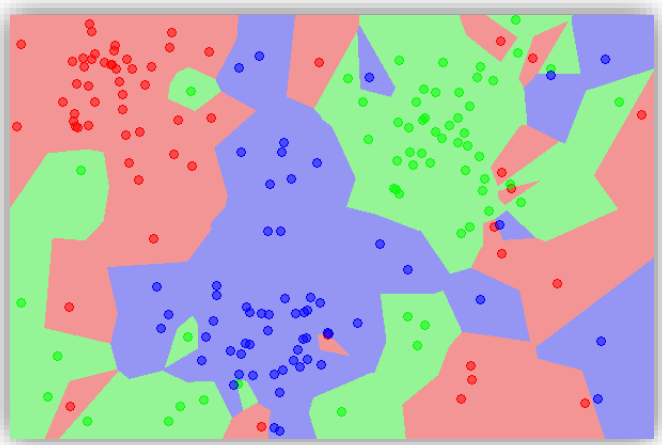
Pontificia Universidad Católica de Chile
Escuela de Ingeniería
Departamento de Ciencia de la Computación

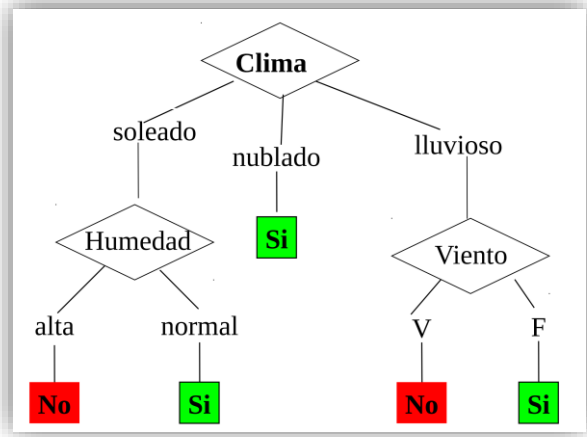
IIC2613 – Inteligencia Artificial

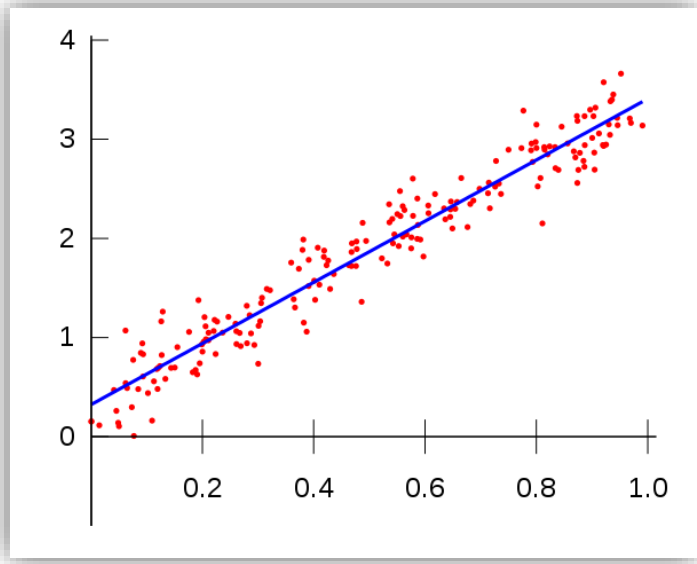
Redes Neuronales

Profesor: Hans Löbel

Reflexionemos un segundo con respecto a las técnicas que hemos visto hasta ahora







¿Cómo podríamos caracterizar las técnicas que hemos analizado hasta ahora?

(datos de entrada)

¿Qué es lo que estamos procesando?

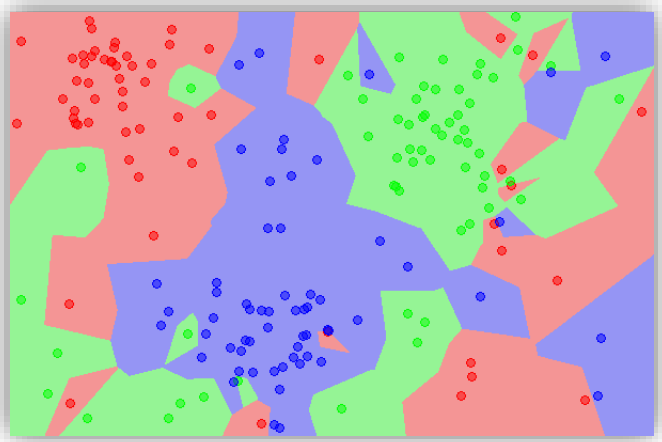
En la práctica, estamos usando características (*features*) de los datos

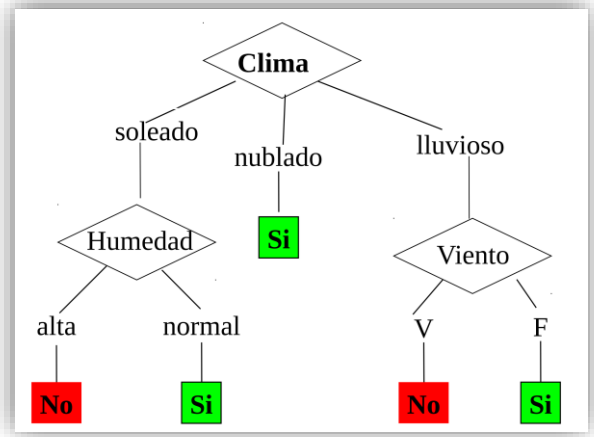
- Entradas seleccionadas tienen que ver más con el conocimiento experto que tengamos (o no) del problema.

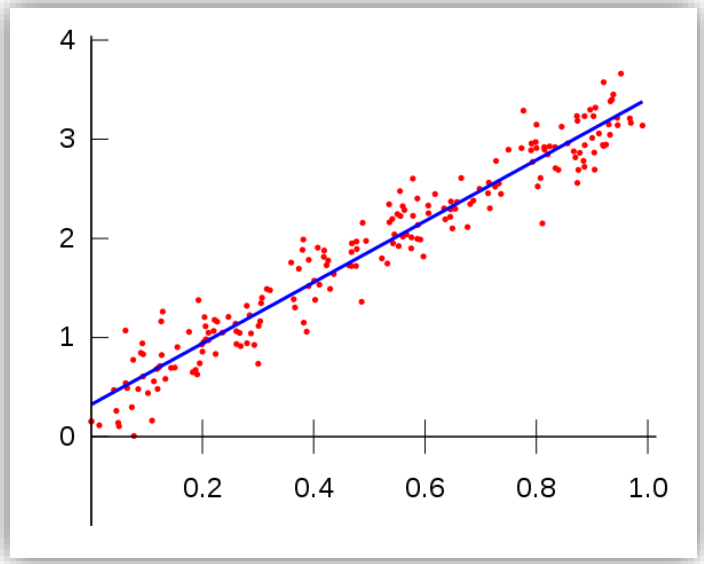
- Esto no es ideal por dos razones principales:
  i. un experto es caro
  ii. nada asegura que este conocimiento sea el mejor.

- ¿Qué es lo que realmente están aprendiendo estos algoritmo?

¿Qué es lo que realmente están aprendiendo estos algoritmos?





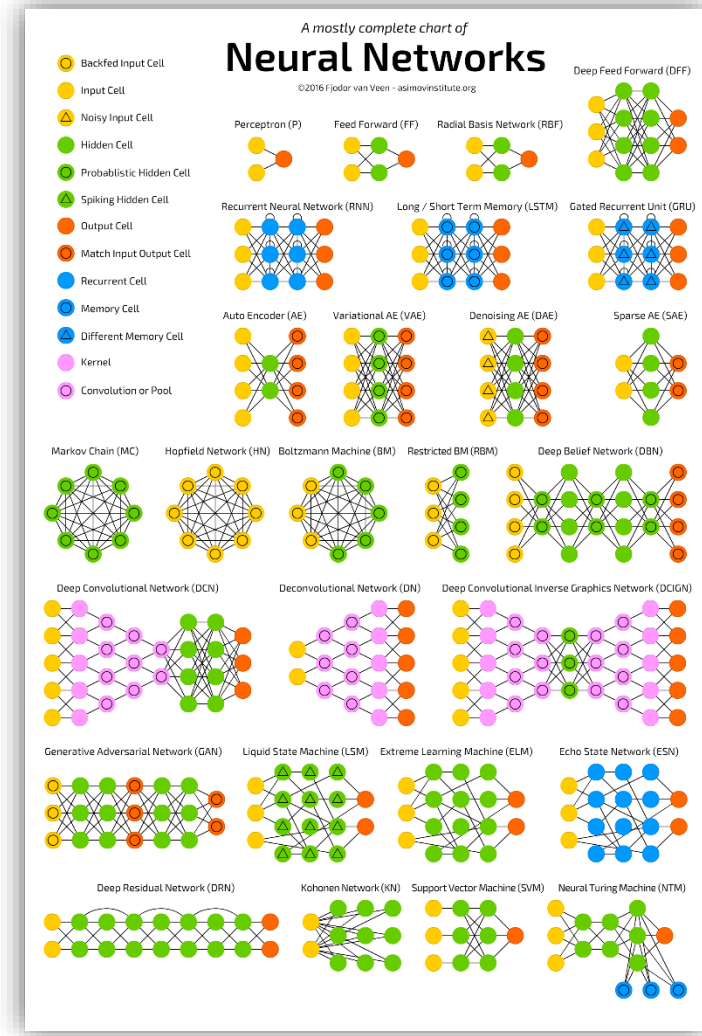


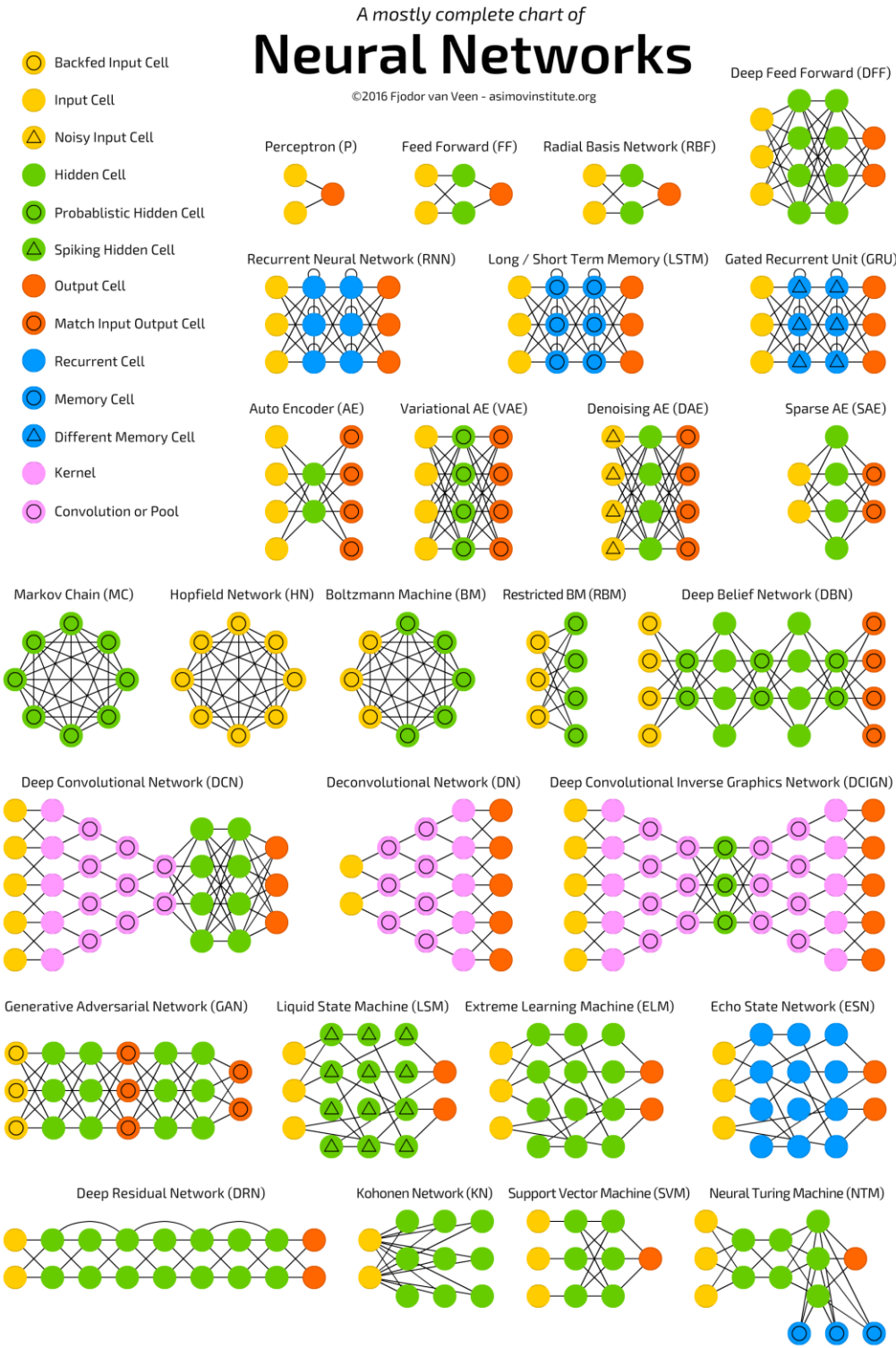
En resumen, hasta ahora no estamos “realmente” aprendiendo de los datos, sólo como separarlos (features)

Necesitamos un mecanismo de aprendizaje, suficientemente general, para aprender aspectos complejos y desconocidos

Redes neuronales son capaces de aprender distintas capas de representaciones de datos

- Método altamente práctico y general para aprender funciones continuas y discretas.
- Brillan en la presencia de grandes volúmenes de datos.
- Existen redes para prácticamente cualquier problema.
- Difíciles de entrenar, interpretabilidad es compleja (caja negra) y sufren de serios problemas de sobreajuste.




A mostly complete chart of
Neural Networks
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Backfed Input Cell
Input Cell
Noisy Input Cell
Hidden Cell
Probablistic Hidden Cell
Spiking Hidden Cell
Output Cell
Match Input Output Cell
Recurrent Cell
Memory Cell
Different Memory Cell
Kernel
Convolution or Pool
Perceptron (P)
Feed Forward (FF)
Radial Basis Network (RBF)
Deep Feed Forward (DFF)
Recurrent Neural Network (RNN)
Long / Short Term Memory (LSTM)
Gated Recurrent Unit (GRU)
Auto Encoder (AE)
Variational AE (VAE)
Denoising AE (DAE)
Sparse AE (SAE)
Markov Chain (MC)
Hopfield Network (HN)
Boltzmann Machine (BM)
Restricted BM (RBM)
Deep Belief Network (DBN)
Deep Convolutional Network (DCN)
Deconvolutional Network (DN)
Deep Convolutional Inverse Graphics Network (DCIGN)
Generative Adversarial Network (GAN)
Liquid State Machine (LSM)
Extreme Learning Machine (ELM)
Echo State Network (ESN)
Deep Residual Network (DRN)
Kohonen Network (KN)
Support Vector Machine (SVM)
Neural Turing Machine (NTM)

A mostly complete chart of

Neural Networks

- Backfed Input Cell
- Input Cell
- Noisy Input Cell
- Hidden Cell
- Probablistic Hidden Cell
- Spiking Hidden Cell
- Output Cell
- Match Input Output Cell
- Recurrent Cell
- Memory Cell
- Different Memory Cell
- Kernel
- Convolution or Pool

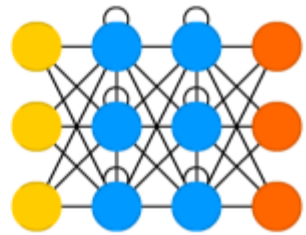
Perceptron (P)

Feed Forward (FF)

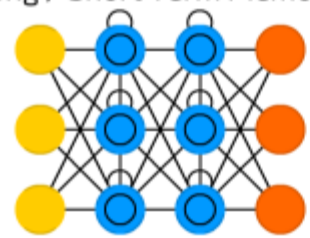
Radial Basis Network (RBF)

Deep Feed Forward (DFF)

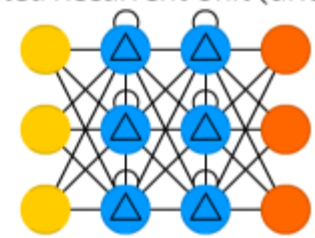
Recurrent Neural Network (RNN)



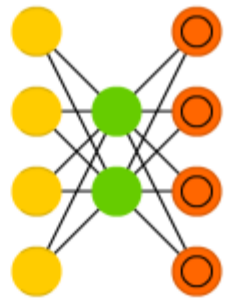
Long / Short Term Memory (LSTM)



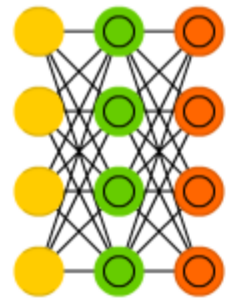
Gated Recurrent Unit (GRU)



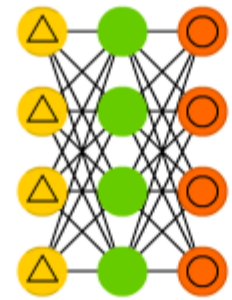
Auto Encoder (AE)



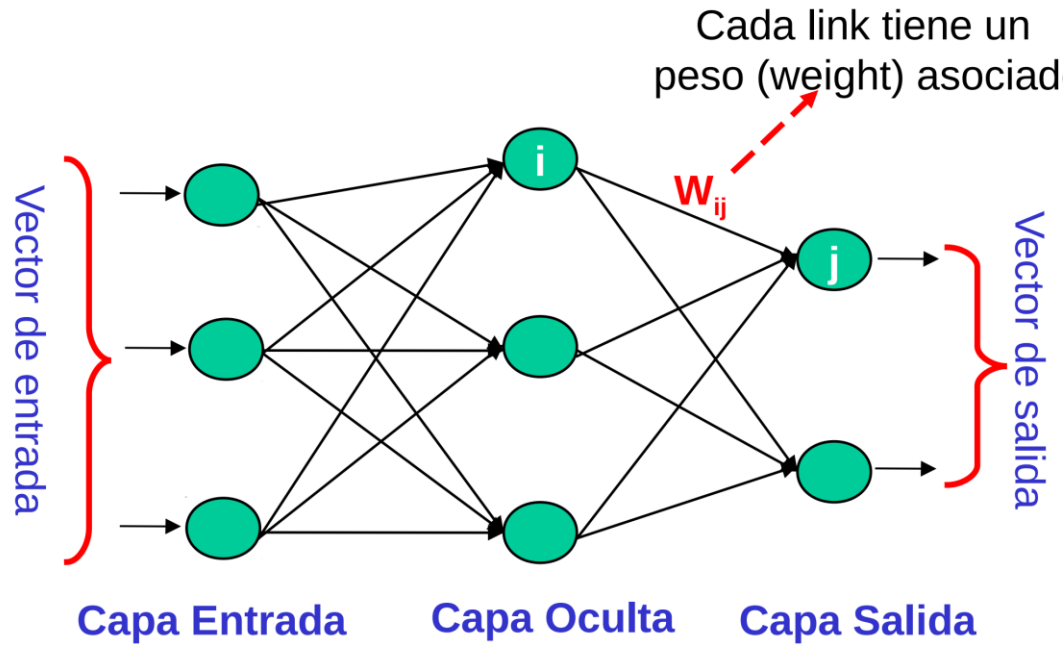
Variational AE (VAE)



Denoising AE (DAE)



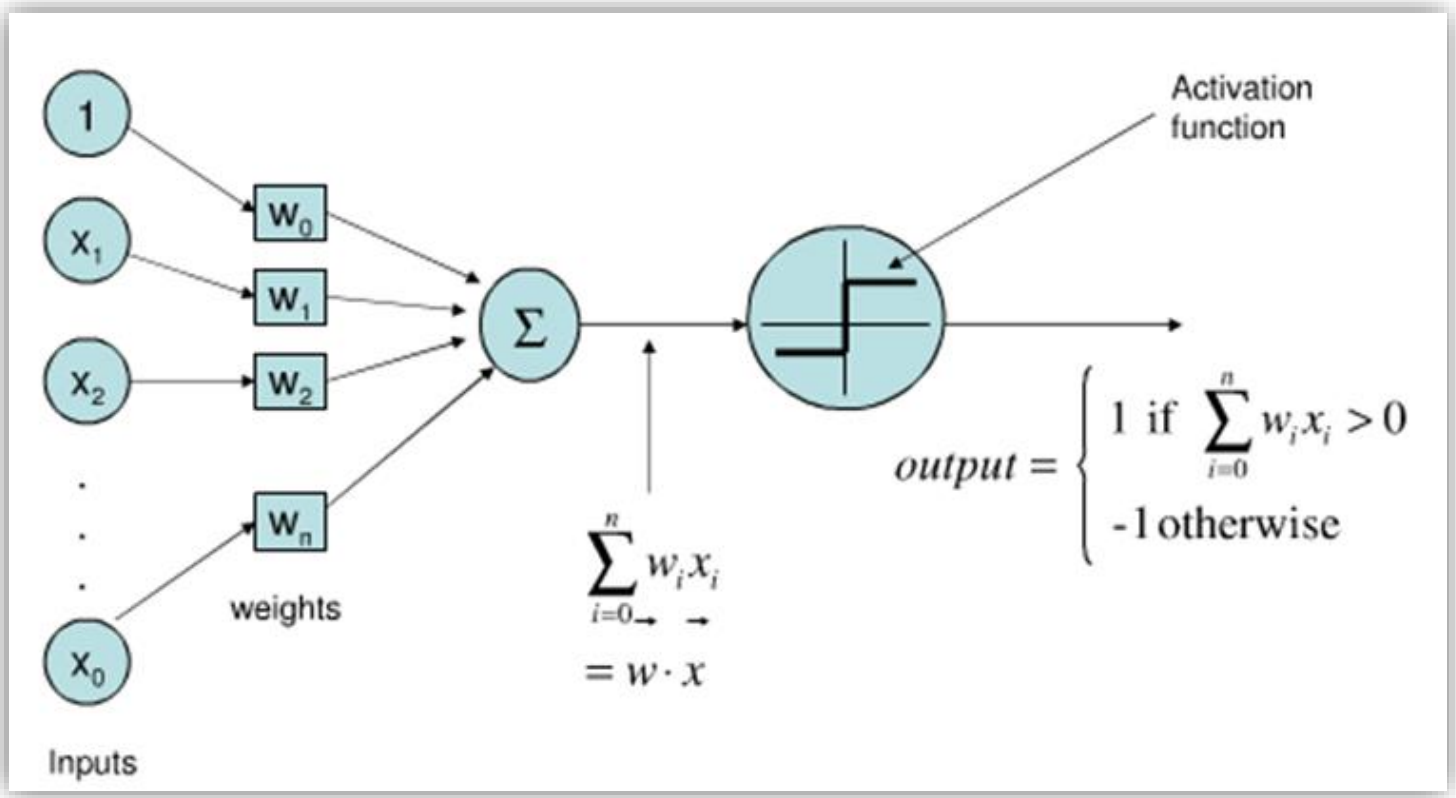
Sparse AE (SAE)



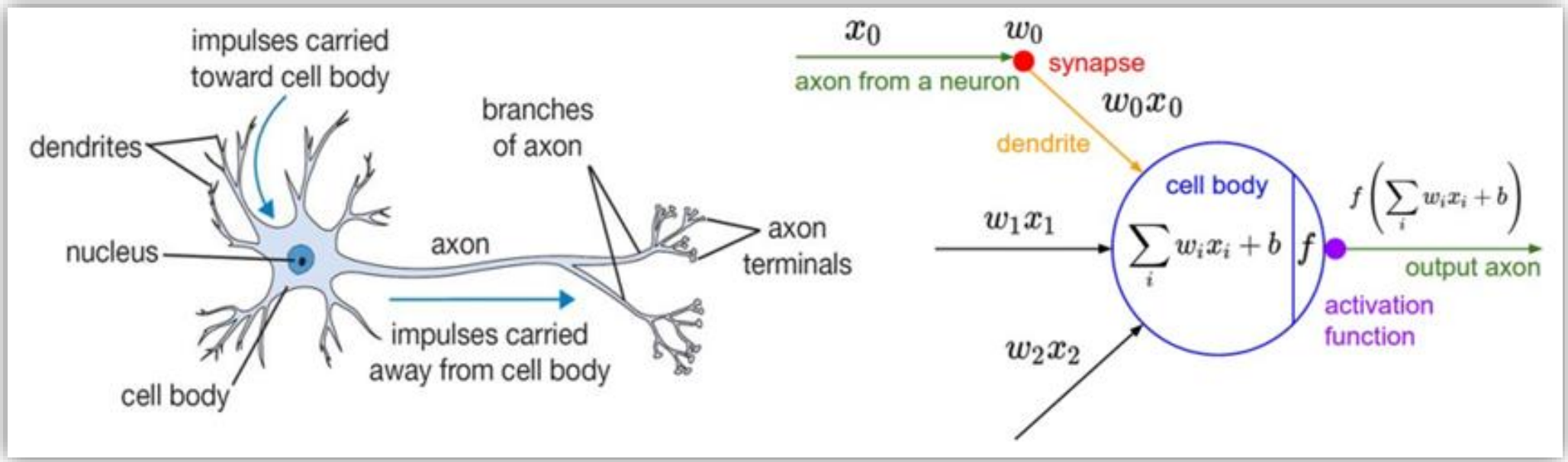
Una ANN es caracterizada por:

1. Estructura de la red, i.e., número de unidades (neuronas en cada) en cada capa y número de capas ocultas.
2. Método para determinar el valor de los pesos W_{ij} que conectan a una neurona i con una neurona j.
3. Función de activación que modula el impulso que envía una neurona a otra.

La unidad fundamental de una red neuronal se conoce como perceptrón

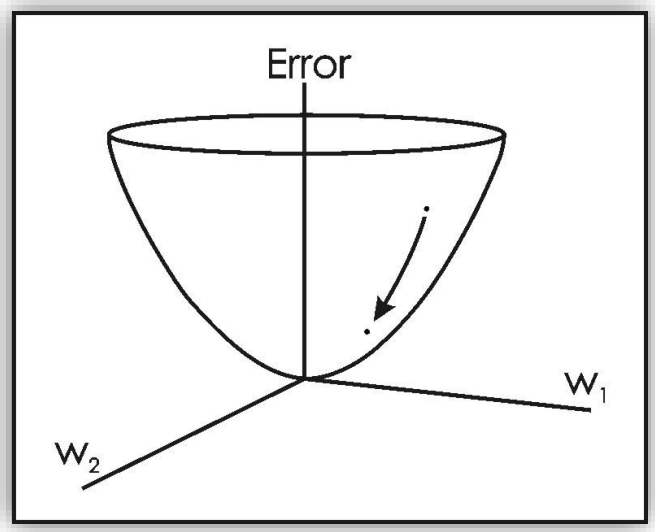



1958 Perceptron


impulses carried
toward cell body
dendrites
branches
of axon
nucleus
axon
axon
terminals
impulses carried
away from cell body
cell body
x_0
w_0
synapse
axon from a neuron
$w_0 x_0$
dendrite
cell body
$w_1 x_1$
$\sum_i w_i x_i + b$
f
$f\left(\sum_i w_i x_i + b\right)$
output axon
activation
function
$w_2 x_2$

¿Cómo podemos entrenar un perceptrón (lineal)?

1. ¿Qué es lo que queremos hacer?
2. ¿Cuál podría ser una buena función objetivo para el problema?
3. ¿Qué características tiene esta función objetivo?
4. ¿Qué algoritmo de optimización podemos utilizar para este problema?



El algoritmo de entrenamiento de un perceptrón lineal es bastante intuitivo

- Inicializar cada peso w_i a un valor aleatorio pequeño (ej. rango [0,1])
- **do**
  - Inicializar gradientes Δw_i a cero
  - **for** (x,y)en set de entrenamiento
    - Aplique (x,y)a perceptron y obtenga salida **out**
    - Para cada peso calcule gradiente y guarde en acumulador:

$$\Delta w_i \leftarrow \Delta w_i + \eta(y - \textbf{out})\, x_i$$

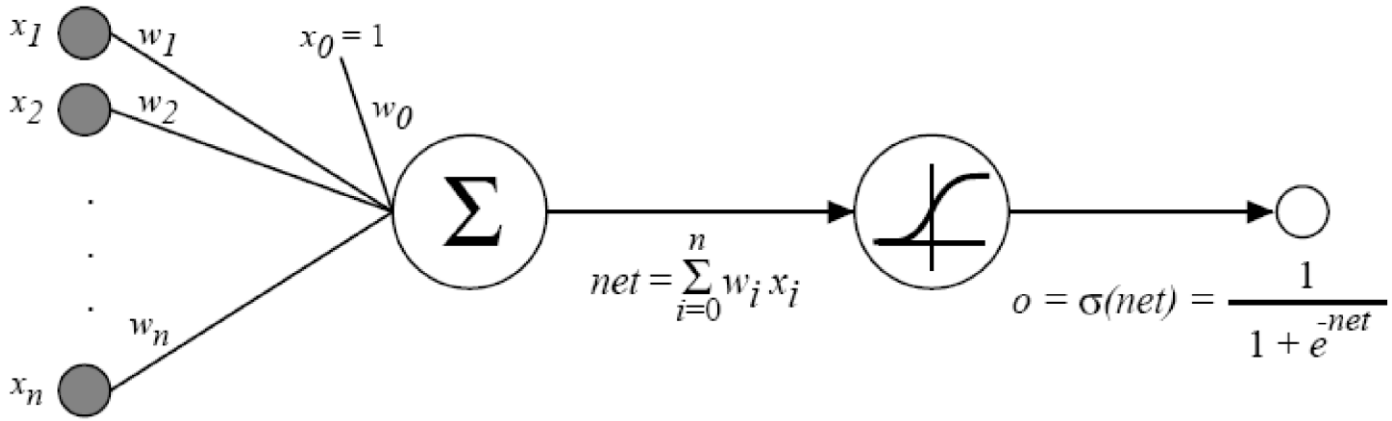
  end for

  - Actualice valor de cada peso:

$$w_i^{new} = w_i^{old} + \Delta w_i$$

- **while** (condición de término ! = TRUE).

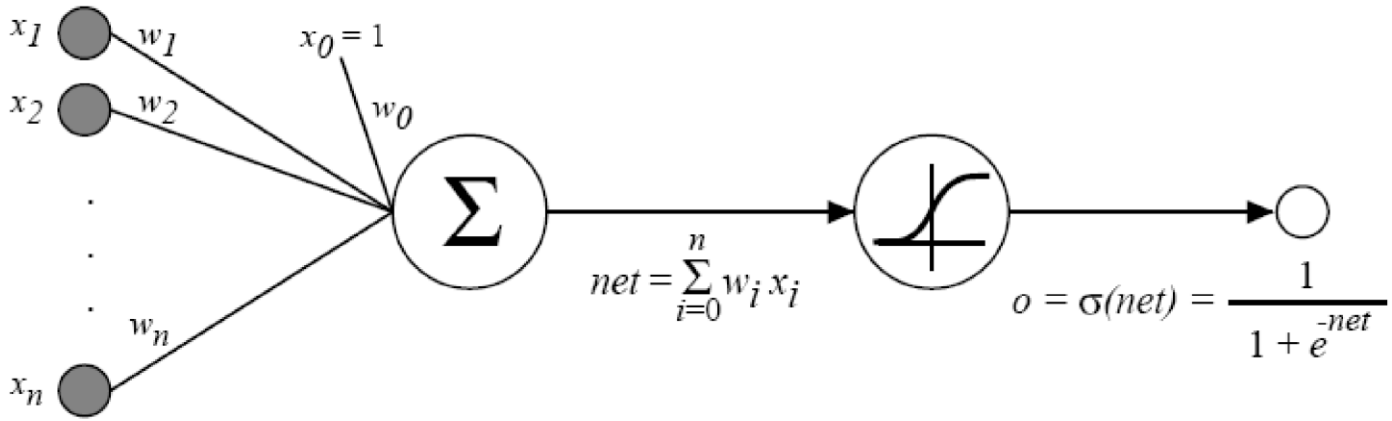
¿Cómo quedaría entonces la regla para un perceptrón sigmoidal?



Regla de entrenamiento

$$\Delta \vec{w} = -\eta \nabla E[\vec{w}]$$

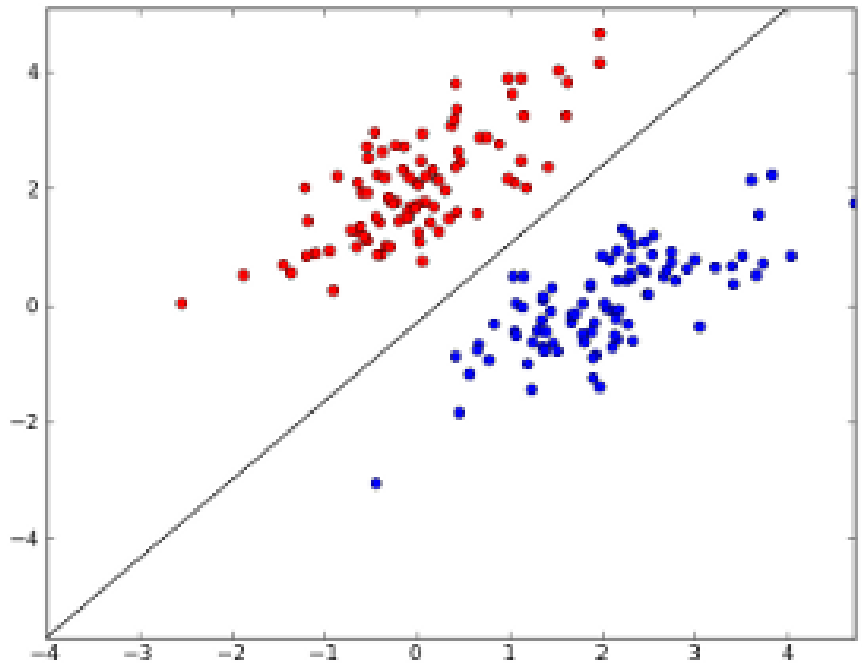
¿Cómo quedaría entonces la regla para un perceptrón sigmoidal?

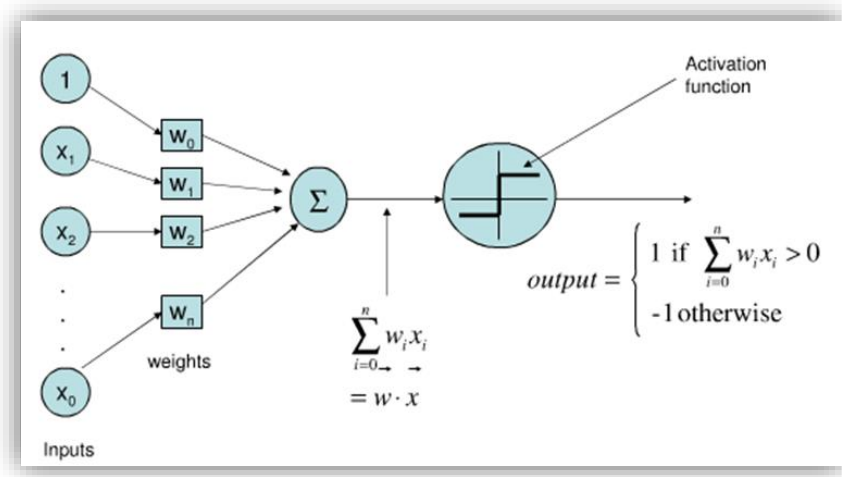


Regla de entrenamiento

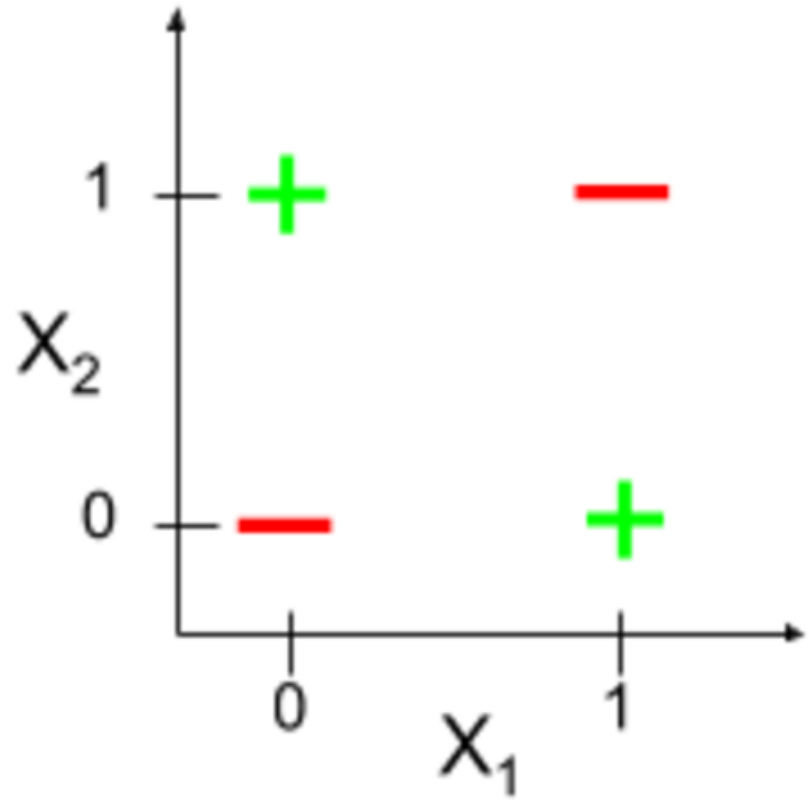
$$\Delta \vec{w} = -\eta \nabla E[\vec{w}]$$

$$\frac{\partial E}{\partial w_i} = -\sum_{d \in D} (t_d - o_d) o_d (1 - o_d) x_{i,d}$$



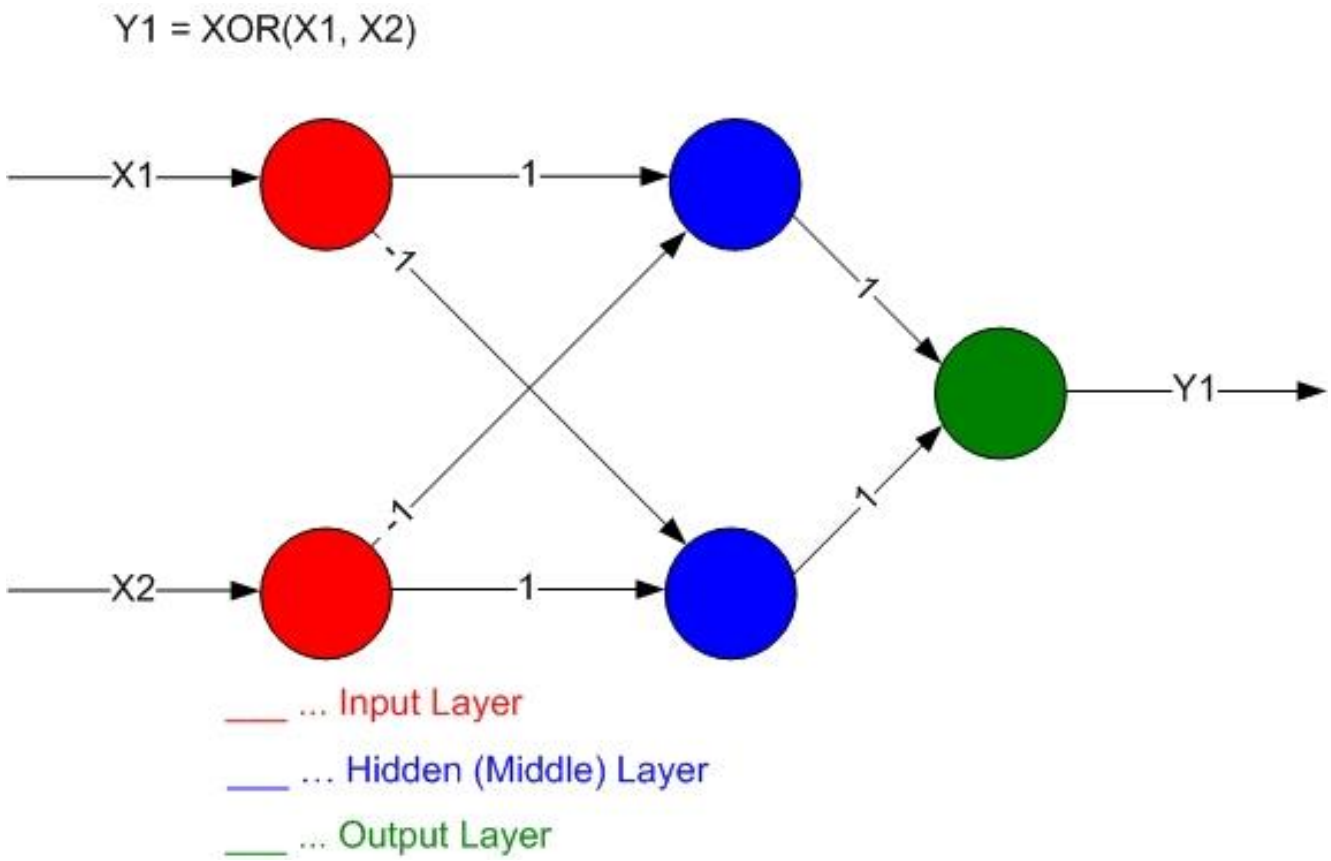


Perceptrón puede clasificar problemas linealmente separables

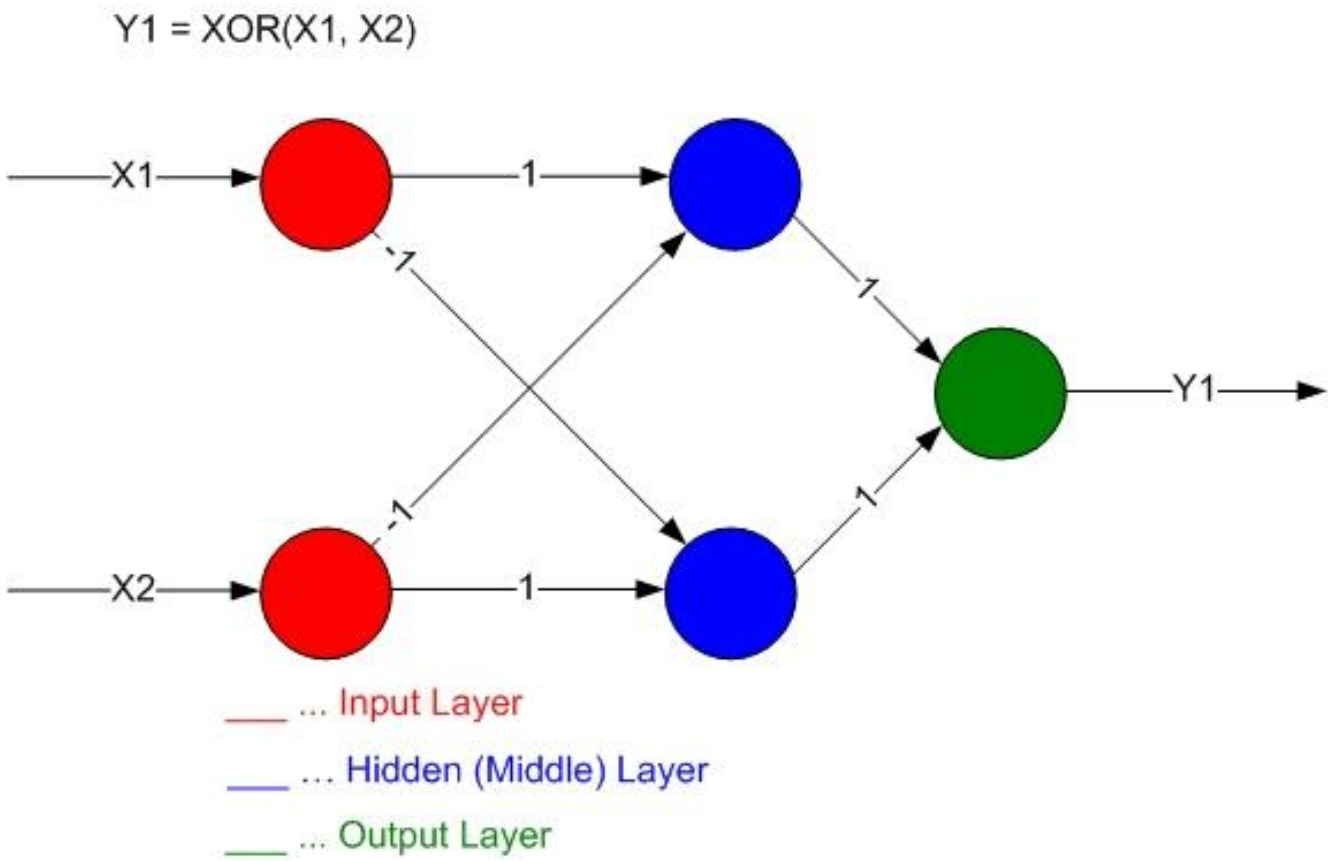


¿Cómo podríamos extender al perceptrón, para que sea capaz de resolver este tipo de problemas (no linealmente separables)?


1958 Perceptron
1969
Perceptron criticized



Al agregar una nueva capa (oculta), podemos representar conceptos intermedios entre el input y el output.



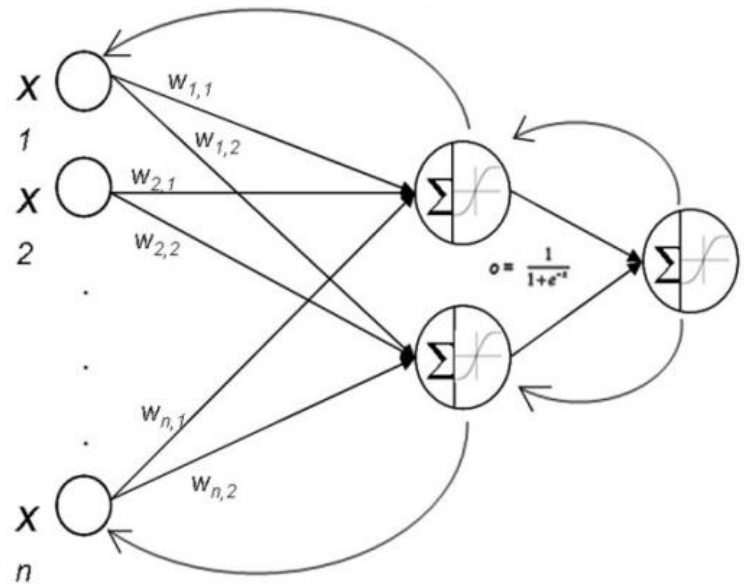
¿Cómo podemos aprender estos nuevos conceptos de nivel intermedios?


1958 Perceptron
1969
Perceptron criticized

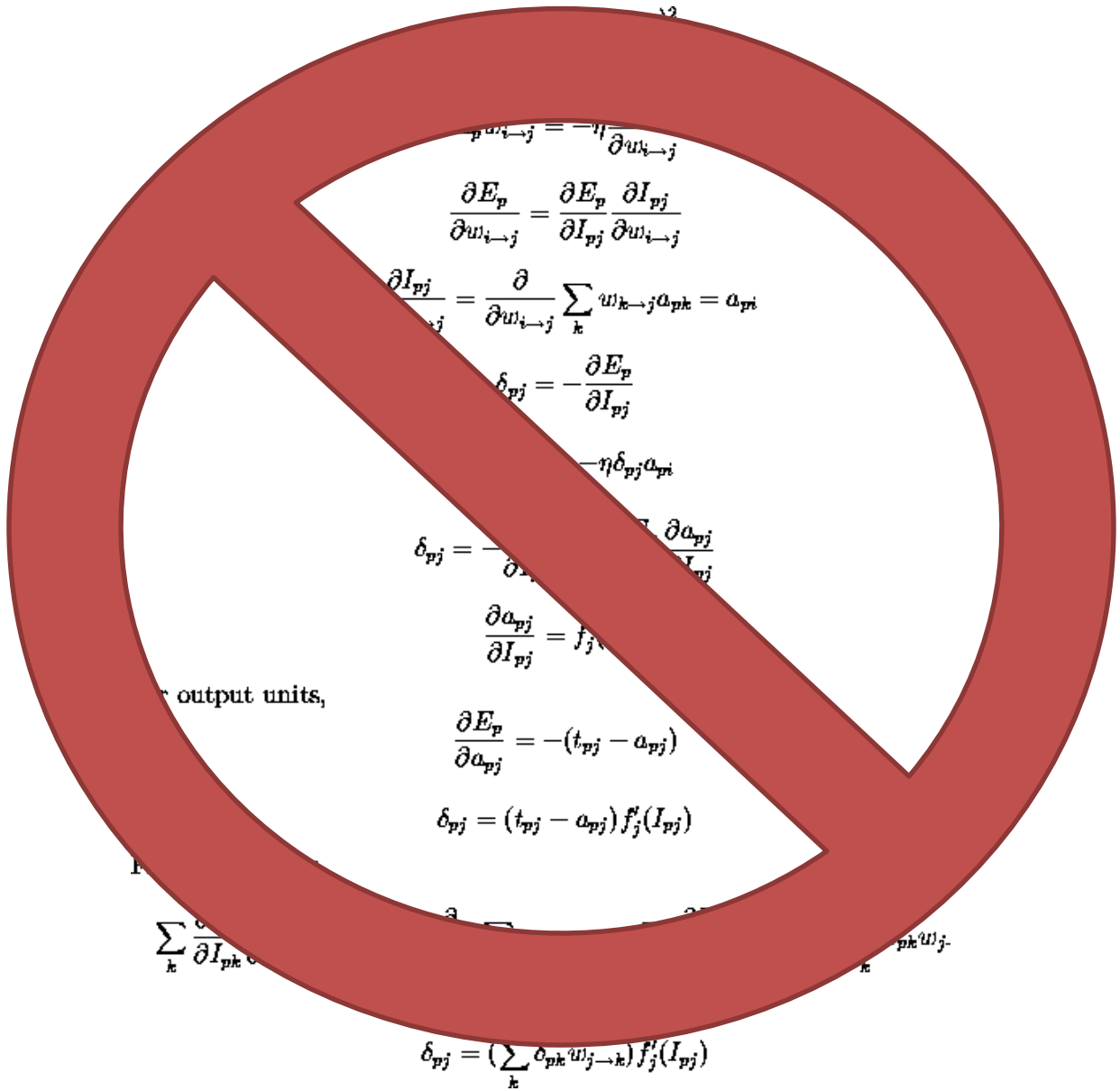

1958 Perceptron
1974 Backpropagation
1969
Perceptron criticized

Backpropagation permite propagar la *señal* del error a todos los nodos de una red para ajustarlos

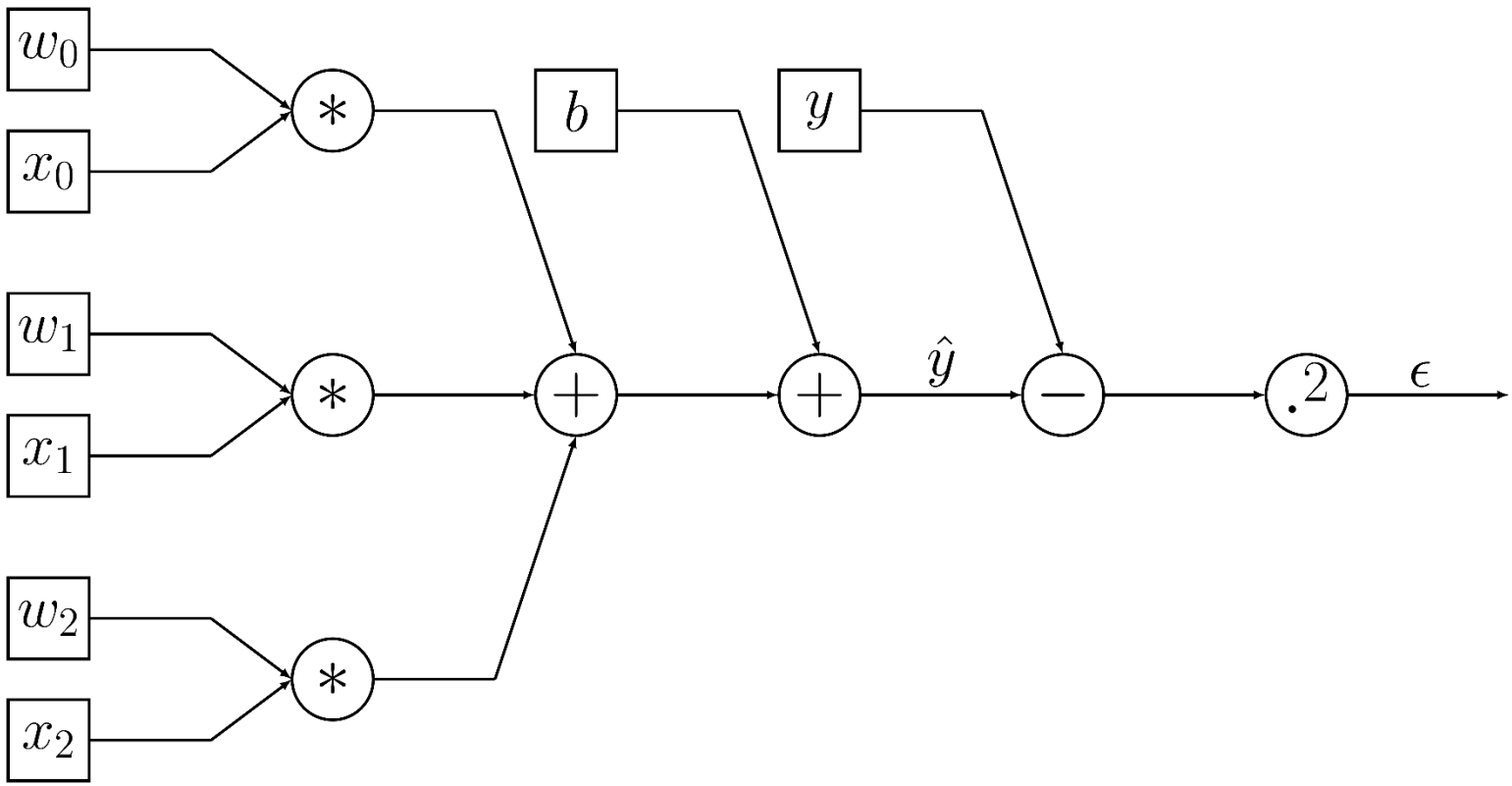
- No es otra cosa que la aplicación recursiva de la regla de la cadena.
- En conjunto con el método del descenso del gradiente, permite entrenar redes de profundidad arbitraria (pero no necesariamente con buen rendimiento).
- Aplicable a cualquier tipo de red y función diferenciable.
- Existen infinitos detalles en su ejecución, que hacen que la probabilidad de fracaso sea muy alta.



En este curso analizaremos backpropagation desde el punto de vista de los grafos de cómputo

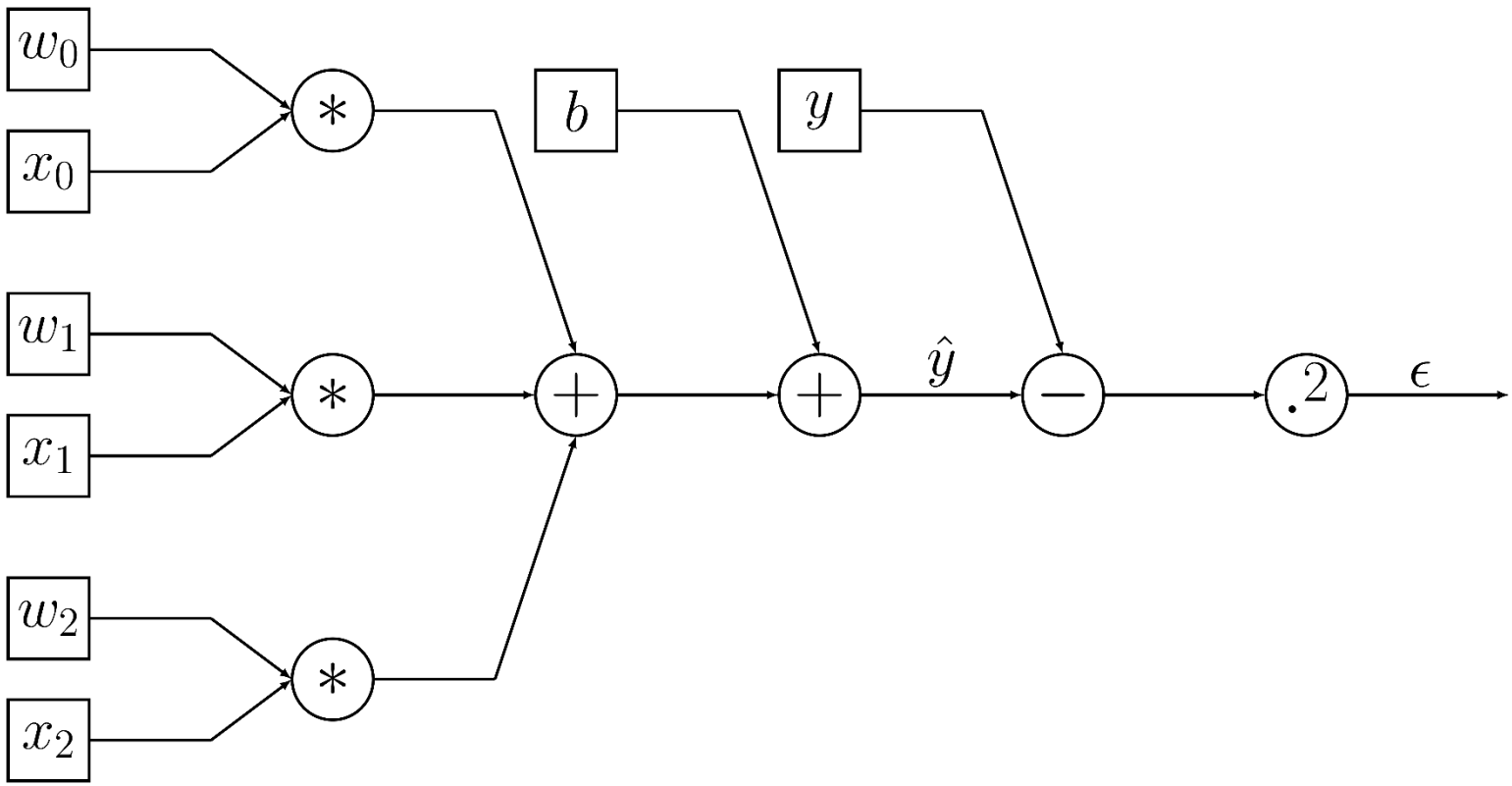


Un grafo de cómputo representa todas las operaciones realizadas hasta llegar al output

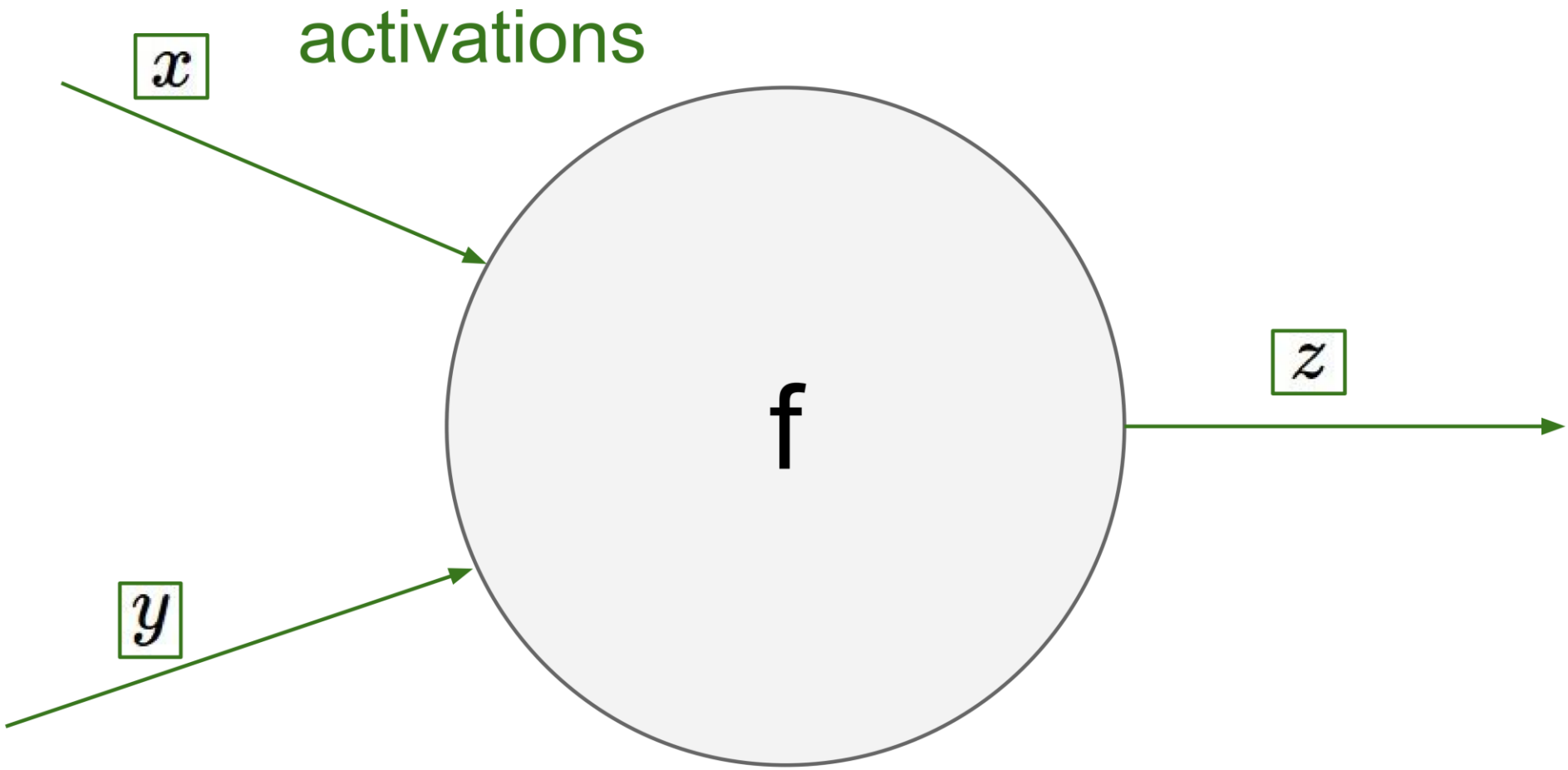


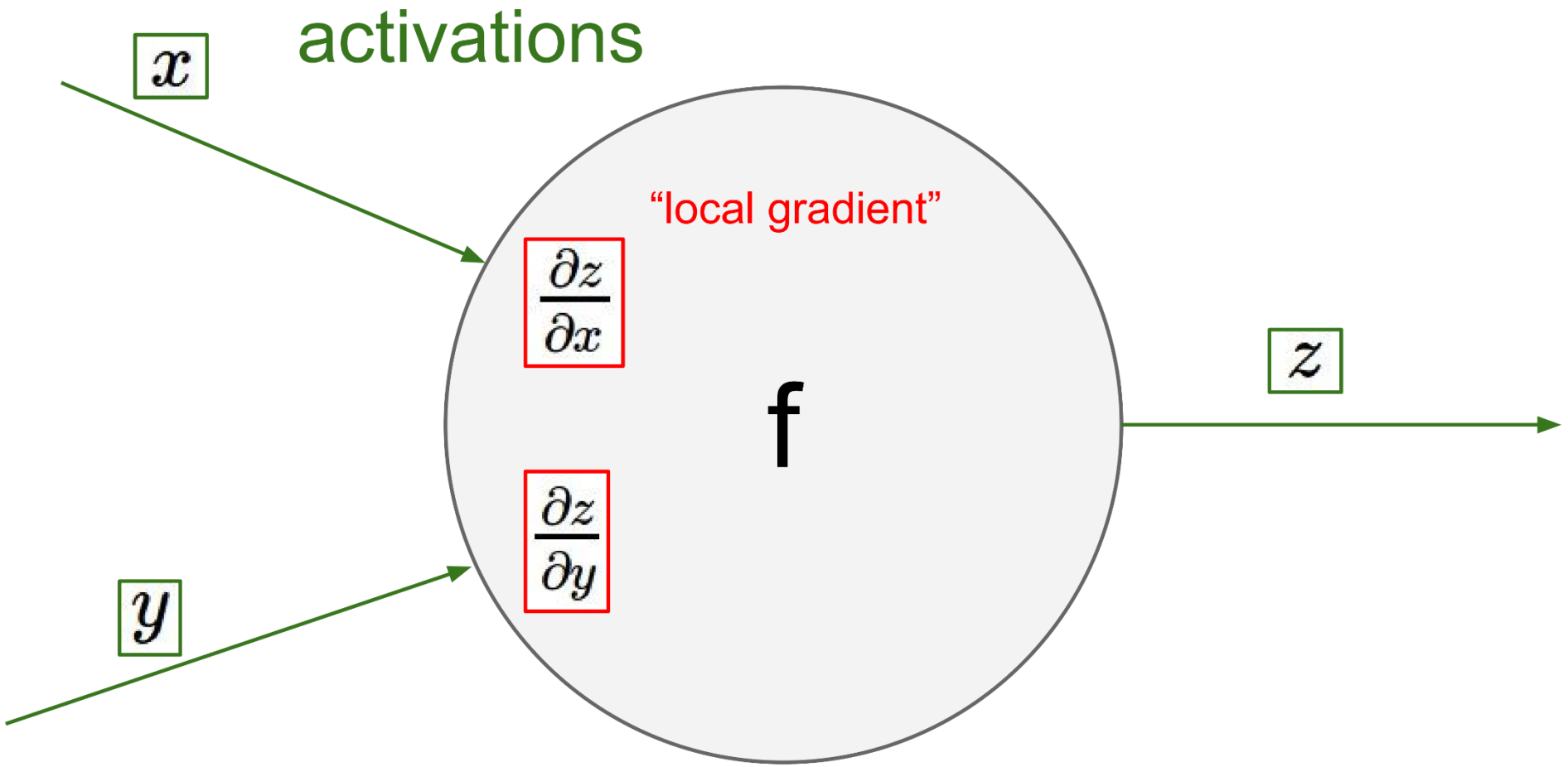
¿Qué función representa este grafo?

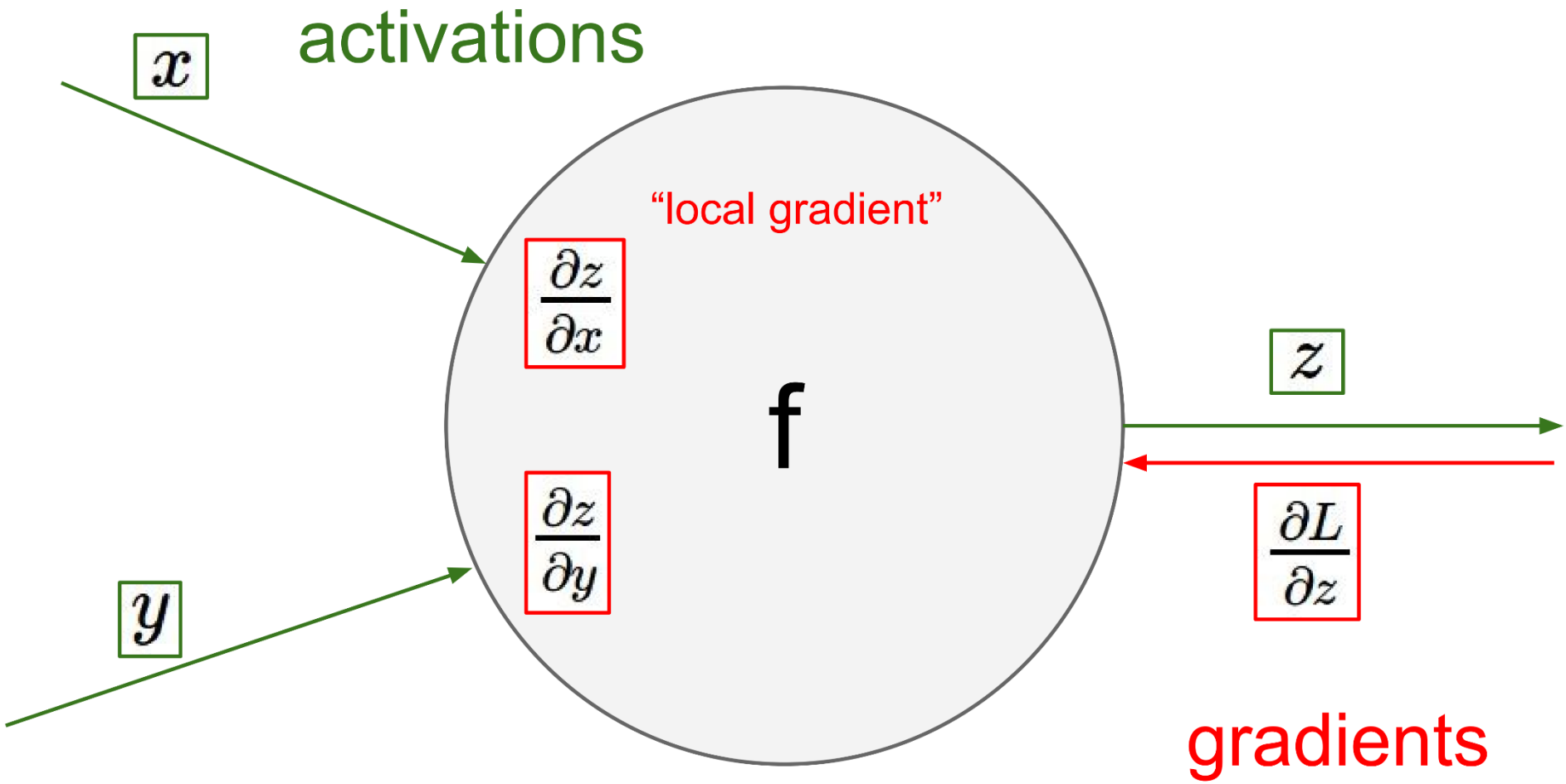
Podemos aprovechar esta estructura junto con la regla de la cadena, para obtener el gradiente completo

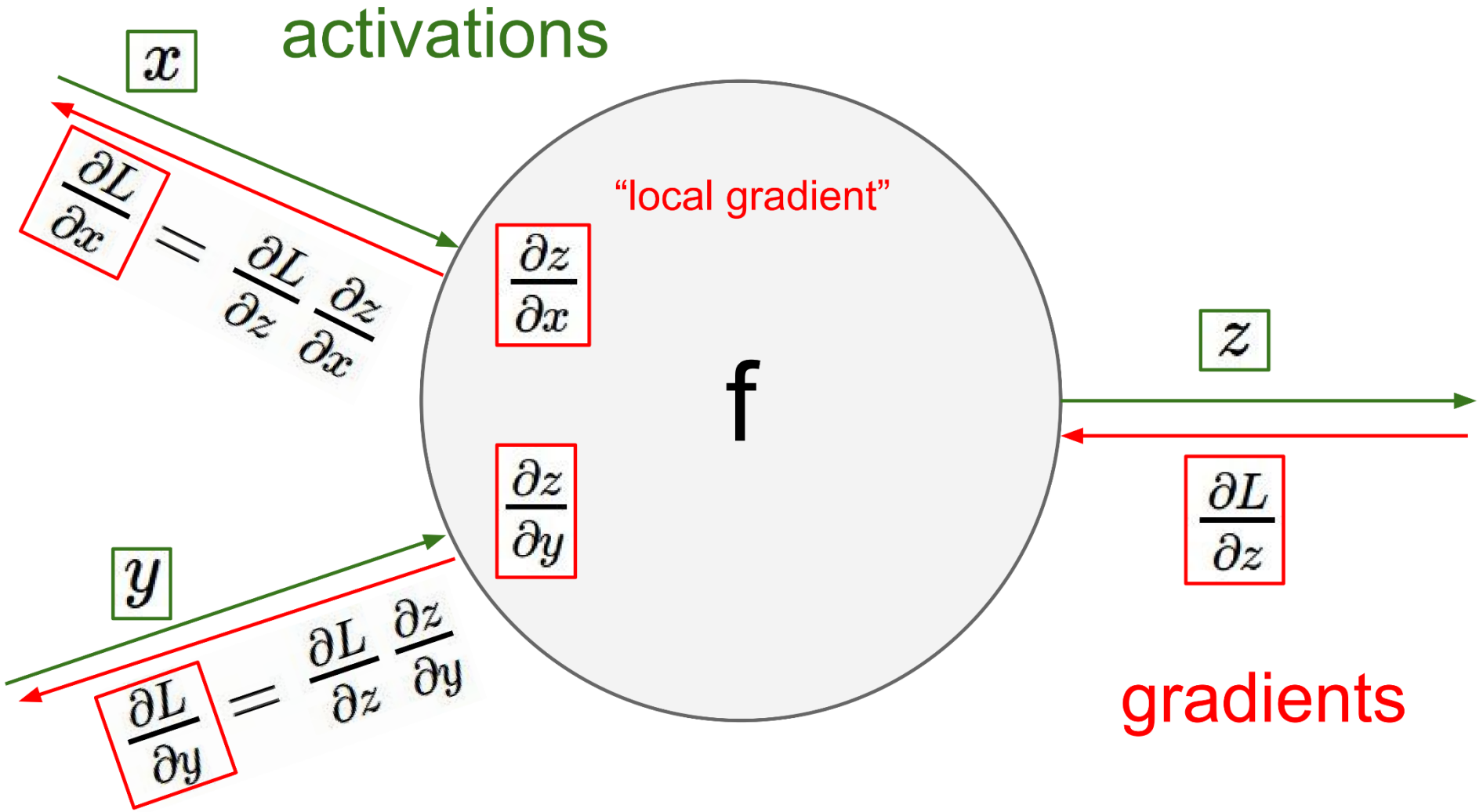


Basta con que sólo analicemos las derivadas locales

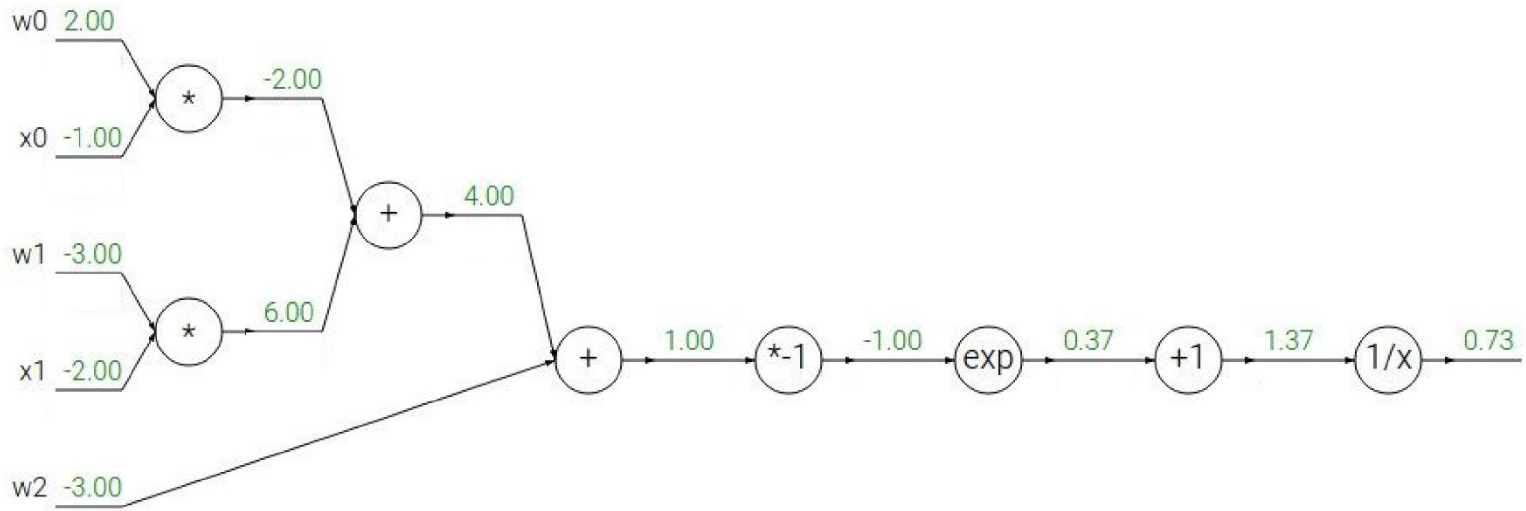



activations
x
y
z
f
"local gradient"
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$


activations
x
y
"local gradient"
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
f
z
$\frac{\partial L}{\partial z}$
gradients


activations
x
y
z
f
"local gradient"
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial y}$
$\frac{\partial L}{\partial z}$
gradients

Another example: $$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



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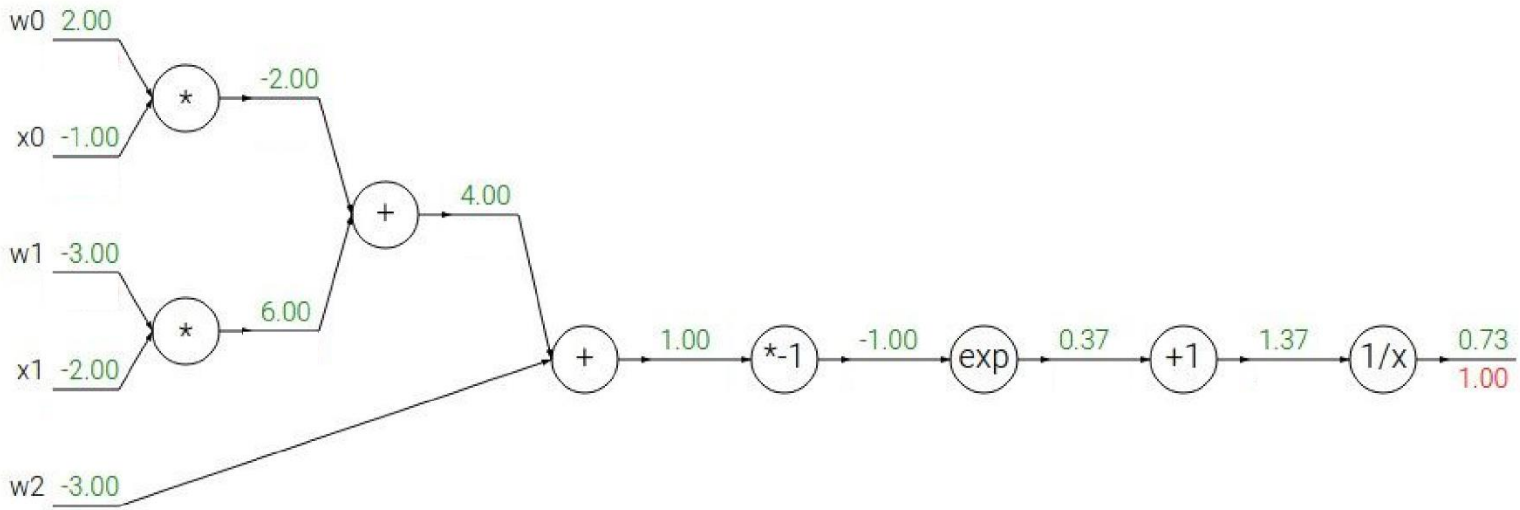


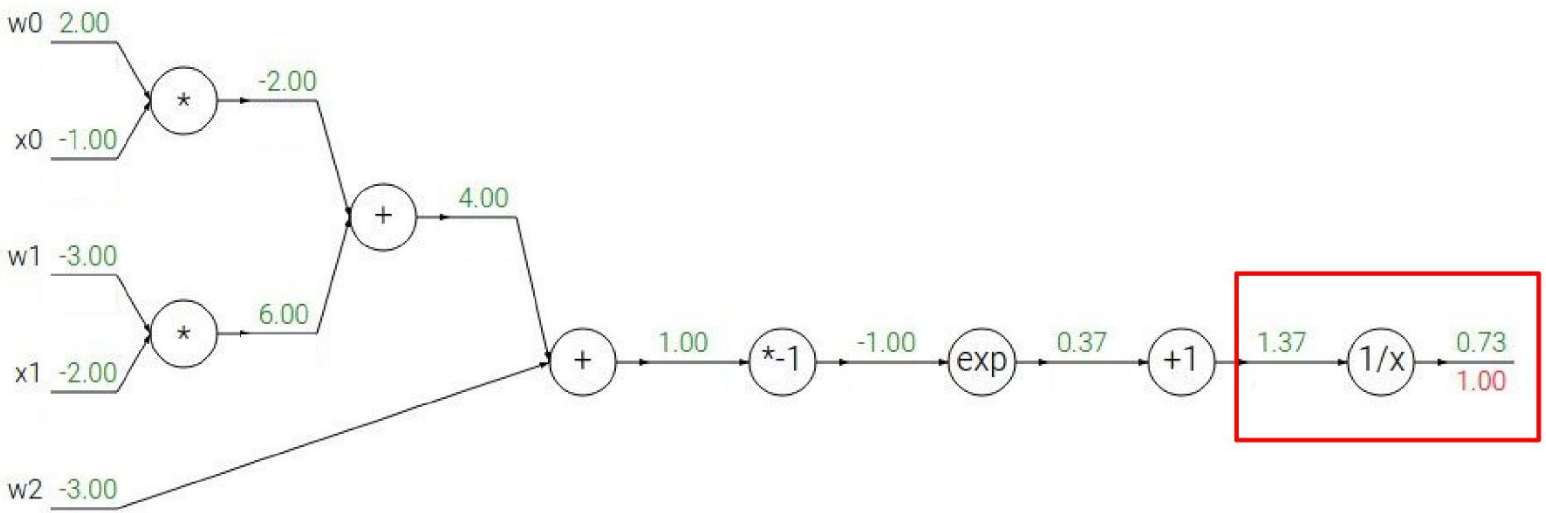
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

Another example: $$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



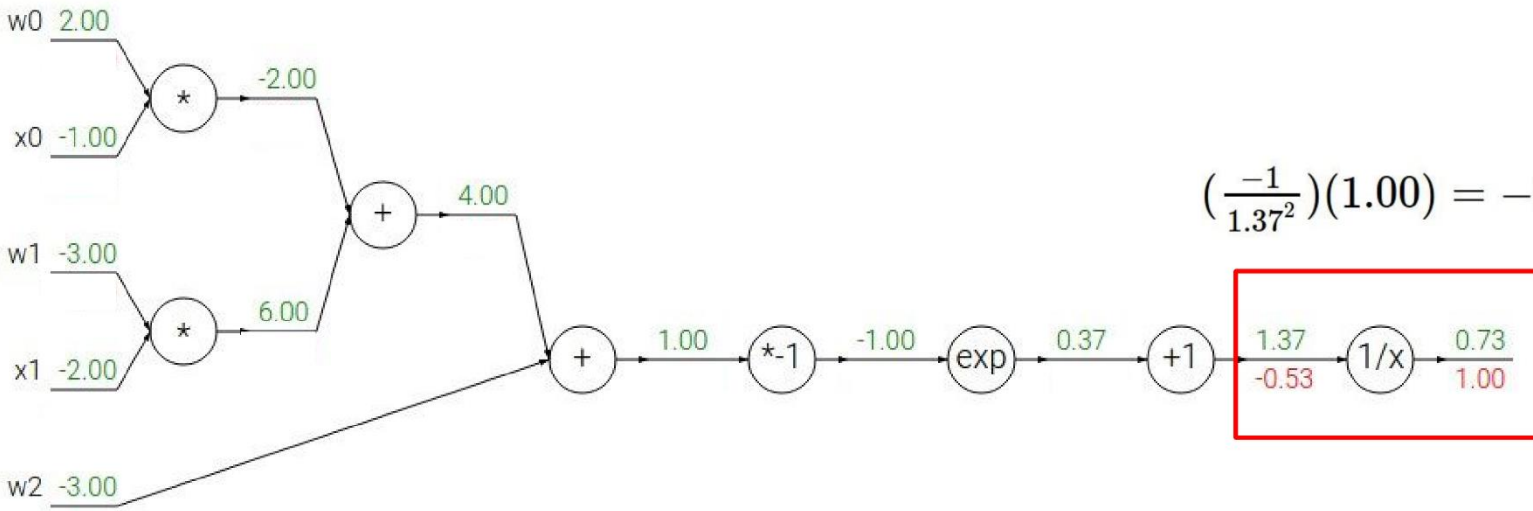
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

Another example: $$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



$$(\frac{-1}{1.37^2})(1.00) = -0.53$$

$$f(x) = e^x \rightarrow \frac{df}{dx} = e^x$$

$$f_a(x) = ax \rightarrow \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \rightarrow \frac{df}{dx} = -1/x^2$$

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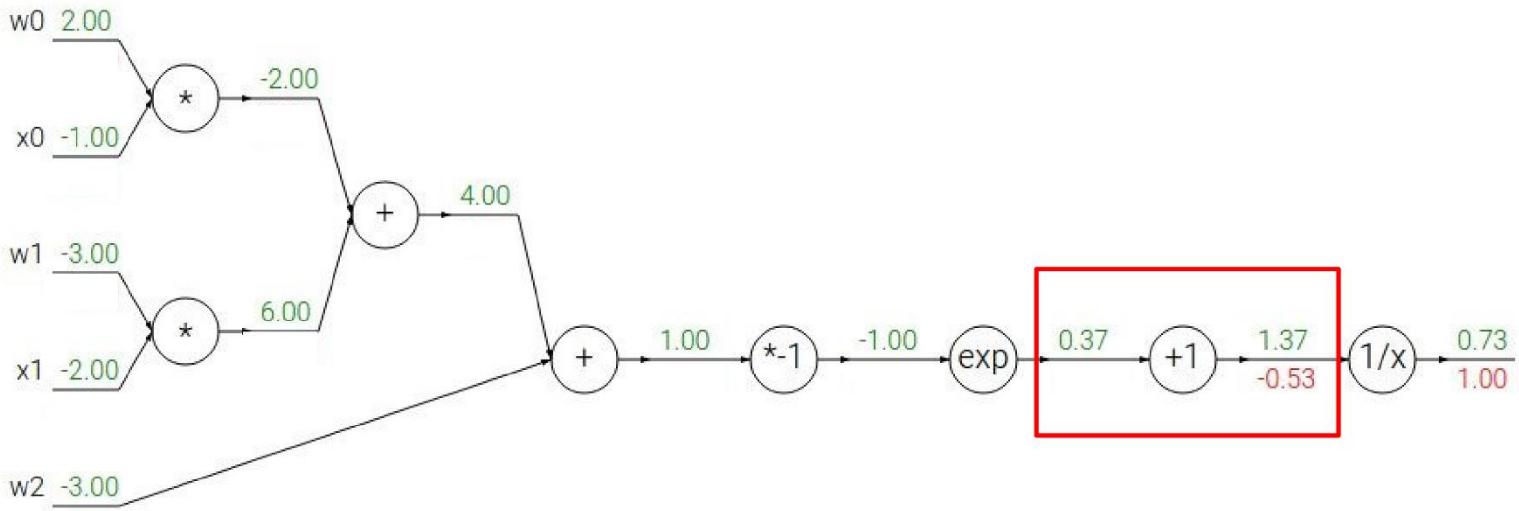

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

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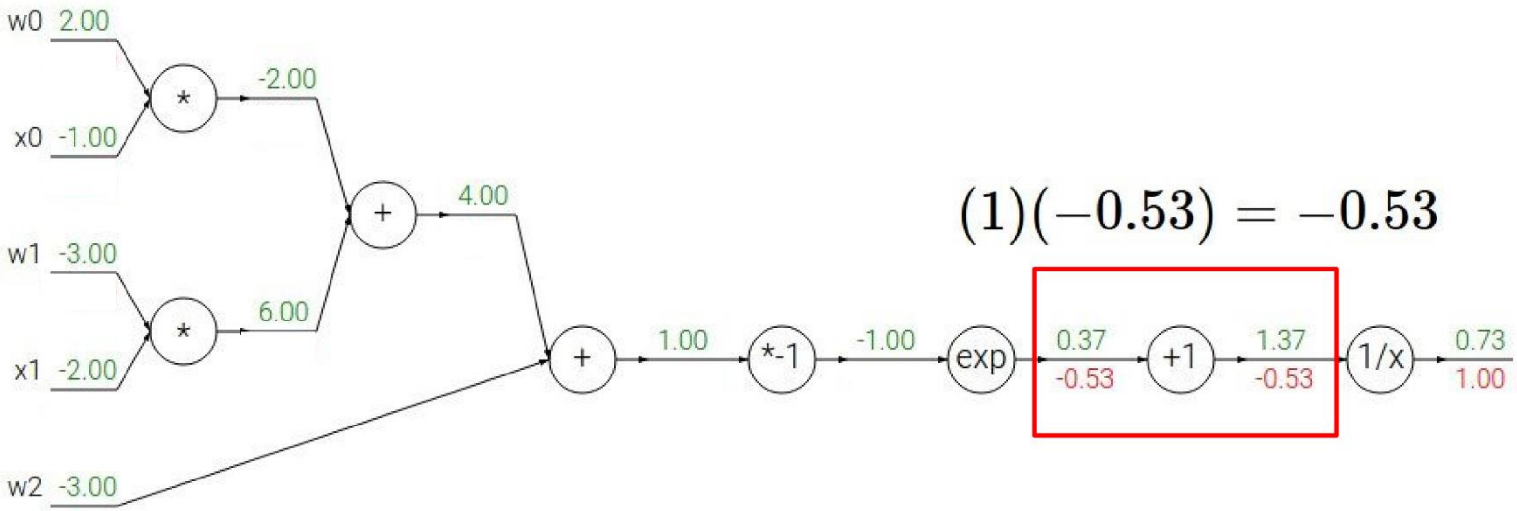
Another example: $$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



$$f(x) = e^x \rightarrow \frac{df}{dx} = e^x$$

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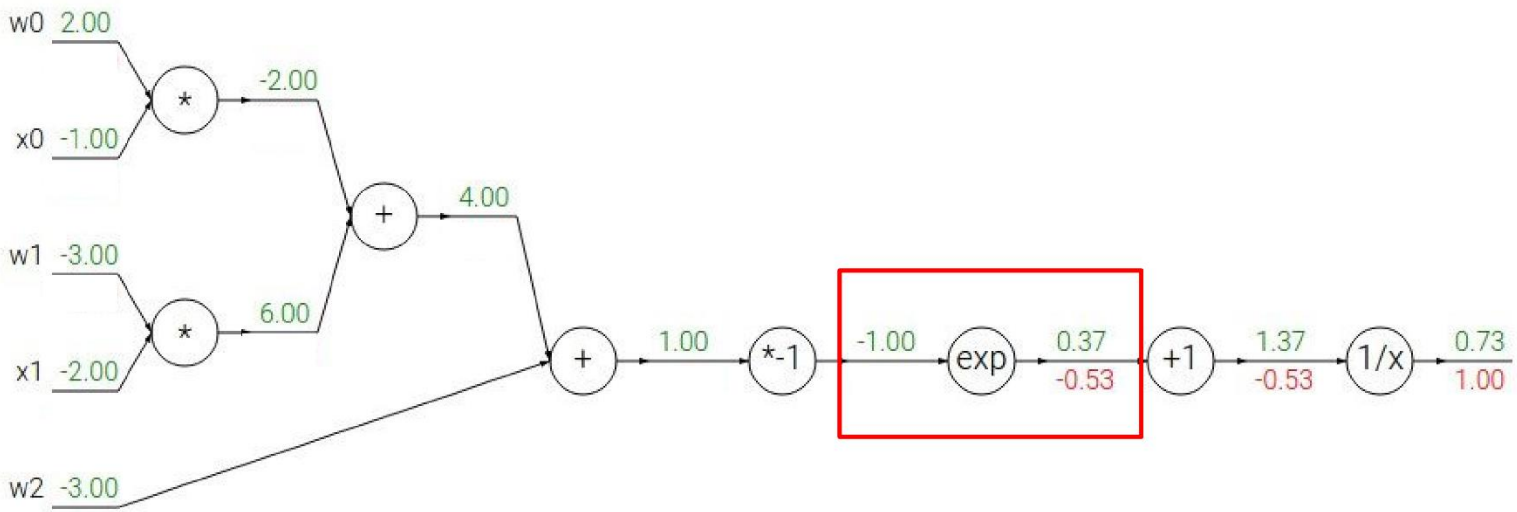

$f(x) = e^x \rightarrow \frac{df}{dx} = e^x$	$f(x) = \frac{1}{x} \rightarrow \frac{df}{dx} = -1/x^2$
$f_a(x) = ax \rightarrow \frac{df}{dx} = a$	$f_c(x) = c + x \rightarrow \frac{df}{dx} = 1$

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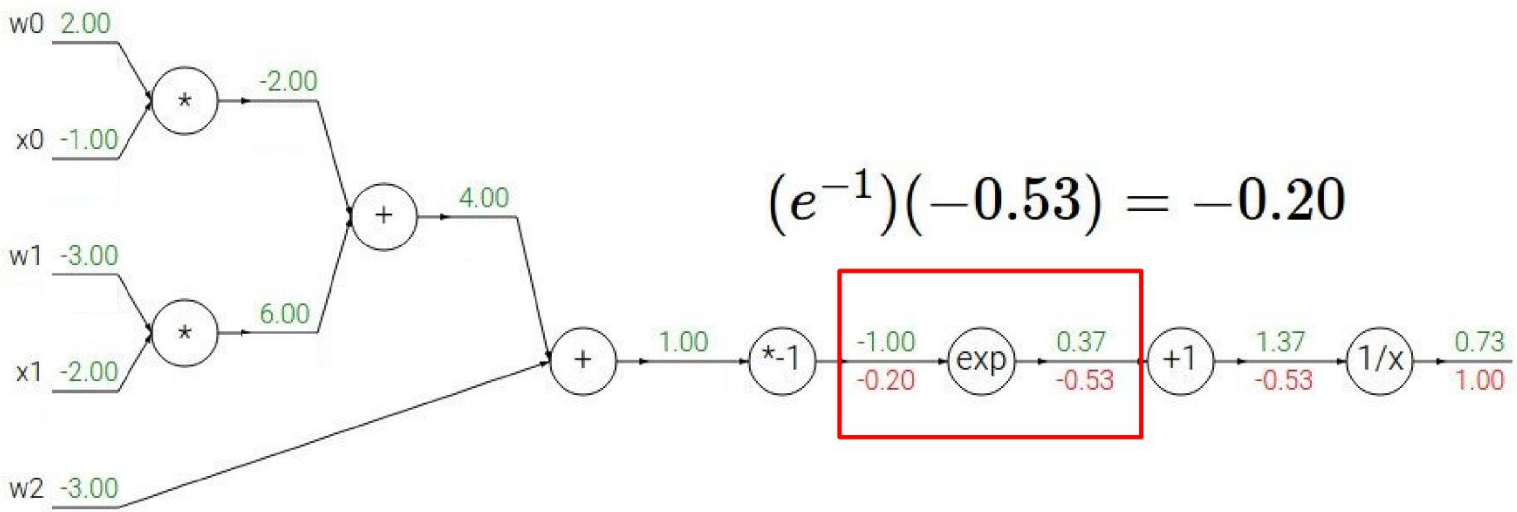

$$(e^{-1})(-0.53) = -0.20$$

$f(x) = e^x \rightarrow \frac{df}{dx} = e^x$	$f(x) = \frac{1}{x} \rightarrow \frac{df}{dx} = -1/x^2$
$f_a(x) = ax \rightarrow \frac{df}{dx} = a$	$f_c(x) = c + x \rightarrow \frac{df}{dx} = 1$

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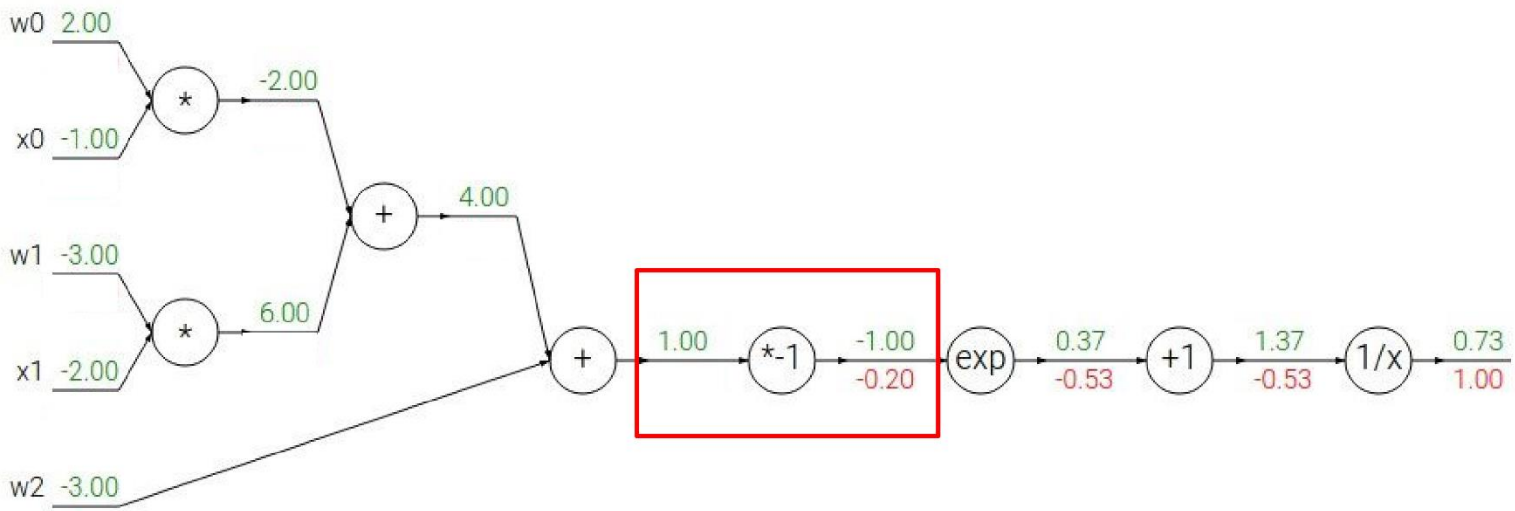

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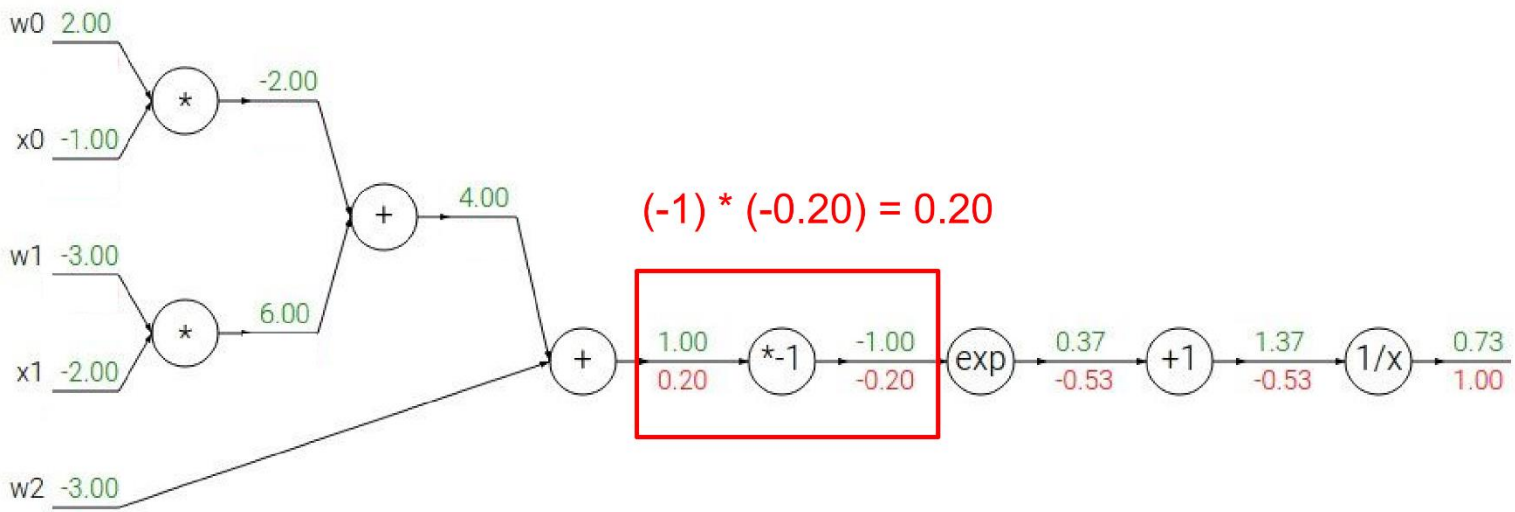

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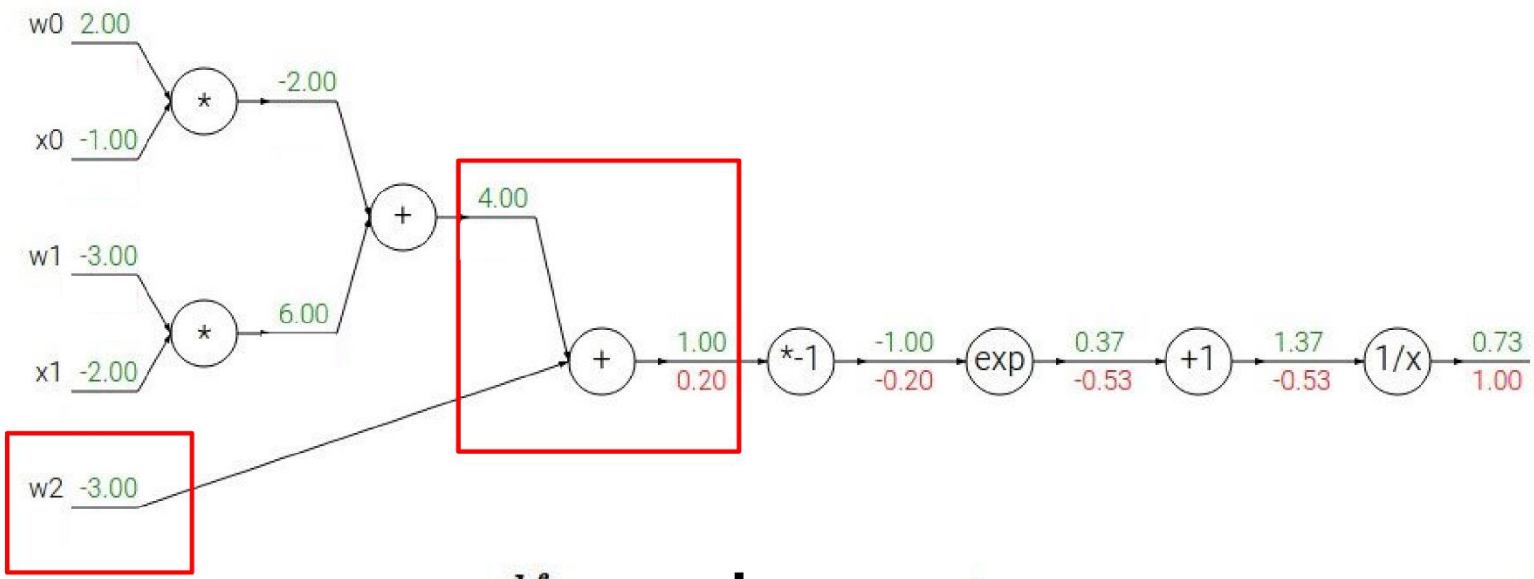
Another example: $$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

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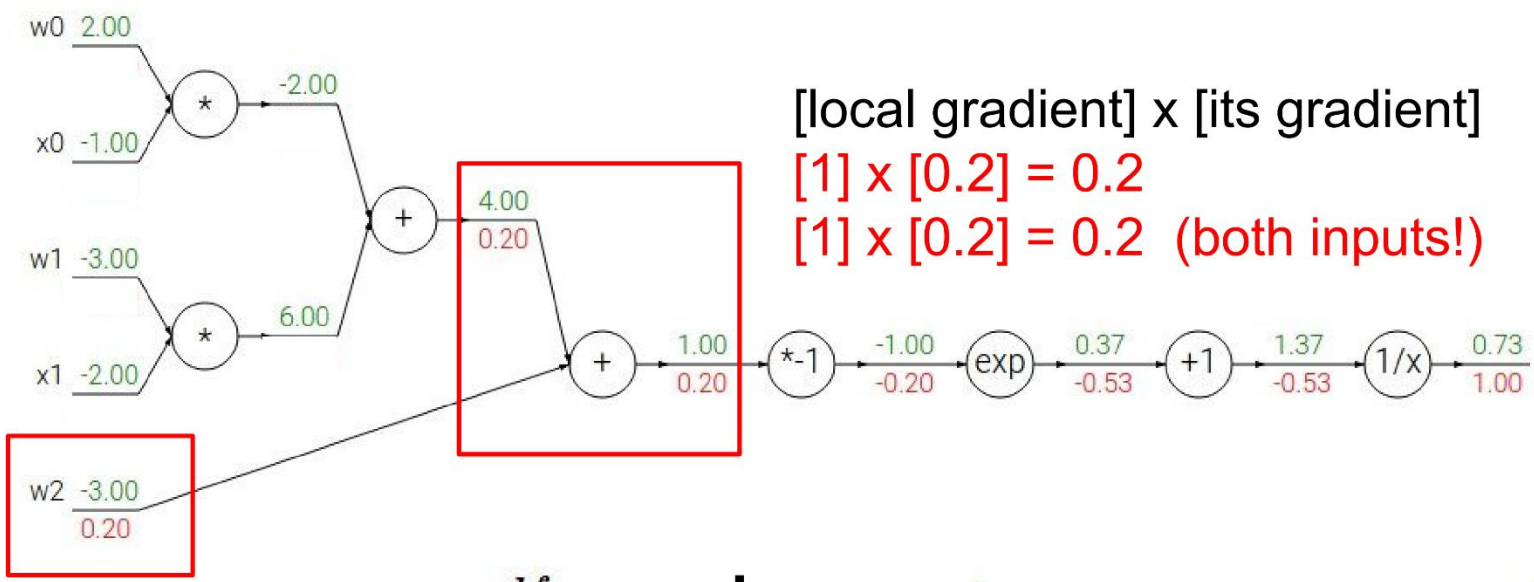


[local gradient] x [its gradient]

[1] x [0.2] = 0.2

[1] x [0.2] = 0.2 (both inputs!)

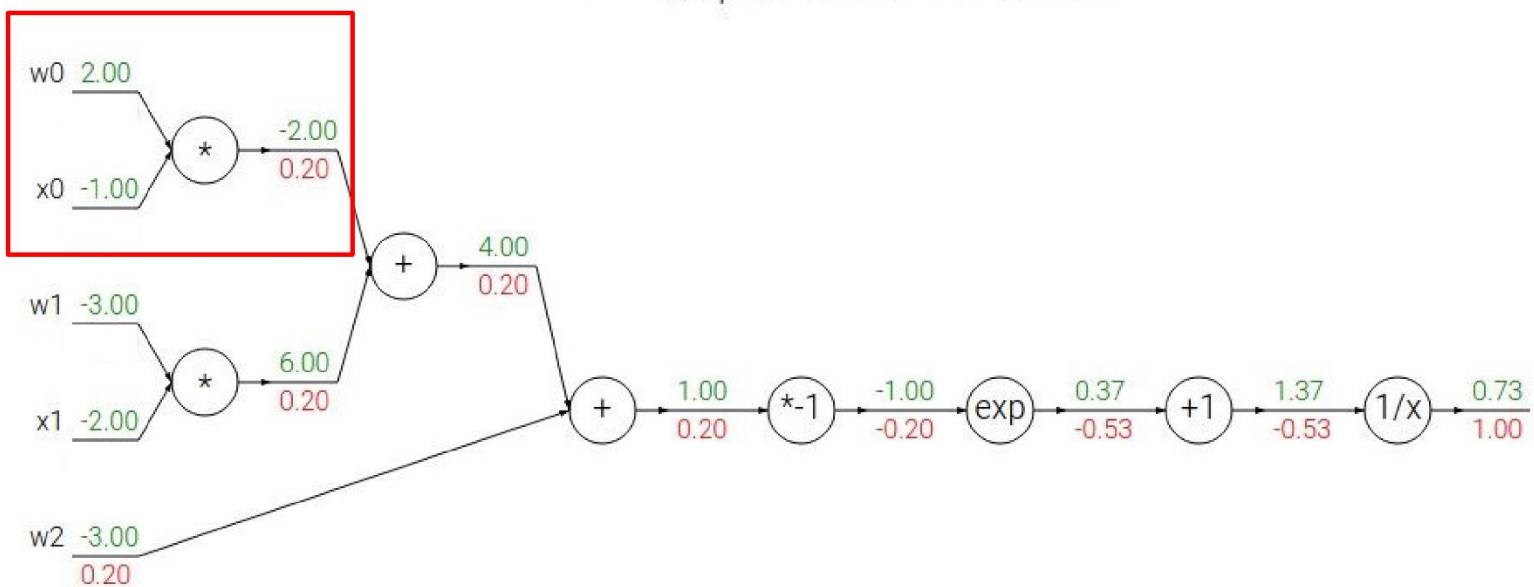
$$f(x) = e^x \rightarrow \frac{df}{dx} = e^x$$

$$f_a(x) = ax \rightarrow \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \rightarrow \frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x \rightarrow \frac{df}{dx} = 1$$

Another example: $$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

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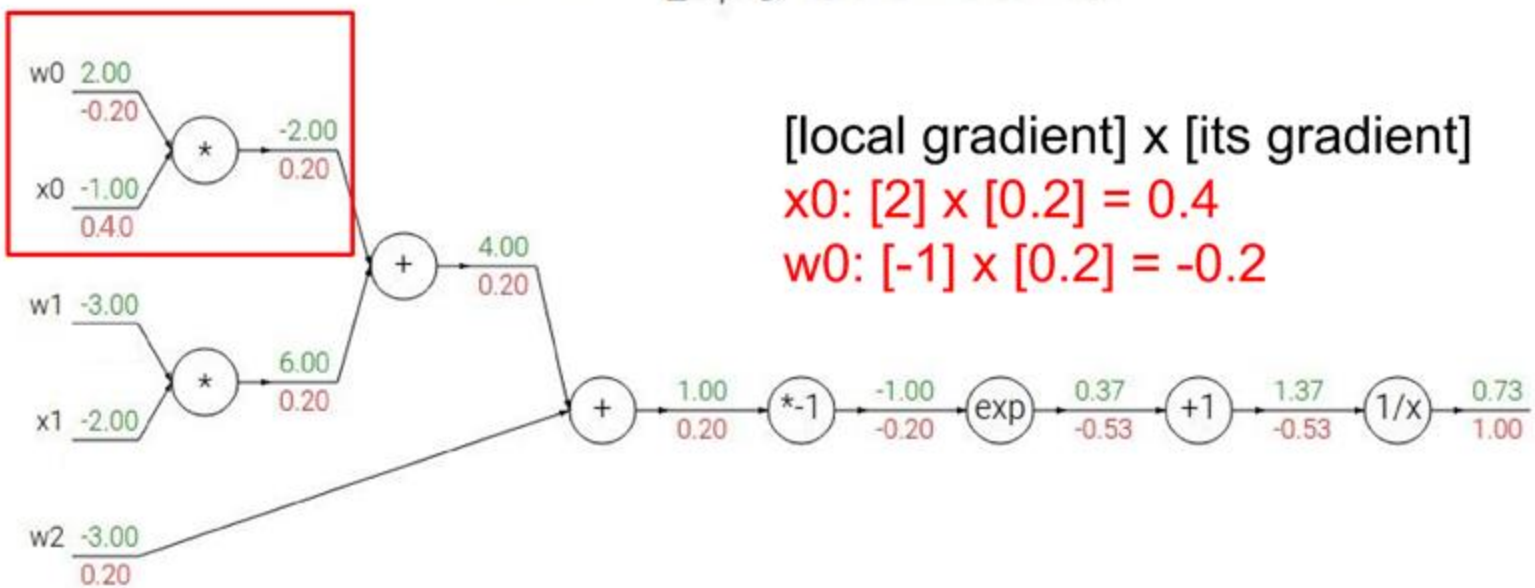
Another example: $$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



[local gradient] x [its gradient]

x0: [2] x [0.2] = 0.4

w0: [-1] x [0.2] = -0.2

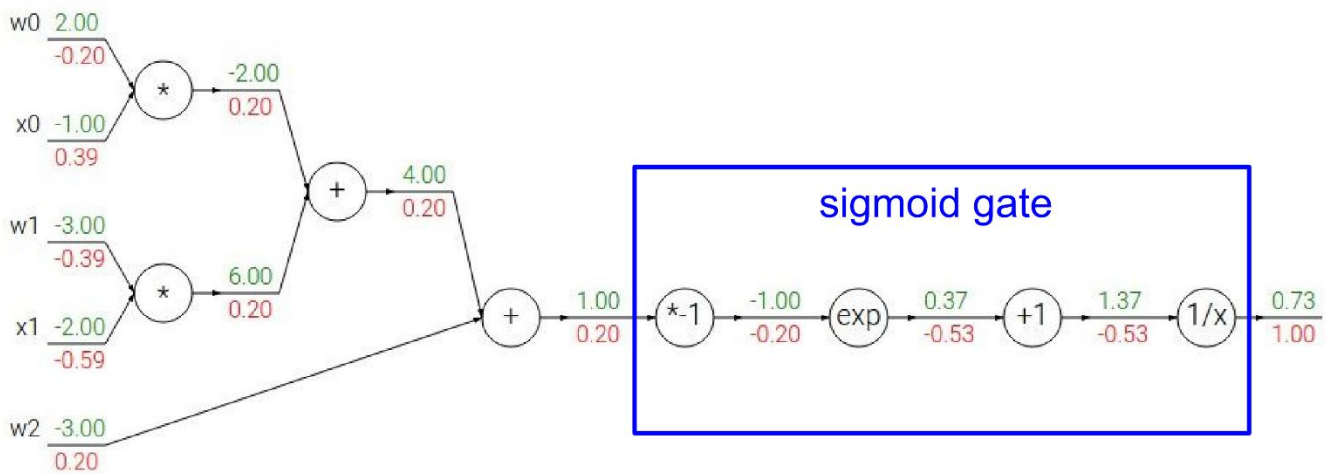
$$f(x) = e^x \rightarrow \frac{df}{dx} = e^x \qquad f(x) = \frac{1}{x} \rightarrow \frac{df}{dx} = -1/x^2$$

$$f_a(x) = ax \rightarrow \frac{df}{dx} = a \qquad f_c(x) = c + x \rightarrow \frac{df}{dx} = 1$$

$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

$$\boxed{\sigma(x) = \frac{1}{1+e^{-x}}}$$ sigmoid function

$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\,\sigma(x)$$



$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

$$\boxed{\sigma(x) = \frac{1}{1+e^{-x}}}$$ sigmoid function

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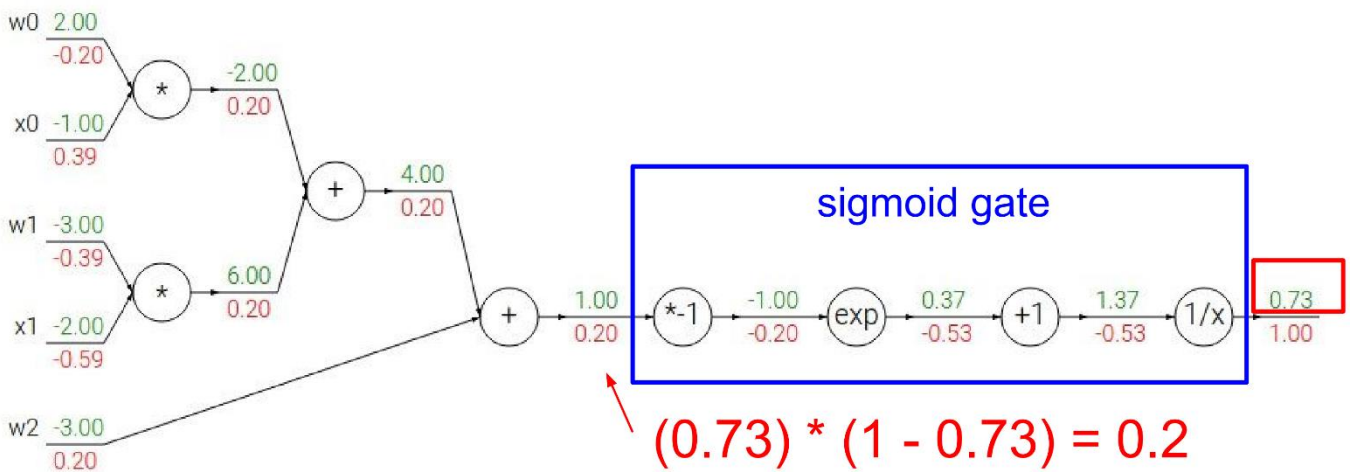
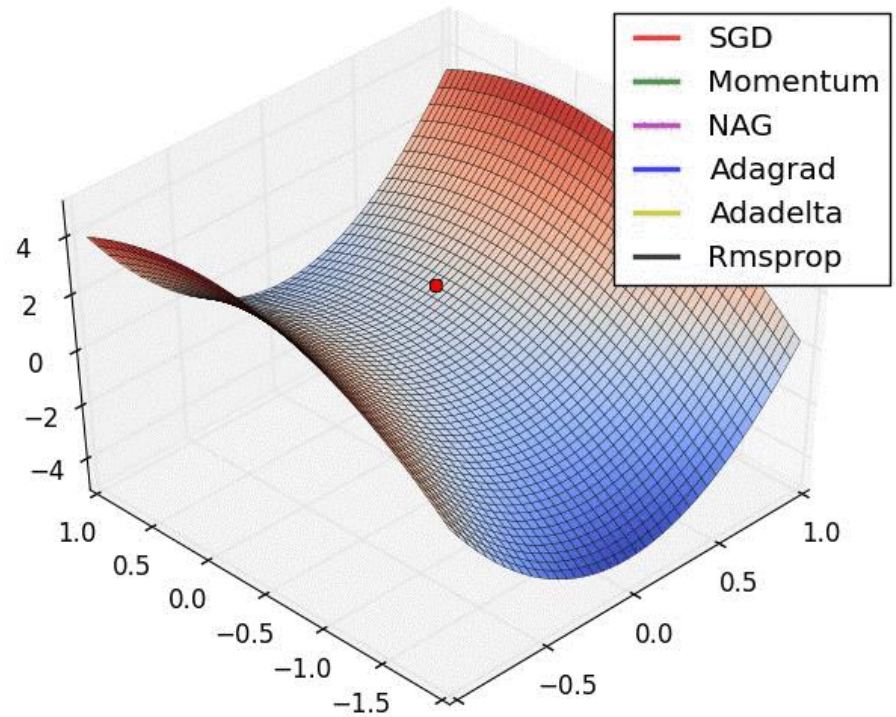


Entrenamiento de redes neuronales (profundas) requiere de muchas consideraciones para que sea exitoso

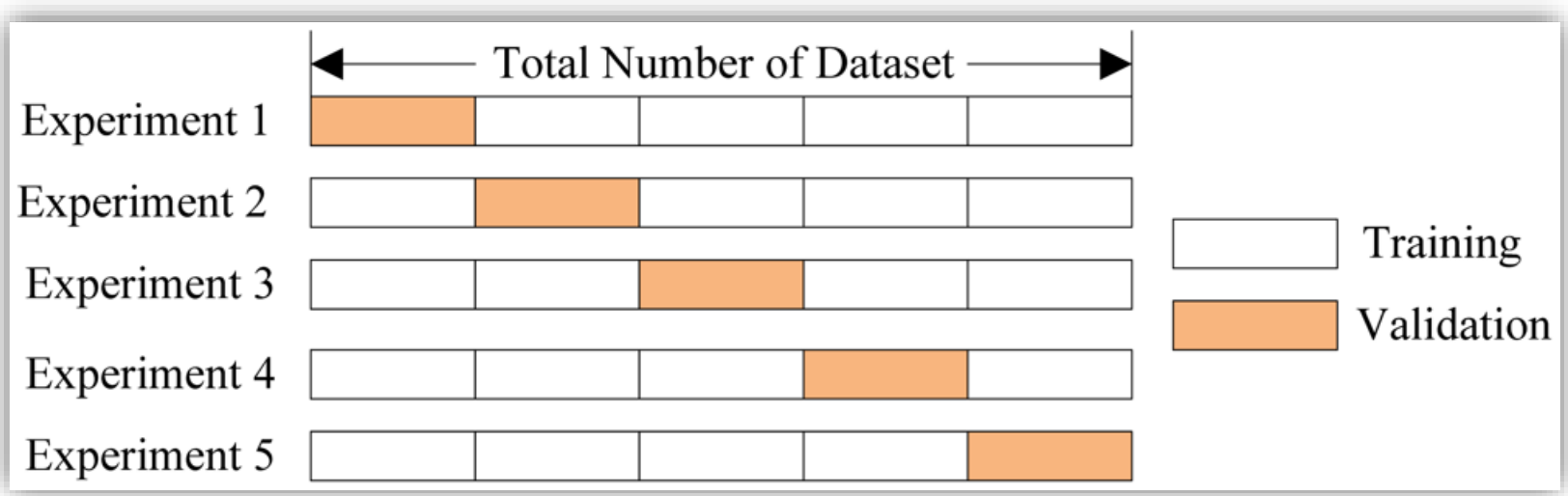
- Momentum permite aminorar riesgo de caer en mínimos locales

$$v = \gamma v + \alpha \nabla_\theta J(\theta; x^{(i)}, y^{(i)})$$
$$\theta = \theta - v$$



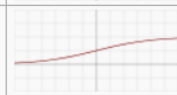
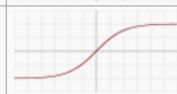
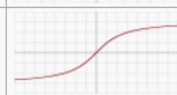
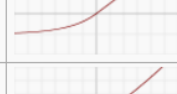
Entrenamiento de redes neuronales (profundas) requiere de muchas consideraciones para que sea exitoso

- Validación cruzada permite detectar sobreentrenamiento



Entrenamiento de redes neuronales (profundas) requiere de muchas consideraciones para que sea exitoso

- Funciones de activación pueden acelerar o frenar el entrenamiento

Name	Plot	Equation	Derivative
Identity		$f(x) = x$	$f'(x) = 1$
Binary step		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x \neq 0 \\ ? & \text{for } x = 0 \end{cases}$
Logistic (a.k.a Soft step)		$f(x) = \frac{1}{1+e^{-x}}$	$f'(x) = f(x)(1-f(x))$
TanH		$f(x) = \tanh(x) = \frac{2}{1+e^{-2x}} - 1$	$f'(x) = 1 - f(x)^2$
ArcTan		$f(x) = \tan^{-1}(x)$	$f'(x) = \frac{1}{x^2+1}$
Rectified Linear Unit (ReLU)		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
Parameteric Rectified Linear Unit (PReLU) [2]		$f(x) = \begin{cases} \alpha x & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} \alpha & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
Exponential Linear Unit (ELU) [3]		$f(x) = \begin{cases} \alpha(e^x - 1) & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} f(x) + \alpha & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
SoftPlus		$f(x) = \log_e(1+e^x)$	$f'(x) = \frac{1}{1+e^{-x}}$

Entrenamiento de redes neuronales (profundas) requiere de muchas consideraciones para que sea exitoso

- Inicialización de pesos: pesos grandes explosión del gradiente, pesos pequeños desvanecimiento del gradiente.
- Normalización de los datos: en general, redes neuronales andan mejor con datos normalizados (media 0, varianza 1).

Incluso con todas estas consideraciones, las redes feed-forward son muy difíciles de hacer funcionar exitosamente.


1958 Perceptron
1974 Backpropagation
awkward silence (AI Winter)
1969
Perceptron criticized

Pontificia Universidad Católica de Chile
Escuela de Ingeniería
Departamento de Ciencia de la Computación

IIC2613 – Inteligencia Artificial

Redes Neuronales

Profesor: Hans Löbel