# Machine Learning

## Neural Networks 2

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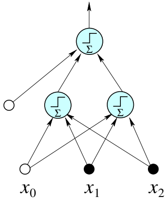
2025

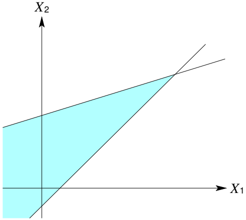
*Ver. 1.0*

# Topics - you should be able to explain after this week

- Neural network with logistic sigmoid activation functions
- Interpretation of the output
- Training of single-layer neural network with MSE / cross entropy
- Gradient descent
- Activation functions
- Training of multi-layer neural network – error back propagation (EBP)
- Relationships with linear regression and logistic regression
- Computation graphs

# Recap: Perceptron structures and decision boundaries



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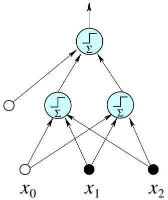


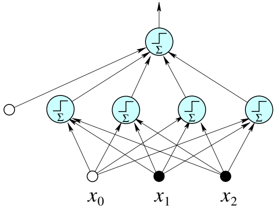


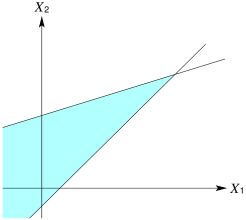


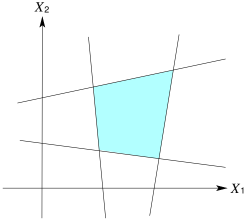

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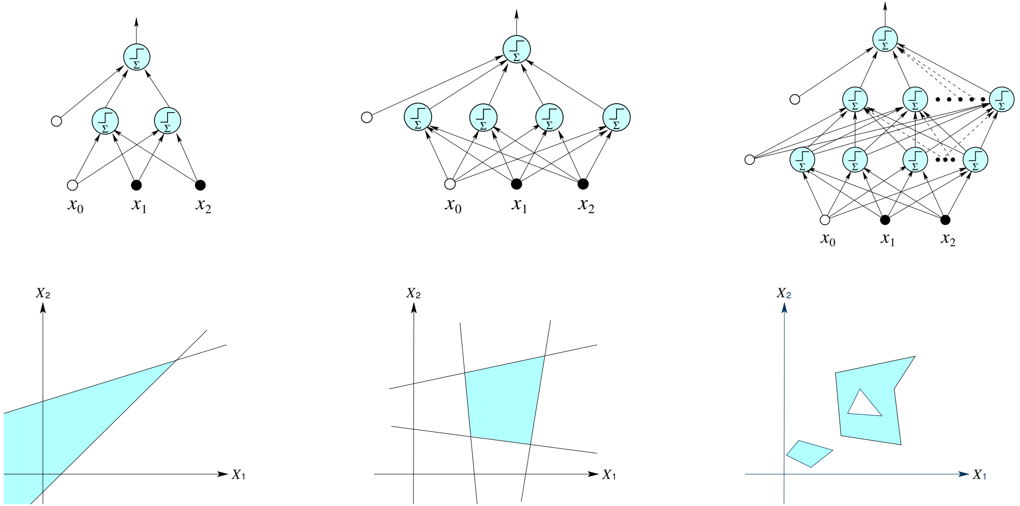
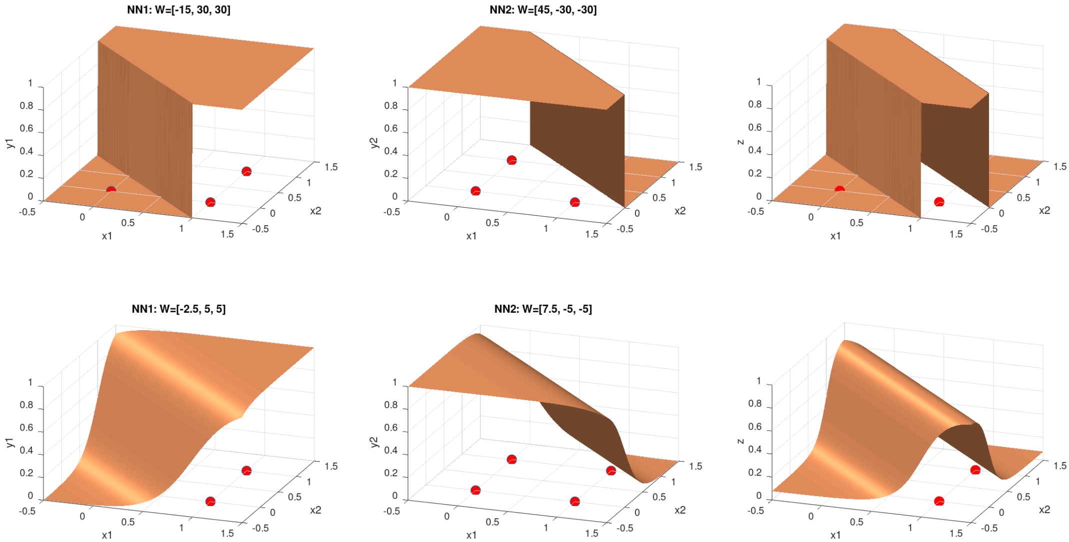


# Recap: Output of NN – threshold func. vs sigmoid func.



# Recap: Ability of neural networks

- Universal approximation theorem
  - "Univariate function and a set of affine functionals can uniformly approximate any continuous function of $n$ real variables with support in the unit hypercube; only mild conditions are imposed on the univariate function. " (G. Cybenko (1989)

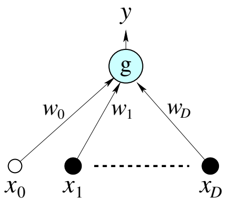
    $\longrightarrow$

    A single-output node neural network with a single hidden layer with a finite neurons can approximate continuous (and discontinuous) functions.
  - K. Hornik (1990) doi:10.1016/0893-6080(91)90009-T
  - N. Guliyev, V. Ismailov (2018) doi:10.31219/osf.io/xgnw8
  - V. Ismailov (2023) "A three layer neural network can represent any multivariate function" https://doi.org/10.1016/j.jmaa.2023.127096

# Output of logistic sigmoid activation function

- Consider a single-layer network with a single output node logistic sigmoid activation function: (cf. logistic regression)

$$
\begin{aligned}
y = g(a) &= \frac{1}{1+\exp(-a)}, \quad \text{where } a = \sum_{i=0}^{d} w_i x_i \\
&= \frac{1}{1+\exp\left(-\sum_{i=0}^{d} w_i x_i\right)}
\end{aligned}
$$



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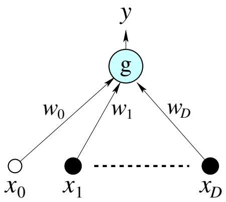


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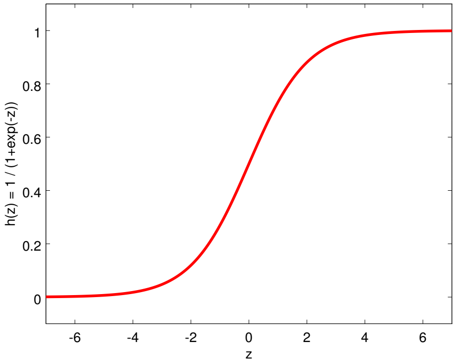
$$= \frac{1}{1+\exp\left(-\sum_{i=0}^{d} w_i x_i\right)}$$

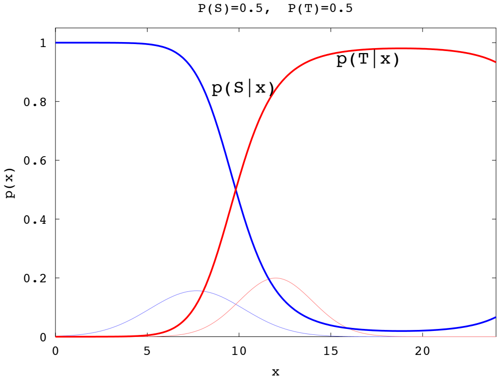
- Consider a two class problem, with classes $C_1$ and $C_2$. The posterior probability of $C_1$:

$$P(C_1|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|C_1)\,P(C_1)}{p(\boldsymbol{x})} = \frac{p(\boldsymbol{x}|C_1)\,P(C_1)}{p(\boldsymbol{x}|C_1)\,P(C_1) + p(\boldsymbol{x}|C_2)\,P(C_2)}$$

$$= \frac{1}{1+\frac{p(\boldsymbol{x}|C_2)\,P(C_2)}{p(\boldsymbol{x}|C_1)\,P(C_1)}} = \frac{1}{1+\exp\left(-\log\frac{p(\boldsymbol{x}|C_1)\,P(C_1)}{p(\boldsymbol{x}|C_2)\,P(C_2)}\right)}$$

# Approximation of posterior probabilities




Logistic sigmoid function:

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

Posterior probabilities of two classes with Gaussian distributions:

# Training single layer neural network with MSE

- Training set : $\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$, where $y_i \in \{0, 1\}$

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- Definition of the training problem as an optimisation problem

$$\min_{\boldsymbol{w}} E_{\text{MSE}}(\boldsymbol{w})$$

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  (scalar form)

$$w_i^{(\text{new})} \leftarrow w_i - \eta \frac{\partial}{\partial w_i} E(\boldsymbol{w}), \qquad (\eta > 0)$$

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- Online/stochastic gradient descent (cf. Batch training)
  Sample $(x_n, y_n)$ from the data set and update the weights at a time.

# Gradient descent

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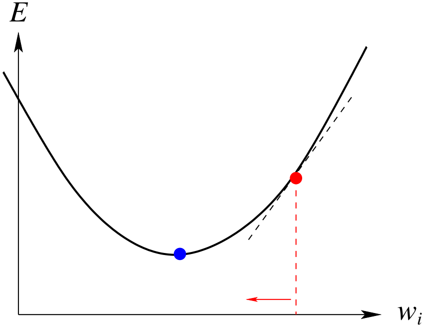


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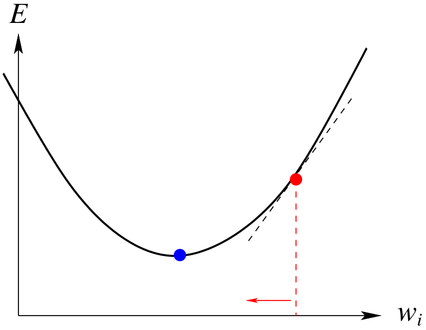


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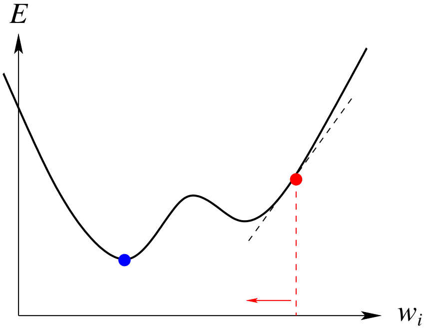


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where $\hat{y}_n = g(a_n), \;\; a_n = \sum_{i=0}^{d} w_i x_{ni}, \quad \frac{\partial\, a_n}{\partial\, w_i} = x_{ni}$

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# Another training criterion – cross-entropy error

- Training problem with the mean squared error (MSE) criterion with the sigmoid function

$$E_{\text{MSE}}(\boldsymbol{w}) = \frac{1}{2}\sum_{n=1}^{N}(\,\hat{y}_n - y_n\,)^2\ , \quad \hat{y}_n = g(a_n)$$

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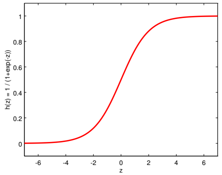
$g'(a) \approx 0$ for such $a$ that $g(a) \approx 0$ or $1$.



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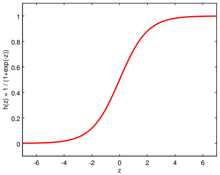


- Cross-entropy error

$$E_{\text{H}}(\boldsymbol{w}) = -\frac{1}{N}\sum_{n=1}^{N}\{\,y_n \log \hat{y}_n + (1-y_n)\log(1-\hat{y}_n)\,\}$$

For multi classes, $E_{\text{H}}(\boldsymbol{w}) = -\frac{1}{N}\sum_{n=1}^{N}\sum_i y_i \log \hat{y}_i$

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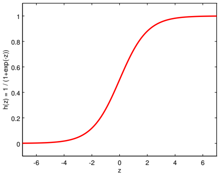


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For multi classes, $E_{\text{H}}(\boldsymbol{w}) = -\frac{1}{N}\sum_{n=1}^{N}\sum_i y_i \log \hat{y}_i$

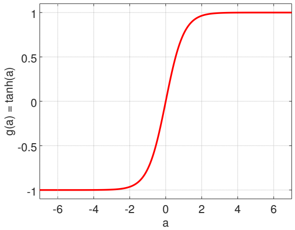
It can be shown that:

$$\frac{\partial\, E_{\text{H}}(\boldsymbol{w})}{\partial\, w_i} = \frac{1}{N}\sum_{n=1}^{N} (\hat{y}_n - y_n)\, x_{ni}$$

# Other activation functions

- Tanh

$$g(a) = \tanh(a) = \frac{1 - e^{-2a}}{1 + e^{-2a}}$$

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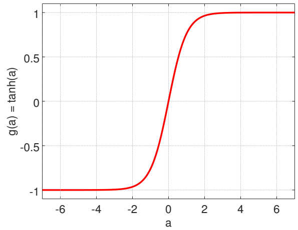


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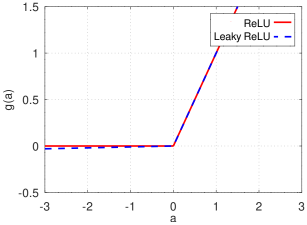
- ReLU (Rectified Linear Unit)

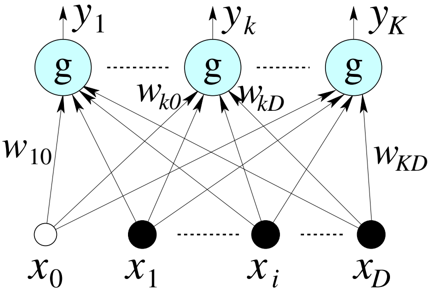
$$g(a) = \max(0, a)$$




  - Several times faster than tanh.
  - 'Dying ReLU' problem – a unit of outputting 0 always $\rightarrow$ use Leaky ReLU instead

For details, see Kevin Murphy, "Probabilistic Machine Learning: An Introduction", Sec. 13.4.3.

# Single-layer network with multiple output nodes




$$y_1(\mathbf{x}) = g(\mathbf{w}_1^T\mathbf{x} + w_{10})$$
$$\vdots$$
$$y_K(\mathbf{x}) = g(\mathbf{w}_K^T\mathbf{x} + w_{K0})$$

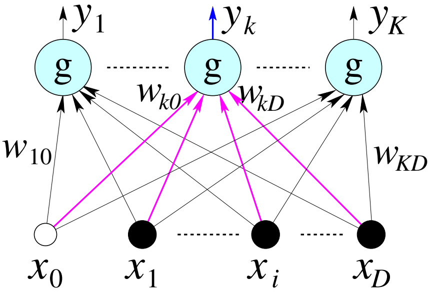
$$\begin{pmatrix} y_1 \\ \vdots \\ y_K \end{pmatrix} = g\left( \begin{pmatrix} w_{10} & w_{11} & \ldots & w_{1d} \\ \vdots & & \ddots & \vdots \\ w_{K0} & w_{K1} & \ldots & w_{Kd} \end{pmatrix} \begin{pmatrix} 1 \\ x_1 \\ \vdots \\ x_d \end{pmatrix} \right)$$

$$\mathbf{y} = g\left(\mathbf{W}\dot{\mathbf{x}}\right)$$

- $K$ output nodes: $y_1, \ldots, y_K$.
- For $\mathbf{x}_n = (x_{n0}, \ldots, x_{nD})^T$,

$$\hat{y}_{nk} = g\left(\sum_{d=0}^{d} w_{kd}\, x_{nd}\right) = g(a_{nk}), \qquad a_{nk} = \sum_{d=0}^{d} w_{kd}\, x_{nd}$$

# Single-layer network with multiple output nodes

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# Training of single-layer network with multiple output nodes

- Training set : $\mathcal{D} = \{(\mathbf{x}_1, \mathbf{y}_1), \ldots, (\mathbf{x}_N, \mathbf{y}_N)\}$

  where $\mathbf{y}_n = (y_{n1}, \ldots, y_{nK})$ and $y_{nk} \in \{0, 1\}$

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- Error function:

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E_{\text{MSE}}(w) &= \frac{1}{2}\sum_{n=1}^{N} \|\hat{\mathbf{y}}_n - \mathbf{y}_n\|^2 \\
&= \sum_{n=1}^{N} E_n, \quad \text{where } \; E_n = \frac{1}{2}\|\hat{\mathbf{y}}_n - \mathbf{y}_n\|^2 \; = \; \frac{1}{2}\sum_{k=1}^{K} (\hat{y}_{nk} - y_{nk})^2
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- Error function:

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

$$= \sum_{n=1}^{N} E_n, \quad \text{where} \;\; E_n = \frac{1}{2}\|\hat{\mathbf{y}}_n - \mathbf{y}_n\|^2 \; = \; \frac{1}{2}\sum_{k=1}^{K} (\hat{y}_{nk} - y_{nk})^2$$

- Training with the gradient descent:

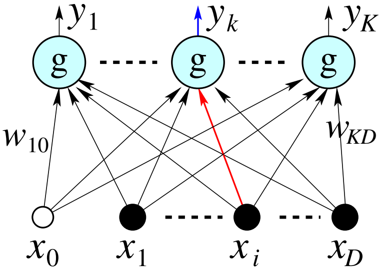
$$w_{ki} \;\leftarrow\; w_{ki} - \eta \frac{\partial E}{\partial w_{ki}}, \qquad (\eta > 0)$$

# The derivatives of the error function (single-layer)

$$E_n = \frac{1}{2}\sum_{k=1}^{K}(\hat{y}_{nk} - y_{nk})^2$$

$$\hat{y}_{nk} = g(a_{nk})$$

$$a_{nk} = \sum_{i=0}^{D} {\color{red} w_{ki}} x_{ni}$$



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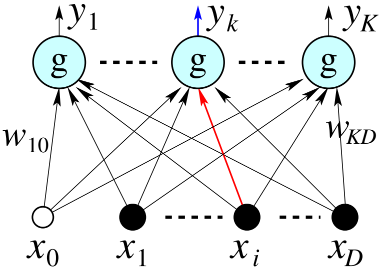
$$\frac{\partial E_n}{\partial w_{ki}} = \frac{\partial E_n}{\partial \hat{y}_{nk}} \frac{\partial \hat{y}_{nk}}{\partial a_{nk}} \frac{\partial a_{nk}}{\partial w_{ki}}$$

$$= (\hat{y}_{nk} - y_{nk})\, g'(a_{nk})\, x_{ni}$$

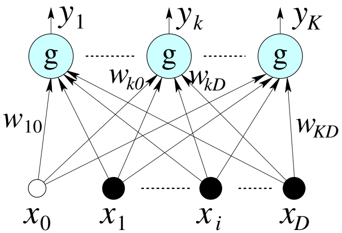


# Normalisation of output nodes - softmax

- Outputs with sigmoid activation function:

$$\sum_{k=1}^{K} y_k \neq 1$$

$$y_k = g(a_k) = \frac{1}{1 + \exp(-a_k)}, \; a_k = \sum_{i=0}^{d} w_{ki} x_i$$



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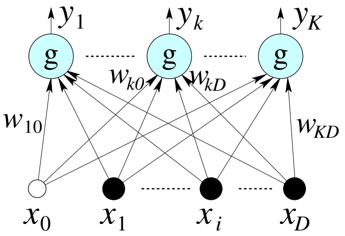


- Softmax activation function:

$$y_k = \frac{\exp(a_k)}{\sum_{\ell=1}^{K} \exp(a_\ell)}$$

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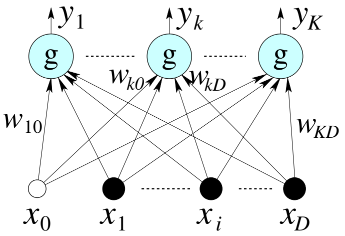


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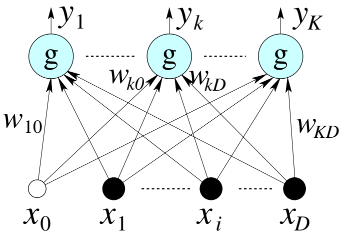


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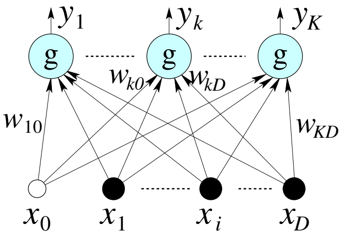


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$$y_k = \frac{\exp(a_k)}{\sum_{\ell=1}^{K} \exp(a_\ell)}$$

- Properties of the softmax function
  (i) $0 \leq y_k \leq 1$
  (ii) $\sum_{k=1}^{K} y_k = 1$

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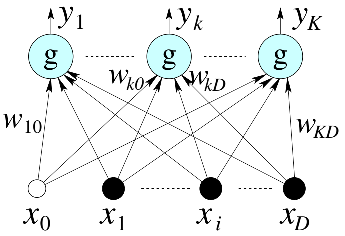


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  (iii) differentiable

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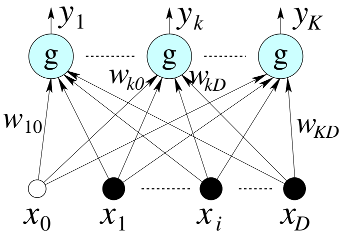


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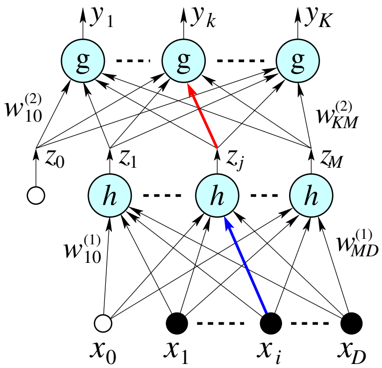
  - (i) $0 \leq y_k \leq 1$
  - (ii) $\sum_{k=1}^{K} y_k = 1$
  - (iii) differentiable
  - (iv) $y_k \approx P(C_k|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|C_k)P(C_k)}{\sum_{\ell=1}^{K} p(\boldsymbol{x}|C_k)P(C_k)}$

# Training of multi-layer neural networks

Multi-layer perceptron (MLP)

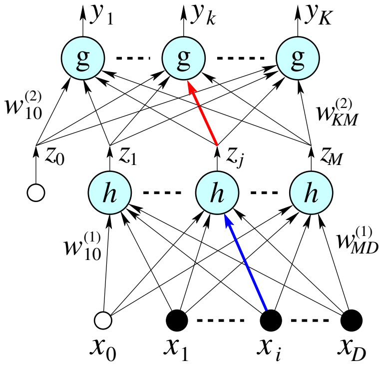


# Training of multi-layer neural networks

Multi-layer perceptron (MLP)

- Hidden-to-output weights:

$$w_{kj}^{(2)} \leftarrow w_{kj}^{(2)} - \eta \frac{\partial E}{\partial w_{kj}^{(2)}}$$



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Multi-layer perceptron (MLP)

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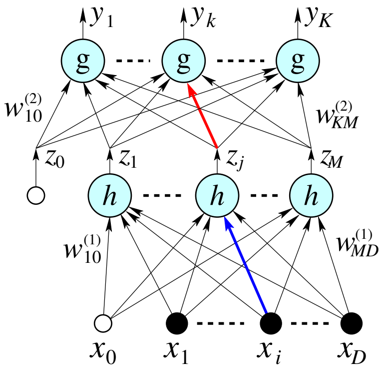
- Input-to-hidden weights:

$$w_{ji}^{(1)} \leftarrow w_{ji}^{(1)} - \eta \frac{\partial E}{\partial w_{ji}^{(1)}}$$



# Training of MLP

| | |
|---|---|
| 1940s | Warren McCulloch and Walter Pitts : 'threshold logic' |
| | Donald Hebb : 'Hebbian learning' |
| 1957 | Frank Rosenblatt : 'Perceptron' |
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| 1986 | D. Rumelhart, G. Hinton, and R. Williams, "Learning representations by back-propagating errors" (1974, Paul Werbos) |

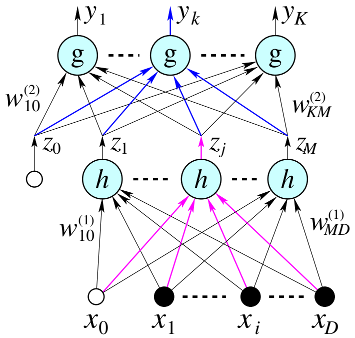


# The derivatives of the error function (two-layers)

$$E_n = \frac{1}{2}\sum_{k=1}^{K}(\hat{y}_{nk} - y_{nk})^2$$

$$\hat{y}_{nk} = g(a_{nk}), \quad a_{nk} = \sum_{j=1}^{M} w_{kj}^{(2)} z_{nj}$$

$$z_{nj} = h(b_{nj}), \quad b_{nj} = \sum_{i=0}^{d} w_{ji}^{(1)} x_{ni}$$



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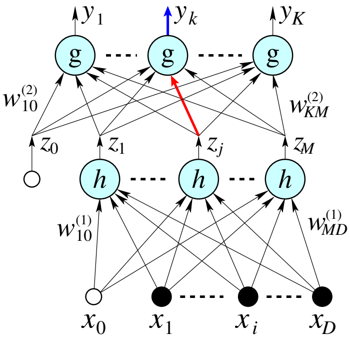

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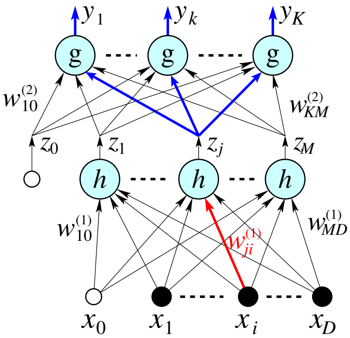



$$\frac{\partial E_n}{\partial w_{ji}^{(1)}} = \frac{\partial E_n}{\partial z_{nj}} \frac{\partial z_{nj}}{\partial b_{nj}} \frac{\partial b_{nj}}{\partial w_{ji}^{(1)}} = \left(\sum_{k=1}^{K} \frac{\partial E_n}{\partial \hat{y}_{nk}} \frac{\partial \hat{y}_{nk}}{\partial z_{nj}}\right) h'(b_{nj})\, x_{ni}$$

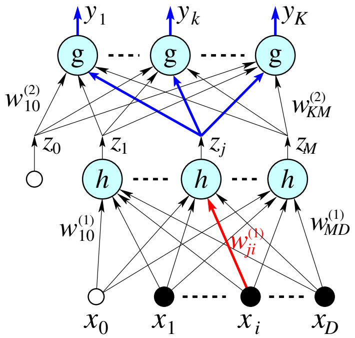
$$= \left(\sum_{k=1}^{K} (\hat{y}_{nk} - y_{nk}) g'(a_{nk}) w_{kj}^{(2)}\right) h'(b_{nj})\, x_{ni}$$

# Error back propagation

$$\frac{\partial E_n}{\partial w_{kj}^{(2)}} = \frac{\partial E_n}{\partial \hat{y}_{nk}} \frac{\partial \hat{y}_{nk}}{\partial a_{nk}} \frac{\partial a_{nk}}{\partial w_{kj}^{(2)}}$$

$$= (\hat{y}_{nk} - y_{nk})\, g'(a_{nk})\, z_{nj}$$

$$= \delta_{nk}^{(2)} z_{nj}, \qquad \delta_{nk}^{(2)} = \frac{\partial E_n}{\partial a_{nk}}$$



# Error back propagation

$$
\begin{aligned}
\frac{\partial E_n}{\partial w_{kj}^{(2)}} &= \frac{\partial E_n}{\partial \hat{y}_{nk}} \frac{\partial \hat{y}_{nk}}{\partial a_{nk}} \frac{\partial a_{nk}}{\partial w_{kj}^{(2)}} \\
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\end{aligned}
$$

$$
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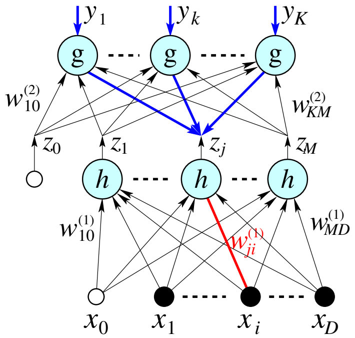
\frac{\partial E_n}{\partial w_{ji}^{(1)}} &= \frac{\partial E_n}{\partial z_{nj}} \frac{\partial z_{nj}}{\partial b_{nj}} \frac{\partial b_{nj}}{\partial w_{ji}^{(1)}} \\
&= \left( \sum_{k=1}^{K} (\hat{y}_{nk} - y_{nk}) g'(a_{nk}) w_{kj}^{(2)} \right) h'(b_{nj})\, x_{ni} \\
&= \left( \sum_{k=1}^{K} \delta_{nk}^{(2)} w_{kj}^{(2)} \right) h'(b_{nj})\, x_{ni}
\end{aligned}
$$



# Practical representations - computation graph

- Consider a two-layer neural network with softmax output
  - 1st layer with sigmoid activation functions:

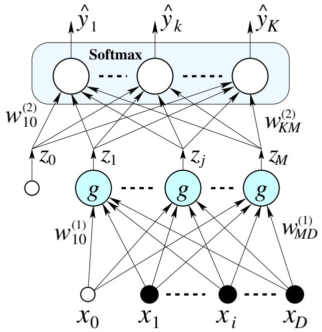
$$\mathbf{z} = g(\mathbf{x}) = \sigma(W_1\, \mathbf{x} + w_{10})$$

  - 2nd layer with a softmax activation function:

$$\hat{\mathbf{y}} = \text{softmax}(W_2\, \mathbf{z} + w_{20})$$

  - Cross-entropy loss function

$$L = -\sum y_i \log \hat{y}_i = -\log \hat{y}_c = -\log \text{softmax}(W_2\, \mathbf{z} + w_{20})_c$$



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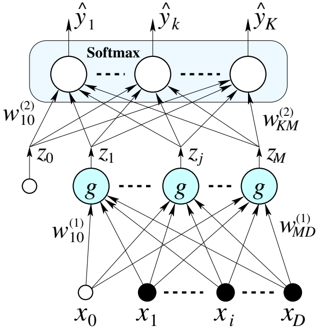


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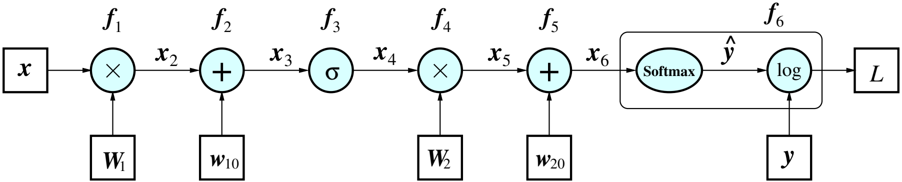
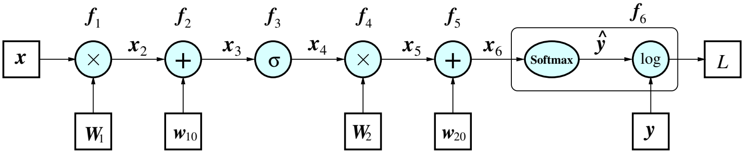


# Computation graph

Represents computation as a directed graph comprising of simple operations on vectors and matrices $\Rightarrow$ Automatic differentiation *(NE)*




$$L = f(\mathbf{x}) = f_6(f_5(f_4(f_3(f_2(f_1(\mathbf{x}))))))$$

$$f = f_6 \circ f_5 \circ f_4 \circ f_3 \circ f_2 \circ f_1$$

$$f_1 : \mathbf{x}_2 = W_1\,\mathbf{x}$$

$$f_2 : \mathbf{x}_3 = \mathbf{x}_2 + w_{10}$$

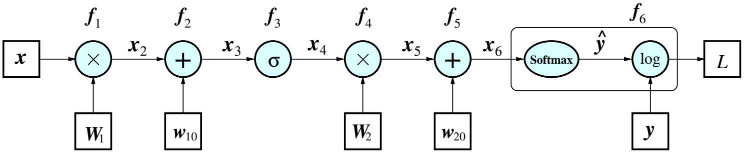
$$f_3 : \mathbf{x}_4 = \sigma(\mathbf{x}_3)$$

$$f_4 : \mathbf{x}_5 = W_2\,\mathbf{x}_4$$

$$f_5 : \mathbf{x}_6 = \mathbf{x}_5 + w_{20}$$

$$f_6 : L = \log \operatorname{softmax}(\mathbf{x}_6)_{i=y}$$

# Computation graph *(cont.)*



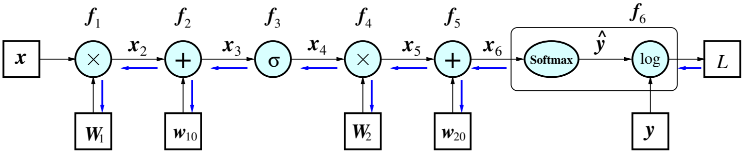

$$\frac{\partial L}{\partial W_2} = \frac{\partial L}{\partial \mathbf{x}_6} \frac{\partial \mathbf{x}_6}{\partial \mathbf{x}_5} \frac{\partial \mathbf{x}_5}{\partial W_2}$$

NB: matrix transpose is omitted for simplicity

$$\frac{\partial L}{\partial W_1} = \frac{\partial L}{\partial \mathbf{x}_6} \frac{\partial \mathbf{x}_6}{\partial \mathbf{x}_5} \frac{\partial \mathbf{x}_5}{\partial \mathbf{x}_4} \frac{\partial \mathbf{x}_4}{\partial \mathbf{x}_3} \frac{\partial \mathbf{x}_3}{\partial W_1}$$

- Forward pass: compute $\mathbf{x}_2, \ldots, \mathbf{x}_6, \hat{\mathbf{y}}, L$.
- Backward pass: compute $\frac{\partial L}{\partial w_{20}}, \frac{\partial L}{\partial W_2}, \frac{\partial L}{\partial w_{10}}, \frac{\partial L}{\partial W_1}$.

# Computation graph *(cont.)*




$$\frac{\partial L}{\partial W_2} = \frac{\partial L}{\partial \mathbf{x}_6} \frac{\partial \mathbf{x}_6}{\partial \mathbf{x}_5} \frac{\partial \mathbf{x}_5}{\partial W_2}$$

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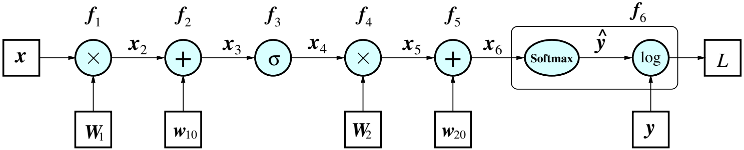
$$\frac{\partial L}{\partial W_1} = \frac{\partial L}{\partial \mathbf{x}_6} \frac{\partial \mathbf{x}_6}{\partial \mathbf{x}_5} \frac{\partial \mathbf{x}_5}{\partial \mathbf{x}_4} \frac{\partial \mathbf{x}_4}{\partial \mathbf{x}_3} \frac{\partial \mathbf{x}_3}{\partial W_1}$$

- Forward pass: compute $\mathbf{x}_2, \ldots, \mathbf{x}_6, \hat{\mathbf{y}}, L$.
- Backward pass: compute $\frac{\partial L}{\partial w_{20}}, \frac{\partial L}{\partial W_2}, \frac{\partial L}{\partial w_{10}}, \frac{\partial L}{\partial W_1}$.

# Computation graph – cross entropy layer




$$L = -\log \hat{y}_c = -\log \frac{e^{a_c}}{\sum_j e^{a_j}}, \quad \text{where } c \text{ is the true class, } \mathbf{a} = \mathbf{x}_4$$

$$\frac{\partial L}{\partial a_i} = \frac{\partial}{\partial a_i}\left(\log(\sum_j e^{a_j}) - a_c\right) = \frac{e^{a_i}}{\sum_j e^{a_j}} - \mathbb{1}_{i=c} = \hat{y}_i - \mathbb{1}_{i=c}$$

$$\frac{\partial L}{\partial \mathbf{x}_6} = \hat{\mathbf{y}} - \mathbf{y}$$

# Quizzes

- On slide 12, show the following:

$$\frac{\partial\, E_{\mathrm{H}}(\boldsymbol{w})}{\partial\, w_i} = \frac{1}{N}\sum_{n=1}^{N}(\hat{y}_n - y_n)\, x_{ni}$$

- On Slide 24, find the following:
  - $\dfrac{\partial\, \mathbf{x}_6}{\partial w_{20}}$
  - $\dfrac{\partial \mathbf{x}_5}{\partial W_2}$
  - $\dfrac{\partial\, \mathbf{x}_4}{\partial\, \mathbf{x}_3}$