
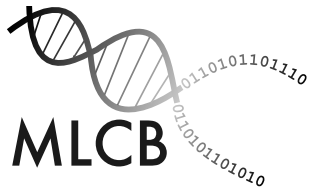


# Neural Networks: A Very Brief Tutorial

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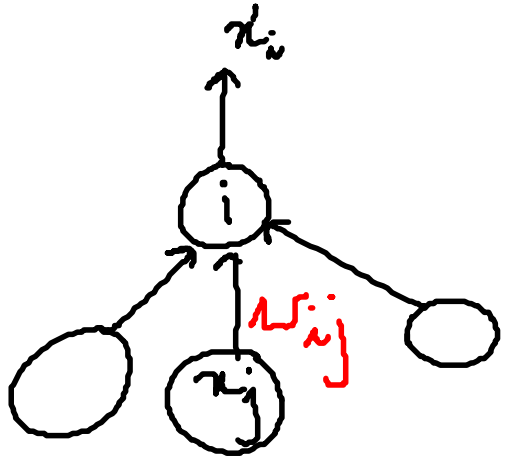
# 1950s – 1970s

# Units




$$x_i' = \varphi(x_1, \dots, x_j, \dots x_m)$$

transfer function

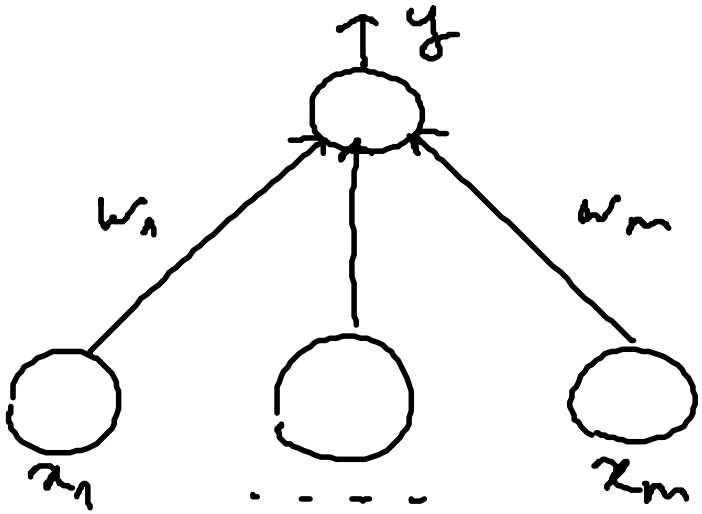
$$= f\left(\sum_{j \in Pr(i)} w_{ij}\, x_j + w_i\right)$$

output; activation; bias

- Linear
- Squashing $x \mapsto \begin{cases} x & \text{if } |x| < \Theta \\ 0 & \text{otherwise} \end{cases}$
- Threshold $x \mapsto \begin{cases} 1 & \text{if } |x| > \Theta \\ 0 & \text{ow} \end{cases}$
- Logistic $1/(1+e^{-x})$
- Sigmoid tanh, etc.
- Softmax (normalized exponential) $\dfrac{e^{-x_i}}{\sum_k e^{-x_k}}$

# Perceptron

Rosenblatt (1958)
Minsky & Papert (1969)




output

$$y = \begin{cases} 1 & \text{if } \sum_i w_i x_i + w_0 > 0 \\ 0 & \text{otw} \end{cases}$$

input

Training rule

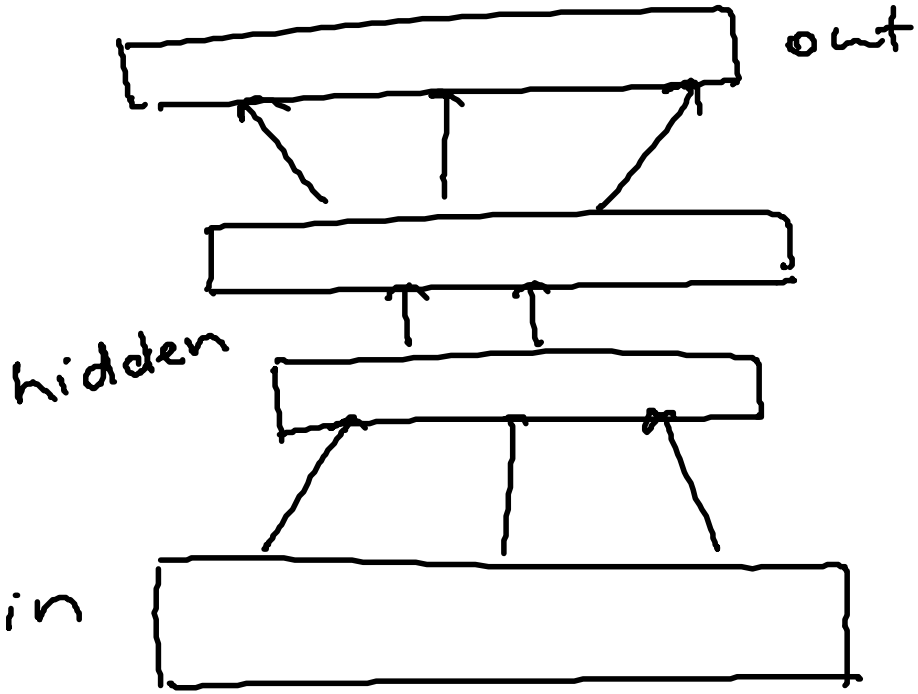
learning rate

$$w_i \leftarrow w_i + \eta\,(\text{true} - y)\,x_i$$

For each training sample,
for each feature

# 1980s – early 1990s

# Multi-Layer Perceptron



# Multi-Layer Perceptron

**Universal approximation**: Any continuous function on a compact subset of $\mathbb{R}^n$ can be approximated to any arbitrary degree of precision by a feed-forward multi-layer perceptron with a single hidden layer containing a finite number of neurons.

Cybenko (1989), Hornik (1991)

# Backpropagation

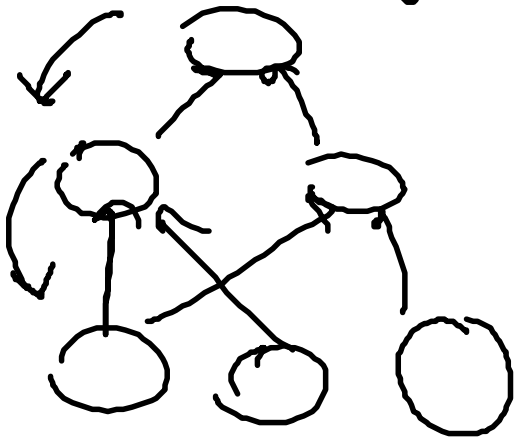
$y_i = f\left(\underbrace{\sum_{k \in rcv(i)} y_k w_{ik}}_{a_i}\right)$

Bryson, Denham & Dreyfus (1969)

Werbos, Rumelhart, Williams & Hinton (1974)

Backwards propagation of errors

$E = y - target$



$\frac{\partial E}{\partial w_{ij}}$

$w_{ij} \leftarrow w_{ij} + \eta \Delta w_{ij}$

$\frac{\partial E}{\partial w_{ij}} = \frac{\partial E}{\partial y_i} \frac{\partial y_i}{\partial w_{ij}}$

$\frac{\partial y_i}{\partial w_{ij}} = f'(a_i) \frac{\partial a_i}{\partial w_{ij}}$

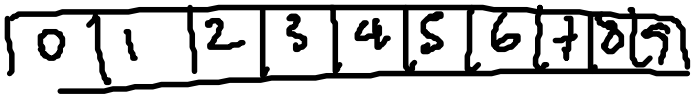
$\frac{\partial a_i}{\partial w_{ij}} = y_j$

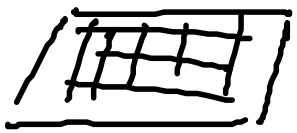
$\frac{\partial E}{\partial y_i} = f'(a_i) y_j$

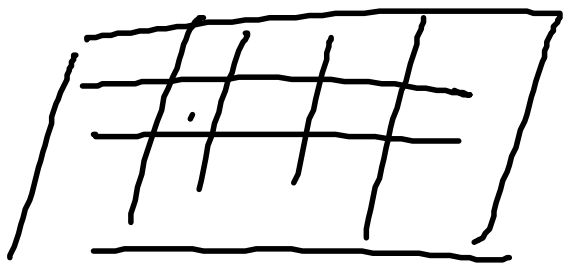
$\frac{\partial E}{\partial y_i} = \sum_{k \in rcv(i)} \frac{\partial E}{\partial y_k} \frac{\partial y_k}{\partial y_i} w_{ki}$

# Handwritten digits recognition

Le Cun et al. (1990)





Shared weights

4 hidden layers

$H_2$, $H_4$: local averaging

# Recurrent Neural Networks

As opposed to **feed-forward** architectures.

Include directed cycles. feedback loops

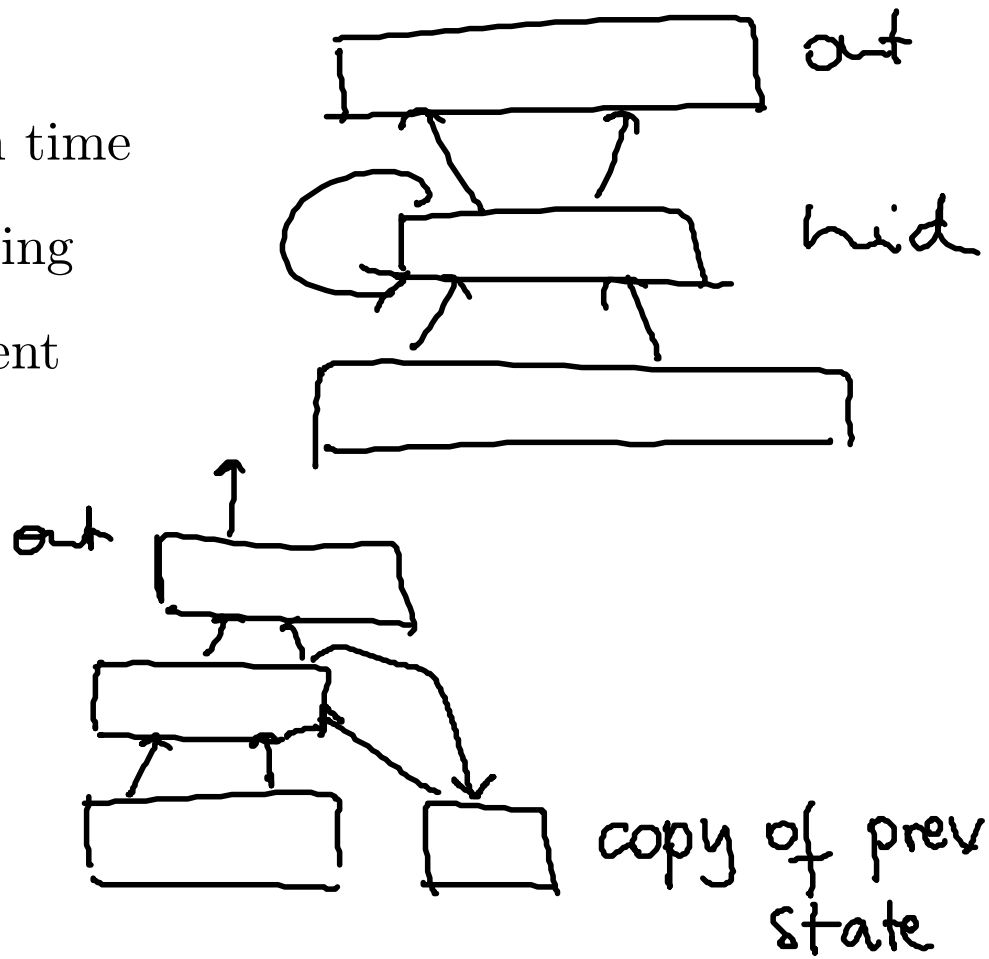
Can encode dynamic temporal behaviour.

Training:

- Backpropagation through time
- Real-time recurrent learning
- High-order gradient descent

Examples:

- Elman networks
- Jordan networks
- Hopfield networks
- Liquid state machines



# Neural Networks (MLPs) in Practice

# Packages

## Matlab

- Neural Network Toolbox
- Deep Learn Toolbox, Deep Belief Networks, and others at `http://deeplearning.net/software_links/`

## Python

- `bpnn.py`
- `fnnet`
- (C bindings) `FANN`
- `PyNN`
- `PyAnn`
- `nnutils` based on `Monte`

## R

- `neuralnet`
- `nnet`

# Neural Network Magic

## Architecture

Start with one hidden layer.

Stop adding layers when you overfit.

Never use more ~~nodes~~ weights than training samples.

## Learning algorithm

Use batch learning.

Use Newton/quasi-Newton methods for small numbers of weights. Prefer Levenberg-Marquardt.

Use conjugate-gradient descent for large numbers of weights.

# Neural Network Magic

## Preconditionning

An **ill-conditionned** network cannot learn.

The best learning rate is typically different for each weight.

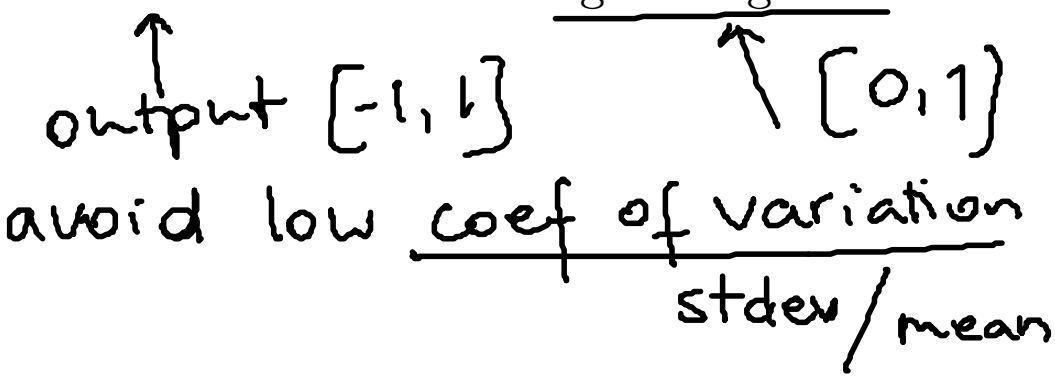
Solutions:

Standardize inputs and targets.

Initialize the weights carefully.

Set local learning rates.

Use *tanh* rather than a logistic sigmoid for hidden layers.



# Neural Network Magic

## Standardization

* Remove outliers

### Features

- Mean 0, standard deviation 1.
- Midrange 0, range 2.
- Orthonormalize. (SVD, PCs ...)

### Targets

- To equalize target importance: mean 0, standard deviation 1.
- To force targets into the range of the output activation function: midrange 0, range 2
  use lower/upper bounds rather than min/max.

### Samples

Standardize to a Euclidean distance of 1 for Kohonen networks or ratio-level data.

# Neural Network Magic

## Escaping saturation

Large weights ⇓ Saturation

### Weight initialization

$$w_{ij} \in [-r, r] \qquad r = \frac{1}{\sqrt{|\mathrm{fan}(i)|}}$$

### Weight decay

regularization

$E \longrightarrow E + \text{weight decay}$

$$\sum w_{ij}^2$$

weight elimination

$$\sum_i \frac{w_i^2}{w_i^2 + 6}$$

# Neural Network Magic

## Escaping local minima

**Online learning** or mini batch

**Momentum**

$$w_{ij} \leftarrow w_{ij} + \eta \Delta w_{ij} + m \Delta^{t-1} w_{ij}$$

**Learning rate adaptation**

$$w_{ij} \leftarrow w_{ij} + \mu_{ij} \Delta w_{ij}$$

1. $\mu$ while the gradient keeps pointing in the same direction
   $\mu_{ij} \leftarrow \mu_{ij} + q \, \Delta^{(t)} w_{ij} \, \Delta^{(t-1)} w_{ij}$
2. Prevent $\mu_{ij} < 0$ => apply to $\log(\mu_{ij})$ instead
3. $\mu_{ij} \leftarrow \mu_{ij} \times \max\left(0.5, 1 + q \, \Delta^{(t)} w_{ij} \, \Delta^{(t-1)} w_{ij}\right)$

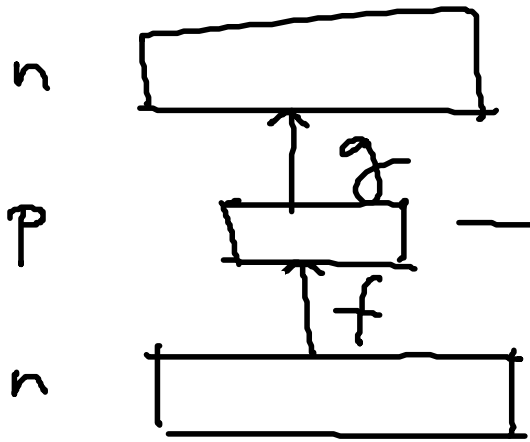
approximate to avoid computing exp

avoid too small $\mu$ etc...

**since 2006**

# Autoencoders

Rumelhart, Hinton & Williams (1986)
Dimensionality reduction with neural networks.




goal: output matches input

compact representation of input

$$\min_{f,g} \sum_x \Delta(f \circ g(x), x)$$

Hinton: sigmoidal neurons + backprop

$$\Delta(y, x) = \|y - x\|_2^2$$

Baldi: Linear autoencoders

$$\min_{A,B} \sum_x \|ABx - x\|_2^2$$

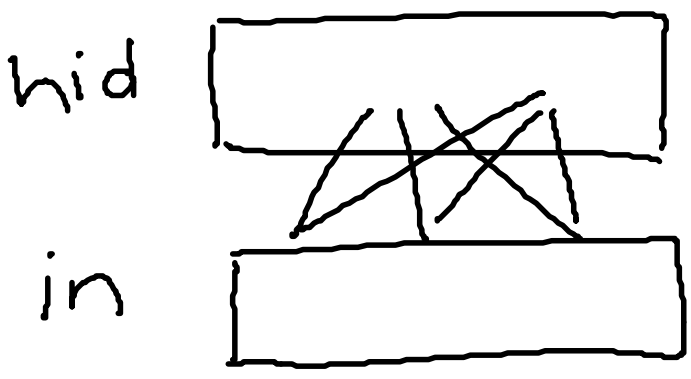
$A, B$ ↑ matrices

# Restricted Boltzmann Machines

Hinton & Sejnowsky (1985) BM

Smolensky (1986) RBM

Unsupervised learning with stochastic neural networks.




activation : probabilistic

bipartite graph: all inputs connected to all hidden

activation energy $E_i = \sum_{j \in ch(i)} w_{ij} x_j$

proba of activation : $p_i = \sigma(E_i)$ ← logistic

# Restricted Boltzmann Machines

**Contrastive divergence** – Hinton (2002)

Given data $V$ (visible units)

$$\underset{W}{\operatorname{argmax}} \sum_{v \in V} \log P(v)$$

$$P(v) \propto e^{-E(v,h)}$$

hidden

$$-E(v,h) = h^T W v - \text{bias}$$

Learning with CD

gradient descent + Gibbs sampling

* compute $P(\text{hidden})$ ← distribution
* sample $h$ from $P(\text{hidden})$
* sample $v'$ (reconstr. of $v$), sample $h'$

$$w_{ij} \leftarrow w_{ij} + \eta \left( v h^T - v' h'^T \right)$$

# Deep Learning

`http://deeplearning.net`

Many (hidden) factors ⇒ many (hidden) layers

2006: "Deep Breakthrough"

Hinton, Osindero & Teh
Bengio, Lamblin, Popovici & Larochelle
Ranzato, Poultney, Chopra & LeCun

Dropout (Hinton, 2012)
Maxout (Goodfellow et al., 2013)

Deep Belief Networks (DBNs)

Convolutional Neural Networks (CNNs)

Stacked auto-encoders

# Deep Learning in Bioinformatics

Predicting protein structure (Di Lena, Nagata & Baldi, 2012).

Predicting aqueous solubility (Lusci, Pollastri & Baldi, 2012).

Predicting protein properties (Qi, Oja, Weston & Noble, 2012).

Predicting drug-target interactions (Wang & Zheng, 2013).

Automating phenotyping (Lasko, Denny & Levy, 2013).

# Resources

Usenet newsgroup `comp.ai.neural-nets` FAQ
`http://www.faqs.org/faqs/ai-faq/neural-nets/`

Introduction to Neural Networks
N. Schraudolph and F. Cummins
`http://www.csi.ucd.ie/staff/fcummins/NNcourse/intro.html`

Neural Networks
C. Stergiou and D. Siganos
`http://www.doc.ic.ac.uk/~nd/surprise_96/journal/vol4/cs11/report.html`

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