Block 11 (Freitag 1.3.2024)

VIDEO: video11a_nn_intro

12 Neural Networks

Fundamental research: how does brain function?

Application: efficient self-learning algorithms (hand writing recognition, optimization, generalisation, . . .)

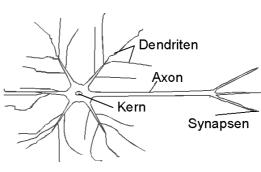
Brain has about 10^{11} neurons. Communication by electrical impulses.

Structure neuron:

Dendritens: input signals, up to 2×10^5 per cell

Axon: output signal

Synapsens: couple axon to dendrites $\overline{}$ of other cells, up to 10^4 per cell, in total about 10^{15} , strengths can be changed.



von www.lunaticpride.de

Modelling by McCulloch/Pitts neurons (W.S. McCulloch and W. Pitts, Bull. Math. Biophys. 1943) [9]

- L inputs $x_i = 0, 1$ (silent/active)
- Strengths $w_i \in \mathbb{R}$ of synapses
- \bullet Threshold value s
- Output signal

$$y = \theta \left(\sum_{i=1}^{L} w_i x_i - s \right) \tag{65}$$

$$\theta(x) = 1$$
 for $x \ge 0$ $\theta(x) = 0$ else.

Logical functions AND/NOT can be realised ⇒ arbitrary logical functions.

Supervised learning: given function $y^{\text{(target)}}(\underline{x})$, and input \underline{x} .

Contribution to weights: Hebb's learning rule (D. Hebb, Wiley, 1949) [10] $(\epsilon > 0)$: "learning parameter")

$$\Delta w_i = \epsilon y^{\text{(target)}}(\underline{x}) x_i \tag{66}$$

Can be performed for many input vectors $\{\underline{x}^{(1)}, \underline{x}^{(2)}, \dots, \underline{x}^{(n)}\}.$

VIDEO: video11b_perceptron

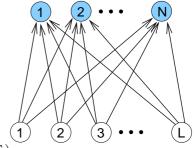
12.1 Perzeptron

(Also) for classification of input petterns \underline{x} and generalisation $\to N$ output $y_r \in \{0, 1\} \ (r = 1, \dots, N)$ according to

$$y_r = \theta \left(\sum_{i=0}^{L} w_{ri} x_i \right) \tag{67}$$

 $(s \leftrightarrow -w_{r0} \text{ via } x_0 = 1)$

Each output is independent of the others, pure layered structure



Perceptron learning algorithm ("training phase")

- start with random weights
- use different training vectors x. For each incorrect output $y_r(x)$ changed weights:

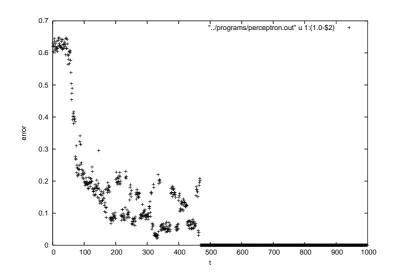
$$\Delta w_{ri} = \epsilon \cdot (y_r^{\text{(target)}}(\underline{x}) - y_r(\underline{x})) \cdot x_i$$
 (68)

As C function (see perceptron.c)

```
/******* perceptron_learning() **********/
/** Peforms 'K' steps of learning algorithm:
/** generate random vector and adjust weights using
                                                     **/
/** parameter 'epsilon' to learn function 'f'
                                                     **/
/** PARAMETERS: (*)= return-paramter
                                                     **/
              L: number of (real) values
/**
                                                     **/
/**
          (*) w: weight vector
/**
        epsilon: learning rate
/**
              f: target function
                                                     **/
/**
              K: number of iterations
                                                     **/
/** RETURNS:
                                                     **/
/**
       (nothing)
void perceptron_learning(int L, double *w, double epsilon,
 int (*f)(int, int *), int K )
{
 int step, t;
                                             /* loop counters */
 int *x;
                                              /* input vector */
 int y, y_wanted;
                                             /* output values */
 x = (int *) malloc( (L+1)*sizeof(int));
 x[0] = 1;
                                       /* bit 0 <-> threshold */
 for(step=0; step<K; step++)</pre>
                                        /* main learning loop */
   random_vector(L, x);
   y = output_neuron(L, x, w);
   y_{\text{wanted}} = f(L, x);
   if(y != y_wanted)
     for(t=0; t<=L; t++)
                                            /* adjust weights */
       w[t] += epsilon*(y_wanted- y)*x[t];
 }
 free(x);
}
Test: function
```

$$f(x) = \begin{cases} 1 & \text{more than half of the bits is 1} \\ 0 & \text{else} \end{cases}$$
 (69)

For L = 10, failure rate as function of number of learning iterations:



resulting weights

```
# w[0] = -1.150000

# w[1] = 0.250000

# w[2] = 0.200000

# w[3] = 0.200000

# w[4] = 0.200000

# w[5] = 0.200000

# w[6] = 0.200000

# w[7] = 0.200000

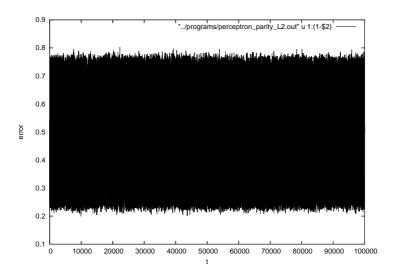
# w[8] = 0.250000

# w[9] = 0.200000
```

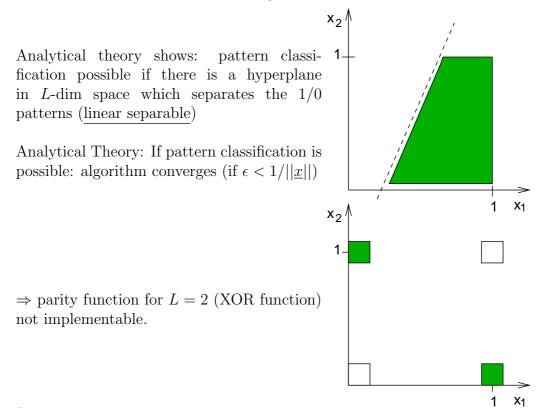
corresponds to exact solution, e.g. $w_0 = 1.1$, $w_i = 0.2$ (i > 0). Test: parity function

$$f(x) = \begin{cases} 1 & \text{number of 1 bits is odd} \\ 0 & \text{else} \end{cases}$$
 (70)

For L=2 (only !), failure rate as function of learning iterations:



Result is "random", all obtained weights close to 0.



Solution: multi-level structures, e.g. a "hidden" layer.

VIDEO: video11c_backpropagation

12.2 Back propagation

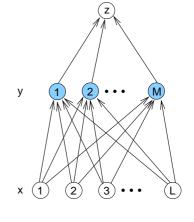
Feed-forward network:

Several layers, here one layer of M <u>hidden</u> Neurons.

w.l.o.g.: 1 output neuron Transfer function $(x_0 = 1)$:

$$y_{j} = \sigma \left(\sum_{k'=0}^{L} w_{jk'} x_{k'} \right) \quad (j = 1 \dots M)(71)$$

$$z = \sigma \left(\sum_{j'=0}^{M} \tilde{w}_{j'} y_{j'} \right) \tag{72}$$

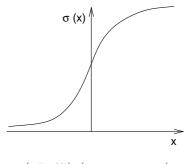


$$\sigma(x) = \frac{1}{1 + \exp(-x)} \in [0, 1]$$

$$\sigma'(x) = (-1)(-1)\frac{\exp(-x)}{(1 + \exp(-x))^2}$$

$$= \frac{1}{1 + \exp(-x)} \frac{1 + \exp(-x) - 1}{1 + \exp(-x)}$$

$$= \sigma(x)(1 - \sigma(x)) \tag{73}$$



Aim: network shall learn p patterns+classifications $(\underline{x}^{\nu}, \hat{z}^{\nu})$ $(\nu = 1, ..., p)$ (e.g. again a function $\hat{z} = f(\underline{x})$, then $\hat{z}^{\nu} = f(\underline{x}^{\nu})$), $\hat{\underline{x}} \in \{0, 1\}^{L}$);

Use as energy function: mean squared error

$$E = \frac{1}{2} \sum_{\nu} (\hat{z}^{\nu} - z(\underline{x}^{\nu}))^2 \tag{74}$$

$$= \frac{1}{2} \sum_{\nu} \left(\hat{z}^{\nu} - \sigma \left(\sum_{j=0}^{M} \tilde{w}_{j} y_{j}(\underline{x}^{\nu}) \right) \right)^{2}$$
 (75)

Look for optimale weights: most simple: gradient descent. Start with some weights, then (ϵ : Parameter):

$$\Delta w_{jk} = -\epsilon \frac{\partial E}{\partial w_{jk}} \tag{76}$$

$$\Delta \tilde{w}_j = -\epsilon \frac{\partial E}{\partial \tilde{w}_j} \tag{77}$$

approximately

$$\Delta E \approx \sum_{\{w\}} \frac{\partial E}{\partial w} \Delta w = -\epsilon \sum_{\{w\}} \left(\frac{\partial E}{\partial w} \right)^2 \le 0$$

 \rightarrow konverges to (local) minimum.

Here, contribution for a single pattern $(\underline{x}^{\nu}, \hat{z}^{\nu}) \to (\underline{x}, \hat{z})$

$$\frac{\partial E}{\partial \tilde{w}_{j}} \stackrel{(74)}{=} -(\hat{z}-z)\frac{\partial z}{\partial \tilde{w}_{j}} \stackrel{(72)}{=} -(\hat{z}-z)\sigma'(\sum_{j'} \tilde{w}_{j'}y_{j'})y_{j}$$

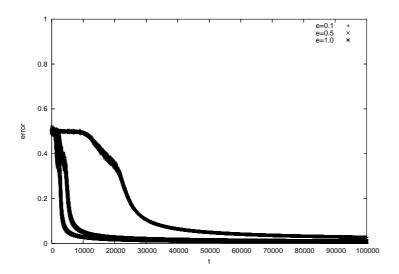
$$\stackrel{(73)}{=} -(\hat{z}-z)z(1-z)y_{j} \qquad (78)$$

$$\frac{\partial E}{\partial w_{jk}} \stackrel{(75)}{=} -(\hat{z}-z)z(1-z)\tilde{w}_{j}\frac{\partial y_{j}}{\partial w_{jk}}$$

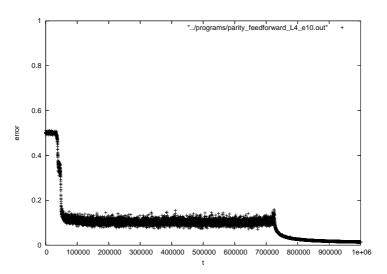
$$\stackrel{(71)}{=} -(\hat{z}-z)z(1-z)\tilde{w}_{j}\sigma'(\sum_{k'} w_{jk'}x_{k'})x_{k}$$

$$\stackrel{(73)}{=} -(\hat{z}-z)z(1-z)\tilde{w}_{j}y_{j}(1-y_{j})x_{k} \qquad (79)$$

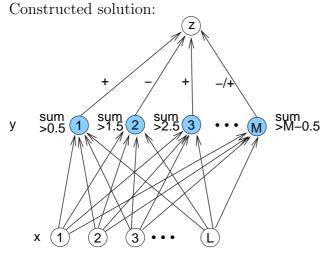
Error rate for parity function L=2



konverges quickly. Error rate for parity function L=4



converges slowly.



Accelerated convergence: better minimization approach: conjugate gradient, Monte Carlo optimisation with Parallel Tempering, ...

So far supervised learning. Unsupervised learning: generalization, not $E = \frac{1}{2} \sum_{\nu} (\hat{z}^{\nu} - z(\underline{x}))^2$ but arbitrary function $f(\hat{z}^{\nu}, z(\underline{x}))$ is minimized. Aim: System learns structures. Weights are adapted, such that set of given

Aim: System learns structures. Weights are adapted, such that set of given patterns is generated. Application: statistical analyses such as clustering of data points, "Deep Learning" (many layers, GO algorithm).

References

[1] A. M. Ferrenberg, D. P. Landau, and Y. J. Wong. Monte Carlo simulations: Hidden errors from "good" random number generators. *Phys.*

- Rev. Lett., 69:3382, 1992.
- [2] B.J.T. Morgan. *Elements of Simulation*. Cambridge University Press, Cambridge, 1984.
- [3] Alexander K. Hartmann. Practical Guide to Computer Simulations. World Scientific, Singapore, 2009.
- [4] D. Stauffer and A. Aharony. *Perkolationstheorie*. Wiley-VCH, Weinheim, 1995.
- [5] A. Dhar. Heat conduction in a one-dimensional gas of elastically colliding particles of unequal masses. *Phys. Rev. Lett.*, 86:3554, 2001.
- [6] P. Grassberger, W. Nadler, and Lei Yang. Heat conduction and entropy production in a one-dimensional hard-particle gas. *Phys. Rev. Lett.*, 89:180601, 2002.
- [7] L.E. Reichl. A Modern Course in Statistical Physics. John Wiley & Sons, New York, 1998.
- [8] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A.H. Teller, and E. Teller. Equation of state calculations by fast computing machines. *J. Chem. Phys.*, 21:1087, 1953.
- [9] W. S. McCulloch and W. Pitts. A logical calculus of the ideas immanent in nervous activity. *Bull. Math. Biophys.*, 5:115–133, 1943.
- [10] D. Hebb. Organisation of Behavior. Wiley, New York, 1949.