Course 395: Machine Learning - Lectures

Lecture 1-2: Concept Learning (M. Pantic)

Lecture 3-4: Decision Trees & CBC Intro (M. Pantic & S. Petridis)

Lecture 5-6: Evaluating Hypotheses (S. Petridis)

Lecture 7-8: Artificial Neural Networks I (S. Petridis)

➢ Lecture 9-10: Artificial Neural Networks II (S. Petridis)

Lecture 11-12: Instance Based Learning (M. Pantic)

Lecture 13-14: Genetic Algorithms (M. Pantic)

Why squared error is not a good choice for sigmoid output activation functions

- See http://neuralnetworksanddeeplearning.com/chap3.html
- For output units: $\Delta w_{ki} = -\eta \frac{\partial E}{\partial o_k} \frac{\partial \sigma(net_k)}{\partial net_k} x_{ki}$
- $\frac{\partial E}{\partial o_k} = -(t_k - o_k)$ when the error function is the squared loss
- $\frac{\partial \sigma(net_k)}{\partial net_k} = \sigma(net_k)(1 - \sigma(net_k)) = o_k(1 - o_k)$

  when σ is sigmoid

Why squared loss is not a good choice for sigmoid output activation functions

- See http://neuralnetworksanddeeplearning.com/chap3.html
- For output units: $\Delta w_{ki} = \eta(t_k - o_k)o_k(1 - o_k)x_{ki}$
- When the output is 0 or 1 then Δw is 0 as well
- If target is 1 and network's output is 1 then Δw = 0 (good)
- If target is 1 and network's output is 0 then Δw = 0 (bad!!!)

Cross Entropy Error as Error Function

- A good error function when the output activation functions are sigmoid is the binary cross entropy defined as follows:

$$E = -\frac{1}{D}\sum_{d=1}^{D}\left(t_d \ln o_d + (1-t_d)\ln(1-o_d)\right)$$

D = number of training examples

- For output units: $\Delta w_{ki} = -\eta \frac{\partial E}{\partial o_k}\frac{\partial \sigma(net_k)}{\partial net_k} x_{ki}$
- $\frac{\partial E}{\partial o_k} = \frac{o_k - t_k}{o_k(1-o_k)}$
- $\frac{\partial \sigma(net_k)}{\partial net_k} = \sigma(net_k)(1-\sigma(net_k)) = o_k(1-o_k)$

Cross Entropy Error as Error Function

- For output units: $\Delta w_{ki} = -\eta \frac{\partial E}{\partial o_k} \frac{\partial \sigma(net_k)}{\partial net_k} x_{ki}$

- $\Delta w_{ki} = -\eta \frac{o_k - t_k}{o_k(1-o_k)} o_k(1-o_k) x_{ki} = \eta(t_k - o_k)\, x_{ki}$

- The higher the error the higher the weight update

Softmax output activation functions

- A popular output activation function for classification is softmax $o_k = \frac{e^{net_k}}{\sum_k e^{net_k}}$
- The output can be interpreted as a discrete probability distribution
- The right error function is the negative log likelihood cost $E = -\sum_k t_k ln o_k$
- Target vectors = [0 0 1 … 0] → $E = -ln o_L$ where L is the position of the active target, i.e., it is 1.
- It is equivalent to the binary cross entropy for 2 classes

Output activation functions: Summary

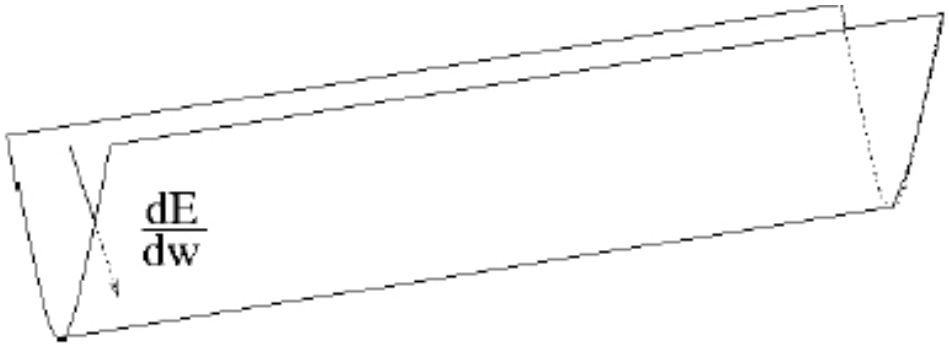
- For each output activation function the right error function should be selected
- Sigmoid → Cross entropy error (useful for classification)
- Softmax → negative log likelihood cost (useful for classification)
- Both combinations work well for classification problems, Softmax has the advantage of producing a discrete probability distribution over the outputs
- Linear → MSE (useful for regression)

Backpropagation with momentum

- Standard backpropagation

$$w_i \leftarrow w_i + \Delta w_i \quad \Delta w_i = -\eta \frac{\partial E}{\partial w_i}$$

- If the error surface is a long and narrow valley, gradient descent goes quickly down the valley walls, but very slowly along the valley floor.



From https://www.cs.toronto.edu/~hinton/csc2515/notes/lec6tutorial.pdf

Backpropagation with momentum

- Standard backpropagation

$$w_i \leftarrow w_i + \Delta w_i \quad \Delta w_i = -\eta \frac{\partial E}{\partial w_i}$$

- Backpropagation with momentum

$$\Delta w_i(t) = \mu\, \Delta w_i(t-1) + (1-\mu)\left(-\eta \frac{\partial E}{\partial w_i(t)}\right) \textbf{ OR}$$

$$\Delta w_i(t) = \mu\, \Delta w_i(t-1) + \left(-\eta \frac{\partial E}{\partial w_i(t)}\right)$$

- $\mu =$ momentum constant, usually $0.9, 0.95$
- It is like giving momentum to the weights
- We do not take into account only the local gradient but also recent trends in the error surface
- Matlab function: **traingdm**

Backpropagation with adaptive learning rate

- It is good that the learning rate is not fixed during training

$$w_i \leftarrow w_i + \Delta w_i \quad \Delta w_i = -\eta \frac{\partial E}{\partial w_i}$$

- Simple heuristic
  1. If error decreases, increase learning rate: $\eta = \eta * \eta_{inc}$
  2. If error increases, decrease learning rate and don't update the weights: $\eta = \eta * \eta_{dec}$

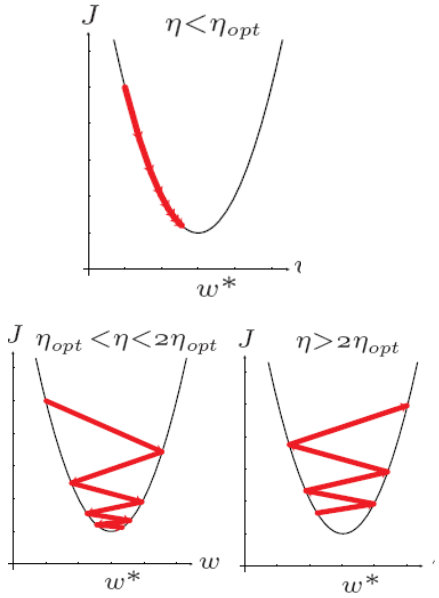
- Typical values for $\eta_{inc} = 1.05, 1.1$
- Typical values for $\eta_{dec} = 0.5, 0.7$
- Matlab function: **traingda**

Resilient Backpropagation

- The weight change depends on the learning rate and the value of the partial derivative. We have no control over the partial derivative.
- The effect of the learning rate can be disturbed by the unforeseeable behaviour of the derivative.
- Resilient backpropagation uses only the sign of the derivative!!
- For each weight w_i we define an individual update value Δ_i which depends only on the sign of the derivative and ignores its actual value

Resilient Backpropagation

$$\Delta_i(t) = \begin{cases} \Delta^{inc} * \Delta_i(t-1) \;\; if \;\; \dfrac{\partial E^{t-1}}{\partial w_i} * \dfrac{\partial E^{t}}{\partial w_i} > 0 \\ \Delta^{dec} * \Delta_i(t-1) \;\; if \;\; \dfrac{\partial E^{t-1}}{\partial w_i} * \dfrac{\partial E^{t}}{\partial w_i} < 0 \end{cases}$$

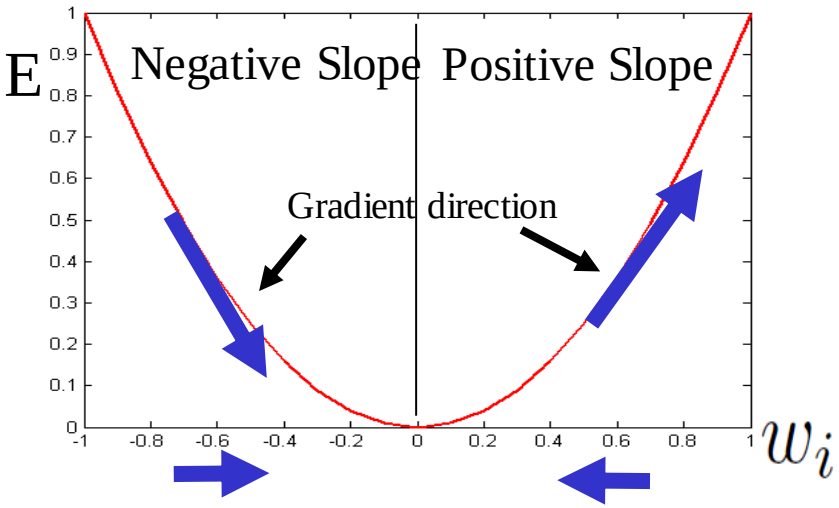


- Every time the partial derivative changes its sign, i.e., last update was too big, the update value is decreased.

- If the derivative retains its sign, the update value is increased in order to accelerate convergence.

Resilient Backpropagation

$$\Delta w_i(t) = \begin{cases} -\Delta_i(t) \;\; if \;\; \dfrac{\partial E^t}{\partial w_i} > 0 \\ \Delta_i(t) \;\; if \;\; \dfrac{\partial E^t}{\partial w_i} < 0 \end{cases}$$



- We also need to initialise the update values Δ_i
- We usually define an upper limit for Δ_i
- Typical values for $\Delta_{inc} = 1.2$
- Typical values for $\Delta_{dec} = 0.5$
- Matlab function: **trainrp**

Other Training Algorithms

- Conjugate gradient
- Levenberg-Marquardt
- Hessian-free
- And many others…not covered in the lecture

Batch/Mini-batch/Stochastic Gradient Descent

- Batch: All examples are fed to the network. Weights are updated only after all examples have been presented to the network
- For each weight the corresponding gradient (or Δw) is computed (for each example).
- The weights are updated based on the average gradient over all examples.
- Stochastic/Incremental/On-line: One example at a time is fed to the network.
- Weights are updated after each example is presented to the network

Batch/Mini-batch/Stochastic Gradient Descent

- Mini-Batch: M (usually 100) randomly examples are fed to the network.
- For each weight the corresponding gradient (or Δw) is computed (for each example).
- The weights are updated based on the average gradient over all M examples.
- Set of M examples is called mini-batch.
- Popular approach in deep neural networks.
- Sometimes called stochastic gradient descent (NOT to be confused with online/incremental gradient descent).

(Hyper)Parameters / Weights

- (Hyper)Parameters are what the user specifies, e.g. number of hidden neurons, learning rate, number of epochs etc
- They need to be optimised
- Weights are the weights of the network
- They are also parameters but they are optimised automatically via gradient descent

Ways to avoid overfitting

- Early stopping (see slide 52)
- L1 Regularisation
- L2 Regularisation
- Dropout
- Max-norm Constraint
- Data augmentation

L2 Regularisation

- $E = E_0 + \lambda \sum_{all\ Weights} w^2$
- E_0 is the original error function, e.g., squared loss, negative log-likelihood
- It is NOT applied to the bias
- We wish to minimise the original error function (E_0)
- We also wish to penalise large weights, keep the weights small (second term)
- Small λ → we prefer to minimise E_0
- Large λ → we prefer small weights

L1 Regularisation

- $E = E_0 + \lambda \sum_{all\ Weights} |w|$
- E_0 is the original error function, e.g., squared loss, negative log-likelihood
- It is NOT applied to the bias
- We wish to minimise the original error function (E_0)
- We also wish to penalise large weights, keep the weights small (second term)
- Small λ → we prefer to minimise E_0
- Large λ → we prefer small weights

L1/L2 Regularisation

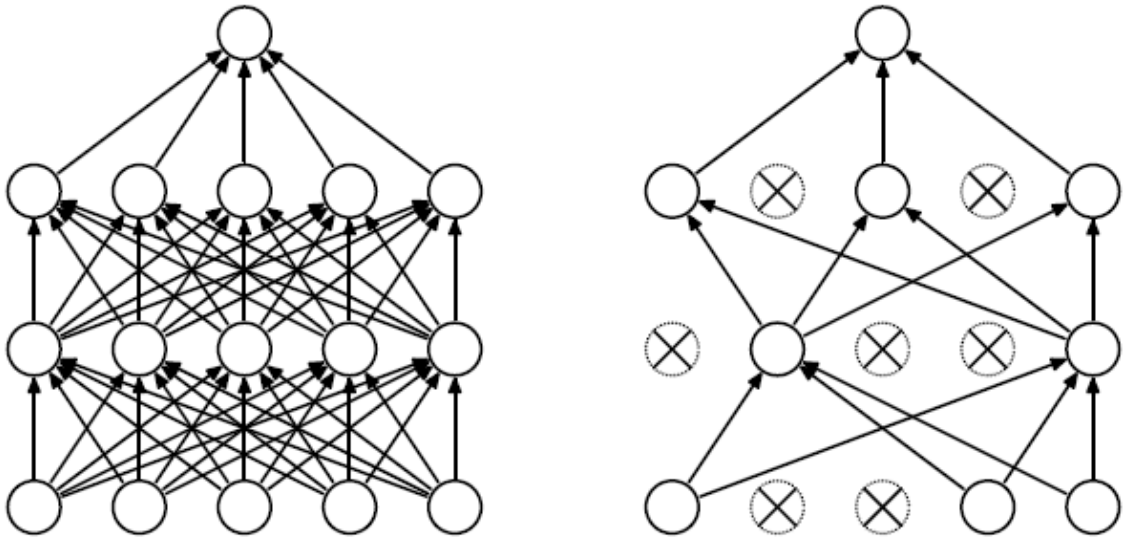
- So what's the difference between L1 and L2 regularisation?
- L2: $\frac{\partial E}{\partial w} = \frac{\partial E_0}{\partial w} + \lambda w \rightarrow \Delta w = -\eta \frac{\partial E_0}{\partial w} - \eta\lambda w$
- L1: $\frac{\partial E}{\partial w} = \frac{\partial E_0}{\partial w} + \lambda sign(w) \rightarrow \Delta w = -\eta \frac{\partial E_0}{\partial w} - \eta\lambda sign(w)$
- L1: The weights shrink by a constant amount towards 0
- L2: The weights shrink by an amount proportional to w
- L1 drives small weights to zero

L1/L2 Regularisation

- Why small weights prevent overfitting?
- When weights are 0 or close to zero this equivalent to removing the corresponding connection between the neurons
- Simpler architecture → avoids overfitting
- Network has the right capacity
- It is like we start with a high capacity (complex) network until we find a network with the right capacity for the problem

Dropout

- We don't modify the error function but the network itself
- During training neurons are randomly dropped out
- The probability that a neuron is present is p

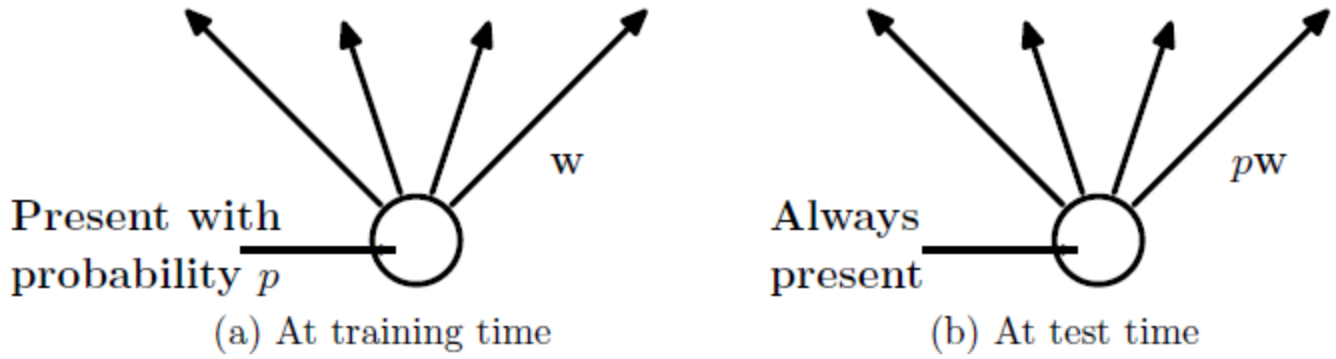


(a) Standard Neural Net (b) After applying dropout.

From Dropout: A simple way to prevent neural networks from overfitting by Srivastava et al., JMLR 2014

Dropout

- Dropout prevents overfitting because it provides a way of approximately combining exponentially many different neural network architectures.
- Typical values for p: 0.8/0.5 for input/hidden neurons
- At test time the outgoing weights of a neuron are multiplied by p



From Dropout: A simple way to prevent neural networks from overfitting by Srivastava et al., JMLR 2014

Max-Norm Regularisation

- Constrain the norm of the incoming weight vector at each hidden unit to be upper bounded by a fixed constant c.
- Weight vector length: $L = \sqrt{{w_{j1}}^2 + {w_{j2}}^2 + \ldots + {w_{jN}}^2}$
- w_{ji} corresponds to incoming weights to neuron j from the N neurons of the previous layer
- If L > c then multiply all the incoming weights by c/L
- The new vector length is c
- Another approach to keep the weights small
- Usually used in combination with dropout

Data Augmentation

- One of the best ways to avoid overfitting is more data
- So we can artificially generate more data, usually a bit noisy, so we introduce more variation
- We should apply operations that correspond to real-world variations.
- For images: flip left-right, rotate, translate, etc

Vanishing/Exploding gradient

$$\Delta w_{ji} = \eta \delta_j x_{ji}$$

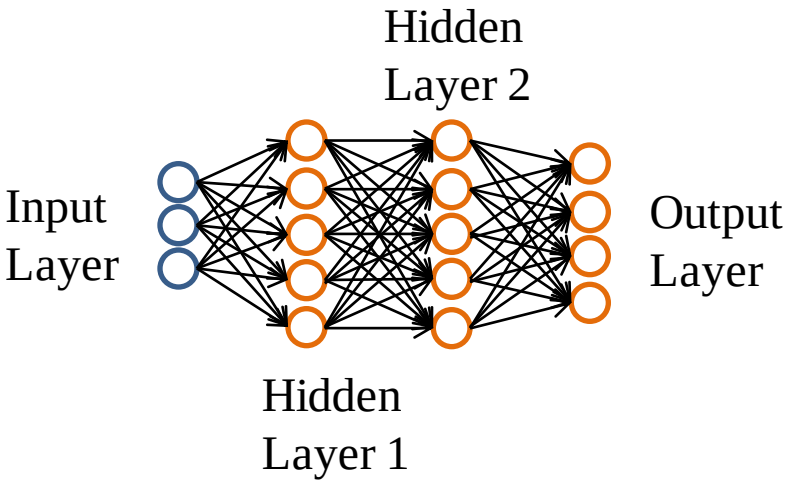
$$\delta_j = \sum_{k=outputNeuronsConnectedToj} \delta_k w_{kj} \frac{\partial \sigma(net_j)}{\partial net_j}$$

- As we backpropagate through many layers:

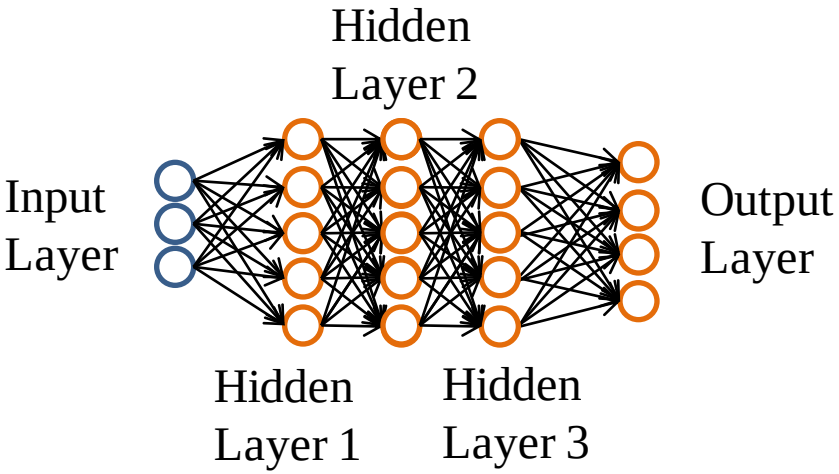
1. If the weights are small -> δ_i shrink exponentially
2. If the weights are big -> δ_i grow exponentially

- So either the network stops learning (case 1) or becomes unstable (case 2)
- That is why it is not possible to train deep networks with backpropagation

Deep NNs



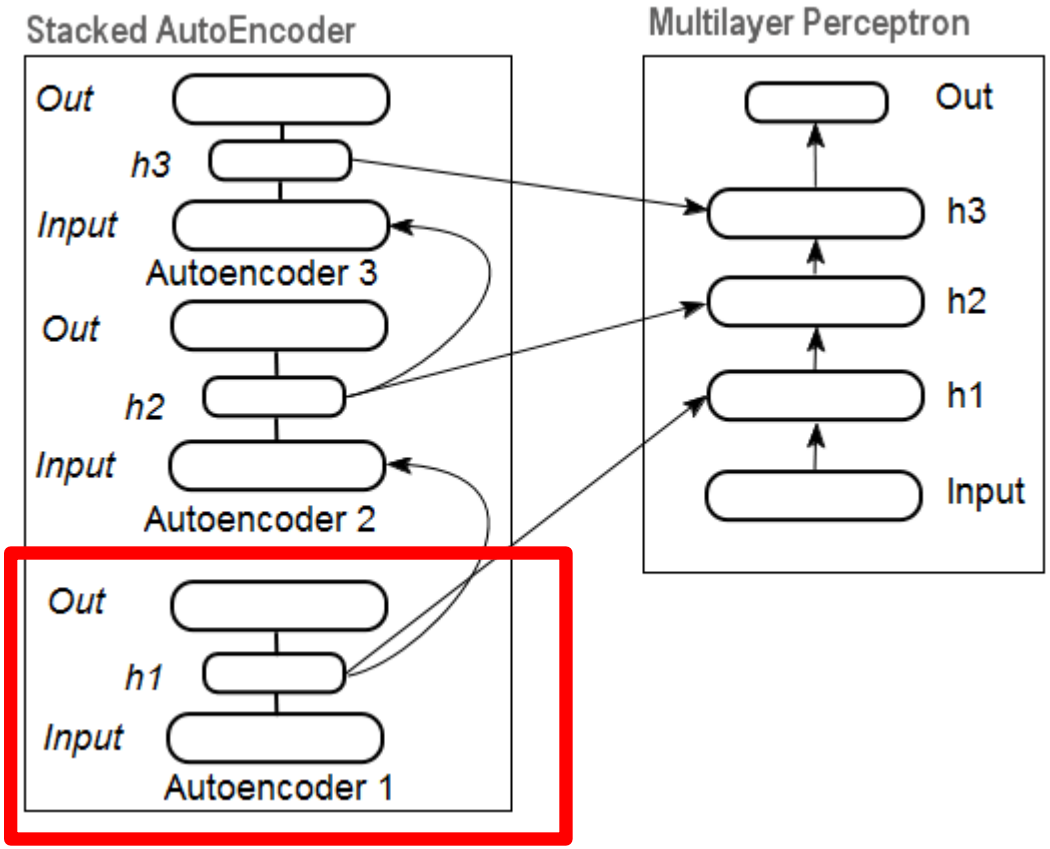
3-layer feed-forward network



4-layer feed-forward network

- There is a pre-training phase where weights are initialised to a good starting point.
- Pre-training is performed per layer using Restricted Boltzmann Machines or Stacked Denoising Autoencoders
- Then backpropagation is used to fine-tune the weights starting from a good initialisation point.

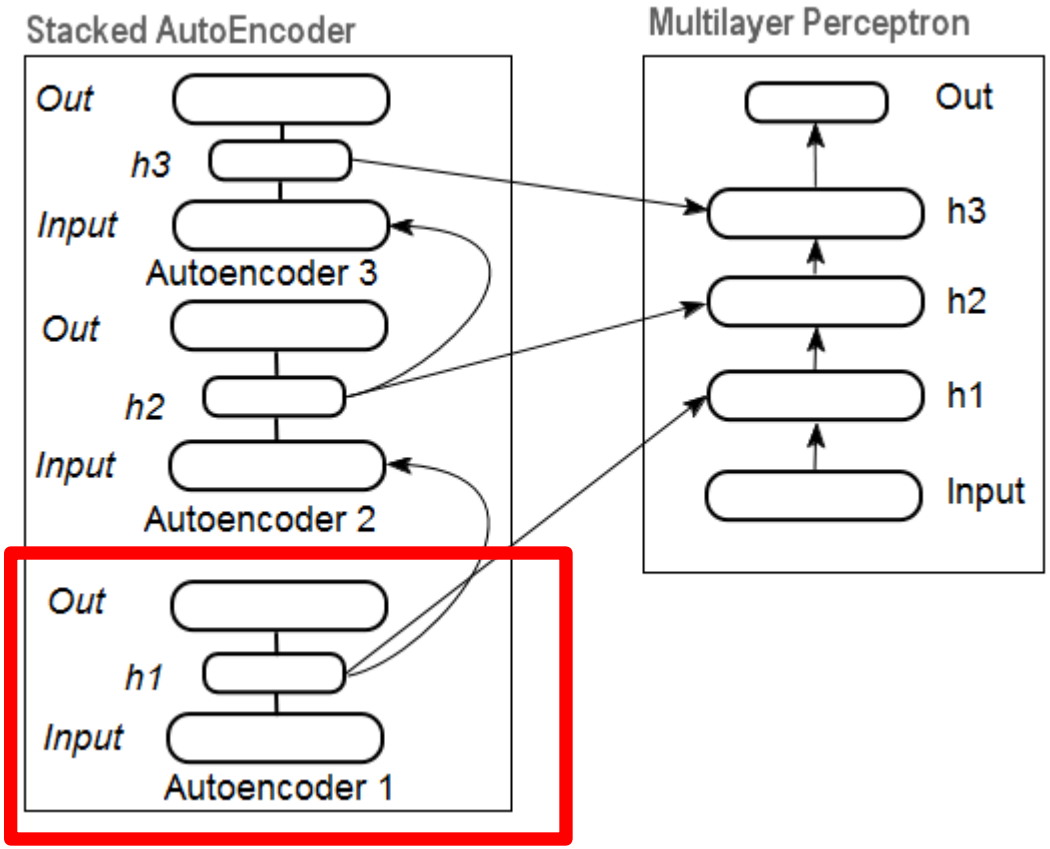
Stacked Denoising Autoencoder



From https://www.mql5.com/en/articles/1103#2_2

- Train a network to reproduce its input
- This network is called an Autoencoder (AE)
- The idea is that the middle layer represents the main variations in the data
- The problem is that the AE may simply learn the identity function

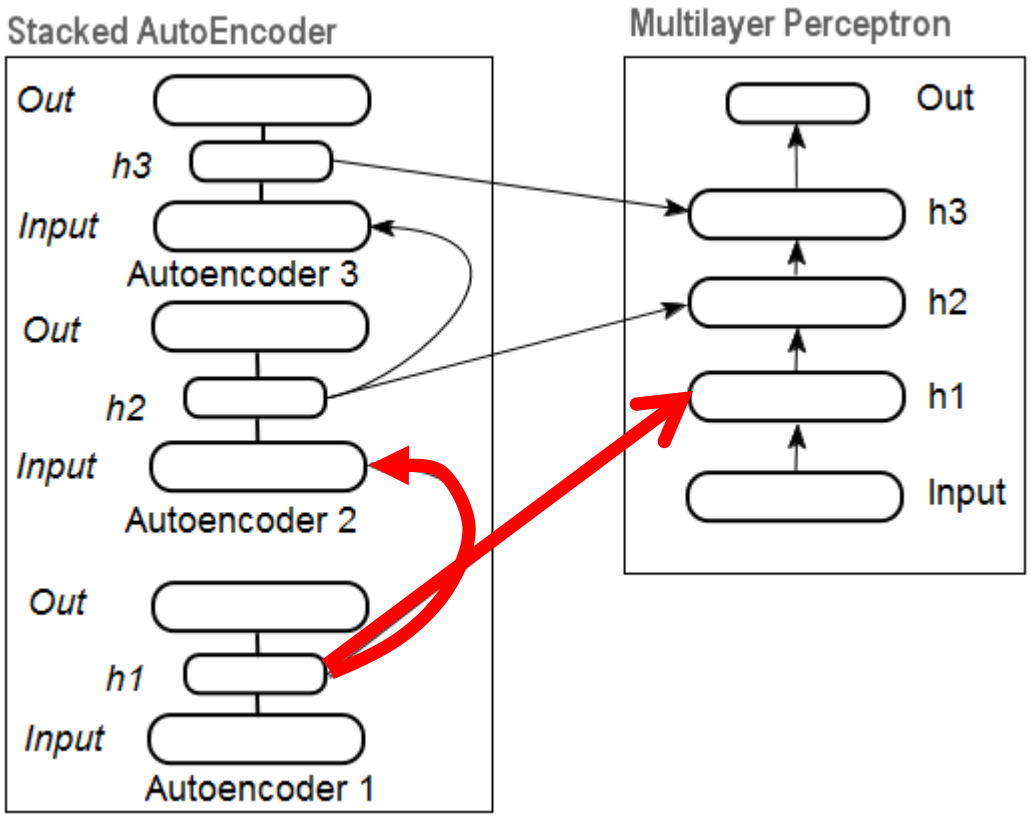
Stacked Denoising Autoencoder



From https://www.mql5.com/en/articles/1103#2_2

- Denoising AE: we add noise to the input so the network learns to reconstruct (output) the "denoised" input
- We usually set as many as half of the inputs to 0
- The network tries to reconstruct the input and undo the effect of noise
- The hidden layer is "forced" to learn the main variations in the data

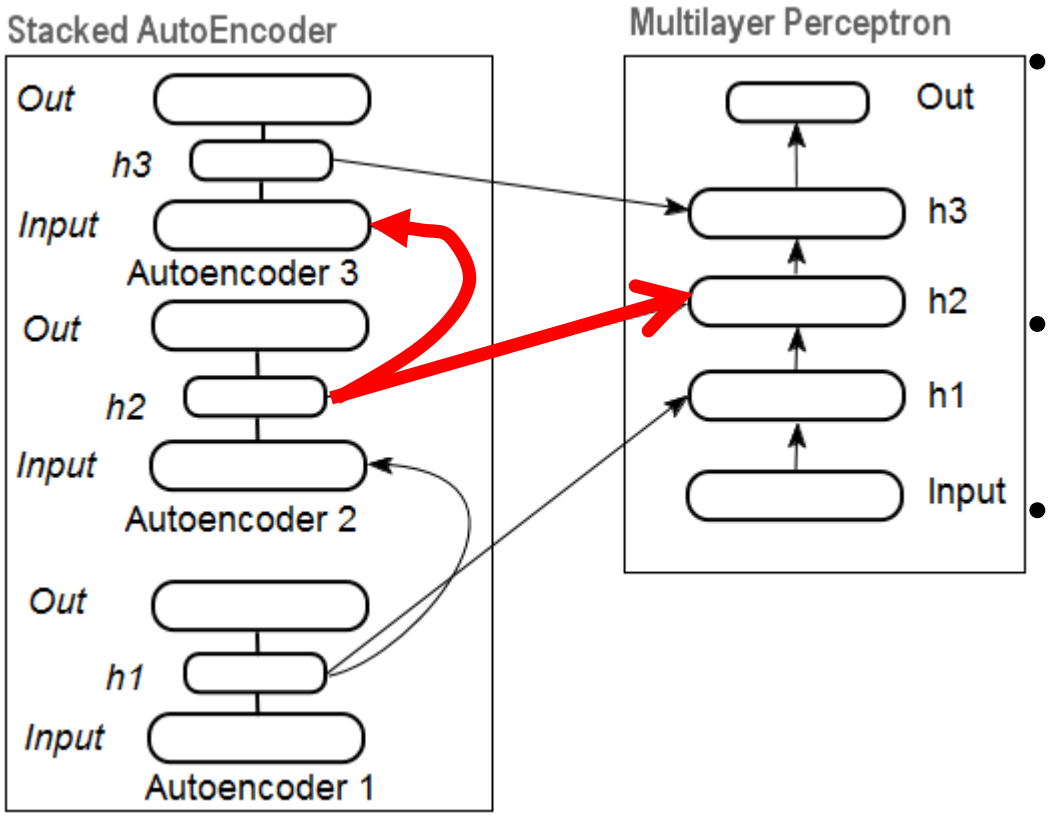
Stacked Denoising Autoencoder



- The hidden layer weights of the AE are copied to the feed-forward NN
- The output of the hidden layer is used as input for the 2nd AE
- Noise is added to this new input and the 2nd AE learns to "denoise" its input

From https://www.mql5.com/en/articles/1103#2_2

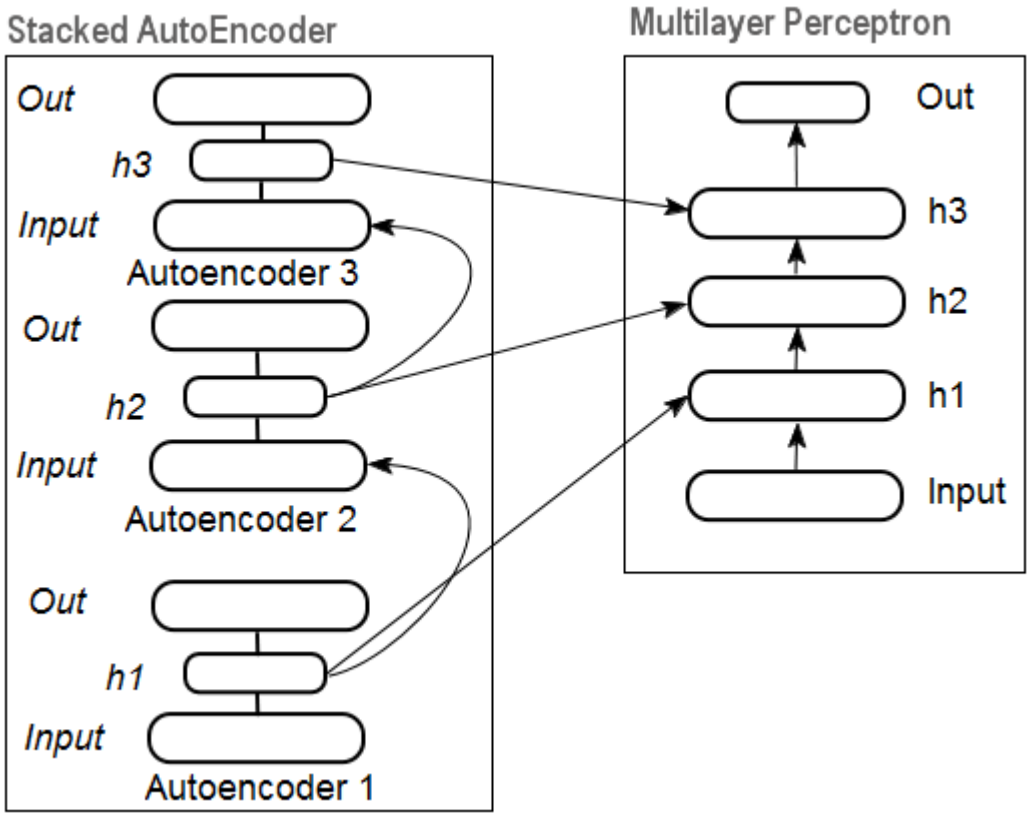
Stacked Denoising Autoencoder



- The hidden layer weights of the 2nd AE are copied to the feed-forward NN
- The output of the hidden layer is used as input for the 3rd AE
- Using this approach we can add as many as layers as we want

From https://www.mql5.com/en/articles/1103#2_2

Stacked Denoising Autoencoder

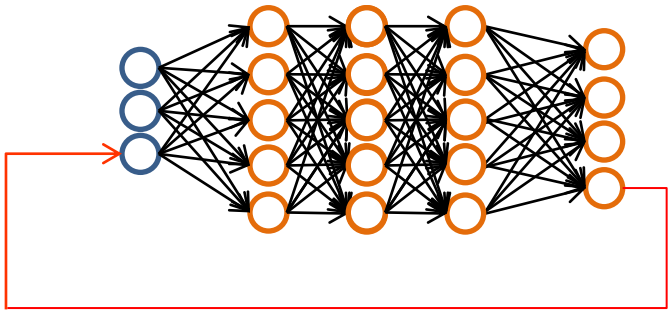


- This approach is used to initialise the NN
- This is called pre-training
- It results in good initialisation of the weights
- Then we fine-tune the network using stochastic gradient descent

From https://www.mql5.com/en/articles/1103#2_2

Deep Networks for Time Series

- Deep feedforward NNs are good at various tasks but not at handling time series data
- Recurrent Neural Networks are suitable for time series
- They also suffer from the vanishing gradient problem



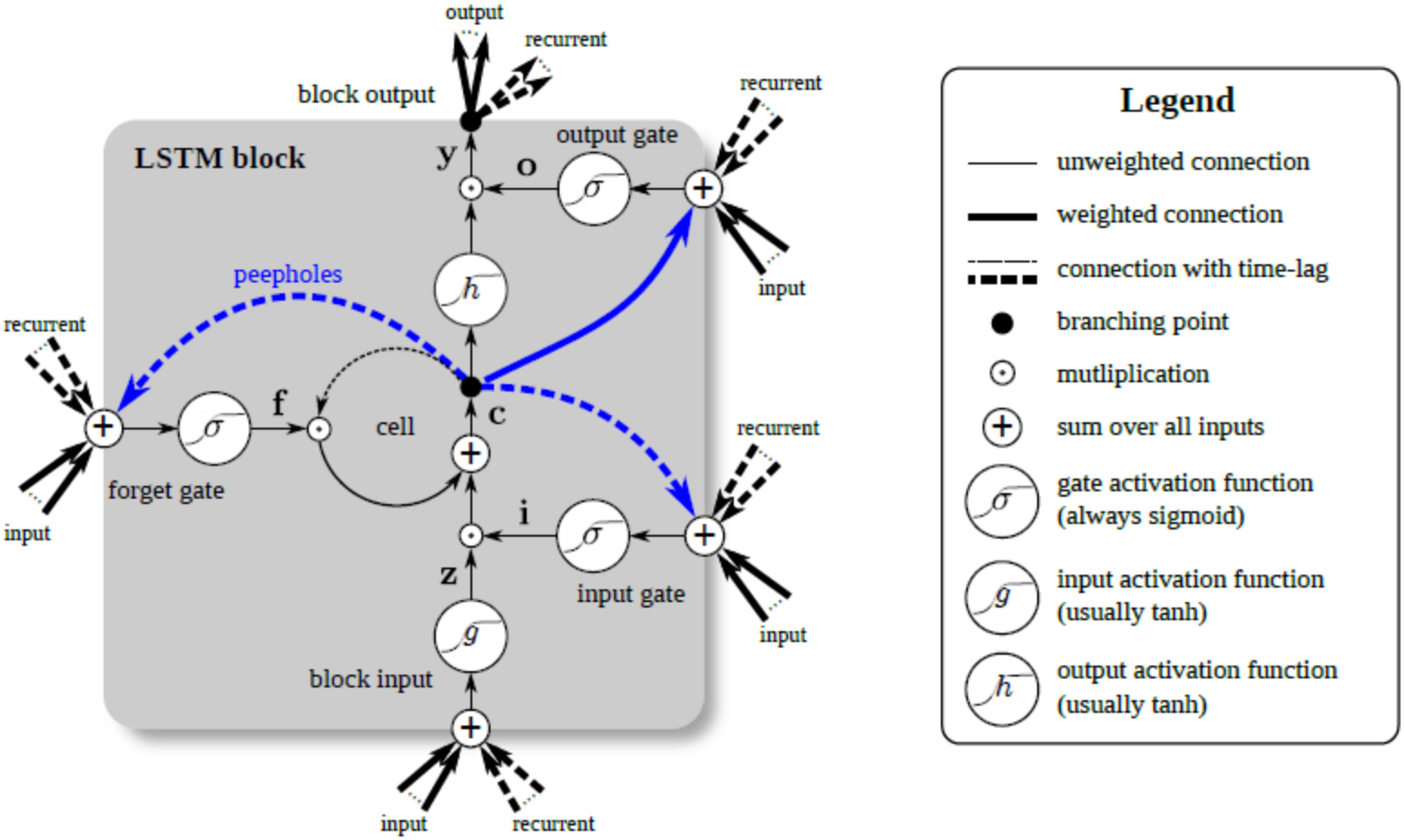
LSTMs

- A type of recurrent network that can be effectively trained is the Long-Short Term Memory Recurrent Neural Network (LSTM-RNN). Introduced in 1990s

- We replace the neuron with a memory cell

- There are input, output and forget gates which control when information flows in / out of the cell and when to reset the state of the cell

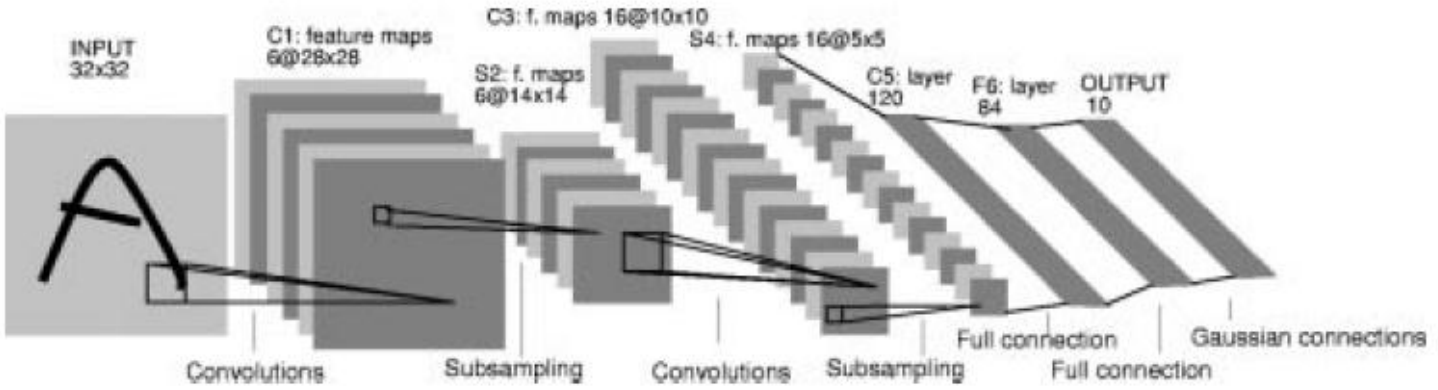
LSTMs



From LSTM: A search space odyssey by Greff et al., arXiv Mar 2015

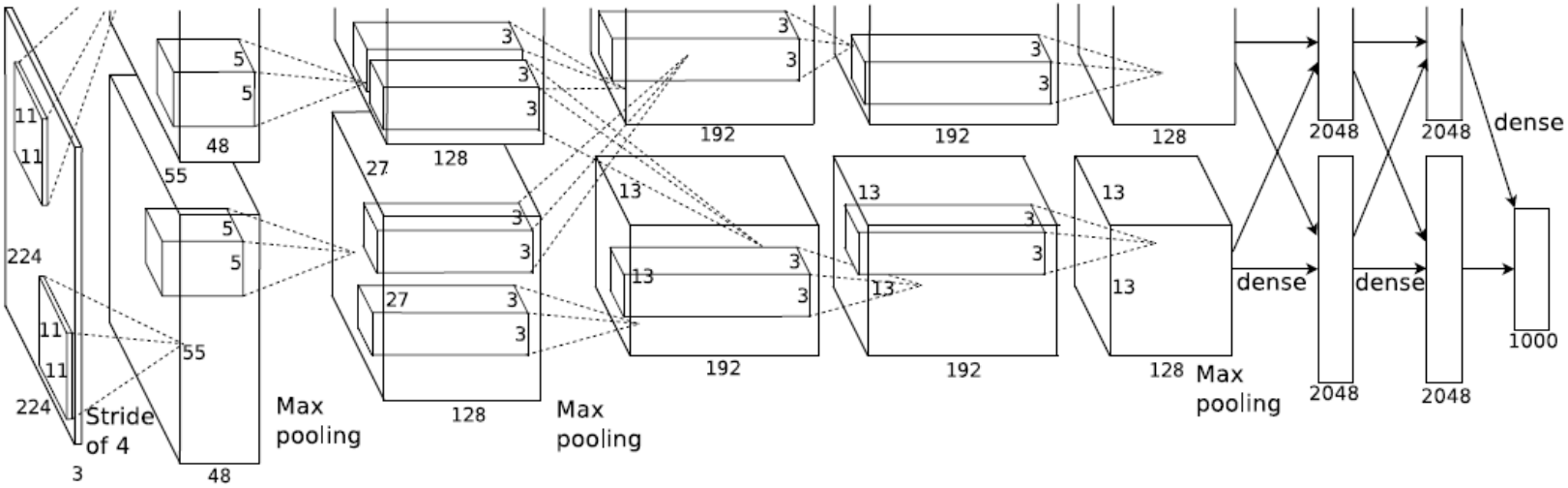
Convolutional Neural Networks

- Convolutional Neural Networks (CNNs) have been very successful in computer vision
- First version was introduced in 1980s (neocognitron)
- Improved in 1998 by LeCun et al., "Gradient-Based Learning Applied to Document Recognition", Proc. IEEE, 1998



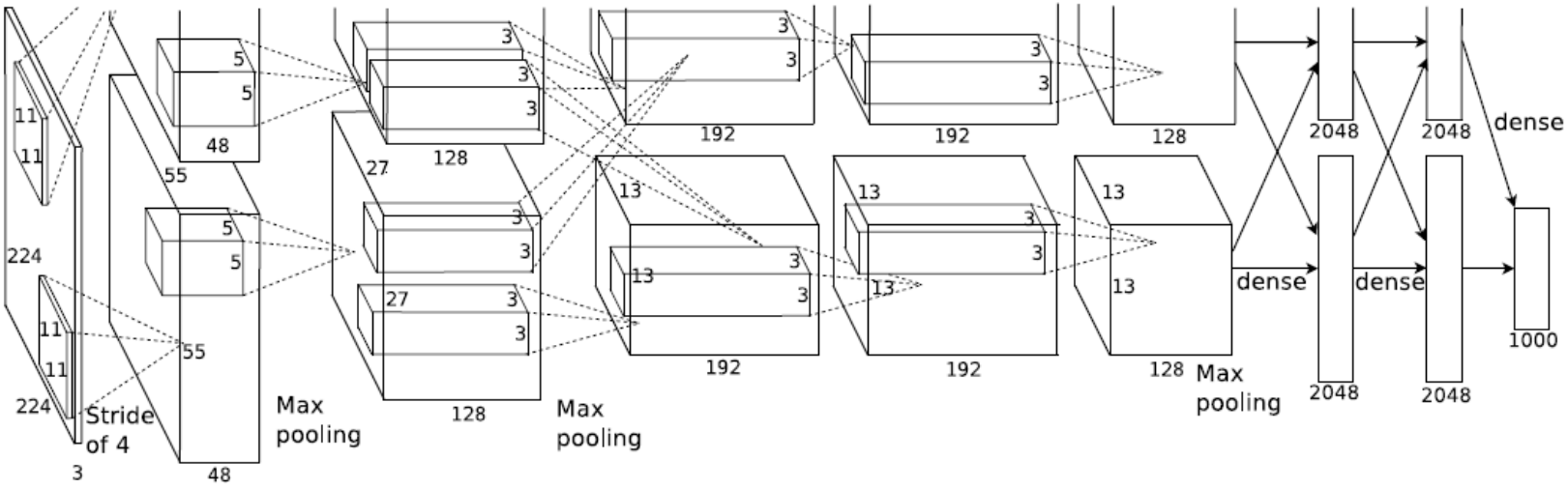
Convolutional Neural Networks

- Became popular in 2012 after winning the ImageNet competition
- "ImageNet Classification with Deep Convolutional Neural Networks", by Krizhevsky et al., NIPS 2012
- Tricks: Data augmentation, Dropout, ReLu + GPUs



Convolutional Neural Networks

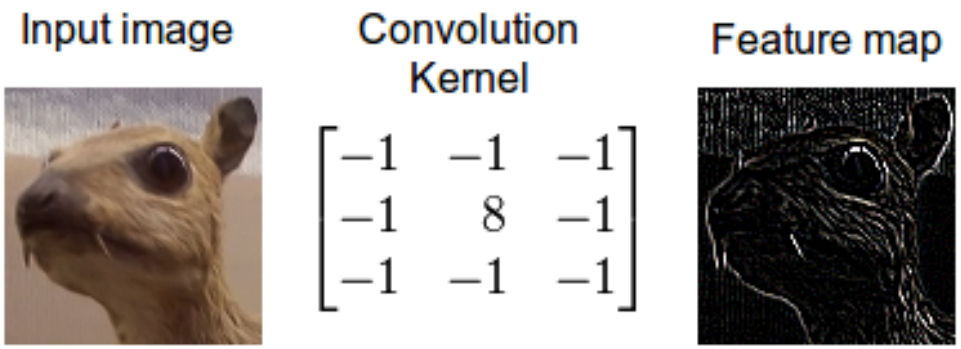
- It's a deep network = many layers
- Each layer is either a convolutional layer or subsampling layer
- Final layers are fully connected layers



Convolutional Layers

- http://deeplearning.stanford.edu/wiki/index.php/Feature_extraction_using_convolution

- The kernel, i.e., weights, are fixed. After convolving the image with the kernel we end up with a feature map

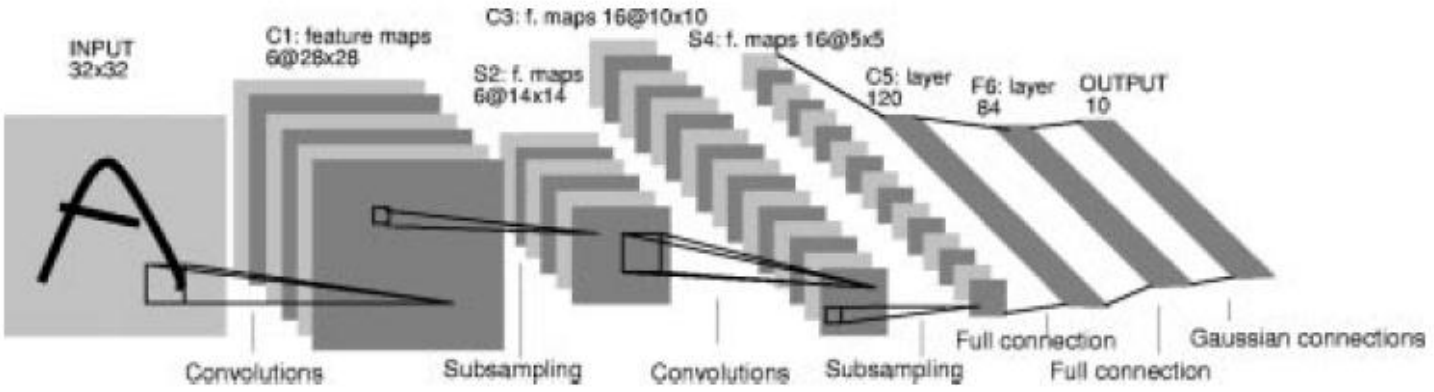


Source: http://en.wikipedia.org/wiki/File:Vd-Orig.png

Convolutional Layers

- Different kernels, i.e., weights, are applied to the image and each of them produces a feature map (kernel is fixed for each feature map)

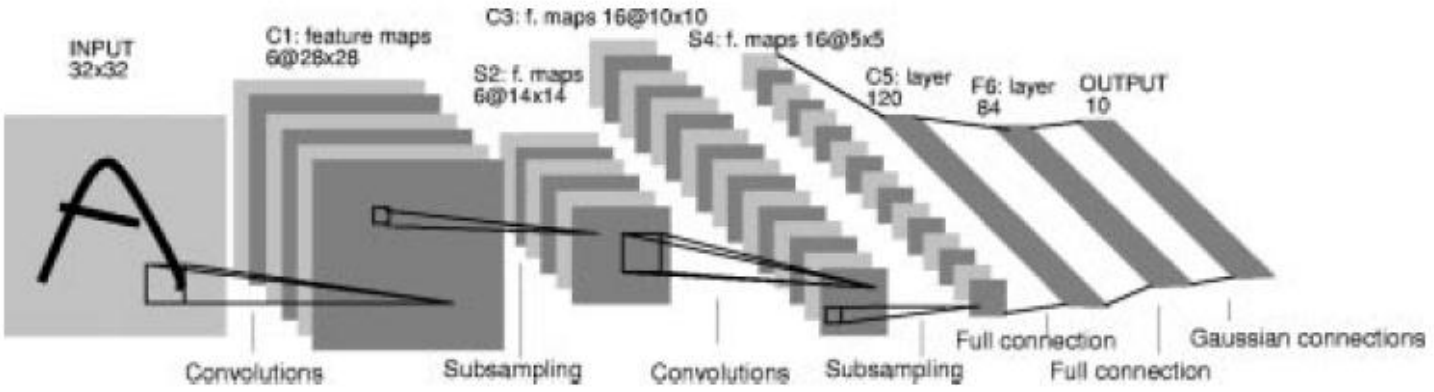
- The weights are learned during training



Subsampling Layers

- Each feature map is downsampled using average pooling or max-pooling

- Use non-overlapping patches of 2x2 and take the average or maximum of the pixels as the output

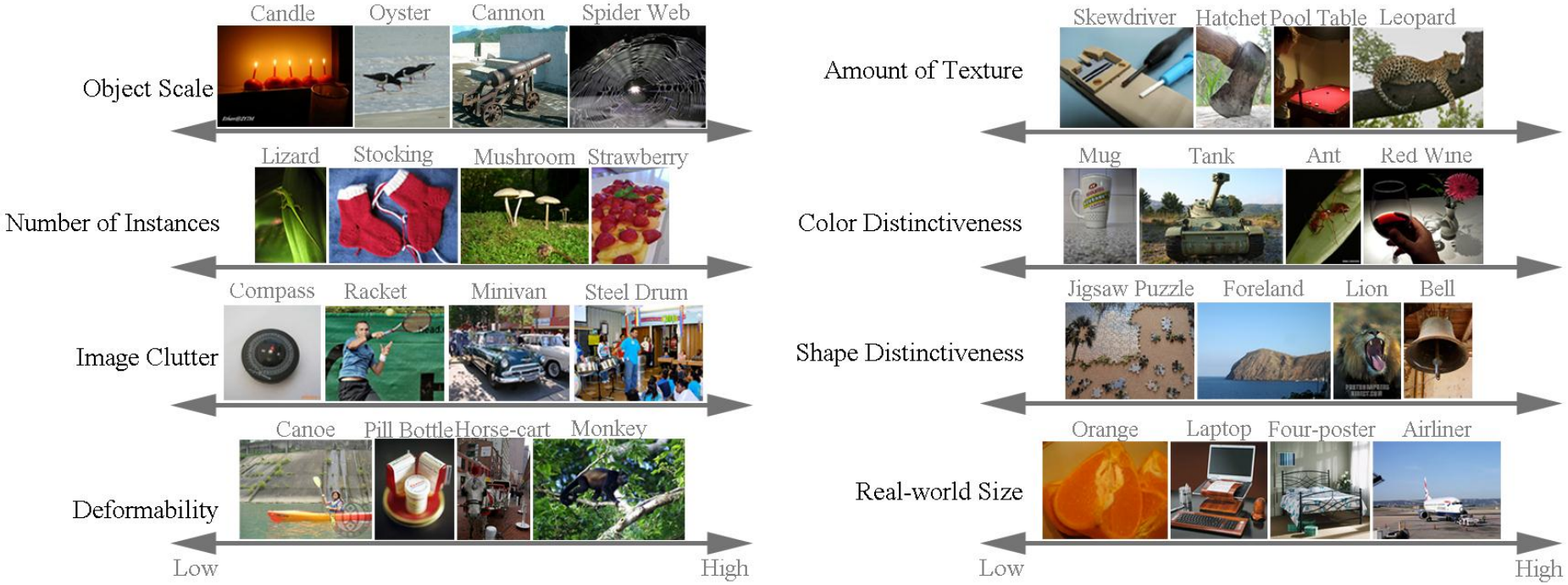


Deep NNs Applications

- Deep Face by Facebook – State of the art in Face verification
  - DeepFace: Closing the Gap to Human-Level Performance in Face Verification, Taigman, Ming, Ranzato, Wolf

- State-of-the-art performance in Speech Recognition
  - Microsoft has done a lot of research on this topic

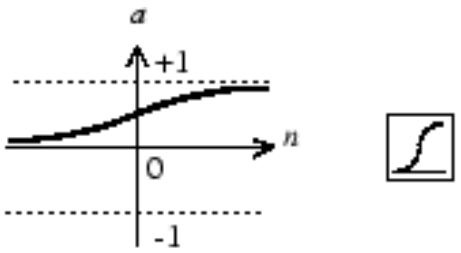
ImageNet Competition – Object Classification



- Classification of 1000+ objects
- State-of-the-art before 2012: ~26%
- New state-of-the-art in 2012 with deep networks: ~15%

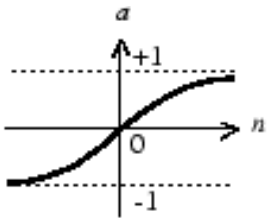
Practical Suggestions: Activation Functions

- Continuous, smooth (essential for backpropagation)
- Nonlinear
- Saturates, i.e. has a min and max value
- Monotonic (if not then additional local minima can be introduced)
- Sigmoids are good candidate (log-sig, tan-sig) or ReLu



$a = logsig(n)$

Log-Sigmoid Transfer Function

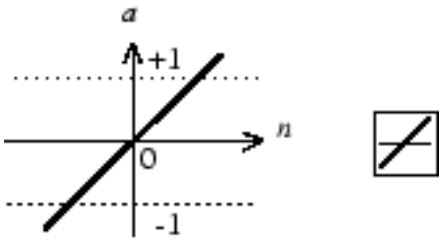


$a = tansig(n)$

Tan-Sigmoid Transfer Function

Practical Suggestions: Activation Functions

- In case of regression then output layer should have linear activation functions



$a = purelin(n)$

Linear Transfer Function

Practical Suggestions: Scaling Inputs

- It is not desirable that some inputs are orders of magnitude larger than other inputs

- Map each input *x(i)* to [-1, +1] using this formula

$$y = 2\frac{x - x_{min}}{x_{max} - x_{min}} - 1$$

- Matlab function: ***mapminmax***
  - Rows: features, columns: examples
  - Normalises each row
  - Useful for continuous inputs/targets

Practical Suggestions: Scaling Inputs

- Standardize inputs to mean=0 and 1 std. dev.=1

  $y = \frac{x - x_{mean}}{x_{std}}$

- Useful for continuous inputs/targets
- Matlab function: ***mapstd***
- Scaling is needed if inputs take very different values. If e.g., they are in the range [-3, 3] then scaling is probably not needed

Practical Suggestions: Scaling Inputs

- The scaling values, x_{min}, x_{max}, x_{mean}, x_{std} are computed on the training set and then applied to the validation and test sets.

- It is not correct to scale each set separately.

Practical Suggestions: Scaling Inputs

- Matlab automatically scales the inputs to [-1, 1] and removes the inputs/outputs that are constant.

- Think if you wish to scale the inputs, if not you should disable the automatic scaling

- Check *http://www.mathworks.co.uk/help/nnet/ug/choose-neural-network-input-output-processing-functions.html*

Practical Suggestions: Target Values

- Binary Classification

  - Target Values : -1/0 (negative) and 1 (positive)

  - 0 for log-sigmoid, -1 for tan-sigmoid

- Multiclass Classification

  - [0,0,1,0] or [-1, -1, 1, -1]

  - 0 for log-sigmoid, -1 for tan-sigmoid

- Regression

  Target values: continuous values [-inf, +inf]

Practical Suggestions: Number of Hidden Layers

- Networks with many hidden layers are prone to overfitting and they are also harder to train
- For most problems one hidden layer should be enough
- 2 hidden layers can sometimes lead to improvement
- If you want to use more layers then you should follow the deep learning methodology to initialise the weights and use strong regularisation (dropout etc)

Division of data

- Matlab automatically divides the dataset into training/validation/test sets.
- You should force matlab to use an empty test set (you have your own) and use the same validation set as yours.
- You can provide the indices of your validation set and your test set (=empty array)
- Check *http://www.mathworks.co.uk/help/nnet/ug/divide-data-for-optimal-neural-network-training.html*

Matlab Examples

- Create feedforward network
  - net = feedforwardnet(hiddenSizes,trainFcn)
  - hiddenSizes = [10, 10, 10] – 3 layer network with 10 hidden neurons in each layer
  - trainFcn = 'trainlm', 'traingdm', 'trainrp' etc
- Configure (set number of input/output neurons)
  - net = configure(net,x,t)
  - x: input data, noFeatures x noExamples
  - t: target data, noClasses x noEx

Matlab Examples

- Train network
  - [net,tr] = train(net,P,T)
  - P: input data
  - T: target data
- Simulate network
  - [Y,Pf,Af,E,perf] = sim(net,P)

Matlab Examples

- Batch training: Train
- Incremental Training: Adapt
- Use Train for the CBC

Questions

- Questions from book: 4..1, 4.2, 4.5, 4.8, 4.10
- You should read chapter 4
- Examinable material: Slides, Manual (part 3A), Chapter 4