, x_N; \theta) = \prod_{i=1}^{N} f_X(x_i; \theta) \underset{\theta}{\rightarrow} \max!$$

here: random variable X $\in$ {1, …, C } with P{ X = i } = q_i (true, but unknown)

→ we use relative frequencies of training set $x_1, \ldots, x_N$ as estimator of q_i

$$\hat{q}_i = \frac{1}{N} \sum_{j=1}^{N} 1_{[x_j = i]}$$ $\Rightarrow$ there are $N \cdot \hat{q}_i$ samples of class i in training set

$\Rightarrow$ the neural network should output $\hat{p}$ as close as possible to $\hat{q}$! [actually: to q]

likelihood $L(\hat{p}; x_1, \ldots, x_N) = \prod_{k=1}^{N} P\{X_k = x_k\} = \prod_{i=1}^{C} \hat{p}_i^{N \cdot \hat{q}_i} \rightarrow \max!$

$$\log L = \log \left(\prod_{i=1}^{C} \hat{p}_i^{N \cdot \hat{q}_i} \right) = \sum_{i=1}^{C} \log \hat{p}_i^{N \cdot \hat{q}_i} = N \underbrace{\sum_{i=1}^{C} \hat{q}_i \cdot \log \hat{p}_i}_{-H(\hat{q}, \hat{p})} \rightarrow \max!$$

$\Rightarrow$ maximizing $\log L$ leads to same solution as minimizing **cross-entropy** $H(\hat{q}, \hat{p})$

in case of *classification*

use softmax function $P\{y = j \,|\, x\} = \dfrac{e^{w_j^T x + b_j}}{\sum_{i=1}^{C} e^{w_i^T x + b_i}}$ in output layer

→ multiclass classification: probability of membership to class j = 1, …, C

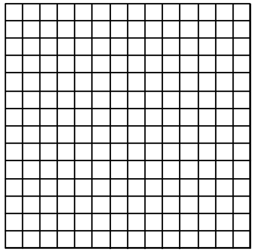
→ class with maximum excitation w'x+b has maximum probabilty

→ decision rule: element x is assigned to class with maximum probability most often used in graphical applications (2-D input; also possible: k-D tensors)

layer of CNN = 3 stages

1. convolution
2. nonlinear activation (e.g. ReLU)
3. pooling

I(x,y)



K(i,j)

$-\delta$		δ	
-1	-2	-1	$-\delta$
1	1	1	
-2	1	-2	δ

example

1. Convolution

local filter / kernel K(i, j) applied to each cell of image I(x, y)

$$S(x,y) = (K * I)(x,y) = \sum_{i=-\delta}^{\delta} \sum_{j=-\delta}^{\delta} I(x+i, y+j) \cdot K(i,j)$$

example: edge detection with Sobel kernel

→ two convolutions

$$K_x = \begin{pmatrix} -1, & 0, & 1 \\ -2, & 0, & 2 \\ -1, & 0, & 1 \end{pmatrix} \quad K_y = \begin{pmatrix} -1, & -2, & -1 \\ 0, & 0, & 0 \\ 1, & 2, & 1 \end{pmatrix}$$

yields S_x yields S_y

$$S(x,y) = \sqrt{S_x(x,y)^2 + S_y(x,y)^2}$$

original image I(x,y)

image S(x,y) after convolution

filter / kernel

well known in image processing; typically hand-crafted!

here: values of filter matrix learnt in CNN !

actually: many filters active in CNN

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 \end{pmatrix}$$

e.g. horizontal line detection

stride

= distance between two applications of a filter (horizontal s_h / vertical s_v)

→ leads to smaller images if s_h or $s_v > 1$

padding

= treatment of border cells if filter does not fit in image

- "valid" : apply only to cells for which filter fits → leads to smaller images
- "same" : add rows/columns with zero cells; apply filter to all cells (→ same size)

2. nonlinear activation

$a(x) = \text{ReLU}(x^T W + c)$

3. pooling

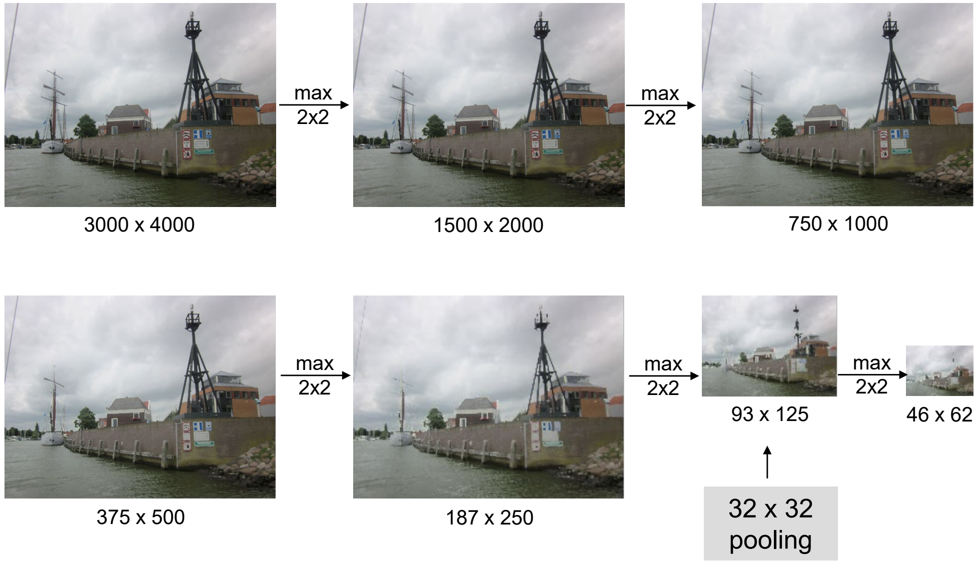
in principle: summarizing statistic of nearby outputs

e.g. **max-pooling** m(i,j) = max(I(i+a, j+b) : a,b = -δ, …, 0, … δ) for δ > 0

- also possible: mean, median, matrix norm, …

- can be used to reduce matrix / output dimensions

example: max-pooling 2x2 (iterated), stride = 2

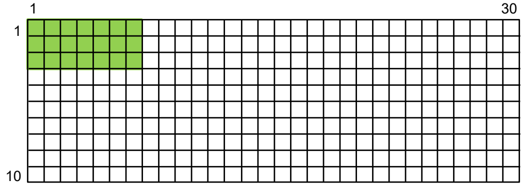


Pooling with Stride

c_{in} : columns of input
r_{in} : rows of input
f_c : columns of filter
f_r : rows of filter
s_c : stride for columns
s_r : stride for rows

image size : $r_{in} \times c_{in}$
filter size : $f_r \times f_c$

<u>assumptions:</u>
$f_c \le c_{in}$
$f_r \le f_{in}$
`padding = valid`



How often fits the filter in image horizontally?

$pos_1 = 1$
$pos_2 = pos_1 + s_c$
$pos_3 = pos_2 + s_c = (pos_1 + s_c) + s_c = pos_1 + 2 \cdot s_c$
⋮
$pos_k = pos_1 + (k-1) \cdot s_c$

thus, find largest k such that

$pos_1 + (k-1) \cdot s_c + (f_c - 1) \le c_{in}$
$\Leftrightarrow \quad (k-1) \cdot s_c + f_c \le c_{in}$
$\Leftrightarrow \quad k \le (c_{in} - f_c) / s_c + 1$ (integer division!)

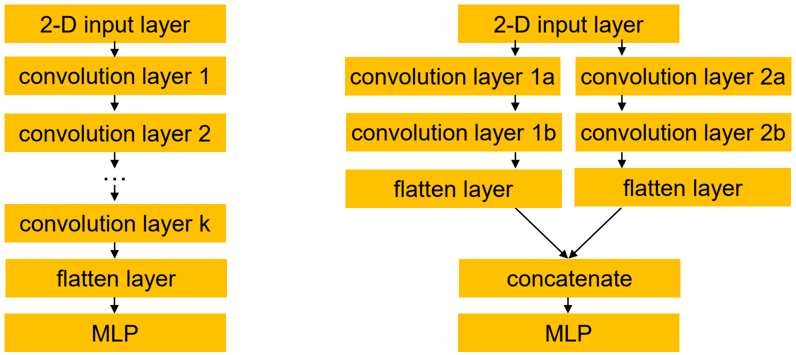
$$\Rightarrow \quad k = \left\lfloor \frac{c_{in} - f_c}{s_c} \right\rfloor + 1 = c_{out}$$

[analog reasoning for rows!]

CNN architecture:

- several consecutive convolution layers (also parallel streams); possibly dropouts
- flatten layer (→ converts k-D matrix to 1-D matrix required for MLP input layer)
- fully connected MLP

examples:



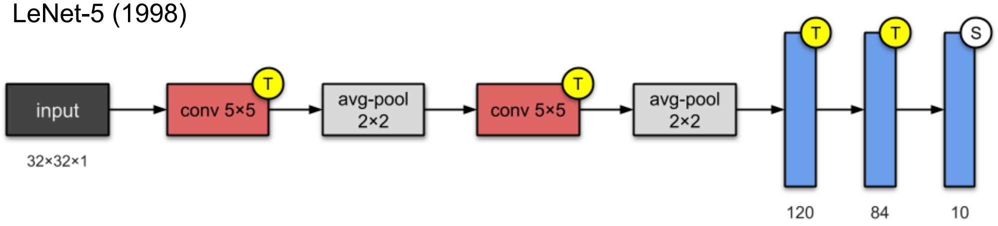
Popular CNN Architectures `https://towardsdatascience.com`

Name	Year	Depth	#Params
LeNet	1998		
AlexNet	2012		> 60 M
VGG16	2014	23	> 23 M
Inception-v1	2014		
ResNet50	2014		> 25 M
Inception-v3	2015	159	
Xception	2016	126	> 22 M
InceptionResNet	2017	572	> 55 M
...			

Popular CNN Architectures

https://towardsdatascience.com

LeNet-5 (1998)

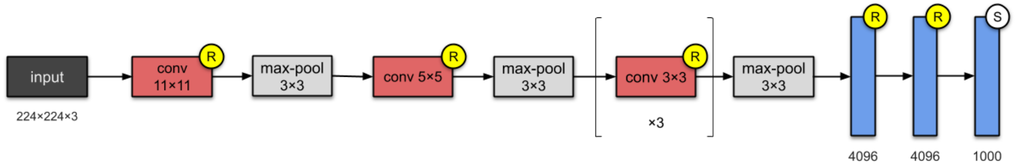


T = tanh
S = softmax

Popular CNN Architectures

https://towardsdatascience.com

AlexNet (2012)



T = tanh
R = ReLU
S = softmax

Used dropout

Popular CNN Architectures

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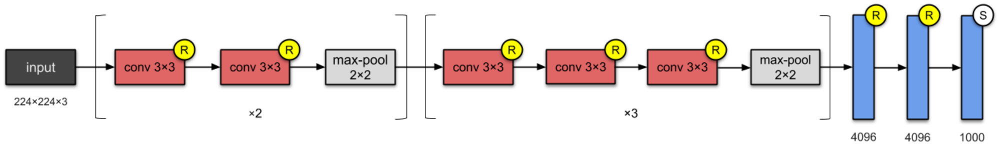
VGG-16 (2014)



T = tanh
R = ReLU
S = softmax

Deeper than AlexNet