TARAN
ADVISORY IN DATA & ANALYTICS

Data Science 2

March 8, 2023

Data Science 2

Faculty of Mathematics and Physics

Agenda

Neural Networks Introduction

Gradient Based Optimization

Activation functions

Regularization

Convolutional neural networks

Convolutional neural network case studies

Classical approaches to NLP

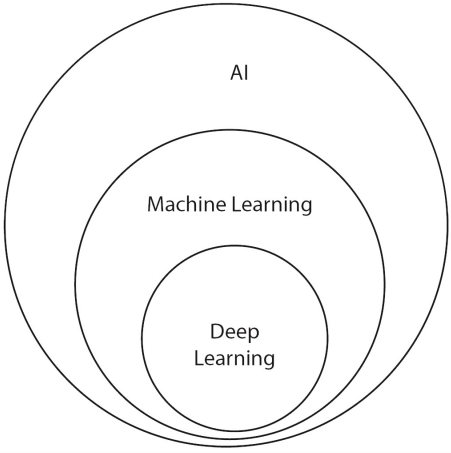
Sequence models

Word embeddings

Neural Networks Introduction

Introduction

- What is artificial intelligence, machine learning and deep learning?
- And how do they relate?



Introduction
Artificial Intelligence

Definition (Artificial intelligence)

Artificial intelligence is an effort to automate intellectual tasks normally performed by humans.

- AI is a superset of machine learning.
- AI includes also algorithms, that are not based on any learning - you can learn computer to play chess by defining set of rules to be obeyed.
- AI was born around 1950s.
- **Symbolic AI** - at the beginning it was believed that human level AI can be achieved by sufficiently large set of rules.

Introduction
Artificial Intelligence

Definition (Artificial intelligence)

Artificial intelligence is an effort to automate intellectual tasks normally performed by humans.

- AI is a superset of machine learning.
- AI includes also algorithms, that are not based on any learning - you can learn computer to play chess by defining set of rules to be obeyed.
- AI was born around 1950s.
- **Symbolic AI** - at the beginning it was believed that human level AI can be achieved by sufficiently large set of rules.

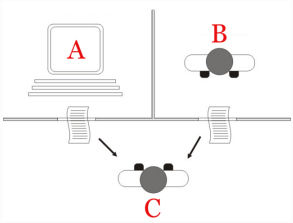
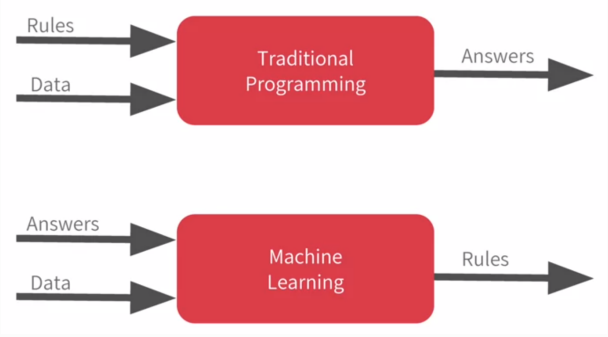


Figure: Turing's test

Definition (Machine Learning)

The use and development of computer systems that are able to learn and adapt without following explicit instructions, by using algorithms and statistical models to analyze and draw inferences from patterns in data.



Introduction
Deep Learning

Definition (Deep learning)

Deep learning is a class of machine learning algorithms that uses multiple layers to progressively extract higher-level features from the raw input. For example, in image processing, lower layers may identify edges, while higher layers may identify the concepts relevant to a human such as digits or letters or faces.

Deep learning achievements:

- Image enhancement
- Image generation
- Object detection
- Text translation
- Chatbots
- Speech recognition
- Optical Character Recognition (OCR)
- Super-human level game playing
- ...

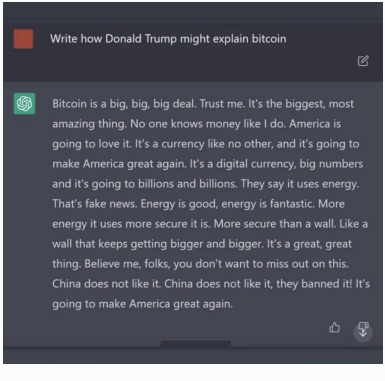
Introduction
Deep Learning

Definition (Deep learning)

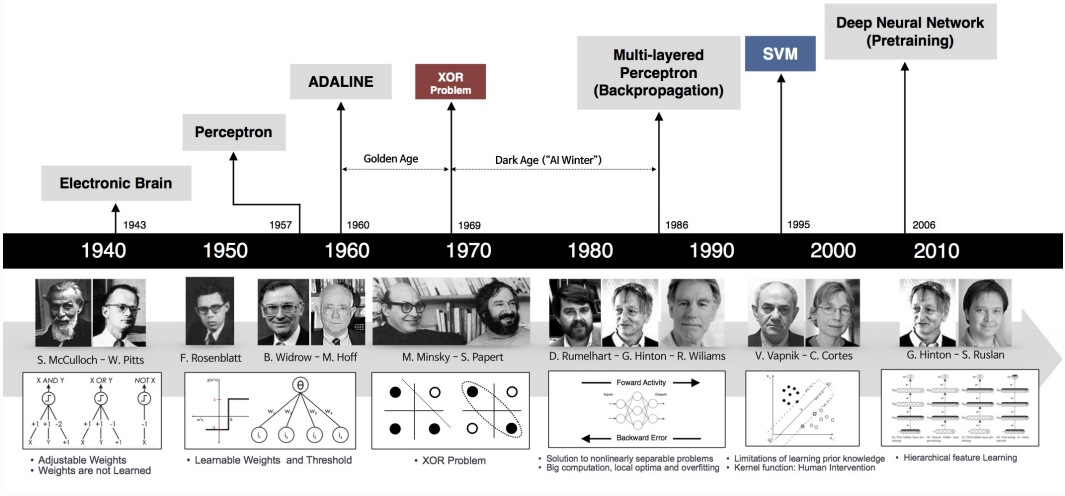
Deep learning is a class of machine learning algorithms that uses multiple layers to progressively extract higher-level features from the raw input. For example, in image processing, lower layers may identify edges, while higher layers may identify the concepts relevant to a human such as digits or letters or faces.

Deep learning achievements:

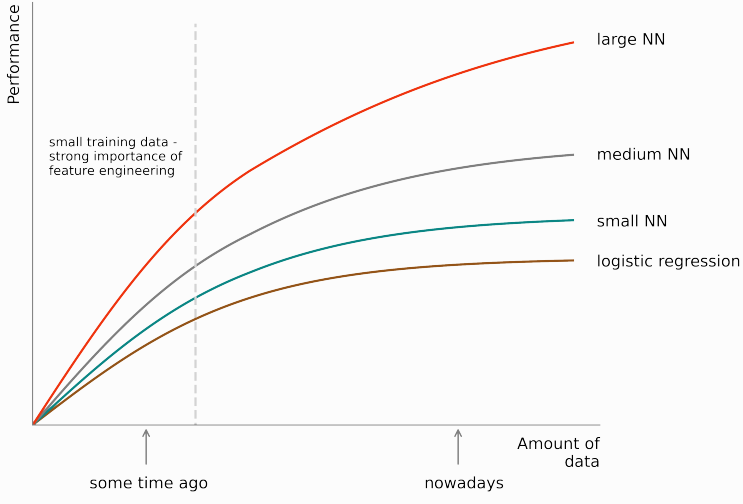
- Image enhancement
- Image generation
- Object detection
- Text translation
- Chatbots
- Speech recognition
- Optical Character Recognition (OCR)
- Super-human level game playing
- ...



Introduction
AI History

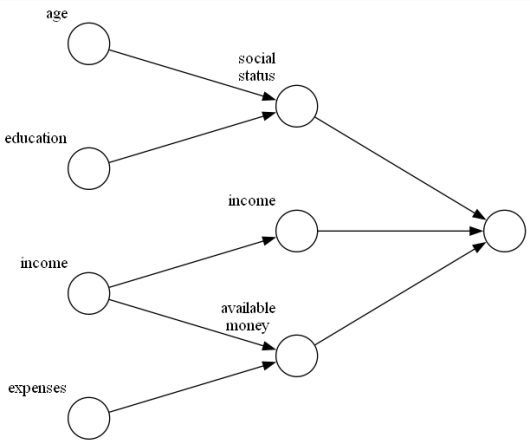


Introduction
Why NN?



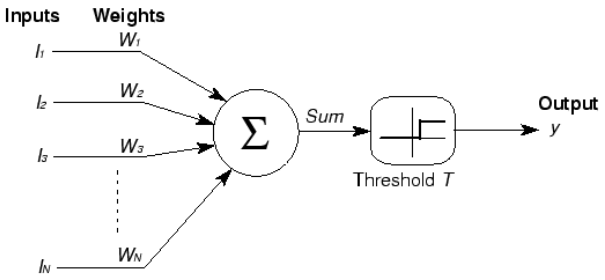
Introduction
Why NN?

Neural Networks do feature engineering automatically.



Neural Networks
Perceptron

In 1958, Frank Rosenblatt introduced an idea of perceptron and called it Mark I Perceptron.

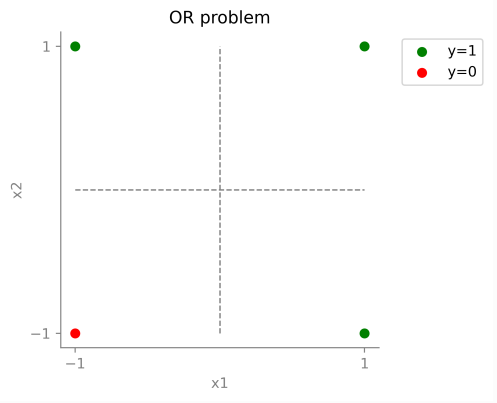


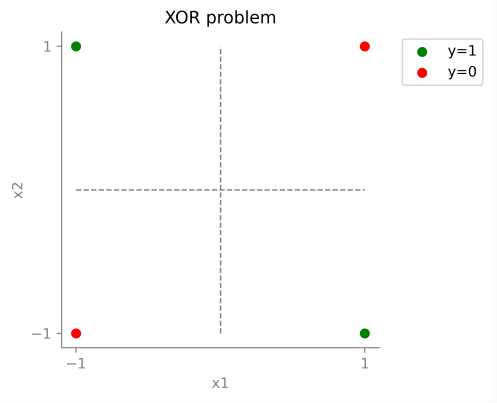
Weights of Mark I Perceptron are 'learnt' through successively passed inputs, while minimizing the difference between desired and actual output.

https://playground.tensorflow.org/

Neural Networks
XOR Problem

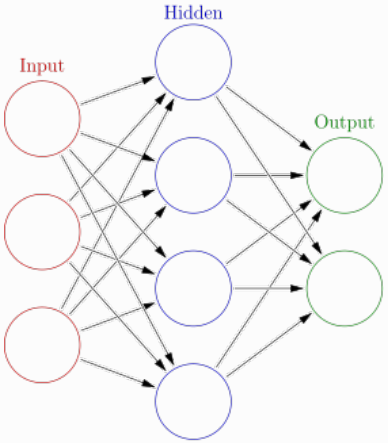
Mark I Perceptron is not capable of solving XOR problem.





Neural Networks
Multi-layer perceptron

To solve XOR problem, we need to use multi-layer perceptron (MLP) neural network.



Neural Networks
Input data

Input data for neural networks are usually passed in form of multi-dimensional Numpy arrays, also called **tensors**:

- Scalars (0D tensors)
- Vectors (1D tensors)
- Matrices (2D tensors)
- 3D and higher dimensional tensors

Tensor is defined by tree key attributes:

- Number of dimensions
- Shape
- Data type

For tensors, dimension is often called an *axis*. First axis is usually allocated for sample axis. In neural network models data are not processed all at once, but in batches.

Gradient Based Optimization

Gradient based optimization

Each neuron transforms input data using following equation:

$$out = f\left(\sum_{j=1}^{N} w_i x_i + b\right) \tag{1}$$

where

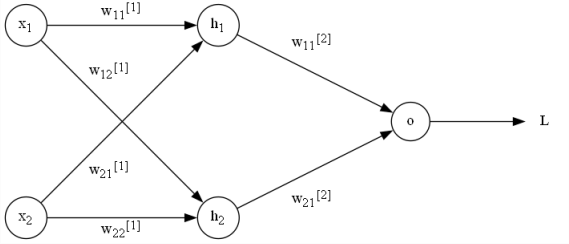
- f ... activation function
- w_i ... weight assigned to a connection coming from i-th input.
- x_i ... value of i-th input
- b ... bias

In multilayer layout weights are represented by weight matrix **W** and biases by bias vector **b**.

Gradient Based Optimization

Backpropagation

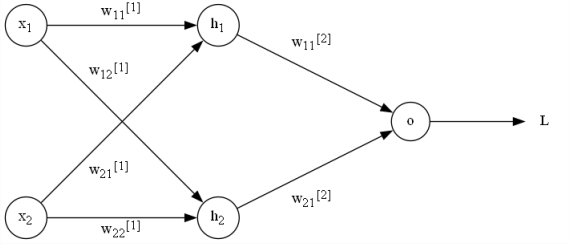
Lets have following network:



Gradient Based Optimization

Backpropagation

Lets have following network:



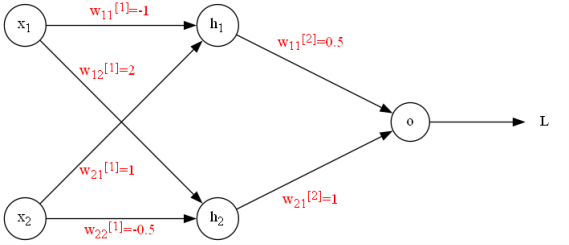
where:

$$
\begin{aligned}
h_1 &= a(w_{11}^{[1]} \cdot x_1 + w_{21}^{[1]} \cdot x_2) \\
h_2 &= a(w_{21}^{[1]} \cdot x_1 + w_{22}^{[1]} \cdot x_2) \\
a(x) &= ReLU(x) = max(0, x) \\
o &= w_{11}^{[2]} \cdot h_1 + w_{21}^{[2]} \cdot h_2 \\
L &= (o - y)^2
\end{aligned}
\tag{2}
$$

Gradient Based Optimization

Backpropagation

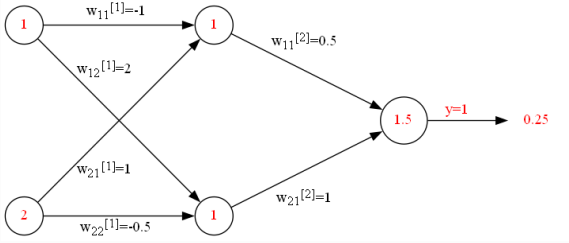
Lets first randomly initialize weights:



Gradient Based Optimization

Backpropagation

Lets first randomly initialize weights:



and calculate forward pass

$$
\begin{aligned}
y &= 1 \\
x_1 &= 1 \\
x_2 &= 2 \\
h_1 &= max(0, -1 \cdot 1 + 1 \cdot 2) = 1 \\
h_2 &= max(0, 1 \cdot 2 + (-0.5) \cdot 2) = 1 \\
o &= 0.5 \cdot 1 + 1 \cdot 1 = 1.5 \\
L &= (1.5 - 1)^2 = 0.25
\end{aligned}
\tag{3}
$$

Gradient Based Optimization

Backpropagation

How do we update weight $w_{11}^{[1]}$? By calculating derivative of loss L with respect to $w_{11}^{[1]}$.

$$\frac{\partial L}{\partial w_{11}^{[1]}} = \frac{\partial L}{\partial o} \frac{\partial o}{\partial h_1} \frac{\partial h_1}{\partial w_{11}^{[1]}} \tag{4}$$

Gradient Based Optimization

Backpropagation

How do we update weight $w_{11}^{[1]}$? By calculating derivative of loss L with respect to $w_{11}^{[1]}$.

$$\frac{\partial L}{\partial w_{11}^{[1]}} = \frac{\partial L}{\partial o}\frac{\partial o}{\partial h_1}\frac{\partial h_1}{\partial w_{11}^{[1]}} \tag{4}$$

$$\begin{aligned}
\frac{\partial L}{\partial o} &= \frac{\partial (o-y)^2}{\partial o} = 2(o-y) = 2(1.5-1) = 1 \\
\frac{\partial o}{\partial h_1} &= \frac{\partial (w_{11}^{[2]} \cdot h_1 + w_{21}^{[2]} \cdot h_2)}{\partial h_1} = w_{11}^{[2]} = 0.5 \\
\frac{\partial h_1}{\partial w_{11}^{[1]}} &= \frac{\partial max(0, w_{11}^{[1]} \cdot x_1 + w_{21}^{[1]} \cdot x_2)}{\partial w_{11}^{[1]}} = (0 \; if \; h_1 <= 0 \; else \; x_1) = 1
\end{aligned} \tag{5}$$

Gradient Based Optimization

Backpropagation

How do we update weight $w_{11}^{[1]}$? By calculating derivative of loss L with respect to $w_{11}^{[1]}$.

$$\frac{\partial L}{\partial w_{11}^{[1]}} = \frac{\partial L}{\partial o}\frac{\partial o}{\partial h_1}\frac{\partial h_1}{\partial w_{11}^{[1]}} \tag{4}$$

$$\begin{aligned}
\frac{\partial L}{\partial o} &= \frac{\partial (o-y)^2}{\partial o} = 2(o-y) = 2(1.5-1) = 1 \\
\frac{\partial o}{\partial h_1} &= \frac{\partial (w_{11}^{[2]} \cdot h_1 + w_{21}^{[2]} \cdot h_2)}{\partial h_1} = w_{11}^{[2]} = 0.5 \\
\frac{\partial h_1}{\partial w_{11}^{[1]}} &= \frac{\partial max(0, w_{11}^{[1]} \cdot x_1 + w_{21}^{[1]} \cdot x_2)}{\partial w_{11}^{[1]}} = (0 \; if \; h_1 <= 0 \; else \; x_1) = 1
\end{aligned} \tag{5}$$

$$\frac{\partial L}{\partial w_{11}^{[1]}} = 1 \cdot 0.5 \cdot 1 = 0.5$$

Gradient Based Optimization

Backpropagation

The update of $w_{11}^{[1]}$ is given by:

$$w_{11}^{[1]} \longleftarrow w_{11}^{[1]} - \alpha \frac{\partial L}{\partial w_{11}^{[1]}} \tag{6}$$

Gradient Based Optimization

Backpropagation

The update of $w_{11}^{[1]}$ is given by:

$$w_{11}^{[1]} \longleftarrow w_{11}^{[1]} - \alpha \frac{\partial L}{\partial w_{11}^{[1]}} \tag{6}$$

We can do the same for all weights:

$$\frac{\partial L}{\partial w_{11}^{[1]}} = \frac{\partial L}{\partial o}\frac{\partial o}{\partial h_1}\frac{\partial h_1}{\partial w_{11}^{[1]}} = 0.5$$

$$\frac{\partial L}{\partial w_{12}^{[1]}} = \frac{\partial L}{\partial o}\frac{\partial o}{\partial h_2}\frac{\partial h_2}{\partial w_{12}^{[1]}} = 1$$

$$\frac{\partial L}{\partial w_{21}^{[1]}} = \frac{\partial L}{\partial o}\frac{\partial o}{\partial h_1}\frac{\partial h_1}{\partial w_{21}^{[1]}} = 1$$

$$\frac{\partial L}{\partial w_{22}^{[1]}} = \frac{\partial L}{\partial o}\frac{\partial o}{\partial h_1}\frac{\partial h_1}{\partial w_{22}^{[1]}} = 2$$

$$\frac{\partial L}{\partial w_{11}^{[2]}} = \frac{\partial L}{\partial o}\frac{\partial o}{\partial w_{11}^{[2]}} = 1$$

$$\frac{\partial L}{\partial w_{21}^{[2]}} = \frac{\partial L}{\partial o}\frac{\partial o}{\partial w_{21}^{[2]}} = 1$$

Gradient Based Optimization

Minibatch Optimization

A/ **Gradient Descent**

- Use all observations to calculate $\vec{g}$
- Most accurate
- High computational costs

B/ **Stochastic Gradient Descent**

- Use only one sample at the time for weights update
- Large variance in $\vec{g}$

C/ **Minibatch**

- Use sub-sample of size M to calculate $\vec{g}$
- Usually, M is power of 2

Minibatches are sampled from the data without replacement. Therefore, after $\lceil \#observation/M \rceil$ every observation contributed to one weights update.

Training neural network

Algorithm (NN training)

Repeat until stopping criterion is met:

1. *Sample a minibatch of n observations from training sample.*
2. *Feed forward step - propagate each observation through neural net and calculate outputs*
3. *Calculate derivatives of loss function with respect to trainable parameters*
4. *Backpropagation step - update trainable parameters based on gradient averaged over batch*

$$\theta^{(t+1)} = \theta^{(t)} - \alpha \cdot \frac{1}{n} \sum_{i=1}^{n} \nabla_{\theta^{(t)}} L(output_i, label_i) \tag{7}$$

- **Minibatch** - Subsample to be used for one update of weights (forward and backward pass)
- **Epoch** - All the training data was used exactly once to update weights

Gradient descent
SGD with momentum

Algorithm (SGD with momentum)

Repeat until stopping criteria is met:

- *Randomly select m samples from training data.*
- $\mathbf{g_t} = \frac{1}{m} \nabla_\theta \sum_i L(f(\mathbf{x}^{(i)}; \boldsymbol{\theta_{t-1}}), y^{(i)})$
- $\mathbf{v_t} = \beta \mathbf{v_{t-1}} - \alpha \boldsymbol{g_t}$
- $\boldsymbol{\theta_t} = \boldsymbol{\theta_{t-1}} + \mathbf{v_t}$

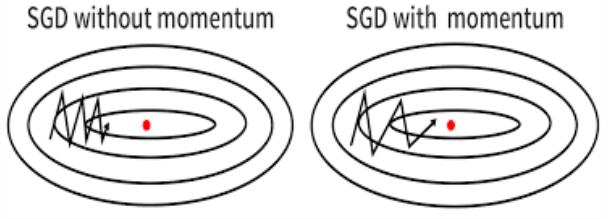
Gradient descent
SGD with momentum

Algorithm (SGD with momentum)

Repeat until stopping criteria is met:

- *Randomly select m samples from training data.*
- $\mathbf{g_t} = \frac{1}{m}\nabla_\theta \sum_i L(f(\mathbf{x}^{(i)}; \boldsymbol{\theta_{t-1}}), y^{(i)})$
- $\mathbf{v_t} = \beta \mathbf{v_{t-1}} - \alpha \boldsymbol{g_t}$
- $\boldsymbol{\theta_t} = \boldsymbol{\theta_{t-1}} + \mathbf{v_t}$

- Good value for β is 0.9



Gradient descent
Nesterov accelerated gradient descent

Algorithm (Nesterov accelerated GD)

Repeat until stopping criteria is met:

- $\boldsymbol{\theta_{t_0}} = \boldsymbol{\theta_{t-1}} + \beta \mathbf{v_{t-1}}$
- *Randomly select m samples from training data.*
- $\mathbf{g_t} = \frac{1}{m} \nabla_\theta \sum_i L(f(\mathbf{x}^{(i)}; \boldsymbol{\theta_{t_0}}), y^{(i)})$
- $\mathbf{v_t} = \beta \mathbf{v_{t-1}} - \alpha \boldsymbol{g_t}$
- $\boldsymbol{\theta_t} = \boldsymbol{\theta_{t_0}} - \alpha \boldsymbol{g_t}$

Gradient descent
Nesterov accelerated gradient descent

Algorithm (Nesterov accelerated GD)

Repeat until stopping criteria is met:

- $\boldsymbol{\theta_{t_0}} = \boldsymbol{\theta_{t-1}} + \beta \mathbf{v_{t-1}}$
- *Randomly select m samples from training data.*
- $\mathbf{g_t} = \frac{1}{m} \nabla_\theta \sum_i L(f(\mathbf{x}^{(i)}; \boldsymbol{\theta_{t_0}}), y^{(i)})$
- $\mathbf{v_t} = \beta \mathbf{v_{t-1}} - \alpha \boldsymbol{g_t}$
- $\boldsymbol{\theta_t} = \boldsymbol{\theta_{t_0}} - \alpha \boldsymbol{g_t}$

- We know we will use momentum, so we can calculate gradient after applying momentum, rather than before.

Gradient descent
Adagrad

Adagrad = Adaptive gradient algorithm

Algorithm (Adagrad)

Repeat until stopping criteria is met:

- *Randomly select m samples from training data.*
- $\mathbf{g_t} = \frac{1}{m} \nabla_\theta \sum_i L(f(\mathbf{x}^{(i)}; \boldsymbol{\theta_{t-1}}), y^{(i)})$
- $\mathbf{r_t} = \mathbf{r_{t-1}} + \boldsymbol{g_t}^2$
- $\boldsymbol{\theta_t} = \boldsymbol{\theta_{t-1}} - \frac{\alpha}{\sqrt{\mathbf{r_t} + \varepsilon}} \mathbf{g_t}$

Gradient descent
Adagrad

Adagrad = Adaptive gradient algorithm

Algorithm (Adagrad)

Repeat until stopping criteria is met:

- *Randomly select m samples from training data.*
- $\mathbf{g_t} = \frac{1}{m} \nabla_\theta \sum_i L(f(\mathbf{x}^{(i)}; \boldsymbol{\theta_{t-1}}), y^{(i)})$
- $\mathbf{r_t} = \mathbf{r_{t-1}} + \boldsymbol{g_t}^2$
- $\boldsymbol{\theta_t} = \boldsymbol{\theta_{t-1}} - \frac{\alpha}{\sqrt{\mathbf{r_t} + \varepsilon}} \mathbf{g_t}$

- Increase learning rate for parameter related to infrequent features
- Decrease learning rate for parameter related to frequent features
- Usually $\varepsilon = 10^{-8}$

Gradient descent
RMSProp

RMSProp = Root mean square propagation

Algorithm (RMSProp)

Repeat until stopping criteria is met:

- *Randomly select m samples from training data.*
- $\mathbf{g_t} = \frac{1}{m} \nabla_\theta \sum_i L(f(\mathbf{x}^{(i)}; \boldsymbol{\theta_{t-1}}), y^{(i)})$
- $\mathbf{r_t} = \beta \mathbf{r_{t-1}} + (1 - \beta) \boldsymbol{g_t}^2$
- $\boldsymbol{\theta_t} = \boldsymbol{\theta_{t-1}} - \frac{\alpha}{\sqrt{\mathbf{r_t} + \varepsilon}} \mathbf{g_t}$

Gradient descent
RMSProp

RMSProp = Root mean square propagation

Algorithm (RMSProp)

Repeat until stopping criteria is met:

- *Randomly select m samples from training data.*
- $\mathbf{g_t} = \frac{1}{m}\nabla_\theta \sum_i L(f(\mathbf{x}^{(i)}; \boldsymbol{\theta_{t-1}}), y^{(i)})$
- $\mathbf{r_t} = \beta \mathbf{r_{t-1}} + (1-\beta)\boldsymbol{g_t}^2$
- $\boldsymbol{\theta_t} = \boldsymbol{\theta_{t-1}} - \frac{\alpha}{\sqrt{\mathbf{r_t}+\varepsilon}}\mathbf{g_t}$

- suppress old gradients and put more weight to new one (in terms of adaptivity)
- Usually $\varepsilon = 10^{-8}$
- Usually $\beta = 0.9$

Gradient descent
Adam

Adam = Adaptive Moment Estimation

Algorithm (Adam)

Set $\mathbf{s_0} = \mathbf{0}$, $\mathbf{r_0} = \mathbf{0}$
Repeat until stopping criteria is met:

- *Randomly select m samples from training data.*
- $\mathbf{g_t} = \frac{1}{m} \nabla_\theta \sum_i L(f(\mathbf{x}^{(i)}; \boldsymbol{\theta_{t-1}}), y^{(i)})$
- $\mathbf{s_t} = \beta_1 \mathbf{s_{t-1}} + (1 - \beta_1) \boldsymbol{g_t}$
- $\mathbf{r_t} = \beta_2 \mathbf{r_{t-1}} + (1 - \beta_2) \boldsymbol{g_t}^2$
- $\hat{\mathbf{s}}_\mathbf{t} = \frac{\mathbf{s_t}}{1-\beta_1^t}$
- $\hat{\mathbf{r}}_\mathbf{t} = \frac{\mathbf{r_t}}{1-\beta_2^t}$
- $\boldsymbol{\theta_t} = \boldsymbol{\theta_{t-1}} - \frac{\alpha}{\sqrt{\hat{\mathbf{r}}_\mathbf{t}} + \varepsilon} \hat{\mathbf{s}}_\mathbf{t}$

- Default values: $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\alpha = 0.001$
- Usually $\varepsilon = 10^{-8}$

Gradient Descent
Algorithms Overview

- SGD with Nesterov Momentum
  - momentum
- AdaGrad (Adaptive Gradient Algorithm)
  - adaptive learning rate
- RMSProp (Root Mean Square Propagation)
  - adaptive learning rate
- Adam (Adaptive Moment Estimation)
  - momentum
  - adaptive learning rate

https://awesomeopensource.com/project/Jaewan-Yun/optimizer-visualization

https://keras.io/api/optimizers/

Learning rate schedules

Even for algorithms with adaptive learning rates, further fine-tuning of learning rate can improve performance. Decreasing learning rate can be performed each batch/epoch/several epochs.

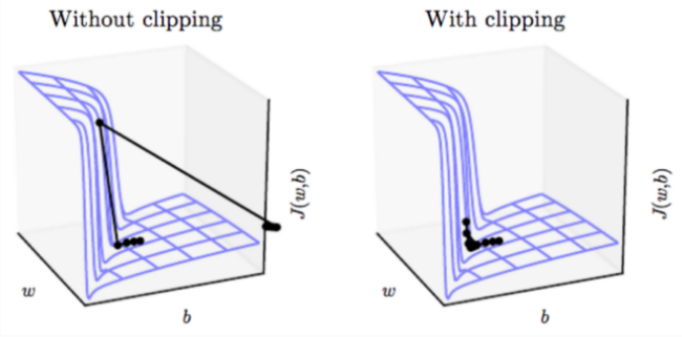
- Exponential decay
  $eta_t = \eta_0 \cdot c^t$
- Polynomial decay
  - Inverse time decay
    $\eta_t = \eta_0 \cdot \frac{1}{t}$
  - Inverse-square decay
    $\eta_t = \eta_0 \cdot \frac{1}{\sqrt{t}}$
- Cosine decay, restarts, ...

https://www.tensorflow.org/api_docs/python/tf/keras/optimizers/schedules/

Gradient clipping

Algorithm (Gradient clipping)

- $\mathbf{g} = \nabla_\theta L(f(\mathbf{x}; \theta), y)$
- *if* $\|\mathbf{g}\| \geq$ *treshold then* $\mathbf{g} =$ **treshold** *end if*



Activation functions

Activation functions

Each neuron transforms input data using following equation:

$$out = f\left(\sum_{j=1}^{N} w_i x_i + b\right) \tag{8}$$

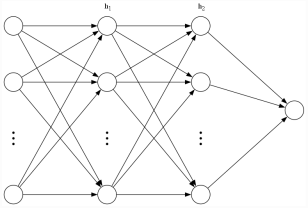
- Activation function adds non-linearity at each neuron
- It helps to control neuron output values range
- Desired features:
  - Differentiability (required)
  - Know analytical solution of first derivative
  - Low computational expense

https://www.tensorflow.org/api_docs/python/tf/keras/activations

Activation Functions

Why Use Non-linear Activation

Let us consider NN with two hidden layers (h_1, h_2), both with no activation function applied.



$$\mathbf{h_1} = \mathbf{W^{[1]}} \cdot \mathbf{x} + \mathbf{b^{[1]}}$$

$$\mathbf{h_2} = \mathbf{W^{[2]}} \cdot \mathbf{h_1} + \mathbf{b^{[2]}} = \mathbf{W^{[2]}} \cdot \left(\mathbf{W^{[1]}} \cdot \mathbf{x} + \mathbf{b^{[1]}}\right) + \mathbf{b^{[2]}} =$$

$$= \underbrace{\mathbf{W^{[2]}} \cdot \mathbf{W^{[1]}}}_{\mathbf{W'}} \cdot \mathbf{x} + \underbrace{\mathbf{W^{[2]}} \cdot \mathbf{b^{[1]}} + \mathbf{b^{[2]}}}_{\mathbf{b'}} \tag{9}$$

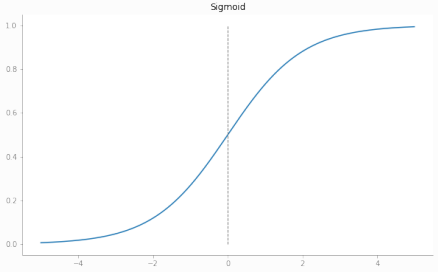
we do not need to have second hidden layer

Activation functions

Sigmoid

Definition:

$$\sigma(x) = \frac{1}{1 + e^{-x}} \tag{10}$$



Derivative:

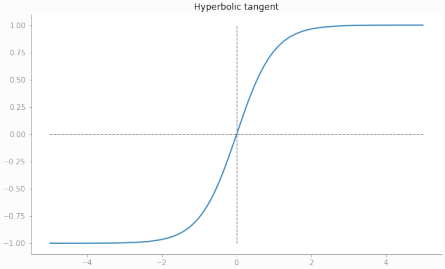
$$\frac{\mathrm{d}\sigma(x)}{\mathrm{d}x} = \sigma(x)(1 - \sigma(x)) \tag{11}$$

Activation functions

Hyperbolic tangent

Definition:

$$\tanh(x) = \frac{e^{2x} - 1}{e^{2x} + 1} \tag{12}$$



Derivative:

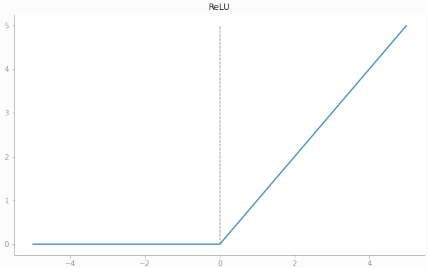
$$\frac{\mathrm{d}\tanh(x)}{\mathrm{d}x} = 1 - \tanh(x)^2 \tag{13}$$

Activation functions

Rectified Linear Unit

Definition:

$$\mathrm{ReLu}(x) = \max(0, x) \tag{14}$$



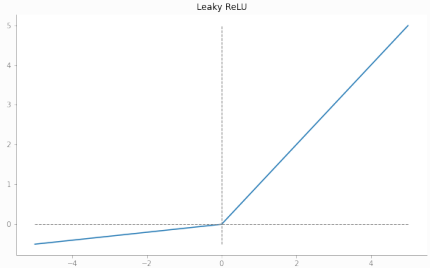
Derivative:

$$\frac{\mathrm{dReLu}(x)}{\mathrm{d}x} = \begin{cases} 1 & \text{if } x > 0 \\ NaN & \text{if } x = 0 \\ 0 & \text{if } x < 0 \end{cases} \tag{15}$$

Activation functions
Leaky ReLU

Definition:

$$\mathrm{LeakyReLU}(x) = \max(\alpha x, x) \tag{16}$$



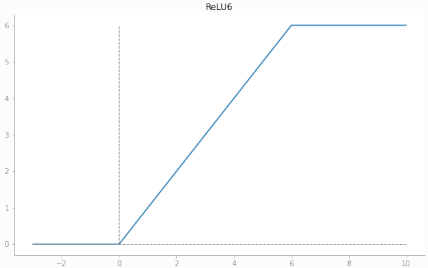
Derivative:

$$\frac{\mathrm{dLeakyReLU}(x)}{\mathrm{d}x} = \begin{cases} 1 & \text{if } x > 0 \\ NaN & \text{if } x = 0 \\ \alpha & \text{if } x < 0 \end{cases} \tag{17}$$

Activation functions
ReLU6

Definition:

$$\mathrm{ReLu6}(x) = \min(\max(0, x), 6) \tag{18}$$



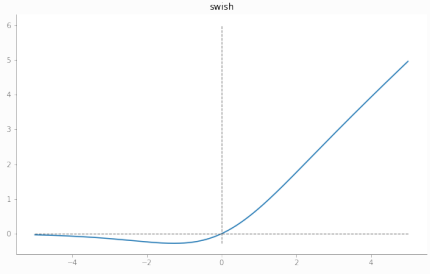
Derivative:

$$\frac{\mathrm{dReLu6}(x)}{\mathrm{d}x} = \begin{cases} 1 & \text{if } x \in (0, 6) \\ NaN & \text{if } x = 0 \text{ or } x = 6 \\ 0 & \text{if } x < 0 \text{ or } x > 6 \end{cases} \tag{19}$$

Activation functions
Swish

Definition:

$$\text{swish}(x) = x\sigma(\beta x) \tag{20}$$



Derivative:

$$\frac{\text{dswish}(x)}{\text{d}x} = \text{swish}(x) + \sigma(x)(\beta - \text{swish}(x)) \tag{21}$$

Activation functions

Activation on output layer

Common activations on output layer:

- None - linear regression if there are no hidden layers
- $\sigma(x)$ - binary classification

$$\sigma(x) = \frac{1}{1 + e^{-x}} \tag{22}$$

- $\mathrm{softmax}$ - multi-class classification

$$\mathrm{softmax}(\mathbf{x})_i = \frac{e^{x_i}}{\sum_j e^{x_j}} \tag{23}$$

Vanishing and exploding gradient

- Vanishing gradient is a consequence of chain rule used in backpropagation algorithm.
- Activation functions such as sigmoid or hyperbolic tangent has derivative in interval $(0, 1)$
- With inappropriate set up derivatives of weights in former layers might **vanish** because of multiplying values lower then 1 in magnitude many times
- If, for instance, the initial loss is big, the gradient might **explode**

Vanishing and exploding gradient

- Vanishing gradient is a consequence of chain rule used in backpropagation algorithm.
- Activation functions such as sigmoid or hyperbolic tangent has derivative in interval $(0, 1)$
- With inappropriate set up derivatives of weights in former layers might **vanish** because of multiplying values lower then 1 in magnitude many times
- If, for instance, the initial loss is big, the gradient might **explode**

Symptoms of vanishing/exploding gradient:

Vanishing gradient

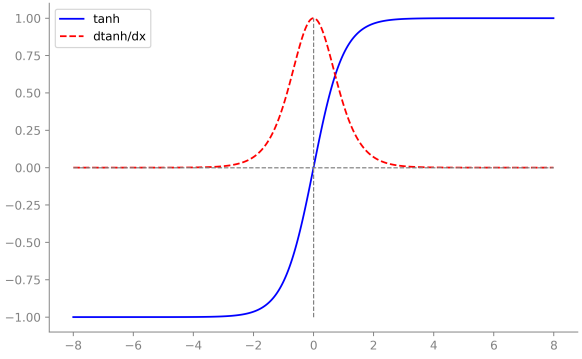
- Model improves very slowly
- Weights closer to output layer changes more dynamically

Exploding gradient

- Large changes in loss
- Model loss is NaN
- Model weights grow exponentially
- Model weights are NaN

Saturating non-linearities

With large input to neuron, derivative of saturating activation functions is close to 0



Weights Initialization

- In general practice biases are initialized with 0.
- Initialization of weights by 0 (or any constant) is not a good idea, since neurons' activation in one layer will never break the symmetry.

Weights Initialization

- In general practice biases are initialized with 0.
- Initialization of weights by 0 (or any constant) is not a good idea, since neurons' activation in one layer will never break the symmetry.

  Let us consider two neurons in hidden layer and weights in network initialized by a constant.

$$h_1 = f\left(\sum_i w_{i1} x_i + b\right)$$
$$h_2 = f\left(\sum_i w_{i2} x_i + b\right) = h_1 \tag{24}$$

Weights Initialization

- In general practice biases are initialized with 0.
- Initialization of weights by 0 (or any constant) is not a good idea, since neurons' activation in one layer will never break the symmetry.

  Let us consider two neurons in hidden layer and weights in network initialized by a constant.

$$\begin{aligned} h_1 &= f\left(\sum_i w_{i1}x_i + b\right) \\ h_2 &= f\left(\sum_i w_{i2}x_i + b\right) = h_1 \end{aligned} \tag{24}$$

$$\frac{\partial h_1}{\partial w_{i1}} = x_i f'(y)|_{y=\sum_i w_{i1}x_i+b} = x_i f'(y)|_{y=\sum_i w_{i2}x_i+b} = \frac{\partial h_2}{\partial w_{i2}} \tag{25}$$

  Weights of connections from one input neuron to hidden neurons of the following layer will be updated by the same amount => activation on following layer neurons remains the same. Neurons in one layer cannot learn different "features".
  https://www.deeplearning.ai/ai-notes/initialization/index.html

Weights initialization

- In general practice biases are initialized with 0.
- Initialization of weights by 0 is not a good idea, since such weights will never break the symmetry inside one layer.
- Glorot initialization is trying to fix the variance of activations as well as gradients across layers:

$$W_{Glorot} \sim U\left[-\sqrt{\frac{6}{m+n}}, \sqrt{\frac{6}{m+n}}\right] \tag{26}$$

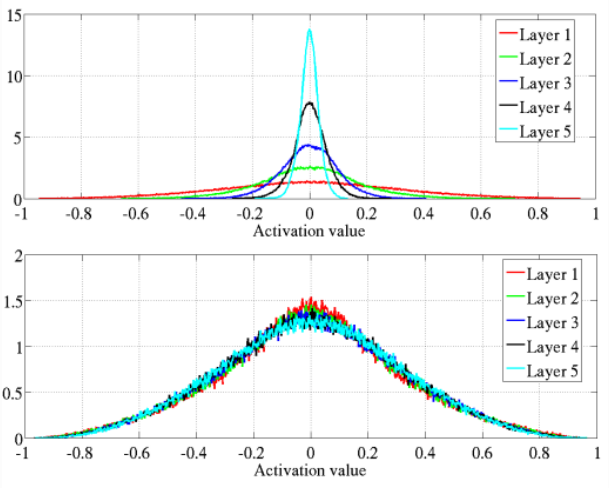
  where n is number of neurons in previous layer and m is a number of neurons in next layer.
- For ReLU activation, HeUniform might be more suitable:

$$W_{He} \sim U\left[-\sqrt{\frac{6}{n}}, \sqrt{\frac{6}{n}}\right] \tag{27}$$

  where n is a number of input units.

https://www.tensorflow.org/api_docs/python/tf/keras/initializers/

Weights initialization



Source: http://proceedings.mlr.press/v9/glorot10a/glorot10a.pdf

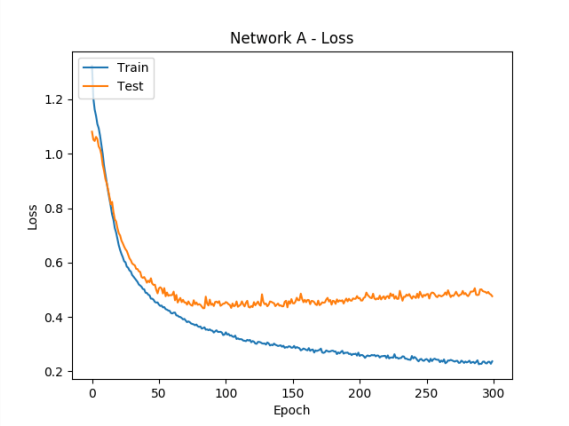
Regularization

Regularization

Regularization allows to control generalization error of model.

- Early stopping
- L2, L1 regularization
- Dataset augmentation
- Ensembling
- Dropout
- Label smoothing

Regularization
Early stopping



- Loss on train set will always decrease
- Stop training once loss on test set stop decreasing

Regularization

L2, L1 regularization

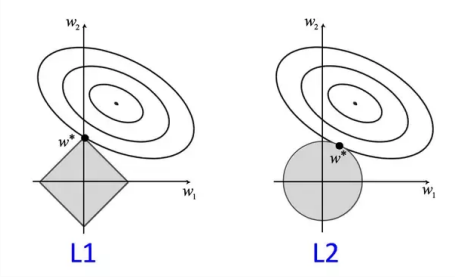
Penalization of large weights. Distribute the model strength amongst more ways in neural net, rather than emphasize one specific way.

- L2 regularization

$$L_{L2}(\boldsymbol{\theta}; \mathbf{X}) = L(\boldsymbol{\theta}; \mathbf{X}) + \lambda \|\boldsymbol{\theta}\|_2^2 \tag{28}$$

- L1 regularization

$$L_{L1}(\boldsymbol{\theta}; \mathbf{X}) = L(\boldsymbol{\theta}; \mathbf{X}) + \lambda \|\boldsymbol{\theta}\|_1 \tag{29}$$



Regularization
Data augmentation

Modifying input data can force model to focus on general patterns rather than focusing on details, which can lead to overfitting.

- Image processing
  - Translation
  - Horizontal flips
  - Scaling
  - Rotation
  - Colour adjustment
  - Mixup - two images are combined using their weighted combination
- Speech recognition
  - Additional noise
  - Frequency change

https://www.tensorflow.org/api_docs/python/tf/keras/preprocessing

Regularization
Ensembling

Model ensembling is a technique to reduce generalization error by combining several models. Usually, model outputs are averaged.

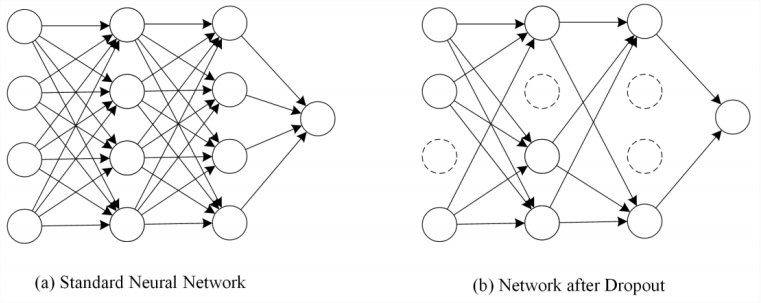
Possible set ups:

- Generate random training samples using sampling with replacement.
- Use different random weight initialization.
- Average model obtained at different time steps (one hour of training, one day of training, ...)

Ensembling often has high computational requirements.

Regularization
Dropout

- Dropout is applied to a layer.
- Each neuron of the layer is randomly excluded with certain probability in each batch.
- Technically, dropout is performed by setting value of the neuron to 0.



(a) Standard Neural Network

(b) Network after Dropout

Regularization
Dropout

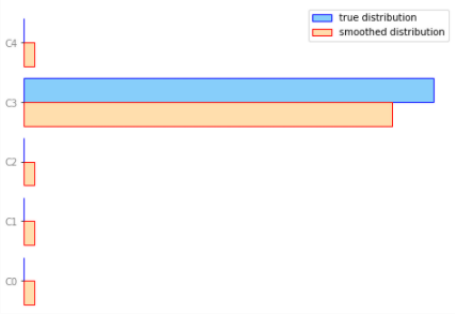
During inference, no neurons are dropped out. This means that neuron receives signal from more neurons than during training. Scaling should be performed:

- Reduce the activation signal during inference by the factor of $1 - p$, where p is a probability of dropout from previous layer.
- Enhance the activation signal during training by the factor of $\frac{1}{1-p}$

Regularization
Label smoothing

In multi-class classification problem, when using softmax, the model is never satisfied with achieved results. If model prediction for the true category is 0.999, it is still trying to improve.
To overcome this, true label distribution is modified from $\mathbf{1}_{true}$ to

$$(1-\alpha)\mathbf{1}_{true} + \alpha\frac{1}{\text{number of classes}}$$



Convolutional neural networks

TARAN

ADVISORY IN DATA & ANALYTICS

Convolutional Neural Networks

Motivation

Convolutional neural networks bring three main advantages:

Convolutional Neural Networks
Motivation

Convolutional neural networks bring three main advantages:

- Local interactions
  - Neighbouring pixels in picture might share an information rather than those far from each other.
  - Neighbouring words in a sentence might have a special meaning.

Convolutional Neural Networks
Motivation

Convolutional neural networks bring three main advantages:

- Local interactions
  - Neighbouring pixels in picture might share an information rather than those far from each other.
  - Neighbouring words in a sentence might have a special meaning.
- Parameter sharing
  - This concept allow to reduce number of trainable parameters.

Convolutional Neural Networks

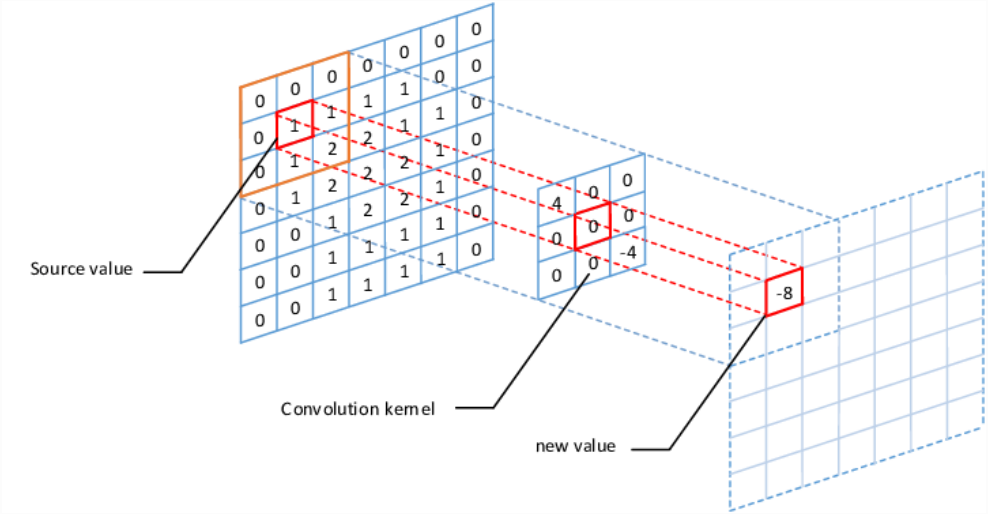
Motivation

Convolutional neural networks bring three main advantages:

- Local interactions
  - Neighbouring pixels in picture might share an information rather than those far from each other.
  - Neighbouring words in a sentence might have a special meaning.
- Parameter sharing
  - This concept allow to reduce number of trainable parameters.
- Shift invariance
  - A pattern should be recognized independently on its position.

Convolutional Neural Networks

Convolution process



Convolutional Neural Networks

Convolution operation

Convolution of two functions is defined as:

$$(f * g)(t) = \int_{\infty}^{\infty} f(\tau) g(t - \tau) \mathrm{d}\tau \tag{30}$$

Convolutional Neural Networks

Convolution operation

Convolution of two functions is defined as:

$$(f * g)(t) = \int_{\infty}^{\infty} f(\tau) g(t - \tau) \mathrm{d}\tau \tag{30}$$

In 2D it takes form:

$$(f * g)(t, u) = \int_{\infty}^{\infty} \int_{\infty}^{\infty} f(\tau, \xi) g(t - \tau, u - \xi) \mathrm{d}\tau \mathrm{d}\xi \tag{31}$$

Convolutional Neural Networks

Convolution operation

Convolution of two functions is defined as:

$$(f * g)(t) = \int_{\infty}^{\infty} f(\tau) g(t - \tau) \mathrm{d}\tau \tag{30}$$

In 2D it takes form:

$$(f * g)(t, u) = \int_{\infty}^{\infty} \int_{\infty}^{\infty} f(\tau, \xi) g(t - \tau, u - \xi) \mathrm{d}\tau \mathrm{d}\xi \tag{31}$$

In discrete domain we have:

$$(\mathbf{w} * \mathbf{x})_t = \sum_i w_i x_{t-i} \tag{32}$$

Or for 2D case:

$$(\mathbf{K} * \mathbf{I})_{i,j} = \sum_{m,n} \mathbf{K}_{m,n} \mathbf{I}_{i-m,j-n} \tag{33}$$

Convolutional Neural Networks

Cross-correlation

CNN actually uses cross-correlation instead of convolution:

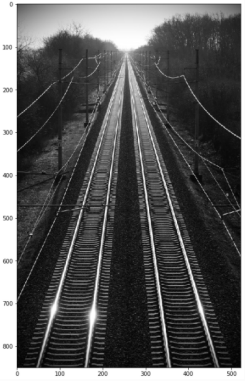
$$(\mathbf{K} \star \mathbf{I})_{i,j} = \sum_{m,n} \mathbf{K}_{m,n} \mathbf{I}_{i+m,j+n} \tag{34}$$

Convolutional Neural Networks
Cross-correlation

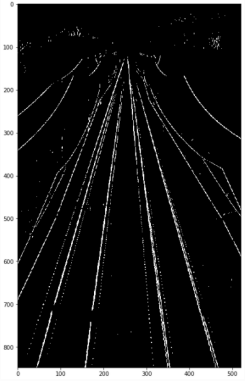
CNN actually uses cross-correlation instead of convolution:

$$(\mathbf{K} \star \mathbf{I})_{i,j} = \sum_{m,n} \mathbf{K}_{m,n} \mathbf{I}_{i+m,j+n} \tag{34}$$

Cross-correlation can be used to detect edges in image. Edge is a space with big differences in pixel values.



-1	0	+1
-2	0	+2
-1	0	+1



Convolutional Neural Networks

Channels

Matrix **K** is called **kernel** or **filter**.

Coloured image consists of three **channels** - RGB. The weights inside the kernel are different for each channel. Thus, we have

$$(\mathbf{K} \star \mathbf{I})_{i,j} = \sum_{m,n,c} \mathbf{K}_{m,n,c} \mathbf{I}_{i+m,j+n,c} \tag{35}$$

Also we want to use more than one kernels - one kernel can detect vertical lines, another horizontal lines and yet another can detect rounded objects. Neural net will decide on its own what shapes are relevant, but we need to provide kernels, whose weights can be trained.

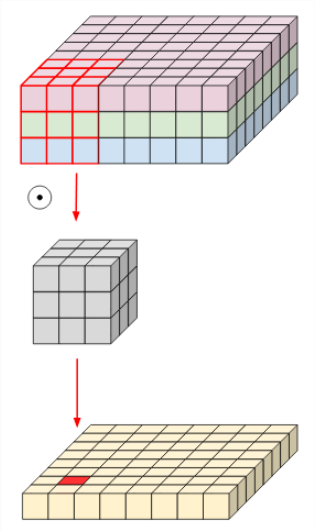
$$(\mathbf{K} \star \mathbf{I})_{i,j,o} = \sum_{m,n,c} \mathbf{K}_{m,n,c,o} \mathbf{I}_{i+m,j+n,c} \tag{36}$$

Kernel is four dimensional tensor with dimensions:

- W ... kernel width
- H ... kernel height
- C ... input channels
- F ... output channels (number of filters we want to train)

Convolutional Neural Networks

Processing multiple input channels

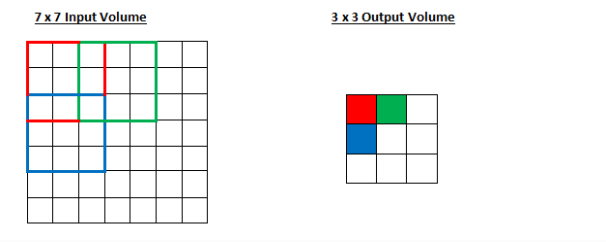


Convolutional Neural Networks

Stride

Stride defines kernel step when computing cross-correlation.

$$(\mathbf{K} \star \mathbf{I})_{i,j,o} = \sum_{m,n,c} \mathbf{K}_{m,n,c,o} \mathbf{I}_{i \cdot S+m, j \cdot S+n, c} \tag{37}$$



Applying stride reduces size of the output. If $S = 2$, then output is half the size of input.

Convolutional Neural Networks

Padding

Padding scheme decides how to behave at the image edges.

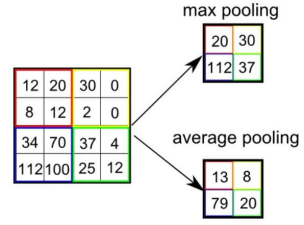
- valid - Only use valid pixels. The kernel cannot overhang the image. Results in output being smaller than the input.
- same - Pad edges of the image with zeros so that resulting output is the same size as input.

0	0	0	0	0	0	0	0
0	**3**	**3**	**4**	**4**	**7**	**0**	0
0	**9**	**7**	**6**	**5**	**8**	**2**	0
0	**6**	**5**	**5**	**6**	**9**	**2**	0
0	**7**	**1**	**3**	**2**	**7**	**8**	0
0	**0**	**3**	**7**	**1**	**8**	**3**	0
0	**4**	**0**	**4**	**3**	**2**	**2**	0
0	0	0	0	0	0	0	0

Convolutional Neural Networks
Pooling

Pooling is an operation that reduces width and height of the image. It is fixed operation - it does not include trainable parameters.

- Max pooling
- Average pooling

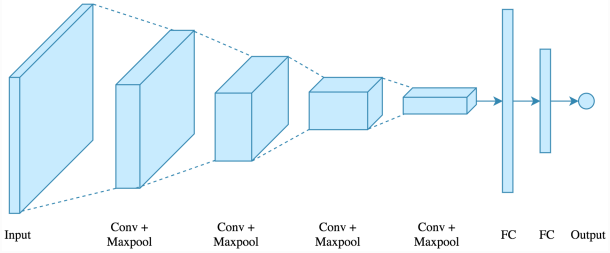


Reducing size of the image allows to detect high level patterns in the picture

Convolutional Neural Networks

CNN architecture

- Double number of channels when performing pooling.
- Some architectures do not use fully connected layers at the end of the network.



Convolutional Neural Networks

Batch normalization

Let us first assume multi layer perceptron neural network. As the weights of the network updates a neuron inside the layer receives different distribution of inputs. This effect is called **internal covariate shift**.

Batch normalization is trying to normalize inputs at each neuron (by normalizing outputs of previous layer). Since we are using minibatch SGD, the inputs are normalized within batches as well.

Empirical mean and variance of the batch B of size m is given by

$$\begin{aligned} \mu_B &= \frac{1}{m}\sum_{i=1}^{m} x_i \\ \sigma_B^2 &= \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_B)^2 \end{aligned} \tag{38}$$

Convolutional Neural Networks

Batch normalization

Batch normalization layer takes the output of each neuron of previous layer $h_i^{(k)}$ (i denotes a layer and k denotes a neuron) and transforms it in two steps:

1. Normalization

$$\hat{h}_i^{(k)} = \frac{h_i^{(k)} - \mu_B^{(k)}}{\sqrt{\sigma_B^{(k)^2} + \varepsilon}} \tag{39}$$

2. Shift and scale

$$x_i^k = \gamma^k \hat{h}_i^{(k)} + \beta^{(k)} \tag{40}$$

γ^k and $\beta^{(k)}$ are trainable parameters.

During inference μ and σ are calculated as a population statistics.

For convolutional networks we don't want to break its properties, mainly the shift invariance. Therefore we perform batch normalization across minibatch and spacial/temporal dimensions.

Convolutional neural network case studies

TARAN

ADVISORY IN DATA & ANALYTICS

Case studies
Networks overview

Motivation:

- Existing networks can help you to select proper architecture and hyperparameters

Case studies
Networks overview

Motivation:

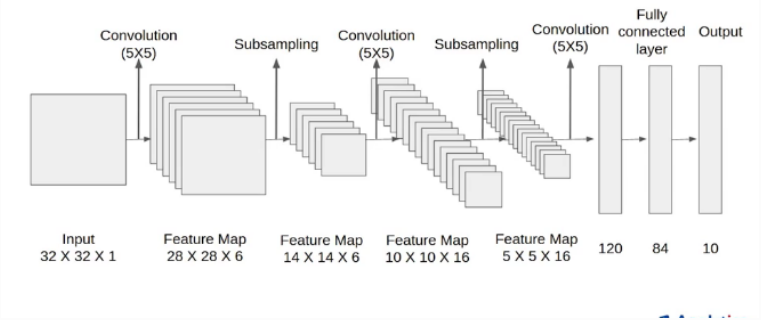
- Existing networks can help you to select proper architecture and hyperparameters

Classic networks:

- LeNet-5
- AlexNet
- VGG-16
- ResNet
- Inception

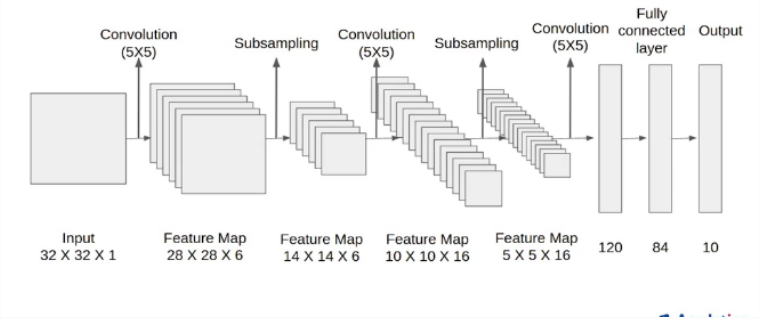
Case studies
LeNet-5

Developed in 1989 by Yann LeCun to classify hand-written digits.



Case studies
LeNet-5

Developed in 1989 by Yann LeCun to classify hand-written digits.

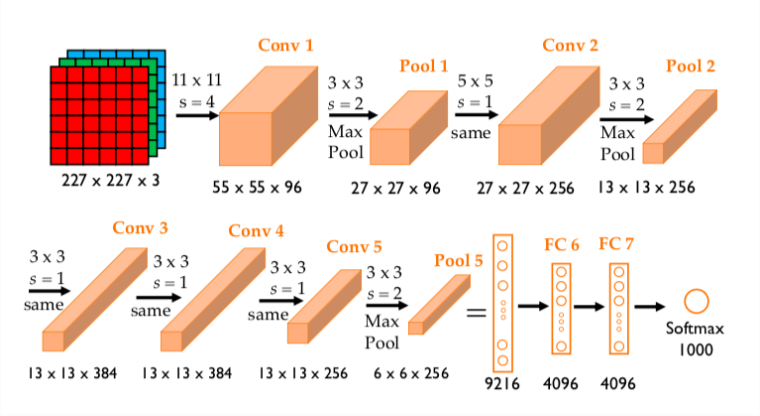


- About 60K trainable parameters

paper: Gradient-Based Learning Applied to Document Recognition (Yann LeCun, Léon Bottou, Yoshua Bengio, Patrick Haffner)

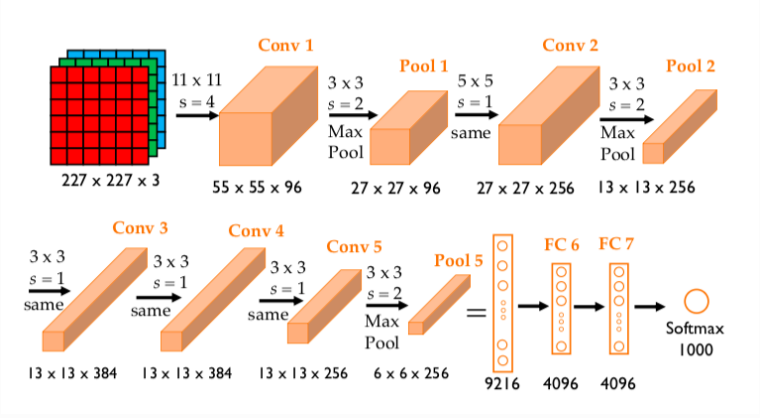
Case studies
AlexNet

Developed in 2012 to compete in the ImageNet Large Scale Visual Recognition Challenge (image classification of 1000 categories).



Case studies
AlexNet

Developed in 2012 to compete in the ImageNet Large Scale Visual Recognition Challenge (image classification of 1000 categories).

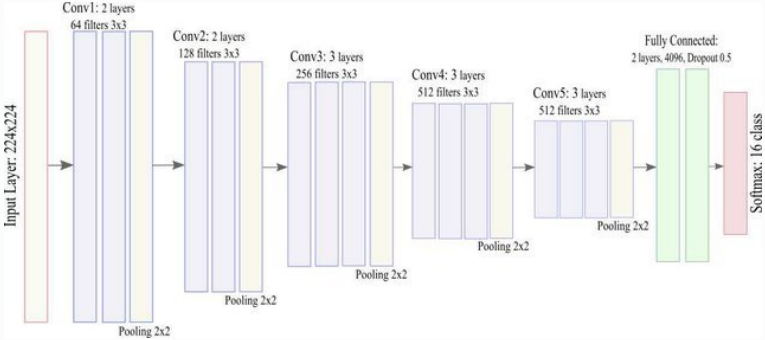


- About 60M trainable parameters

paper: ImageNet Classification with Deep Convolutional Neural Networks (Alex Krizhevsky, Ilya Sutskever, Geoffrey E. Hinton)

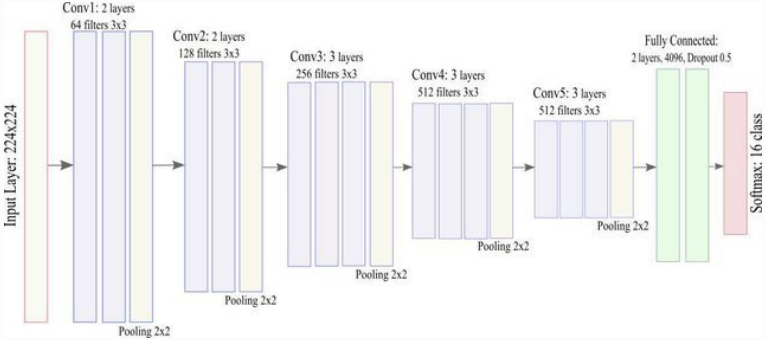
Case studies
VGG-16

Developed in 2014.



Case studies
VGG-16

Developed in 2014.



- About 138M trainable parameters

paper: Very deep convolutional networks for large-scale image recognition (Karen Simonyan, Andrew Zisserman)

Case studies
ResNet

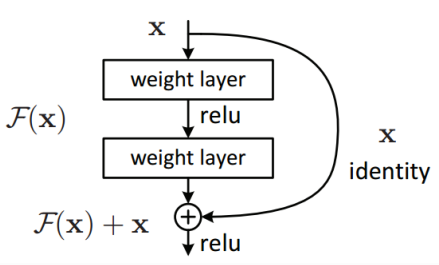
Residual neural networks utilizes skip connections.

- Residual networks allows to train deep networks.
- Skip connections help with vanishing gradient problem.

Case studies
ResNet

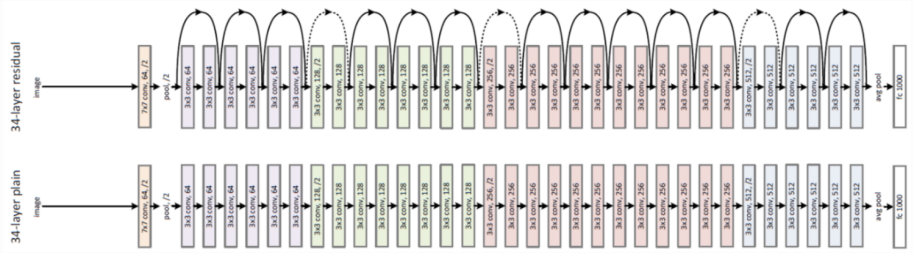
Residual neural networks utilizes skip connections.

- Residual networks allows to train deep networks.
- Skip connections help with vanishing gradient problem.



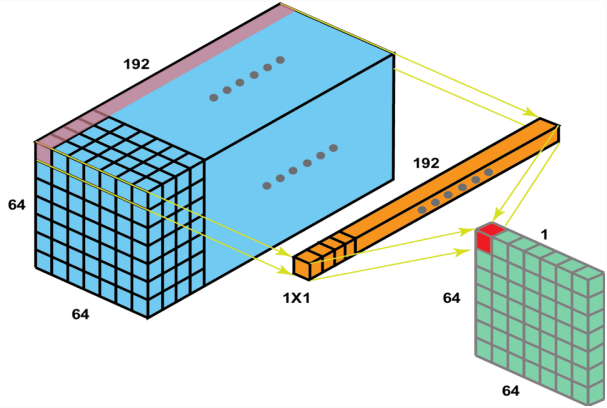
paper: Deep Residual Learning for Image Recognition (Kaiming He, Xiangyu Zhang, Shaoqing Ren, Jian Sun)

Case studies
Residual connections

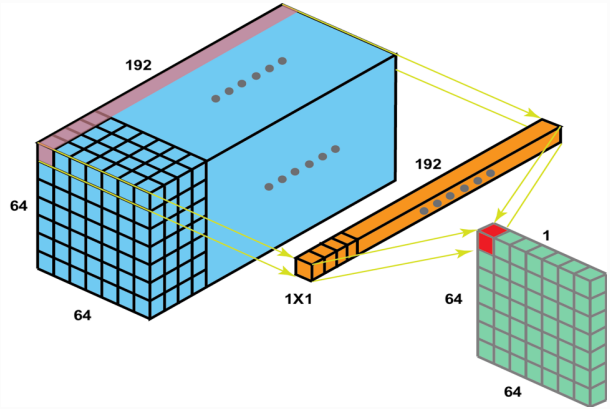


Case studies

1x1 convolution



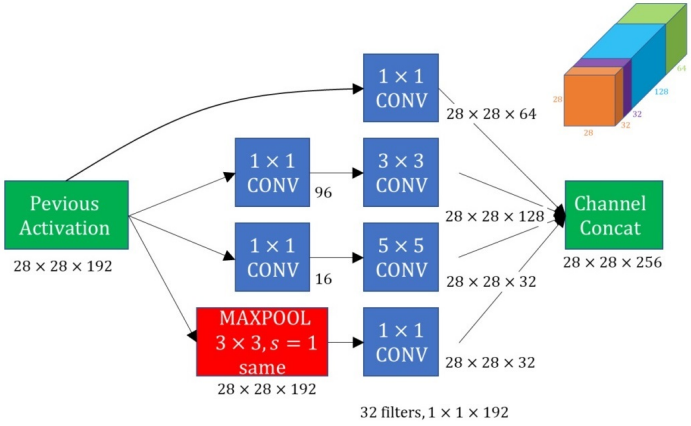
Case studies
1x1 convolution



- Can be used to shrink channels
- Can add additional non-linearity (keeping channel dimensionality)
- Can reduce computational costs

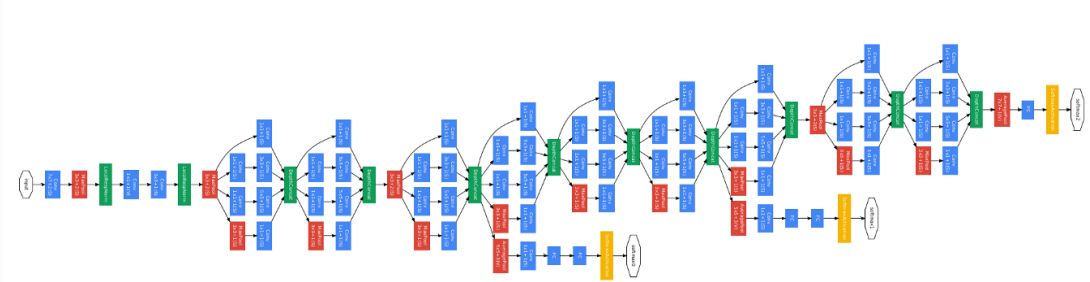
Case studies
Inception module

An example of an Inception module



Case studies
Inception network

Developed in 2014.



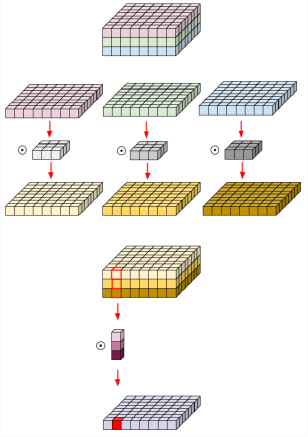
paper: Going Deeper with Convolutions (Szegedy et al.)

Case studies

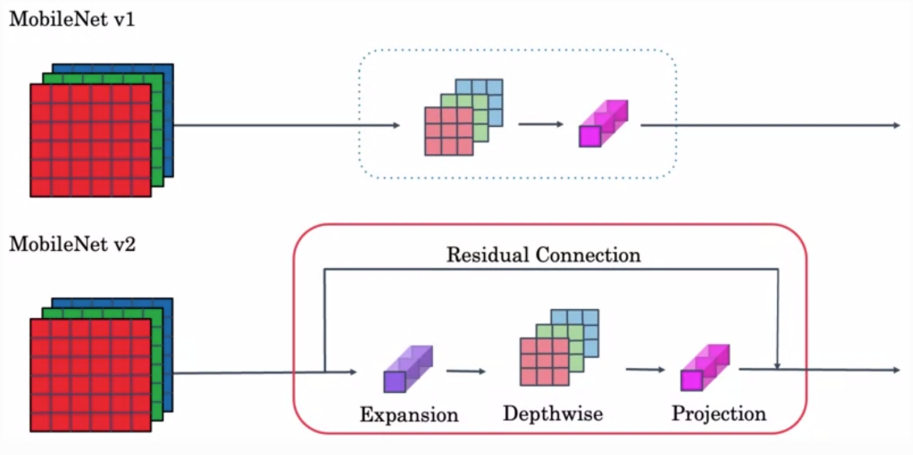
Depth-wise separable convolution

This convolution originated from the idea that depth and spatial dimension of a filter can be separated. For instance Sobel filter for edge detection can be written as vector multiplication.

$$\begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix} * \begin{bmatrix} -1 & 0 & 1 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 1 \\ -2 & 0 & 2 \\ -1 & 0 & 1 \end{bmatrix} \tag{41}$$



Case studies
MobileNet



Convolutional Neural Networks

Transfer learning

It might be useful to utilize network trained on different dataset.

- First layers of pre-trained network capture low level features such as horizontal lines and vertical lines.
- Pre-trained network harvested large dataset.
- Using pre-trained network can save lot of computational costs.

Convolutional Neural Networks

Transfer learning

It might be useful to utilize network trained on different dataset.

- First layers of pre-trained network capture low level features such as horizontal lines and vertical lines.
- Pre-trained network harvested large dataset.
- Using pre-trained network can save lot of computational costs.

We can:

- Retrain only classification layer (low amount of data).

Convolutional Neural Networks

Transfer learning

It might be useful to utilize network trained on different dataset.

- First layers of pre-trained network capture low level features such as horizontal lines and vertical lines.
- Pre-trained network harvested large dataset.
- Using pre-trained network can save lot of computational costs.

We can:

- Retrain only classification layer (low amount of data).
- Unfreeze last n layers of pre-trained network (larger dataset).

Convolutional Neural Networks

Transfer learning

It might be useful to utilize network trained on different dataset.

- First layers of pre-trained network capture low level features such as horizontal lines and vertical lines.
- Pre-trained network harvested large dataset.
- Using pre-trained network can save lot of computational costs.

We can:

- Retrain only classification layer (low amount of data).
- Unfreeze last n layers of pre-trained network (larger dataset).
- Unfreeze all layers and keep only architecture (very large dataset).

Classical approaches to NLP

Overview

Terminology:

- NLP = Natural Language Processing
- Corpus - Set of texts (documents) to be used for training
  - Set of emails
  - ...
- Document - A text unit to be processed
  - Single email
  - ...

Since lot of methods are based on word frequency analysis, data preprocessing is of essence:

- Stemming/lemmatisation
- Collocation detection
- Synonyms replacement

Other techniques used in NLP:

- TF-IDF (term frequency - inverse document frequency) - for words encoding
- SVD (singular value decomposition) - for dimensionality reduction

Text pre-processing
Stemming

Stemming is a process of reducing inflected words to their word stem.

Example:

- fishing -> fish
- fished -> fish
- fisher -> fish

Text pre-processing
Stemming

Stemming is a process of reducing inflected words to their word stem.

Example:

- fishing -> fish
- fished -> fish
- fisher -> fish
- argued -> argu
- arguing -> argu

Text pre-processing
Stemming

Stemming is a process of reducing inflected words to their word stem.

Example:

- fishing -> fish
- fished -> fish
- fisher -> fish
- argued -> argu
- arguing -> argu

How to do stemming:

a/ Use predefined mapping
- simple, fast
- new and unfamiliar words are not handled

b/ Automated mapping
- suffix stripping - remove "ed", "ing", "ly"
- works poorly for exceptional relations such as "run" and "ran"

Text pre-processing
Lemmatisation

lemma = canonical form

Lemmatisation replaces inflected words with their canonical form.

Lemmatisation uses vocabulary and morphological analysis:

- Lemmatisation uses part-of-speech (POS) tagging (recognition of nouns, verbs and other types)
- Lemmatisation uses vocabulary to determine word lemma
- Lemma for "saw" will be either "saw" or "see" - depending on the word was a noun or a verb

Text pre-processing
Collocations

Collocation refers to a group of two or more words that usually go together.

Examples:

- post office
- fast food

Collocation can be detected automatically using normalized point-wise mutual information (NPMI):

$$\begin{aligned} PMI &= \log\left[\frac{p(x,y)}{p(x)p(y)}\right] \\ NPMI &= \frac{PMI}{-\log p(x,y)} = \frac{\log[p(x)p(y)]}{\log p(x,y)} - 1 \end{aligned} \tag{42}$$

Words encoding
TF-IDF

TF-IDF = term frequency - inverse document frequency

- term frequency - frequency of a word in a document

$$TF(t,d) = \frac{\text{frequency of t in d}}{\text{number of words in d}} \tag{43}$$

- document frequency - measures document importance in a corpus

$$DF(t) = \text{number of documents with presence of t} \tag{44}$$

- inverse document frequency - measures informativeness of t

$$IDF(t) = \log \frac{N}{DF(t)+1} \tag{45}$$

- tf-idf

$$TF - IDF(t,d) = \frac{TF(t,d)}{IDF(t)} \tag{46}$$

Text pre-processing
Other tips

- stop words - most common words with low informative value. Remove them.
  - the
  - is
  - to
  - ...
- n grams - sequence of contiguous words
- To improve performance synonyms can be replaced

Dimensionality reduction
SVD

Let's assume we have TF-IDF matrix A with m rows that stand for terms and n columns that stands for documents. Rank of the matrix is $r \leq min(m, n)$.

Singular value decomposition of A is given by:

$$A = U\Sigma V^T \tag{47}$$

where U is an $m \times r$ orthogonal matrix, Σ is $r \times r$ diagonal matrix singular values on diagonal and V is $r \times n$ orthogonal matrix.

- Singular values in Σ are greater than zero
- Largest singular value is in upper left corner of Σ

Dimensionality reduction
SVD

SVD can be viewed as sum of rank one matrices:

$$A = \sum_{i=1}^{r} \Sigma_{ii} U_{,i} V_{i,}^T \tag{48}$$

where $U_{,i}$ is i-th column of U and $V_{i,}$ is i-th row of V.
We can approximate A using only $k < r$ strongest singular values:

$$A \approx A_k = \sum_{i=1}^{k} \Sigma_{ii} U_{,i} V_{i,}^T = U_k \Sigma_k V_k^T \tag{49}$$

To project a document d represented by m-dimensional vector to k-dimensional space, we can use:

$$\hat{d} = U_k^T d \tag{50}$$

Sequence models

Sequence models
Examples

Examples of sequence data:

- Speech recognition
- Music generation
- Sentiment classification
  The food was awful. $\mapsto$ ● ○ ○ ○ ○
- Machine translation
  La nourriture était horrible. $\mapsto$ *The food was awful.*
- Video recognition
- Name entity recognition
  Yesterday, Harry met Hermione. $\mapsto$ *Yesterday, Harry met Hermione.*

Sequence models
Notation

We will use following notation:

- x ... input sequence
- $x^{<i>}$ ... i-th element of sequence x
- T_x ... total number of elements in x
- y ... output sequence
- $y^{<i>}$ ... i-th element of sequence y
- T_y ... total number of elements in y
- $X^{(i)<t>}$ ... t-th element of i-th training sequence
- $Y^{(i)<t>}$ ... t-th element of output sequence for i-th training sequence
- $T_x^{(i)}$ ... total number of elements in i-th training sequence
- $T_y^{(i)}$ ... total number of elements in output sequence for i-th training sequence

Sequence models
Vocabulary

How do we represent words in a sentence?

Vocabulary is enumerated list of known words.

- It can include punctuation.
- $<$ *UNKNOWN* $>$ can be added to represent word not included in vocabulary.

Each word can be transformed using one-hot encoding.

Sequence models

Forward propagation

Usually:

$$a^{<0>} = \mathbf{0} \tag{51}$$

After first layer:

$$\begin{aligned} a^{<1>} &= g_1\left(W_{aa}a^{<0>} + W_{ax}x^{<1>} + b_a\right) \\ \hat{y}^{<1>} &= g_2\left(W_{ya}a^{<1>} + b_y\right) \end{aligned} \tag{52}$$

Note: In W_{ax}, first subscript (a) means that W_{at} is used to calculate a-like quantity, while second subscript (x) means that W_{ax} will be multiplied by x

Simplified notation:

$$\begin{aligned} W_a &= [W_{aa} \mid W_{ax}] \\ W_y &= W_{ya} \end{aligned} \tag{53}$$

Thus:

$$\begin{aligned} a^{<t>} &= g_1\left(W_a[a^{<t-1>}, x^{<t>}] + b_a\right) \\ \hat{y}^{<t>} &= g_2\left(W_y a^{<t>} + b_y\right) \end{aligned} \tag{54}$$

Sequence models
RNN types

Different types of RNN:

(a) **one-to-one**
This is standard neural network

(b) **many-to-many ($T_x = T_y$)**
example: name entity recognition

(c) **many-to-many ($T_x \neq T_y$)**
example: machine translation

(d) **many-to-one**
example: semantic classification

Sequence models
Language model

Let's assume speech recognition system:

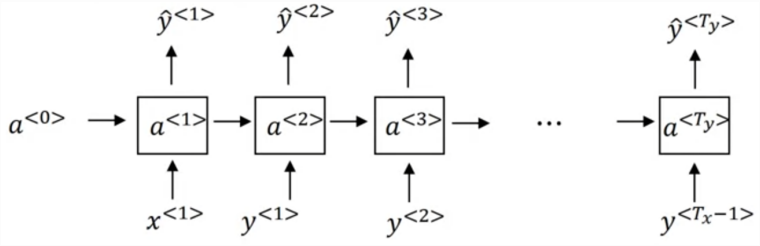
Most crimes are committed at night.
Most crimes are committed at knight.

Both sentences have the same pronunciation.

Language model assigns probability to each word given preceding words in a sentence.

$$\mathbb{P}\left[night \mid Most, crimes, are, committed, at\right] > \mathbb{P}\left[knight \mid Most, crimes, are, committed, at\right] \tag{55}$$

Sequence models
Language model

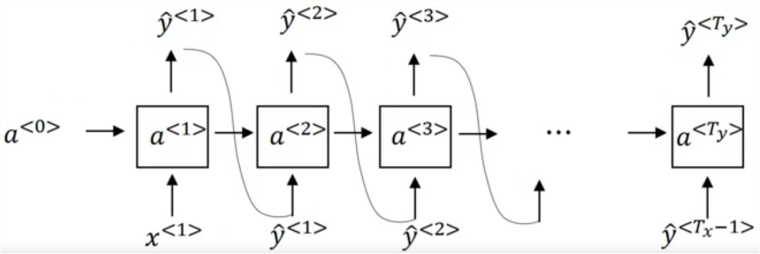


- $\hat{y}^{<t>}$ predicts probability of each word in vocabulary given previous words.
- $x^{<1>} = a^{<0>} = \mathbf{0}$
- loss function:

$$l^{<t>}(y_i^{<t>}, \hat{y}_i^{<t>}) = -\sum_i y_i^{<t>} \log \hat{y}_i^{<t>}$$
$$L = \sum_t l^{<t>}(y_i^{<t>}, \hat{y}_i^{<t>}) \tag{56}$$

Sequence models

Sampling novel sequence



- Stop generating sequence if $< EOS >$ or after fixed number of iteration
- $x^{<1>} = a^{<0>} = \mathbf{0}$
- $\hat{y}^{<t>}$ is drawn from distribution given be words probabilities
- Character level language model can be trained

Sequence models
Vanishing gradient problem

The cat, which ate ..., was full.

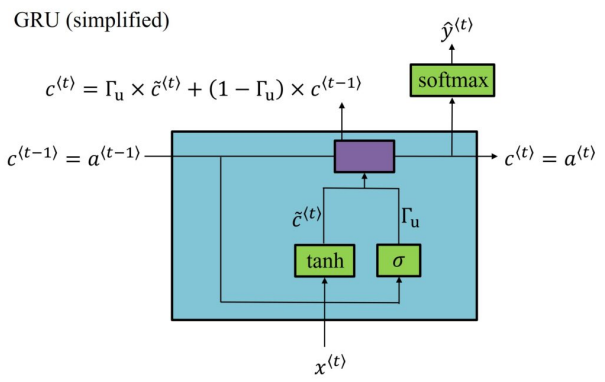
The cats, which ate ..., were full.

Sometimes probability of a word depends on very distant positions.

- Output $\hat{y}^{<t>}$ is strongly influenced by close inputs ($x^{<t>}$, $x^{<t-1>}$).
- It is not easy to propagate gradient from the end of sequence to the beginning.
- Exploding gradient can be dealt with by gradient clipping.
- What about vanishing gradient?

Sequence models
Gated recurrent unit

$$
\begin{aligned}
c^{<t-1>} &= a^{<t-1>} \\
\tilde{c}^{<t>} &= \tanh\left(W_c[c^{<t-1>}, x^{<t>}] + b_c\right) \\
\Gamma_u &= \sigma\left(W_u[c^{<t-1>}, x^{<t>}] + b_u\right) \\
c^{<t>} &= \Gamma_u \times \tilde{c}^{<t>} + (1 - \Gamma_u) \times c^{<t-1>}
\end{aligned}
\tag{57}
$$



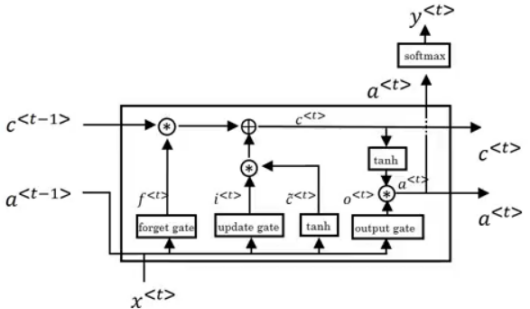
Sequence models
Gated recurrent unit

Full GRU:

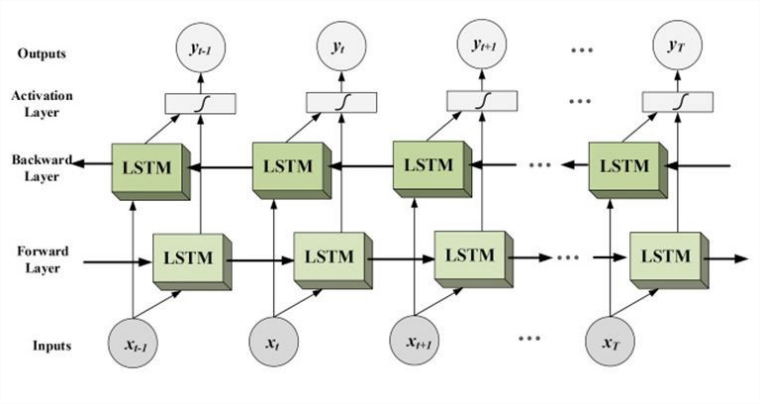
$$
\begin{aligned}
c^{<t-1>} &= a^{<t-1>} \\
\tilde{c}^{<t>} &= \tanh\left(W_c[\Gamma_r \times c^{<t-1>}, x^{<t>}] + b_c\right) \\
\Gamma_u &= \sigma\left(W_u[c^{<t-1>}, x^{<t>}] + b_u\right) \\
\Gamma_r &= \sigma\left(W_r[c^{<t-1>}, x^{<t>}] + b_u\right) \\
c^{<t>} &= \Gamma_u \times \tilde{c}^{<t>} + (1 - \Gamma_u) \times c^{<t-1>}
\end{aligned}
\tag{58}
$$

Sequence models
Long Short Term Memory

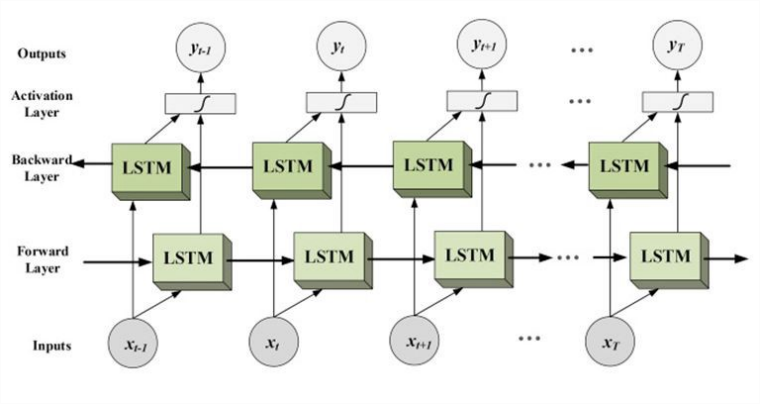
$$
\begin{aligned}
\tilde{c}^{<t>} &= \tanh\left(W_c[a^{<t-1>}, x^{<t>}] + b_c\right) \\
\Gamma_u &= \sigma\left(W_u[a^{<t-1>}, x^{<t>}] + b_u\right) \\
\Gamma_f &= \sigma\left(W_f[a^{<t-1>}, x^{<t>}] + b_f\right) \\
\Gamma_o &= \sigma\left(W_o[a^{<t-1>}, x^{<t>}] + b_o\right) \\
c^{<t>} &= \Gamma_u \times \tilde{c}^{<t>} + \Gamma_f \times c^{<t-1>} \\
a^{<t>} &= \Gamma_o \times \tanh(c^{<t>})
\end{aligned}
\tag{59}
$$



Sequence models
Bidirectional RNN

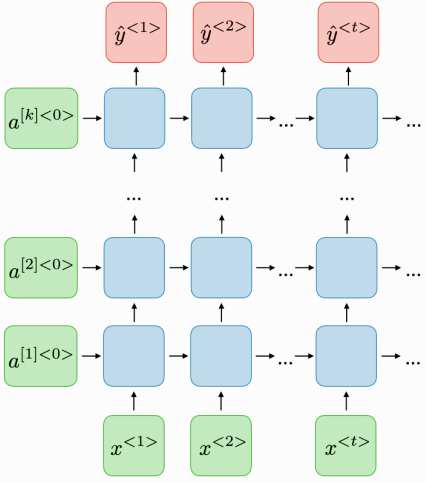


Sequence models
Bidirectional RNN



+ To predict $\hat{y}^{<t>}$ the whole sequence is used, not just sequence up to $x^{<t>}$
- To calculate prediction, you need to wait until the whole sequence is finished

Sequence models
Deep RNN



- Each layer has one weight matrix assigned
- Because of time dimension, three layer network might be already quite large
- Deep RNN can be build using RNN, GRU, LSTM or BRNN layers

Word embeddings

TARAN

ADVISORY IN DATA & ANALYTICS

Word embeddings

Word representation

So far we were using one-hot encoding for words representation.

Man (5391)	Woman (9853)	King (4914)	Queen (7157)	Water (9532)	Beer (982)
0	0				
⋮					
1	⋮				
		⋮	⋮	⋮	⋮
⋮	1				
	⋮				
0	0				

Word embeddings

Word representation

Instead one-hot, we might want to use feature representation.

	Man (5391)	Woman (9853)	King (4914)	Queen (7157)	Water (9532)	Beer (982)
Gender	-0.97	0.98	-0.95	0.93	0.02	0.01
Royal	0.04	-0.02	0.96	0.95	0.01	-0.04
Beverage	-0.03	0.01	0.02	- 0.04	0.97	0.98
⋮						

- Features in embeddings don't have nice meaning like in the table above
- Vectors for similar things (water and beer) are similar in feature space

Word embeddings
t-SNE

t-SNE = t-distributed stochastic neighbour embedding

Let us have a set of N high-dimensional objects $\mathbf{x}_1, \ldots, \mathbf{x}_N$.

$$p_{j|i} = \frac{\frac{\exp(-\|\mathbf{x_i}-\mathbf{x_j}\|^2)}{2\sigma_i^2}}{\sum_{k\neq i}\frac{\exp(-\|\mathbf{x_i}-\mathbf{x_k}\|^2)}{2\sigma_i^2}} \qquad \forall i \neq j$$
$$p_{i|i} = 0 \tag{60}$$

"The similarity of datapoint x_j to datapoint x_i is the conditional probability $p_{j|i}$ that x_i would pick x_j as its neighbour if neighbours were picked in proportion to their probability density under a Gaussian centred at x_i."

$$p_{ij} = \frac{p_{j|i} + p_{i|j}}{2N}$$
$$p_{ii} = 0 \tag{61}$$

Word embeddings
t-SNE

We want to learn d-dimensional representation $\mathbf{y}_1, ..., \mathbf{y}_N$ of $\mathbf{x}_1, ..., \mathbf{x}_N$.

$$q_{ij} = \frac{\left(1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2\right)^{-1}}{\sum_k \sum_{l \neq k} \left(1 + \|\mathbf{y}_k - \mathbf{y}_l\|^2\right)^{-1}} \qquad (62)$$
$$q_{ii} = 0$$

Locations of $\mathbf{y}_1, ..., \mathbf{y}_N$ are given by minimization of distance between distributions P and Q.

$$KL(P\|Q) = \sum_{i \neq j} p_{ij} \log \frac{p_{ij}}{q_{ij}} \qquad (63)$$

Word embeddings
Similarity functions

What if, for a given word w, we want to find a most similar word in embedding space:

$$\underset{w_i}{\operatorname{argmax}}\, sim(e_w, e_{w_i}) \tag{64}$$

Similarity functions can be:

- Cosine similarity

$$sim(u, v) = \frac{u^T v}{\|u\|_2 \|v\|_2} \tag{65}$$

- Negative Euclidean distance

$$sim(u, v) = -\|u - v\|^2 \tag{66}$$

Word embeddings
Learning embeddings

Let's o_i be the one-hot encoding of i-th word in vocabulary.

$$o_i = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} \leftarrow i - th\ position \tag{67}$$

Embedded vector for i-th word is given by embedding matrix E.

$$e_i = E \cdot o_i = \begin{bmatrix} e_{11} & \dots & e_{1m} \\ \vdots & \ddots & \vdots \\ e_{n1} & \dots & e_{nm} \end{bmatrix} \cdot \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} \tag{68}$$

For vocabulary size 10000 and 300-dimensional embedding space, $E \in \mathbb{R}^{300x10000}$

Word embeddings
Learning embeddings

Let's have a language model.

I want a glass of orange juice.

Based on "I want a glass of orange", we want to predict "juice".

Word embeddings
Learning embeddings

Let's have a language model.

I want a glass of orange juice.

Based on "I want a glass of orange", we want to predict "juice".

Model:

- Start with on-hot encoding
- Apply embedding
- Add output layer with softmax activation (output layer size is given by vocabulary size)

Embedding matrix is learned through model training (*E* consists of trainable parameters).

Word embeddings
Learning embeddings

Let's have a language model.

I want a glass of orange juice.

Based on "I want a glass of orange", we want to predict "juice".

Model:

- Start with on-hot encoding
- Apply embedding
- Add output layer with softmax activation (output layer size is given by vocabulary size)

Embedding matrix is learned through model training (*E* consists of trainable parameters).

Words used for predicting target word are called context.

- n words left from target word
- n words left + n word right from target word
- 1 word left
- nearby one word (skip-gram)

Word embeddings
Learning embeddings

I want a glass of orange juice.

context	target
glass	orange
glass	of
glass	want
⋮	⋮

$$\mathbb{P}[t|c] = \frac{e^{\theta_t^T e_c}}{\sum_{j=1}^{10000} e^{\theta_j^T e_c}} \tag{69}$$

Loss function:

$$L(\hat{y}, y) = -\sum_{i=1}^{10000} y_i \log \hat{y}_i \tag{70}$$

Word embeddings
Word2vec

Problem with previous approach is the computational cost.

We will use negative sampling to create a training sample:

context	target	y
orange	juice	1
orange	football	0
orange	paper	0
⋮	⋮	0
orange	of	0

For one positive context-target pair we added K negative pairs.

The output layer will still be of size of vocabulary size, but each neuron will calculate sigmoid instead of softmax.

$$\mathbb{P}[y = 1|c, t] = \sigma(\theta_t^T e_c) \tag{71}$$

Word embeddings
Word2vec

How to choose negative samples:

- x We can draw negative samples based on distribution over word frequencies
  Leads to high presence of words such as "the", "of", "a"
- x We can sample words uniformally
  This is very non-representative
- √ Use following distribution (discovered empirically)

$$\mathbb{P}[w_i] = \frac{f(w_i)^{3/4}}{\sum_j f(w_j)^{3/4}} \tag{72}$$