Machine Learning

Lecture 11: Neural Networks 3

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Ver. 1.0

Topics - you should be able to explain after this week

- Problems with multi-layer neural networks trained with EBP
- Overfitting and generalisation
- Techniques to mitigate the overfitting
- Convolutional neural networks
- Recurrent neural networks
- Other neural network models
- Sequence to sequence models

History of artificial neural networks till 1990

1940s	Warren McCulloch and Walter Pitts : 'threshold logic'
	Donald Hebb : 'Hebbian learning'
1957	Frank Rosenblatt : 'Perceptron'
1969	Marvin Minsky and Seymour Papert : limitations of neural networks
1980	Kunihiro Fukushima: 'Neocognitoron'
1986	D. Rumelhart, G. Hinton, and R. Williams, "Learning representations by back-propagating errors" (1974, Paul Werbos)

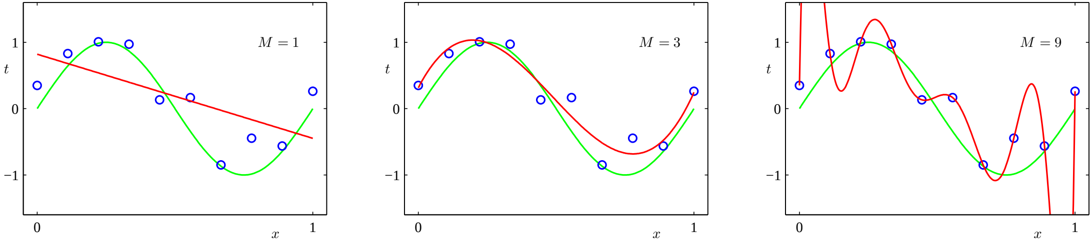
Problems with multi-layer neural networks trained with EBP

- Still difficult to train
  - Computationally very expensive (e.g. weeks of training)
  - Slow convergence ('vanishing gradients')
  - Difficult to find the optimal network topology
- Poor generalisation
  - Very good performance on the training set
  - Poor performance on the test set

Overfitting and generalisation

Example of curve fitting by a polynomial function:

$$y(x, \boldsymbol{w}) = w_0 + w_1\, x + w_2\, x^2 + \ldots + w_M\, x^M = \sum_{k=0}^{M} w_k\, x^k$$



(after Fig 1.4 in PRML C. M. Bishop (2006))

- cf. memorisation of the training data

Generalisation in neural networks

- How many hidden units (or, how many weights) do we need?
- Optimising training set performance does not necessarily optimise test set performance
  - Network too "flexible": Too many weights compared with the number of training examples
  - Network not flexible enough: Not enough weights (hidden units) to represent the desired mapping
- **Generalisation Error**: The predicted error on unseen data. How can the generalisation error be estimated?
  - Training error?

$$E_{\text{train}} = \frac{1}{2} \sum_{\text{trainingset}} \sum_{k=1}^{K} (y_k - t_k)^2$$

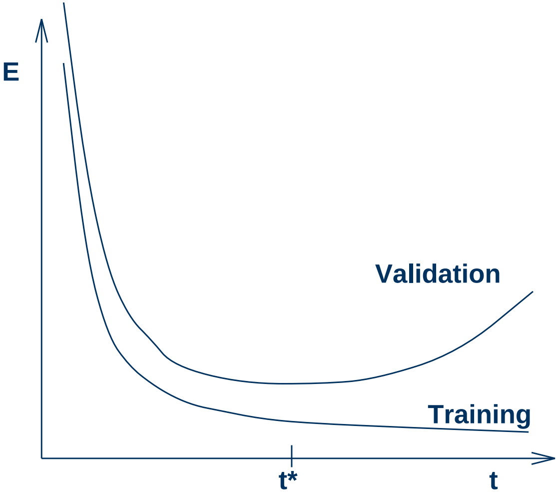
  - Cross-validation error?

$$E_{\text{xval}} = \frac{1}{2} \sum_{\text{validationset}} \sum_{k=1}^{K} (y_k - t_k)^2$$

Overtraining in neural networks

- Overtraining (overfitting) corresponds to a network function too closely fit to the training set (too much flexibility)
- Undertraining corresponds to a network function not well fit to the training set (too little flexibility)
- Solutions
  - If possible increasing both network complexity in line with the training set size
  - Use prior information/knowledge to constrain the network functions: Structural Stabilisation
  - Control the effective flexibility: **early stopping** and **regularisation**

Early stopping



Early stopping (*cont.*)

- Use validation set to decide when to stop training
- Training-set error monotonically decreases as training progresses
- Validation-set error will reach a minimum then start to increase
- "Effective Flexibility" increases as training progresses
- Network has an increasing number of "effective degrees of freedom" as training progresses
- Network weights become more tuned to training data
- Very effective — used in many practical applications such as speech recognition and optical character recognition

Regularisation – penalising complexity

- Original error function

$$E(\boldsymbol{w}) = \frac{1}{2}\sum_{n=1}^{N}||\hat{\mathbf{y}}_n - \mathbf{y}_n||^2$$

- Regularised error function (aka weight decay)

$$\tilde{E}(\boldsymbol{w}) = \frac{1}{2}\sum_{n=1}^{N}||\hat{\mathbf{y}}_n - \mathbf{y}_n||^2 \, + \, \frac{\beta}{2}\sum||\boldsymbol{w}||^2$$

Breakthrough

1957 Frank Rosenblatt : 'Perceptron'

1986 D. Rumelhart, G. Hinton, and R. Williams: 'Backpropagation'

2006 G. Hinton etal (U. Toronto)

"Reducing the dimensionality of data with neural networks", Science, July 2006

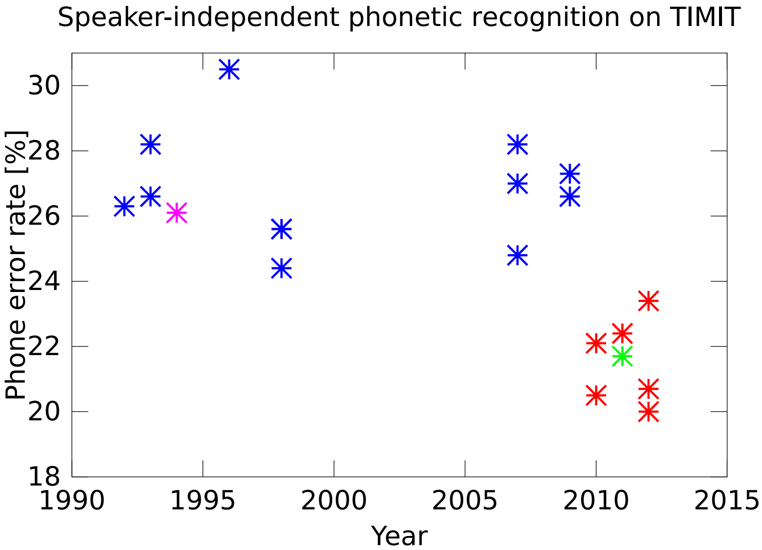
2009 J. Schmidhuber (Swiss AI Lab IDSIA)

Winner at ICDAR2009 handwriting recognition competition

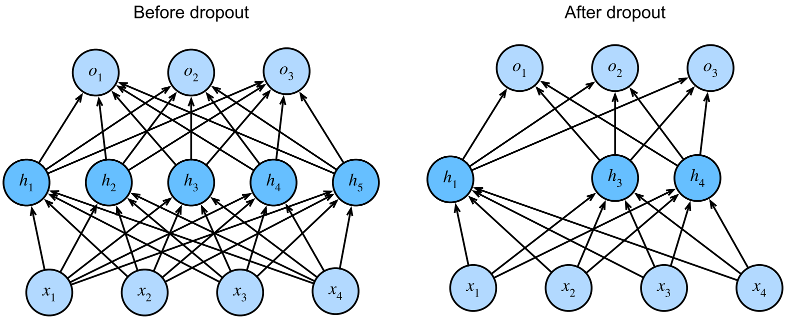
2011- many papers from U.Toronto, Microsoft, IBM, Google, ...

- What's the idea?
  - Pretraining
    - A single layer of feature detectors $\rightarrow$ Stack it to form several hidden layers
  - Fine-tuning, dropout
  - GPU
  - Convolutional network (CNN), Long short-term memory (LSTM)
  - Rectified linear unit (ReLU)

Speech recognition



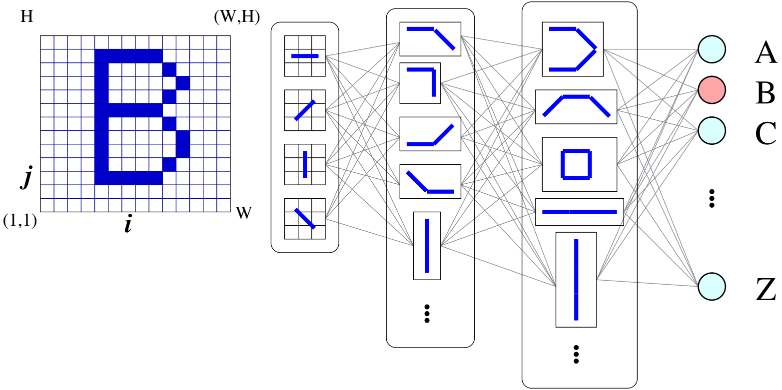
Another regularisation - dropout



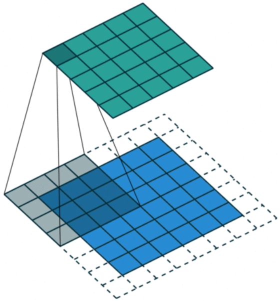
After Figure 5.6.1 MLP before and after dropout of Dive into Deep Learning

Background of convolutional neural networks

- Primary visual cortex (D. Hubel and T. Wiesel in 1959)
- Neocognitron (K. Fukushima in 1979)
- Nice to have shift/scale/rotation invariant classifiers
- Hard to train fully-connected neural networks on image data



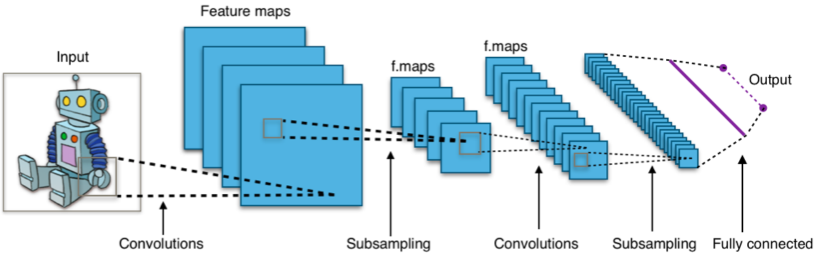
Convolutional neural networks (CNNs)



After Convolution arithmetic - Arbitrary padding no strides of Wikimedia common

Components of CNNs

- Convolutional layers
- Pooling layers
- Normalisation layers
- (Fully connected layers)



After Typical CNN architecture of Wikimedia common

Convolution *(NE)*

- The output of applying a filter $w(n)$ to an input $x(n)$ is given as convolution, denoted as $[\mathbf{w} \circledast \mathbf{x}](n)$ or $w(n) \circledast x(n)$:

$$y(n) = [\mathbf{w} \circledast \mathbf{x}](n) = \sum_{\ell=-\infty}^{\infty} w(\ell)\, x(n-\ell)$$

- If $w(n)$ is defined in $[-L, L]$,

$$\begin{aligned} y(n) &= \sum_{\ell=-L}^{L} w(\ell)\, x(n-\ell) \\ &= \sum_{k=-L}^{L} w(k)\, x(n+k) \quad \text{where } k = -\ell \end{aligned}$$

- Further simplification by assuming w(n) is defined in $[0, L-1]$ yields:

$$y(n) = \sum_{k=0}^{L-1} w(k)\, x(n+k)$$

CNNs – Convolutional layers

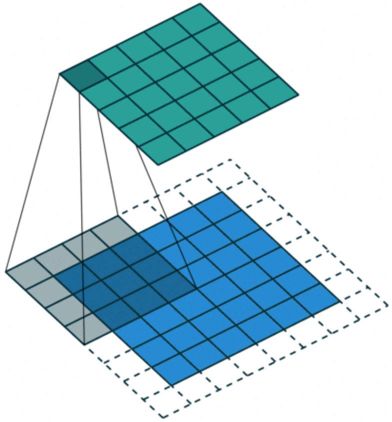
- 1D convolution

$$[\mathbf{w} \circledast \mathbf{x}](i) = \sum_{u=0}^{L-1} w_u \, x_{i+u}$$

- 2D convolution

$$[\mathbf{W} \circledast \mathbf{X}](i,j) = \sum_{u=0}^{H-1}\sum_{v=0}^{W-1} w_{u,v} \, x_{i+u,j+v}$$

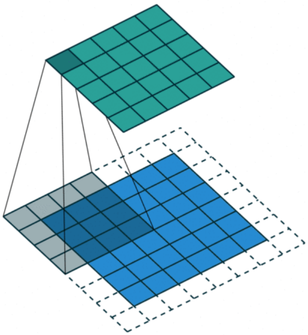
- filters (aka kernels)
  - Assuming local correlation / connectivity
  - Parameter sharing (shared weights)
- Parameters for convolution
  - Stride
  - Padding



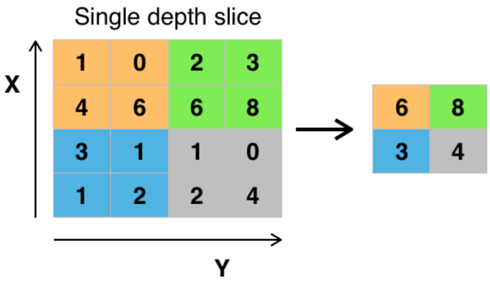
After Convolution arithmetic - Arbitrary padding no strides of Wikimedia common

CNNs – Pooling layers

- Downsampling → increase robustness against small shift
- Types of pooling
  - Max pooling
  - Average pooling



After Convolution arithmetic - Arbitrary padding no strides *of* Wikimedia common



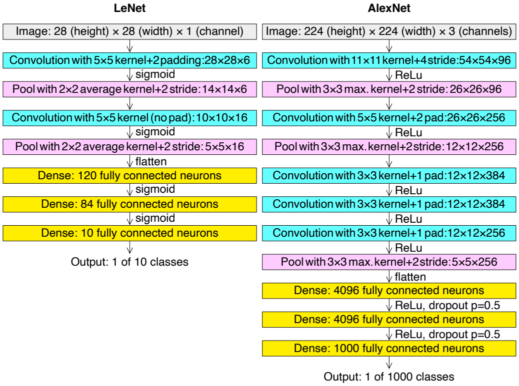
After Max pooling *of* Wikimedia common

CNNs – Normalisation layers

- Batch normalisation *(S. Loffe and C. Szebedy, Google, 2015)*
  - Normalise the output distribution of a layer for each mini-batch – zero mean and a unit variance.

CNN based systems

- LeNet (LeCun *et al.*, 1998)
- AlexNet (Alex Sutskever *et al.*, 2017)
- VGG16 (K.Simonyan and A.Zisserman, 2014)
- ResNet (He *et al.*, 2016)



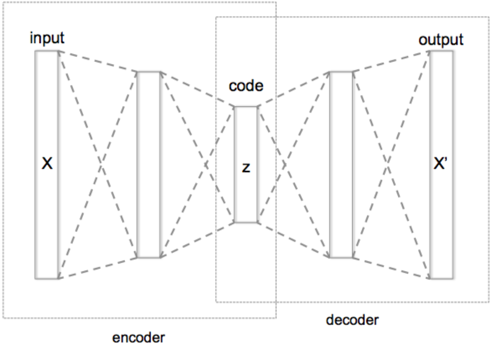
After Comparison image neural networks of Wikimedia common

Other neural networks

- Autoencoder

$$\min_{\theta,\phi} \frac{1}{N}\sum_{i=1}^{N} \|\mathbf{x}_i - \mathrm{Decoder}_\theta(\mathrm{Encoder}_\phi(\mathbf{x}_i))\|^2$$

  $\mathbf{z}$:
  - Embedded features, bottleneck features
  - Latent representation
  - cf. PCA

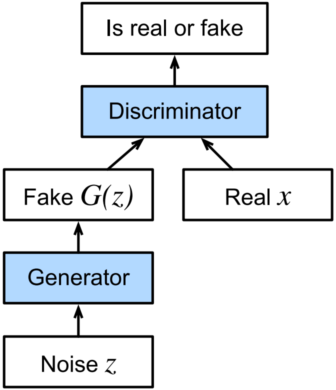


After Autoencoder structure of Wikimedia common

- Variational Auto Encoder (VAE)
  [D.Kingma and M.Welling, 2013]

Other neural networks (*cont.*)

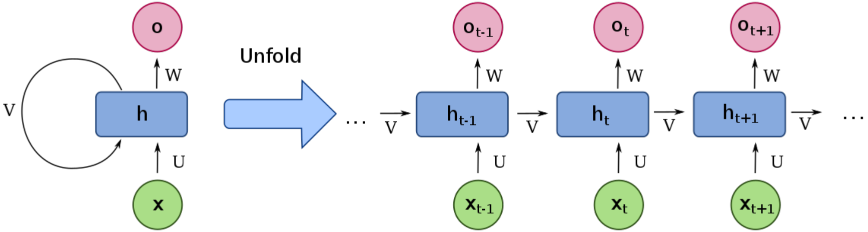
- Generative adversarial network (GAN) [I. Goodfellow *et al.*, 2014]



After Figure 18.1.1 Generative Adversarial Networks of Dive into Deep Learning

Neural networks for sequences

- Recurrent Neural Network (RNN)

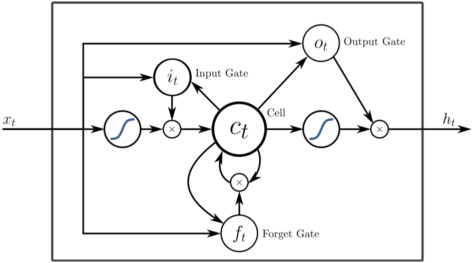


After Recurrent neural network unfold of Wikimedia common

- Vanishing/exploding gradients problem

Neural networks for sequences *(cont.)*

- Long short-term memory (LSTM) S.Hochreiter and J.Schmidhuber, 1995

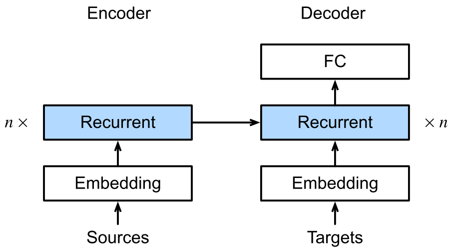


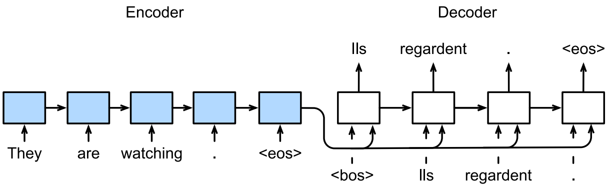
After A peephole LSTM unit with input (i.e. i), output (i.e. o), and forget (i.e. f) gates of Wikimedia common

- https://arxiv.org/abs/1409.1259 Kyunghyun Cho *et al.*, 2014

Sequence to sequence models

- seq2seq $\cdots$ encoder-decoder model with attention





From Figures 10.7.1 and 10.7.2 of Dive into Deep Learning

Sequence to sequence models

- Transformer
  - BERT (Bidirectional Encoder Representations from Transformers) J.Devlin *et al.*, Google, 2018
    question answering, natural language interface
  - GPT-2 (Generative Pre-trained Transformer 2) , A.Radford *et al.*, OpenAI, 2019) $\cdots$ 1.5 billion parameters.
    text translation/generation/summarisation, question answering
  - GPT-3 $\cdots$ 175 billion parameters
  - DALL-E $\cdots$ 12-billion parameter version of GPT-3 trained to generate images from text descriptions

Other topics *(NE)*

- Transfer learning
- Multi-task learning
- Data augmentation
- Domain adaptation
- Zero-shot learning