Machine Learning

Neural Networks 2

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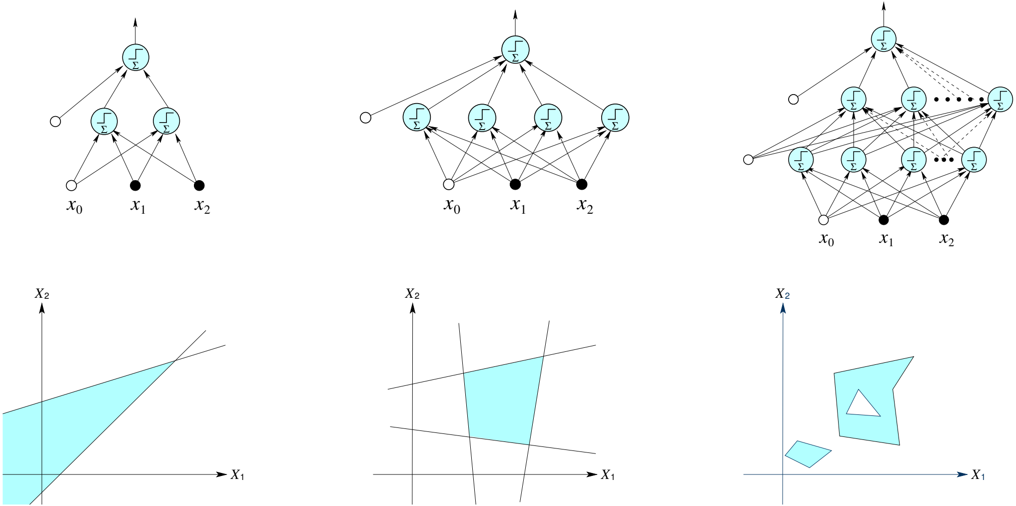
Ver. 1.0

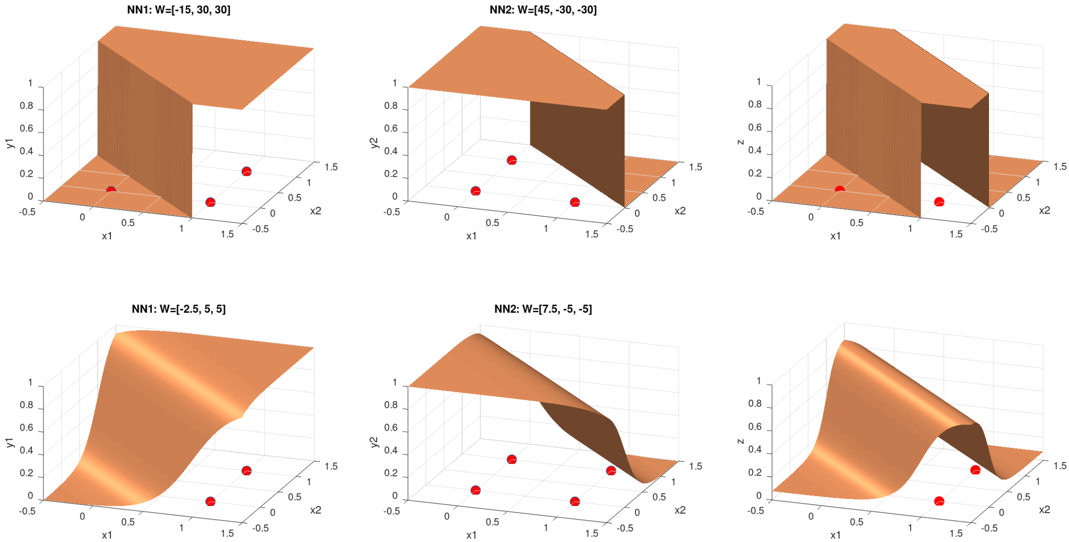
Topics - you should be able to explain after this week

- 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



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)

    $\longrightarrow$

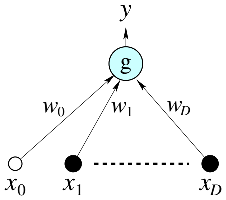
    A single-output node neural network with a single hidden layer with a finite neurons can approximate continuous (and discontinuous) functions.
  - K. Hornik (1990) doi:10.1016/0893-6080(91)90009-T
  - N. Guliyev, V. Ismailov (2018) doi:10.31219/osf.io/xgnw8
  - V. Ismailov (2023) “A three layer neural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

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

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

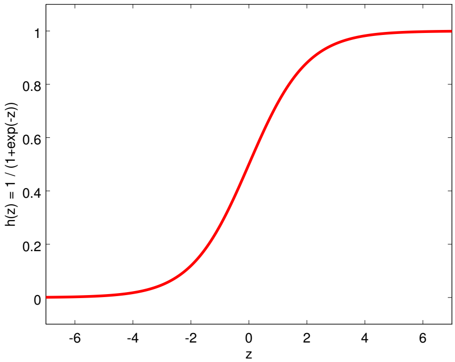


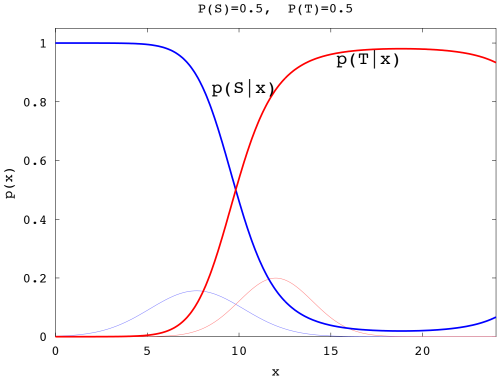
- Consider a two class problem, with classes C_1 and C_2. The posterior probability of C_1:

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

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

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 $y_i \in \{0, 1\}$
- Error function:

$$E_{\text{MSE}}(\boldsymbol{w}) = \frac{1}{2}\sum_{n=1}^{N}\left(\hat{y}_n - y_n\right)^2 = \frac{1}{2}\sum_{n=1}^{N}\left(g(\boldsymbol{w}^T\mathbf{x}_n) - y_n\right)^2 = \frac{1}{2}\sum_{n=1}^{N}\left(g\left(\sum_{i=0}^{d} w_i x_{ni}\right) - y_n\right)^2$$

- Definition of the training problem as an optimisation problem

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

Training single layer neural network with MSE *(cont.)*

- Optimisation problem: $\min_{\boldsymbol{w}} E_{\text{MSE}}(\boldsymbol{w})$
- No analytical (closed-form) solutions
- Employ an iterative method (requires initial values)
  e.g. Gradient descent, Newton's method, Conjugate gradient methods
- Gradient descent

  (scalar form)

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

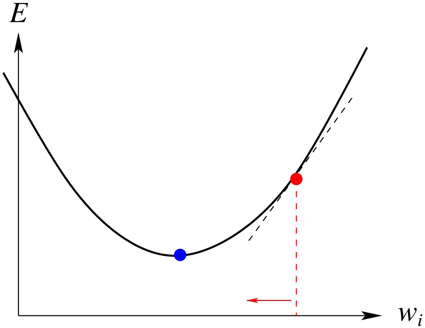
  (vector form)

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

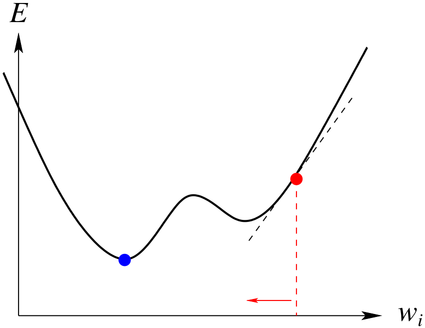
- Online/stochastic gradient descent (cf. Batch training)
  Sample (x_n, y_n) from the data set and update the weights at a time.

Gradient descent

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



global minimum



local minimum

Training single layer neural network with MSE *(cont.)*

$$E_{\text{MSE}}(\boldsymbol{w}) = \sum_{n=1}^{N} E_n, \quad \text{where } E_n = \frac{1}{2}\left(\hat{y}_n - y_n\right)^2 = \frac{1}{2}\left(g\left(\sum_{i=0}^{d} w_i x_{ni}\right) - y_n\right)^2$$

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

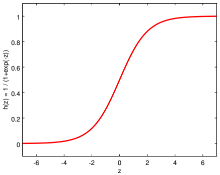
$$\begin{aligned}
\frac{\partial E_n(\boldsymbol{w})}{\partial w_i} &= \frac{\partial E_n(\boldsymbol{w})}{\partial \hat{y}_n} \frac{\partial \hat{y}_n}{\partial a_n} \frac{\partial a_n}{\partial w_i} \\
&= (\hat{y}_n - y_n) \frac{\partial g(a_n)}{\partial a_n} \frac{\partial a_n}{\partial w_i} \\
&= (\hat{y}_n - y_n)\, g'(a_n)\, x_{ni} \\
&= (\hat{y}_n - y_n)\, g(a_n)\,(1 - g(a_n))\, x_{ni} \quad \text{if } g(\,) \text{ is a sigmoid function}
\end{aligned}$$

Another training criterion – cross-entropy error

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

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

$$\frac{\partial\, E_{\mathrm{MSE}}(\boldsymbol{w})}{\partial\, w_i} = \sum_{n=1}^{N}(\hat{y}_n - y_n)\, g'(a_n)\, x_{ni}\,, \qquad g'(a) = g(a)(1-g(a))$$



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

- Cross-entropy error

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

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

It can be shown that:

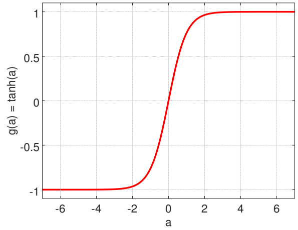
$$\frac{\partial\, E_{\mathrm{H}}(\boldsymbol{w})}{\partial\, w_i} = \frac{1}{N}\sum_{n=1}^{N}(\hat{y}_n - y_n)\, x_{ni}$$

Other activation functions

- Tanh

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

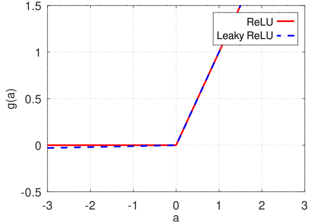
  - Mapping $(-\infty, +\infty) \rightarrow (-1, 1)$
  - 0 (zero) centred $\rightarrow$ faster convergence than sigmoid



- ReLU (Rectified Linear Unit)

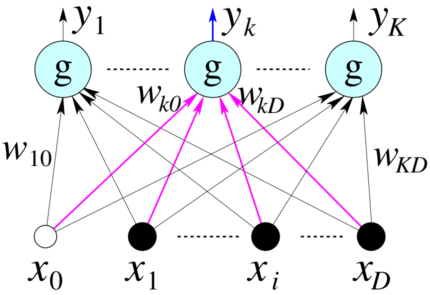
$$g(a) = \max(0, a)$$

  - 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



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

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

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

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

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

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 $y_{nk} \in \{0, 1\}$

- Error function:

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

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

- Training with the gradient descent:

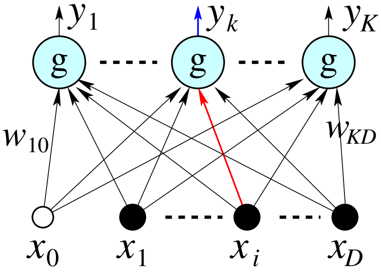
$$w_{ki} \leftarrow w_{ki} - \eta \frac{\partial E}{\partial w_{ki}}, \qquad (\eta > 0)$$

The derivatives of the error function (single-layer)

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

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

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



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

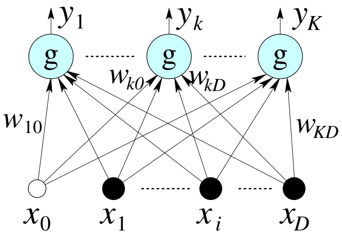
$$= (\hat{y}_{nk} - y_{nk})\, g'(a_{nk})\, x_{ni}$$

Normalisation of output nodes - softmax

- Outputs with sigmoid activation function:

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

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



- Softmax activation function:

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

- Properties of the softmax function

(i) $0 \leq y_k \leq 1$

(ii) $\sum_{k=1}^{K} y_k = 1$

(iii) differentiable

(iv) $y_k \approx P(C_k|\mathbf{x}) = \frac{p(\mathbf{x}|C_k)P(C_k)}{\sum_{\ell=1}^{K} p(\mathbf{x}|C_k)P(C_k)}$

Training of multi-layer neural networks

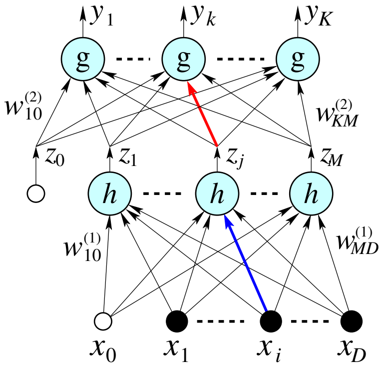
Multi-layer perceptron (MLP)

- Hidden-to-output weights:

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

- 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'
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)

The derivatives of the error function (two-layers)

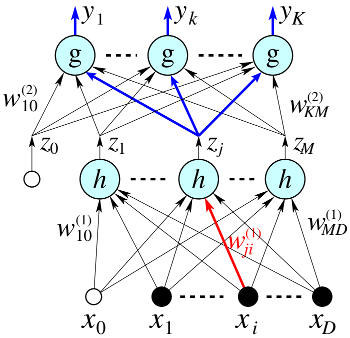
$$E_n = \frac{1}{2}\sum_{k=1}^{K}(\hat{y}_{nk} - y_{nk})^2$$

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

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

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

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



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

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

Error back propagation

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

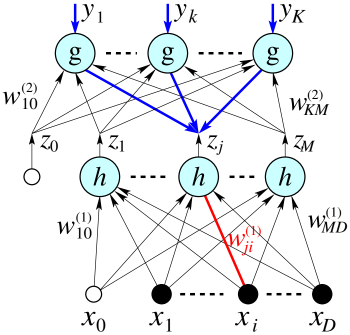
$$= (\hat{y}_{nk} - y_{nk})\, g'(a_{nk})\, z_{nj}$$

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

$$\frac{\partial E_n}{\partial w_{ji}^{(1)}} = \frac{\partial E_n}{\partial z_{nj}} \frac{\partial z_{nj}}{\partial b_{nj}} \frac{\partial b_{nj}}{\partial w_{ji}^{(1)}}$$

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

$$= \left(\sum_{k=1}^{K} \delta_{nk}^{(2)} w_{kj}^{(2)} \right) h'(b_{nj})\, x_{ni}$$



Practical representations - computation graph

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

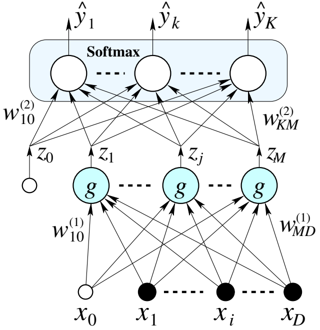
    $$\mathbf{z} = g(\mathbf{x}) = \sigma(W_1\,\mathbf{x} + w_{10})$$

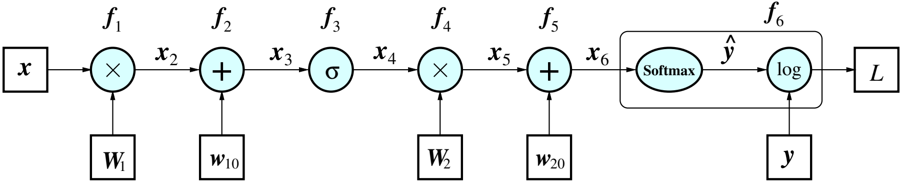
  - 2nd layer with a softmax activation function:

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

  - Cross-entropy loss function

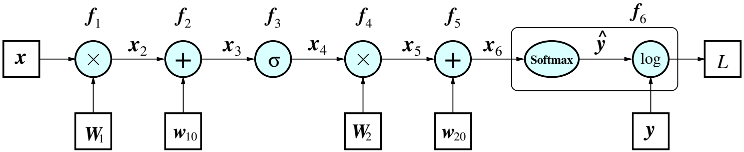
    $$L = -\sum y_i \log \hat{y}_i = -\log \hat{y}_c = -\log \text{softmax}(W_2\,\mathbf{z} + w_{20})_c$$





Computation graph

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



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

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

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

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

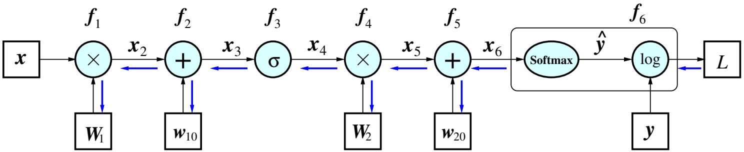
$$f_3 : \mathbf{x}_4 = \sigma(\mathbf{x}_3)$$

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

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

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

Computation graph *(cont.)*



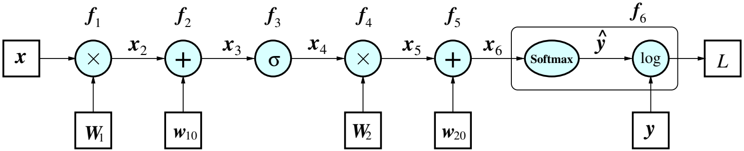
$$\frac{\partial L}{\partial W_2} = \frac{\partial L}{\partial \mathbf{x}_6}\frac{\partial \mathbf{x}_6}{\partial \mathbf{x}_5}\frac{\partial \mathbf{x}_5}{\partial W_2}$$

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 – 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:
  - $\frac{\partial \mathbf{x}_6}{\partial w_{20}}$
  - $\frac{\partial \mathbf{x}_5}{\partial W_2}$
  - $\frac{\partial \mathbf{x}_4}{\partial \mathbf{x}_3}$

Appendix – derivatives

- Derivatives of functions of one variable

$$\frac{\mathrm{d}f}{\mathrm{d}x} = f'(x) = \lim_{\epsilon \to 0} \frac{f(x+\epsilon) - f(x)}{\epsilon}$$

e.g., $f(x) = 4x^3,\ f'(x) = 12x^2$

- Partial derivatives of functions of more than one variable

$$\frac{\partial f}{\partial x} = \lim_{\epsilon \to 0} \frac{f(x+\epsilon, y) - f(x, y)}{\epsilon}$$

e.g., $f(x, y) = y^3 x^2,\ \frac{\partial f}{\partial x} = 2y^3 x$

Derivative rules

	Function	Derivative
Constant	c	0
	x	1
Power	x^n	nx^{n-1}
	$\frac{1}{x}$	$-\frac{1}{x^2}$
	$\sqrt{x}$	$\frac{1}{2}x^{-\frac{1}{2}}$
Exponential	e^x	e^x
Logarithms	$\ln(x)$	$\frac{1}{x}$
Sum rule	$f(x) + g(x)$	$f'(x) + g'(x)$
Product rule	$f(x)g(x)$	$f'(x)g(x) + f(x)g'(x)$
Reciprocal rule	$\frac{1}{f(x)}$	$-\frac{f'(x)}{f^2(x)}$
	$\frac{f(x)}{g(x)}$	$-\frac{f'(x)g(x)-f(x)g'(x)}{g^2(x)}$
Chain rule	$f(g(x))$	$f'(g(x))g'(x)$
	$z = f(y), y = g(x)$	$\frac{\mathrm{d}z}{\mathrm{d}x} = \frac{\mathrm{d}z}{\mathrm{d}y}\frac{\mathrm{d}y}{\mathrm{d}x}$

Vectors of derivatives

Consider $f(\boldsymbol{x})$, where $\boldsymbol{x} = (x_1, \ldots, x_d)^T$

Notation: all partial derivatives put in a vector:

$$\nabla_{\boldsymbol{x}} f(\boldsymbol{x}) = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \cdots, \frac{\partial f}{\partial x_d} \right)^T$$

Example: $f(\boldsymbol{x}) = x_1^3 x_2^2$

$$\nabla_{\boldsymbol{x}} f(\boldsymbol{x}) = \begin{pmatrix} 3x_1^2 x_2^2 \\ 2x_1^3 x_2 \end{pmatrix}$$

Fact: $f(\boldsymbol{x})$ changes most quickly in direction $\nabla_{\boldsymbol{x}} f(\boldsymbol{x})$