INTRODUCTION TO NEURAL NETWORKS

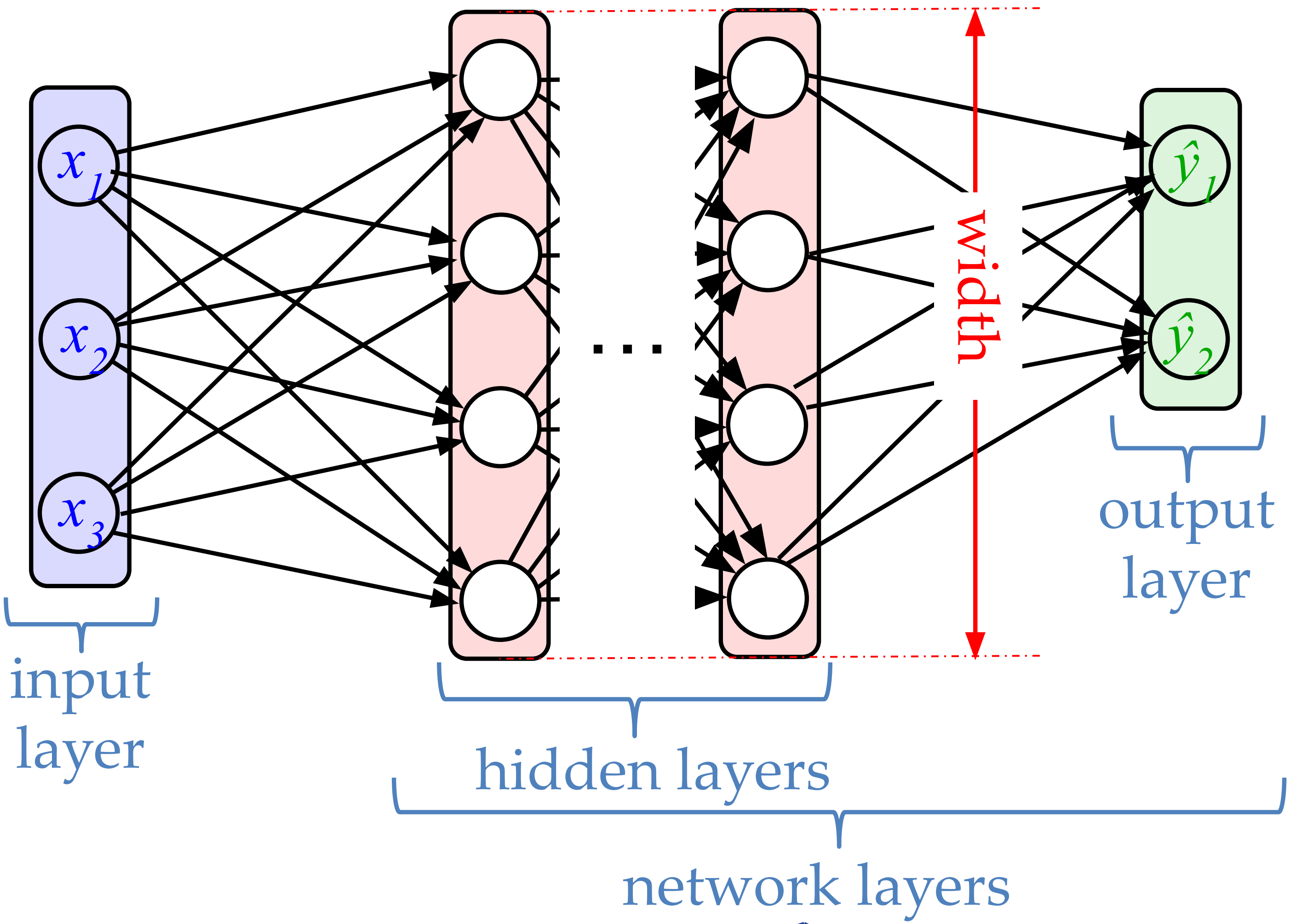
Backpropagation

Pascal Germain*, 2019

Translated to English by Vera Shalaeva, 2020

* Thanks to Philippe Giguère for his permit to reuse some of his slides.

Illustration and notions



$$\hat{y} = f^{(3)}\left(f^{(2)}\left(f^{(1)}\left(x\right)\right)\right)$$

Parameters to choose

- Architecture
  - # layers
  - # neurones (hidden) by layer
  - type of layer
- Output neuron function
- Loss function
- Optimizer
  - and other « *details* »

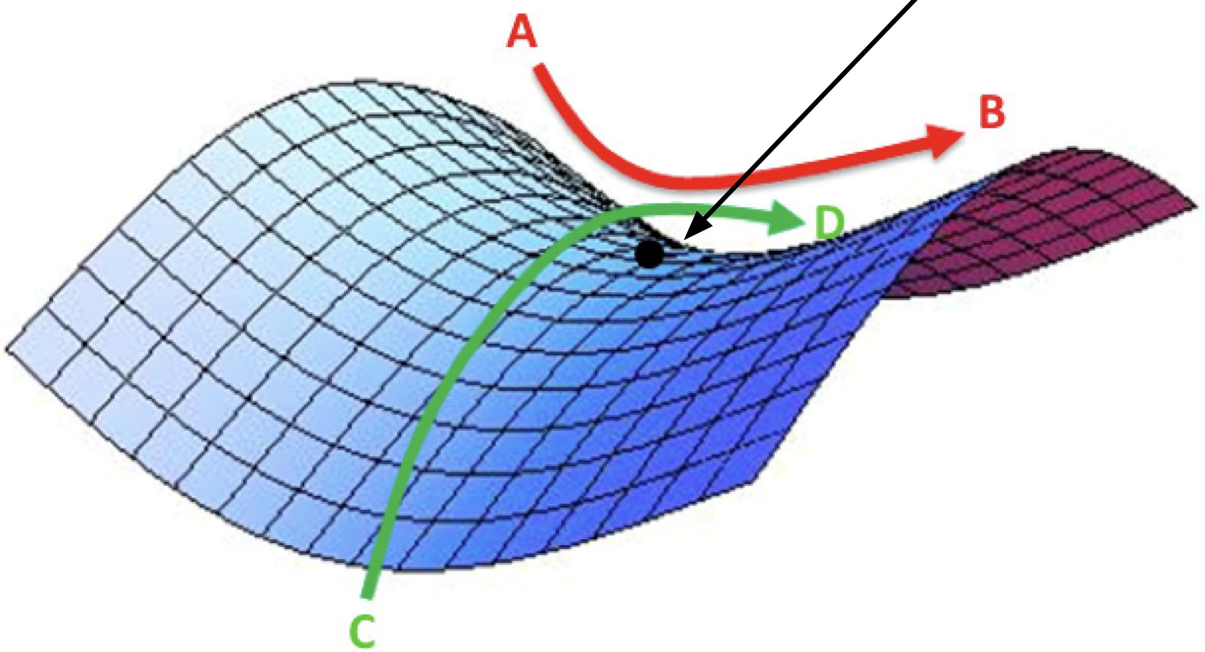
Comparison with classical methods

- Many learning methods are convex
  - Least squares
  - Logistic regression
  - SVM
- Neural Networks are not convex
  - Challenging to get theoretical guarantees.
  - Result varies according to initialization of the gradient descent.
  - We have to accept that local minimum might be a good solution.
  - Research shows that solutions are often saddle points
    - ratio (saddle points)/(local minimum) increase exponentially with the number of parameters to estimate

See Goodfellow et al. Section 8.2.3

Saddle point example

- Partial derivative is equal to zero at a saddle point.



https://www.safaribooksonline.com/library/view/fundamentals-of-deep/9781491925607/ch04.html

Profile of a loss function

Adapté de
cs231n

Backpropagation algorithm
(«*backprop*»)

The chain rule.

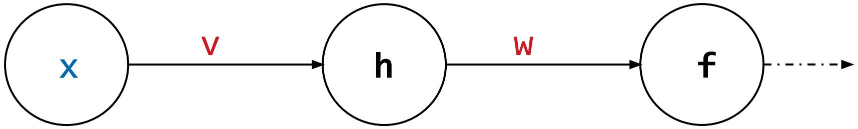
$$\boxed{\begin{aligned}\frac{\partial f(h(x))}{\partial x} &= \frac{\partial f(h(x))}{\partial h(x)}\frac{\partial h(x)}{\partial x}\\ &= \left[\frac{\partial f(a)}{\partial a}\right]_{a=h(x)}\frac{\partial h(x)}{\partial x}\end{aligned}}$$

For example:

$$\begin{aligned}F(x) &= (2x+3)^2\\ &= f(2x+3) \quad \text{where: } f(x) = x^2\\ &= f(h(x)) \quad \text{where: } h(x) = 2x+3.\end{aligned}$$

Then :

$$\begin{aligned}\frac{\partial F(x)}{\partial x} &= \frac{\partial f(h(x))}{\partial h(x)}\frac{\partial h(x)}{\partial x}\\ &= 2\,h(x) \times 2\\ &= 4(2x+3)\end{aligned}$$



$$\boxed{\frac{\partial f(h(x))}{\partial x} = \left[\frac{\partial f(a)}{\partial a}\right]_{a=h(x)} \frac{\partial h(x)}{\partial x}}$$

$$R_{v,w}(x) = f(w \cdot h(v \cdot x))$$

$$\frac{\partial L(R_{v,w}(x), y)}{\partial w} = \left[\frac{\partial L(r, y)}{\partial r}\right]_{r=R_{v,w}(x,y)} \cdot \frac{\partial R_{v,w}(x)}{\partial w}$$

The chain rule.

$$\frac{\partial f(h(x))}{\partial x} = \frac{\partial f(h(x))}{\partial h(x)} \frac{\partial h(x)}{\partial x}$$
$$= \left[\frac{\partial f(a)}{\partial a}\right]_{a=h(x)} \frac{\partial h(x)}{\partial x}$$

We can also write:

$$(f \circ h)' = (f' \circ h) \times h'$$

$$(\, f(h(x))\,)' = f'(h(x)) \times h'(x)$$

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial h} \frac{\partial h}{\partial x}$$

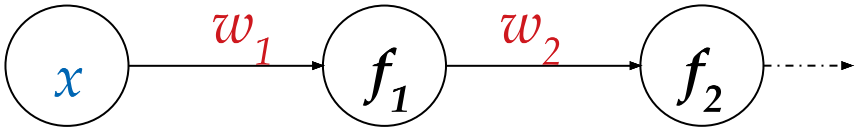
$$x \xrightarrow{v} h \xrightarrow{w} f \dashrightarrow$$

$$\boxed{\frac{\partial f(h(x))}{\partial x} = \left[\frac{\partial f(a)}{\partial a}\right]_{a=h(x)} \frac{\partial h(x)}{\partial x}}$$

$$R_{v,w}(x) = f(w \cdot h(v \cdot x))$$

$$\begin{aligned}
\frac{\partial L(R_{v,w}(x),y)}{\partial w} &= \left[\frac{\partial L(r,y)}{\partial r}\right]_{r=R_{v,w}(x,y)} \cdot \frac{\partial R_{v,w}(x)}{\partial w} \\
&= \left[\frac{\partial L(r,y)}{\partial r}\right]_{r=R_{v,w}(x,y)} \cdot \left[\frac{\partial f(a)}{\partial a}\right]_{a=w \cdot h(v \cdot x)} \cdot \frac{\partial w \cdot h(v \cdot x)}{\partial w} \\
&= \boxed{\left[\frac{\partial L(r,y)}{\partial r}\right]_{r=R_{v,w}(x,y)} \cdot \left[\frac{\partial f(a)}{\partial a}\right]_{a=w \cdot h(v \cdot x)}} \cdot h(v \cdot x)
\end{aligned}$$

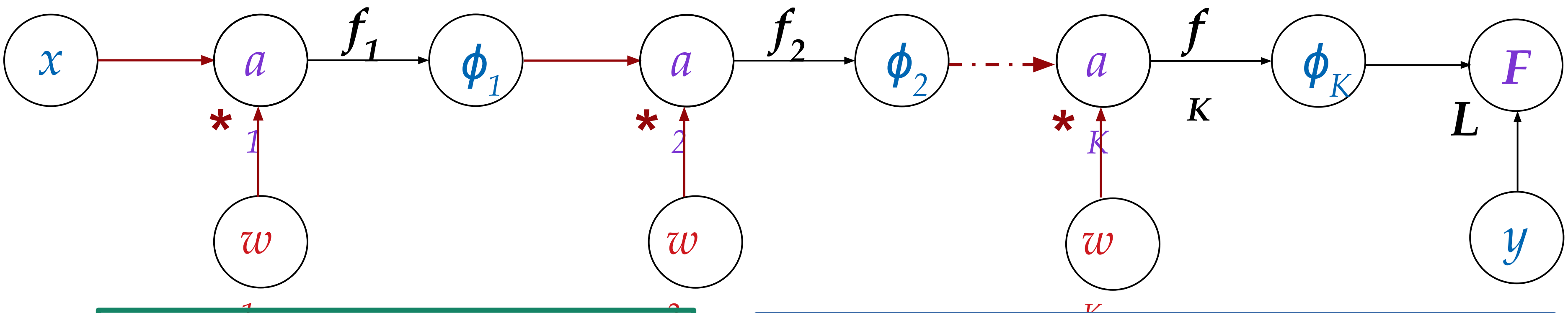
$$\begin{aligned}
\frac{\partial L(R_{v,w}(x),y)}{\partial v} &= \left[\frac{\partial L(r,y)}{\partial r}\right]_{r=R_{v,w}(x,y)} \cdot \frac{\partial R_{v,w}(x)}{\partial v} \\
&= \left[\frac{\partial L(r,y)}{\partial r}\right]_{r=R_{v,w}(x,y)} \cdot \left[\frac{\partial f(a)}{\partial a}\right]_{a=w \cdot h(v \cdot x)} \cdot \frac{\partial w \cdot h(v \cdot x)}{\partial v} \\
&= \left[\frac{\partial L(r,y)}{\partial r}\right]_{r=R_{v,w}(x,y)} \cdot \left[\frac{\partial f(a)}{\partial a}\right]_{a=w \cdot h(v \cdot x)} \cdot w \cdot \frac{\partial h(v \cdot x)}{\partial v} \\
&= \left[\frac{\partial L(r,y)}{\partial r}\right]_{r=R_{v,w}(x,y)} \cdot \left[\frac{\partial f(a)}{\partial a}\right]_{a=w \cdot h(v \cdot x)} \cdot w \cdot \left[\frac{\partial h(b)}{\partial b}\right]_{b=v \cdot x} \cdot \frac{\partial v \cdot x}{\partial v} \\
&= \boxed{\left[\frac{\partial L(r,y)}{\partial r}\right]_{r=R_{v,w}(x,y)} \cdot \left[\frac{\partial f(a)}{\partial a}\right]_{a=w \cdot h(v \cdot x)}} \cdot w \cdot \left[\frac{\partial h(b)}{\partial b}\right]_{b=v \cdot x} \cdot x
\end{aligned}$$



$$\frac{\partial f(h(x))}{\partial x} = \left[\frac{\partial f(a)}{\partial a}\right]_{a=h(x)} \frac{\partial h(x)}{\partial x}$$

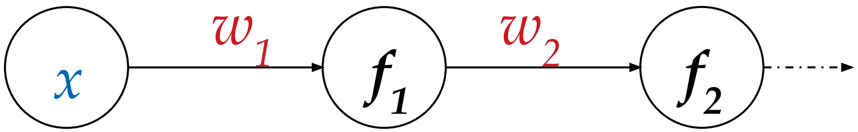
$$R(x) = f_2(w_2 \cdot f_1(w_1 \cdot x))$$

$$F = L\Big(R(x), y\Big)$$



Step 1: Forward propagation

Step 2: Backpropagation of gradient



$$\frac{\partial f(h(x))}{\partial x} = \left[\frac{\partial f(a)}{\partial a}\right]_{a=h(x)} \frac{\partial h(x)}{\partial x}$$

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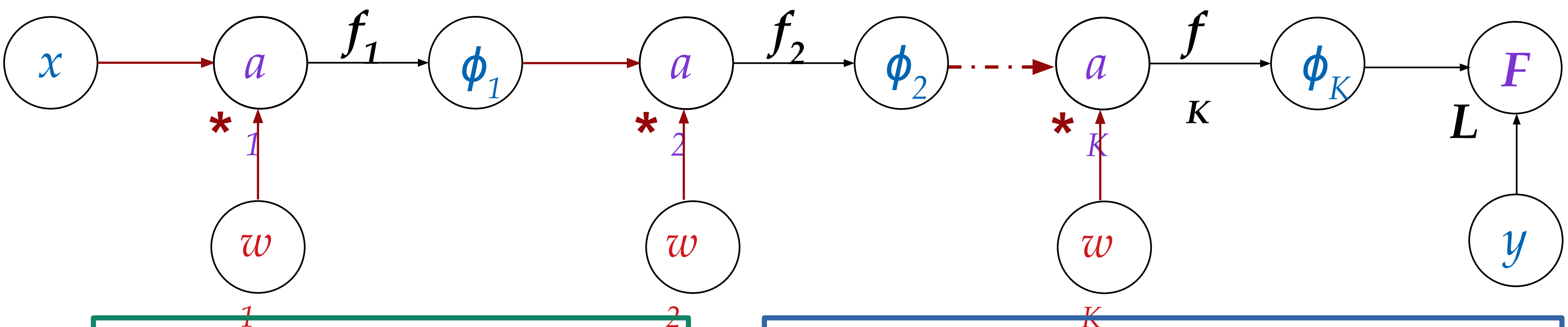
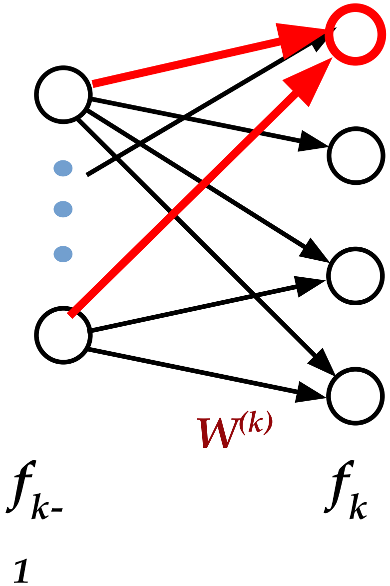
$$F = L\Big(R(x), y\Big)$$

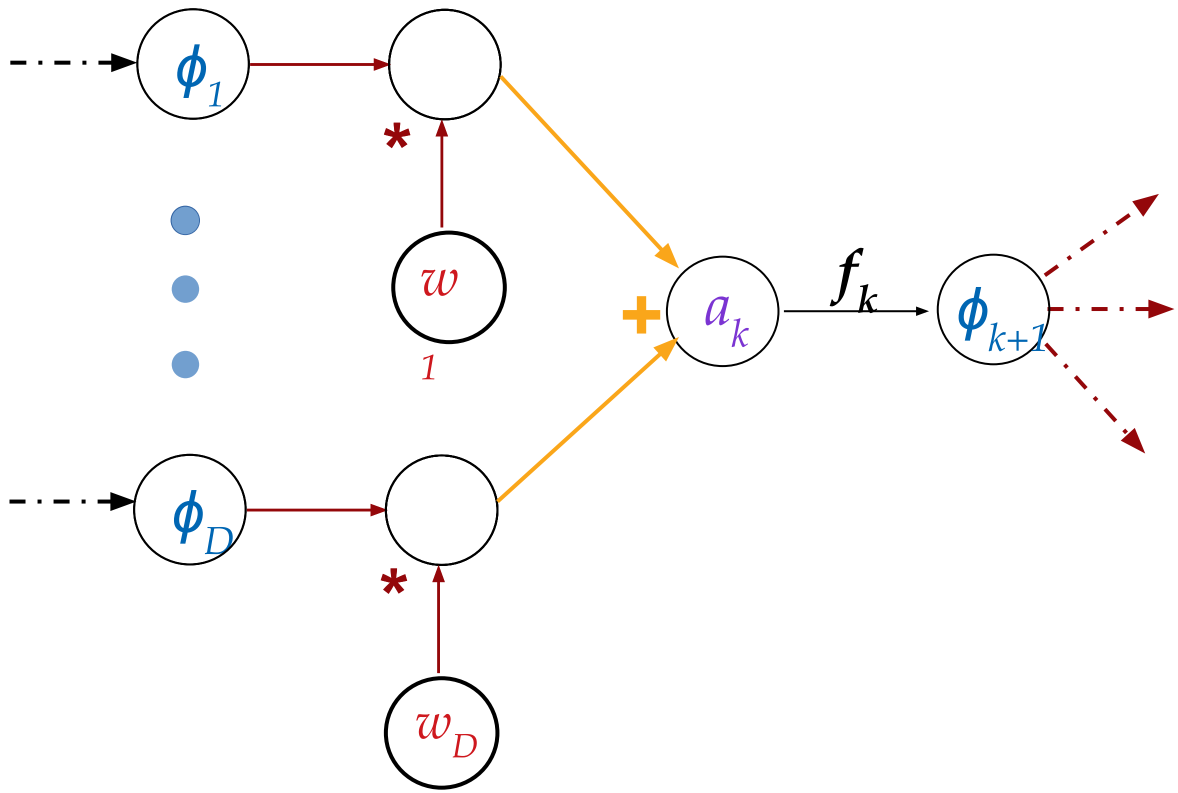


- $\phi_0 = x$
- **For** $k = 1, 2, \ldots K$:
  - $a_k = w_k \cdot \phi_{k-1}$
  - $\phi_k = f_k(a_k)$
- $F = L(\phi_K, y)$

- $\phi_K^\delta = \frac{\partial F}{\partial \phi_K} = L'(\phi_k, y)$
- **For** $k = K, K{-}1, \ldots, 1$:
  - $a_k^\delta = \frac{\partial F}{\partial \phi_k} \frac{\partial \phi_k}{\partial a_k} = \phi_k^\delta \, f_k'(a_k)$
  - $w_k^\delta = \frac{\partial F}{\partial a_k} \frac{\partial a_k}{\partial w_k} = a_k^\delta \, \phi_{k-1}$
  - $\phi_{k-1}^\delta = \frac{\partial F}{\partial a_k} \frac{\partial a_k}{\partial \phi_{k-1}} = a_k^\delta \, w_k$



$$\frac{\partial f(h(x))}{\partial x} = \left[\frac{\partial f(a)}{\partial a}\right]_{a=h(x)} \frac{\partial h(x)}{\partial x}$$



A network R of K hidden layers

- Activation functions: $f_1, \dots f_K$
- Weight matrices: $\mathbf{W}^{(1)}, \dots \mathbf{W}^{(K)}$
  - Each matrix $\mathbf{W}^{(k)}$ of size $d_k \times d_{k-1}$
  - d_k is the number of neurons at a layers k
  - $k = 0$ corresponds to the input layer $\mathbf{x} \in \mathbb{R}^{d_0}$

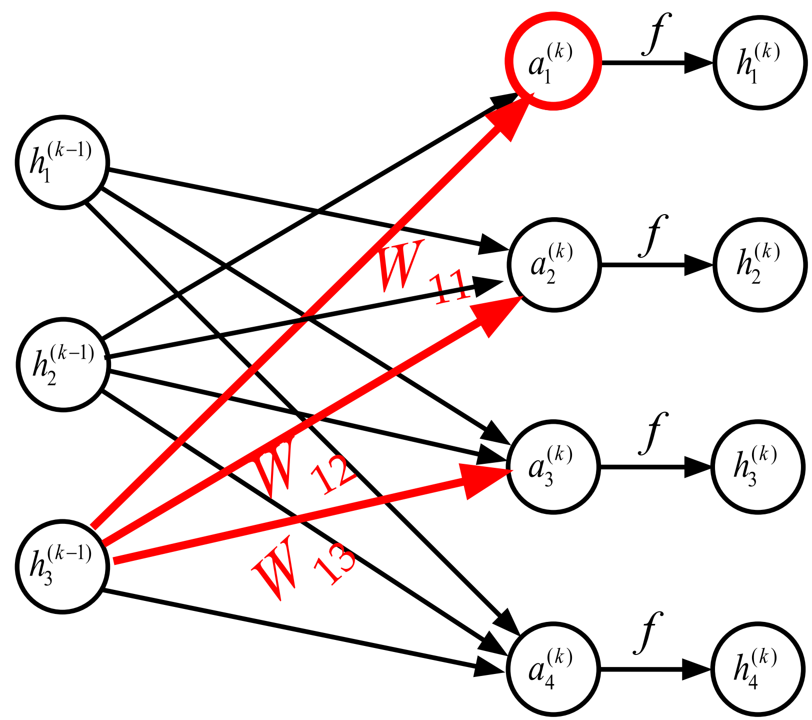
$$\mathbf{W}^{(k)} = \begin{bmatrix} W_{11} & \cdots & W_{1d_{K-1}} \\ \vdots & \ddots & \vdots \\ W_{d_K 1} & \cdots & W_{d_K d_{K-1}} \end{bmatrix}$$

Algorithm: Forward pass.

Input: A network *R*, Observation **x**

- $\mathbf{h}[0] \leftarrow \mathbf{x}$
- **For** k **from 1 to K:**
  - $\mathbf{a}[k] \leftarrow \mathbf{W}^{(k)} \mathbf{h}^{(k-1)}$
  - $\mathbf{h}[k] \leftarrow f_k(\mathbf{a}[k])$

Output: $\mathbf{h}[K]$



Algorithm: Forward pass.

Input: A network R, Observation $\mathbf{x}$

- $\mathbf{h}[0] \leftarrow \mathbf{x}$
- For k de 1 à K:
  - $\mathbf{a}[k] \leftarrow \mathbf{W}^{(k)}\mathbf{h}^{(k-1)}$
  - $\mathbf{h}[k] \leftarrow f_k(\mathbf{a}[k])$

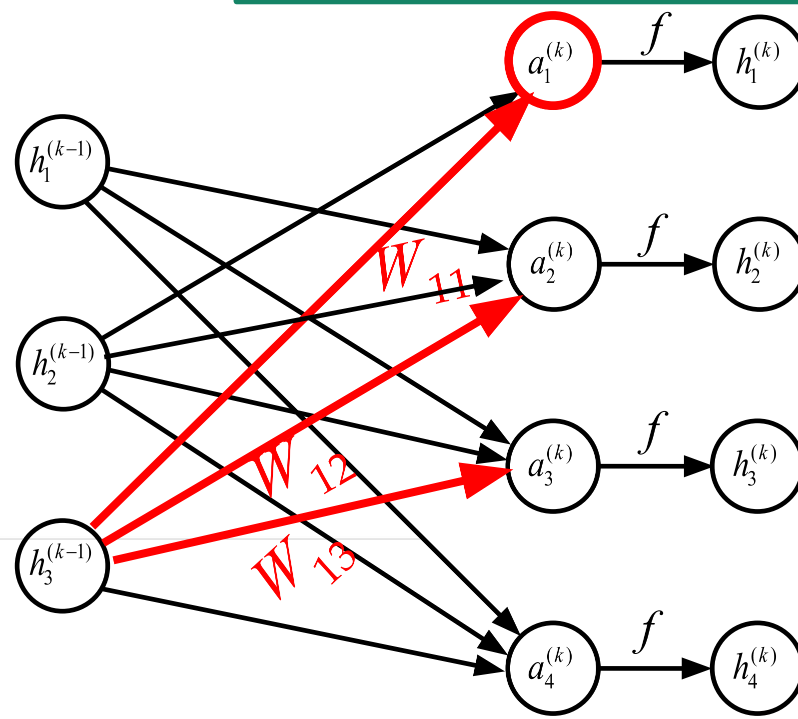
Output: $\mathbf{h}[K]$

Algorithm: Backpropagation.

Input: A network R, Observation $\mathbf{x}$, Loss L, output $\mathbf{y}$

- $\mathbf{g} \leftarrow L'(h[K], \mathbf{y})$
- For k from K to 1:
  - $\mathbf{g} \leftarrow \mathbf{g} \odot f'_k(\mathbf{a}[k])$
  - $\nabla_{\mathbf{W}}[k] \leftarrow \mathbf{g}\,\mathbf{h}[k]^T$
  - $\mathbf{g} \leftarrow \mathbf{W}^{(k)T}\mathbf{g}$

Output: $\nabla_{\mathbf{W}}$



Automatic differentiation of the computational graph.

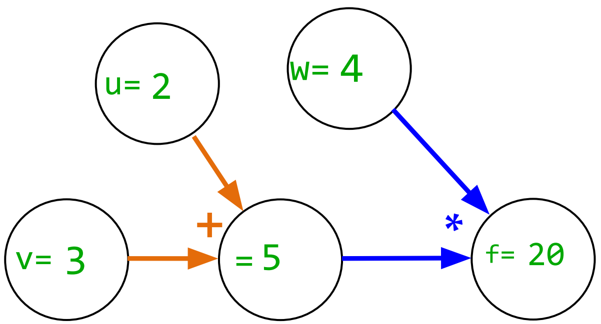
«Backprop» and automatic differentiation

- Algorithm that computes all gradients in a graph.
- **It is not optimization algorithm!**
- But all algorithm of neural network optimization use gradients computed by *backprop*.
- It is based on the chain rule.
- The modern libraries do the computations automatically (*pyTorch* et *TensorFlow*).

Example of computations on a simple graph

$$f = \boxed{\boxed{(u+v)}w}$$

node : variable
arrow : operation

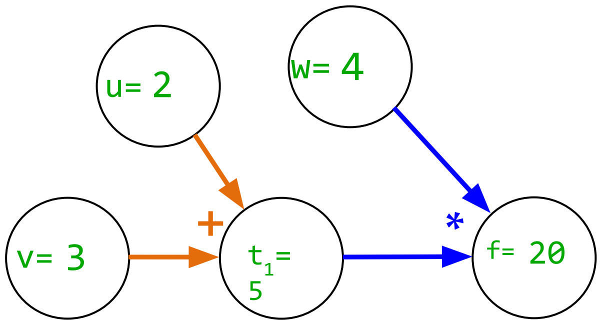


Initial values of variables:
u=2
v=3
w=4

Evaluation of graph to get f: **Forward pass**

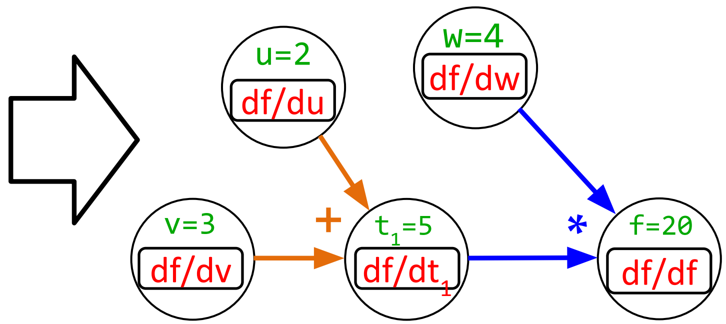
Example of computations on a simple graph

From a forward pass graph computations:



$$f=(u+v)w$$

We add a variable to save the gradients:



$$\boxed{\frac{\partial f}{\partial x} = \frac{\partial f}{\partial h}\frac{\partial h}{\partial x}}$$

Example of computations on a simple graph

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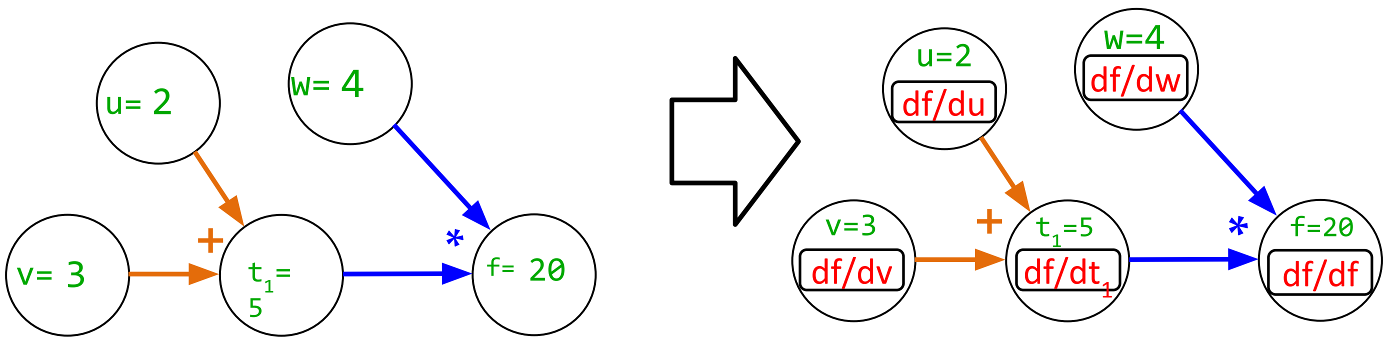


$$f=(u+v)w$$

$$f=t_1 w,\ t_1=u+v$$

$$\boxed{\frac{\partial f}{\partial x} = \frac{\partial f}{\partial h}\frac{\partial h}{\partial x}}$$

$$\frac{\partial f}{\partial f} = 1$$

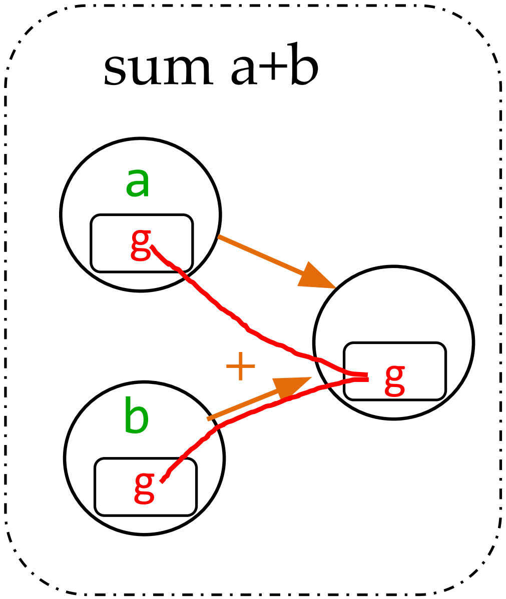
$$\frac{\partial f}{\partial w} = \frac{\partial}{\partial w}(t_1 w)\frac{\partial f}{\partial f} = t_1 \cdot 1$$

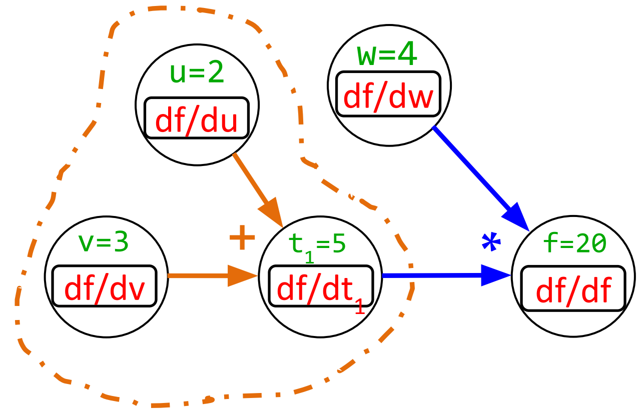
$$\frac{\partial f}{\partial t_1} = \frac{\partial}{\partial t_1}(t_1 w)\frac{\partial f}{\partial f} = w \cdot 1$$

$$\frac{\partial f}{\partial u} = \frac{\partial t_1}{\partial u}\frac{\partial f}{\partial t_1} = 1 \cdot \frac{\partial f}{\partial t_1} = 4$$

$$\frac{\partial f}{\partial v} = \frac{\partial t_1}{\partial v}\frac{\partial f}{\partial t_1} = 1 \cdot \frac{\partial f}{\partial t_1} = 4$$

Deriving the basic rules





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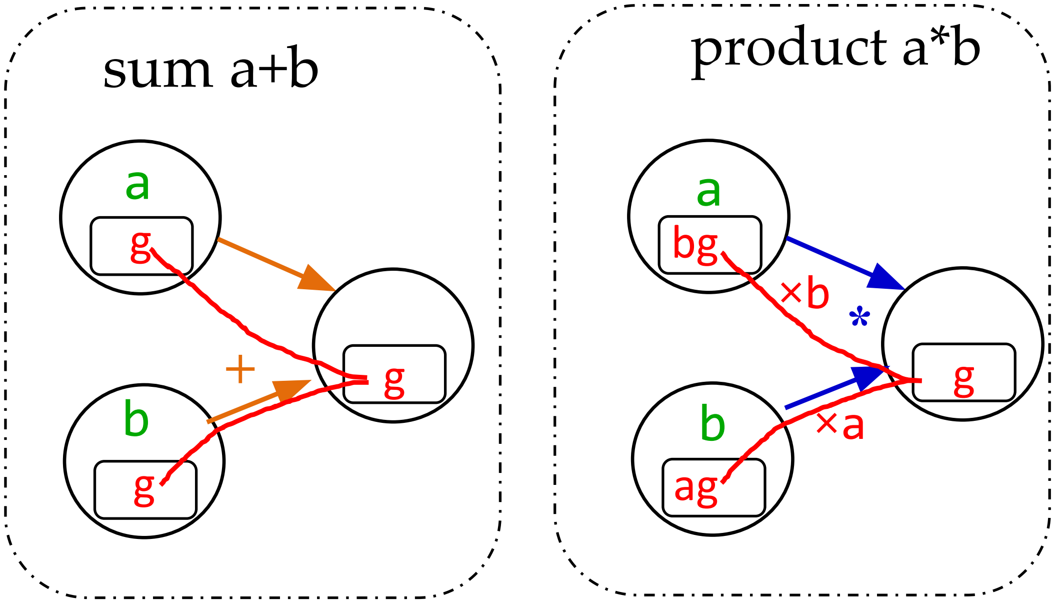
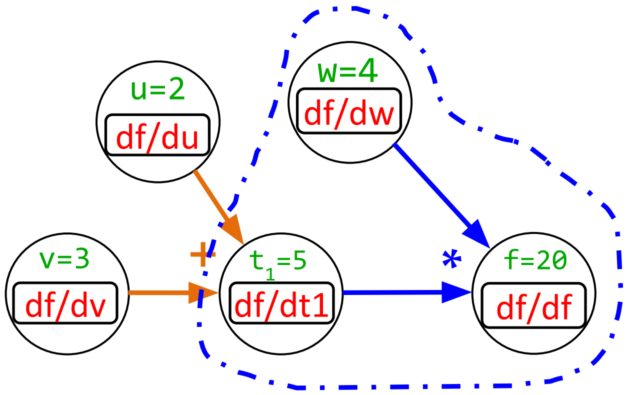
Deriving the basic rules





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$$\frac{\partial f}{\partial v} = \frac{\partial t_1}{\partial v}\frac{\partial f}{\partial t_1} = 1 \cdot \frac{\partial f}{\partial t_1} = 4$$

Derivative of activation functions and classical loss functions.

Derivative of loss functions.

Quadratic loss

$$L_{\text{quad}}(\hat{y}, y) = (\hat{y} - y)^2$$

$$\begin{aligned} L'_{\text{quad}}(\hat{y}, y) &= \frac{\partial L_{\text{quad}}(\hat{y}, y)}{\partial \hat{y}} \\ &= 2(\hat{y} - y) \end{aligned}$$

Derivative of loss functions.

Quadratic loss.

$$L_{\mathrm{quad}}(\hat{y}, y) = (\hat{y} - y)^2$$

$$\begin{aligned} L'_{\mathrm{quad}}(\hat{y}, y) &= \frac{\partial L_{\mathrm{quad}}(\hat{y}, y)}{\partial \hat{y}} \\ &= 2(\hat{y} - y) \end{aligned}$$

Negative log likelihood.

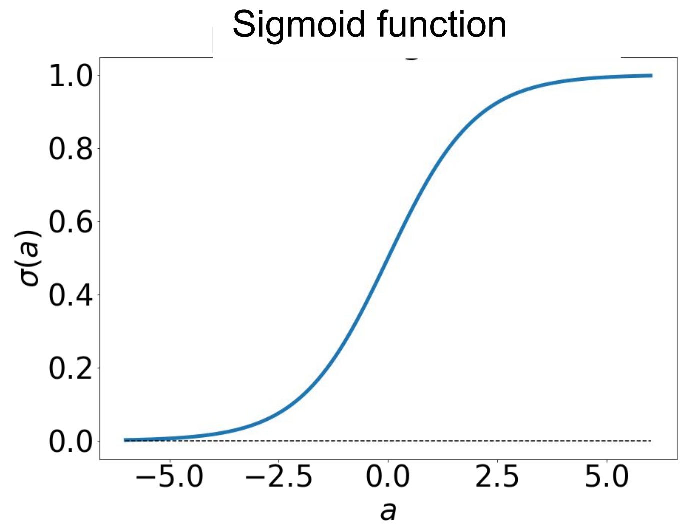
$$L_{\mathrm{nlv}}(\hat{y}, y) = -y \log(\hat{y}) - (1 - y) \log(1 - \hat{y})$$

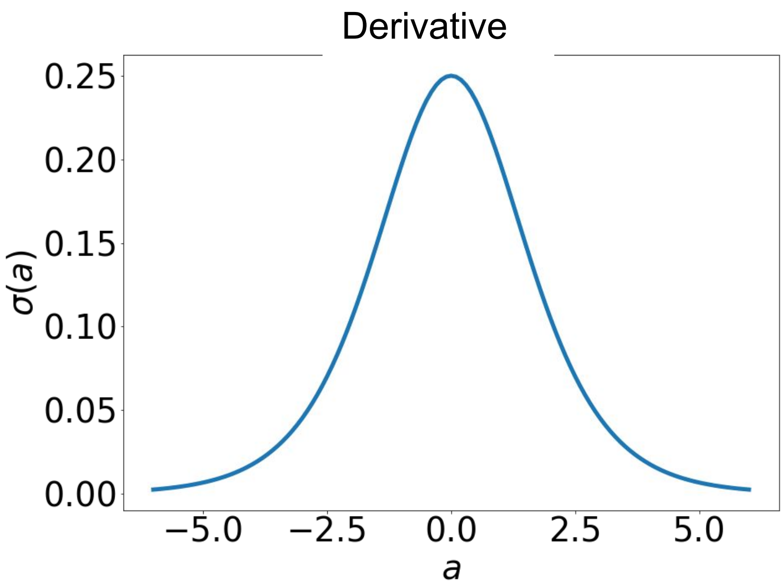
$$\begin{aligned} L'_{\mathrm{nlv}}(\hat{y}, y) &= \frac{\partial L_{\mathrm{nlv}}(\hat{y}, y)}{\partial \hat{y}} \\ &= -\frac{y}{\hat{y}} - \frac{1 - y}{1 - \hat{y}} \end{aligned}$$

Derivative of activation functions.

$$\sigma(a) = \frac{1}{1+e^{-a}}$$

$$\begin{aligned}
\sigma'(a) &= \frac{\partial}{\partial a}(1+e^{-a})^{-1} \\
&= -(1+e^{-a})^{-2}\,\frac{\partial}{\partial a}(1+e^{-a}) \\
&= -\frac{1}{(1+e^{-a})^2}\left[-\frac{\partial}{\partial a}e^{a}\right] \\
&= \frac{e^{a}}{(1+e^{-a})^2}
\end{aligned}$$





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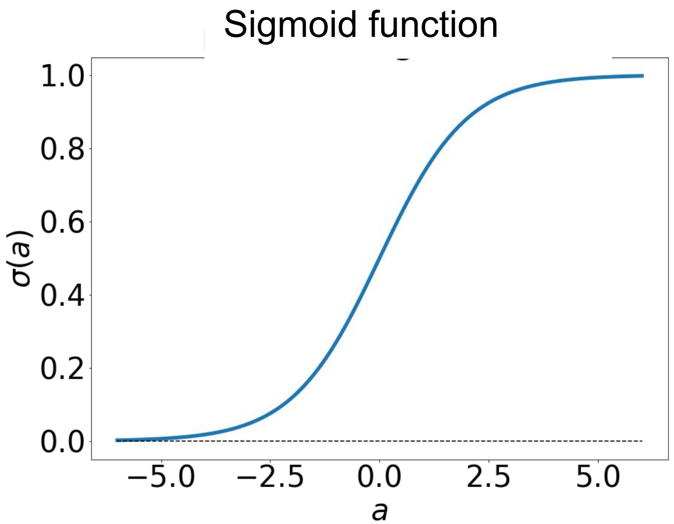
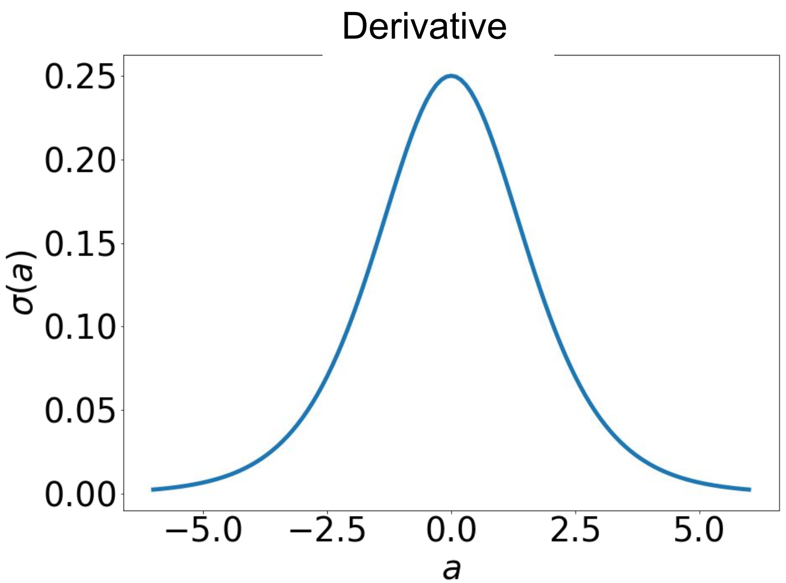
&= -(1+e^{-a})^{-2}\,\frac{\partial}{\partial a}(1+e^{-a}) \\
&= -\frac{1}{(1+e^{-a})^2}\left[-\frac{\partial}{\partial a}e^{a}\right] \\
&= \frac{e^{a}}{(1+e^{-a})^2} \\
&= \frac{1+e^{a}}{(1+e^{-a})^2} - \frac{1}{(1+e^{-a})^2} \\
&= \frac{1}{1+e^{-a}} - \left(\frac{1}{1+e^{-a}}\right)^2 \\
&= \sigma(a) - \Big(\sigma(a)\Big)^2 \\
&\boxed{= \sigma(a)\Big(1-\sigma(a)\Big)}
\end{aligned}$$

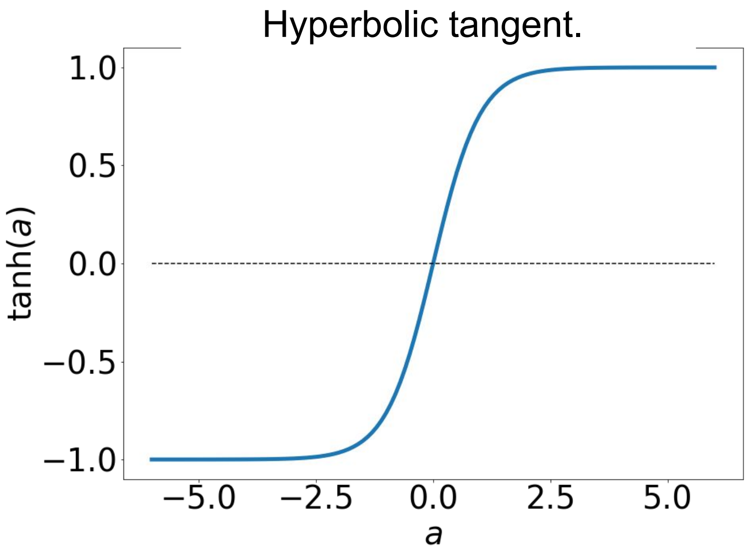


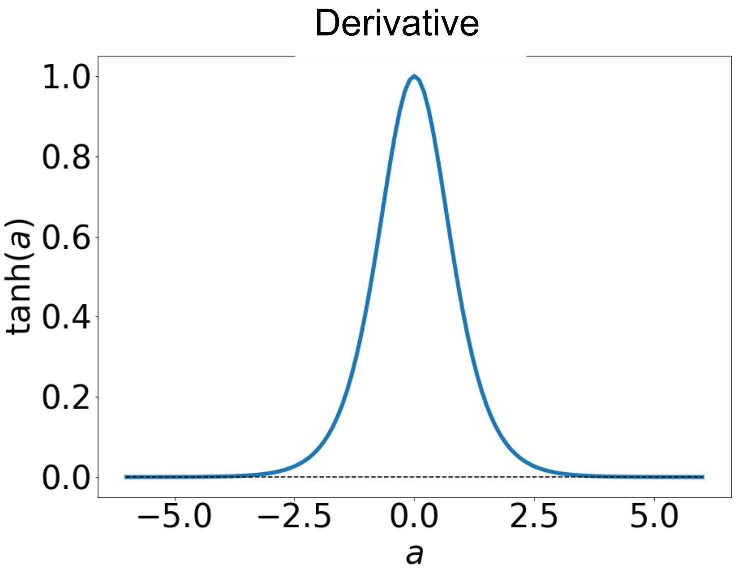


Derivative of activation functions.

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

$$\tanh'(a) = \frac{\partial \tanh(a)}{\partial a}$$
$$= 4\,\sigma'(2a)$$
$$= 1 - \Big(\tanh(a)\Big)^2$$





Derivative of activation functions.

$$\mathrm{relu}(a) = \max(0, a)$$

$$\mathrm{relu}'(a) = \frac{\partial\, \mathrm{relu}(a)}{\partial a} = \mathbb{1}_{a>0}$$