IIC 2433 Minería de Datos

https://github.com/marcelomendoza/IIC2433

- BACKPROPAGATION -

El perceptrón multicapa (Multi-Layer Perceptron)

Forward propagation

$$\mathbf{x} = \mathbf{x}^{(0)} \xrightarrow{\mathrm{W}^{(1)}} \mathbf{s}^{(1)} \xrightarrow{\theta} \mathbf{x}^{(1)} \xrightarrow{\mathrm{W}^{(2)}} \mathbf{s}^{(2)} \xrightarrow{\theta} \mathbf{x}^{(2)} \cdots \xrightarrow{\mathrm{W}^{(L)}} \mathbf{s}^{(L)} \xrightarrow{\theta} \mathbf{x}^{(L)} = h(\mathbf{x}).$$

Forward propagation

$\mathbf{x}^{(0)} \leftarrow \mathbf{x}$

for $\ell = 1$ to L **do**

  $\mathbf{s}^{(\ell)} \leftarrow (\mathrm{W}^{(\ell)})^{\mathrm{T}} \mathbf{x}^{(\ell-1)}$

  $\mathbf{x}^{(\ell)} \leftarrow \begin{bmatrix} 1 \\ \theta(\mathbf{s}^{(\ell)}) \end{bmatrix}$

end for

$h(\mathbf{x}) = \mathbf{x}^{(L)}$

Objetivo supervisado:

$$E_{\text{in}}(h) = E_{\text{in}}(\mathrm{W}) = \frac{1}{N} \sum_{n=1}^{N} (h(\mathbf{x}_n) - y_n)^2$$

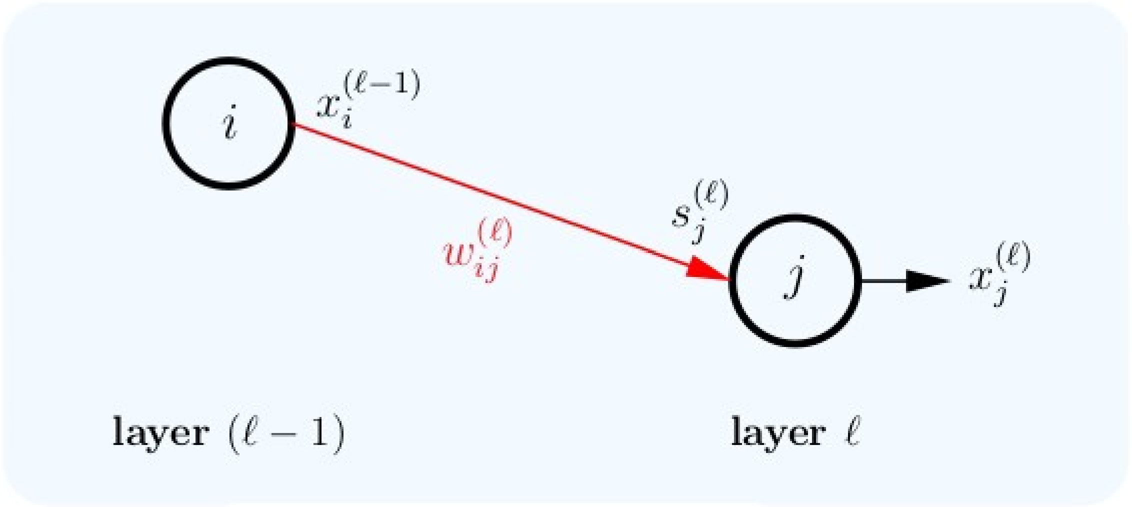
Dado que $\theta = \tanh$, E_{in} es diferenciable usando GD sobre

$$\underbrace{\mathrm{W} = \{\mathrm{W}^{(1)}, \mathrm{W}^{(2)}, \ldots, \mathrm{W}^{(L)}\}}_{\text{Parámetros del modelo}}$$

Feed-Forward

$$\mathbf{x} = \mathbf{x}^{(0)} \xrightarrow{\mathrm{W}^{(1)}} \mathbf{s}^{(1)} \xrightarrow{\theta} \mathbf{x}^{(1)} \xrightarrow{\mathrm{W}^{(2)}} \mathbf{s}^{(2)} \xrightarrow{\theta} \mathbf{x}^{(2)} \cdots \xrightarrow{\mathrm{W}^{(L)}} \mathbf{s}^{(L)} \xrightarrow{\theta} \mathbf{x}^{(L)} = h(\mathbf{x}).$$

Nodo a nodo:

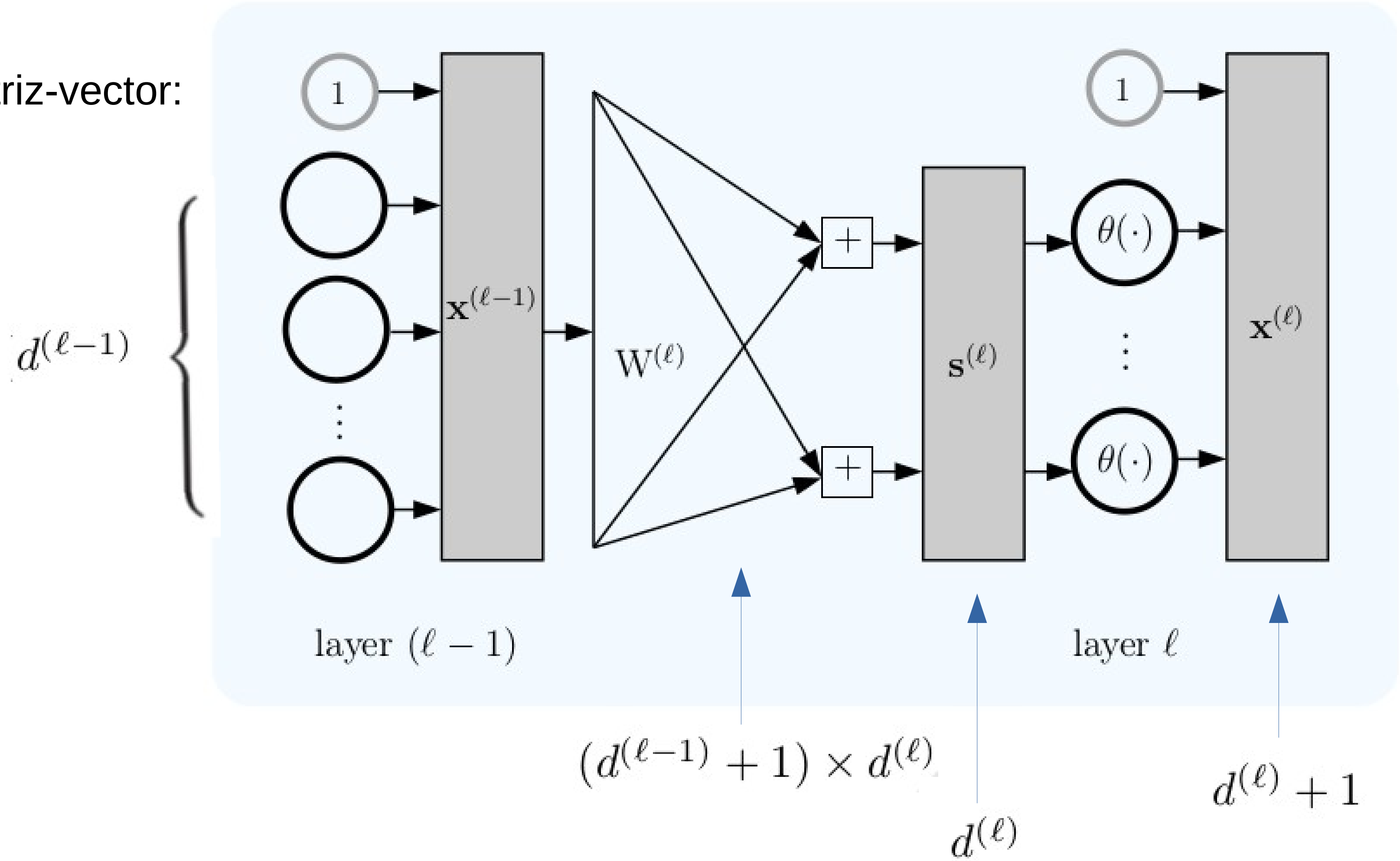


Feed-Forward

$$\mathbf{x} = \mathbf{x}^{(0)} \xrightarrow{\mathrm{W}^{(1)}} \mathbf{s}^{(1)} \xrightarrow{\theta} \mathbf{x}^{(1)} \xrightarrow{\mathrm{W}^{(2)}} \mathbf{s}^{(2)} \xrightarrow{\theta} \mathbf{x}^{(2)} \cdots \xrightarrow{\mathrm{W}^{(L)}} \mathbf{s}^{(L)} \xrightarrow{\theta} \mathbf{x}^{(L)} = h(\mathbf{x}).$$

$$\mathbf{s}^{(\ell)} \leftarrow (\mathrm{W}^{(\ell)})^{\mathrm{T}}\mathbf{x}^{(\ell-1)}$$

Matriz-vector:



Backpropagation

Minimizar: $$E_{\text{in}}(h) = E_{\text{in}}(\mathrm{W}) = \frac{1}{N}\sum_{n=1}^{N}(h(\mathbf{x}_n) - y_n)^2$$

Podemos usar la idea de gradiente descendente:

$$\mathrm{W}(t+1) = \mathrm{W}(t) - \eta \nabla E_{\text{in}}(\mathrm{W}(t))$$

Dado que:

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}\overbrace{\mathsf{e}}^{\mathsf{e}_n}(h(\mathbf{x}_n), y_n)$$

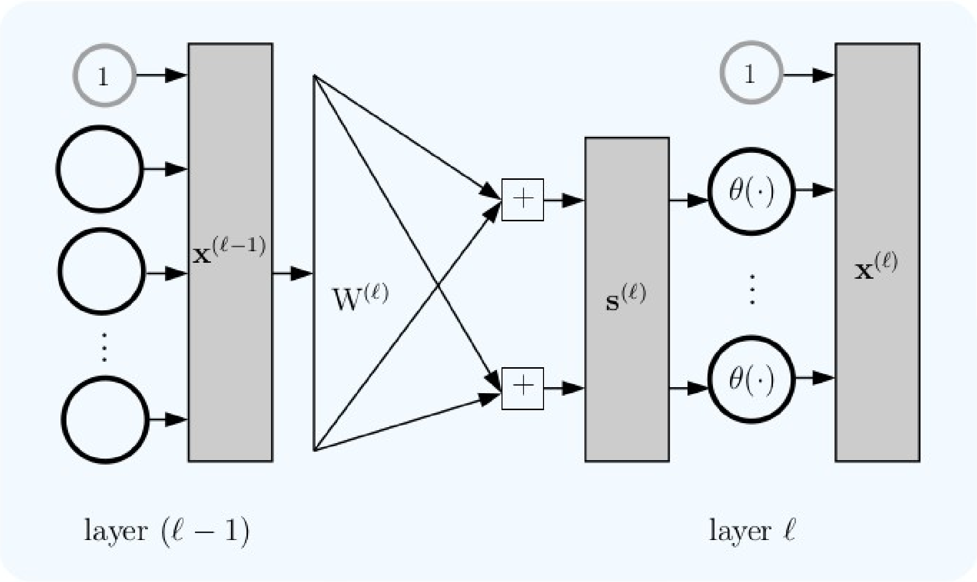
$$\frac{\partial E_{\text{in}}(\mathbf{w})}{\partial \mathrm{W}^{(\ell)}} = \frac{1}{N}\sum_{n=1}^{N}\frac{\partial \mathsf{e}_n}{\partial \mathrm{W}^{(\ell)}}$$

Necesitamos:

$$\frac{\partial \mathsf{e}(\mathbf{x})}{\partial \mathrm{W}^{(\ell)}}$$

Backpropagation

Vamos a usar la **regla de la cadena** para expresar las derivadas parciales de la capa $(\ell-1)$ en función de las derivadas parciales de la capa ℓ .



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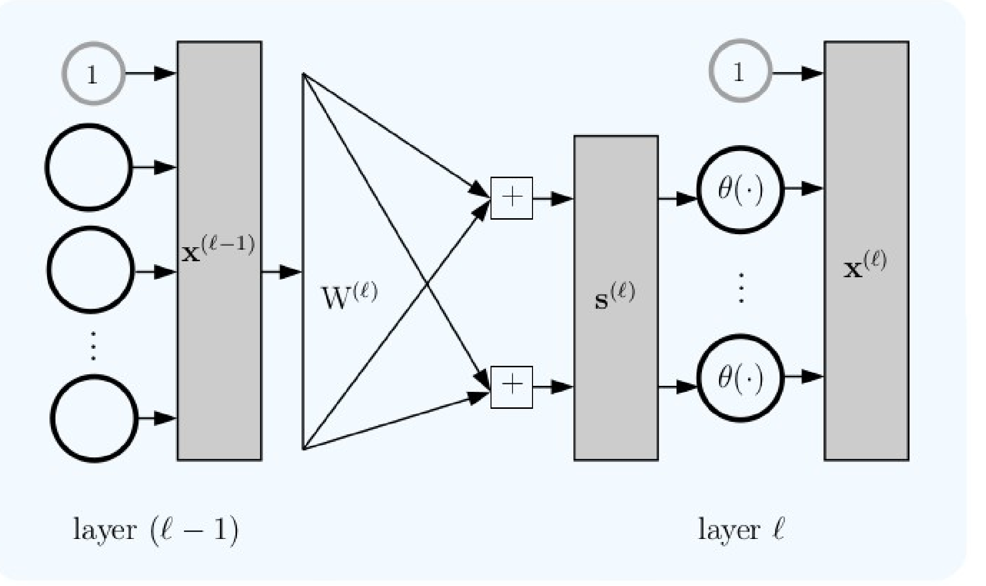
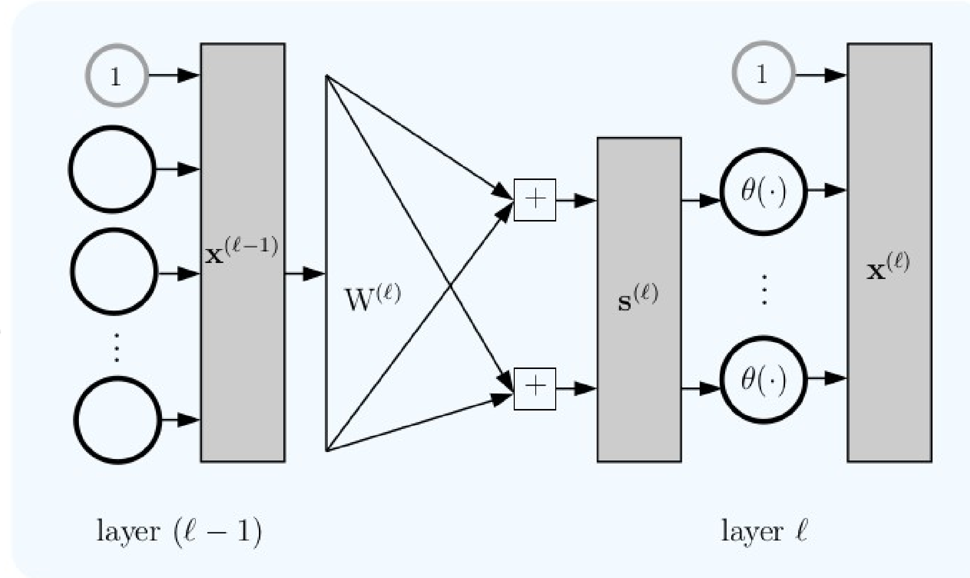


Tenemos: $\mathbf{s}^{(\ell)} = (\mathrm{W}^{(\ell)})^{\mathrm{T}}\mathbf{x}^{(\ell-1)}$

Definimos la sensibilidad de la capa ℓ :

$$\boldsymbol{\delta}^{(\ell)} = \frac{\partial \mathrm{e}}{\partial \mathbf{s}^{(\ell)}}$$

Backpropagation



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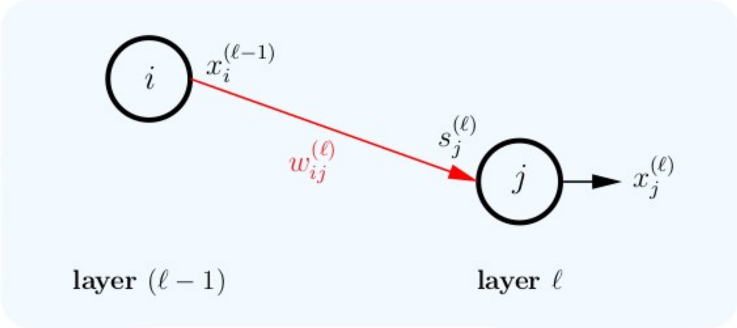
Aplicando la regla de la cadena:

$$\frac{\partial \mathrm{e}}{\partial \mathrm{W}^{(\ell)}} = \frac{\partial \mathbf{s}^{(\ell)}}{\partial \mathrm{W}^{(\ell)}} \cdot \left(\frac{\partial \mathrm{e}}{\partial \mathbf{s}^{(\ell)}}\right)^{\mathrm{T}}$$

$$= \mathbf{x}^{(\ell-1)}(\boldsymbol{\delta}^{(\ell)})^{\mathrm{T}}$$

?

Backpropagation



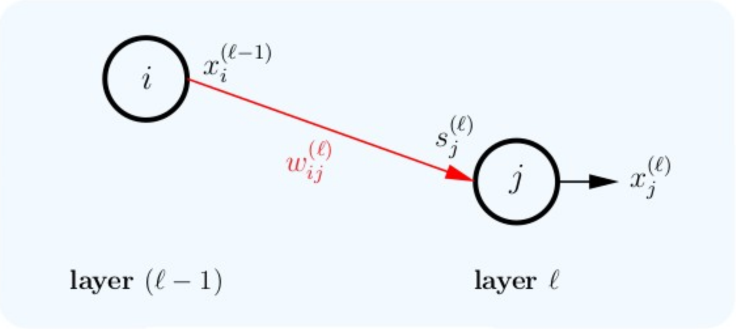
Miremos esto:

$$\frac{\partial \mathrm{e}}{\partial \mathrm{W}^{(\ell)}} = \frac{\partial \mathbf{s}^{(\ell)}}{\partial \mathrm{W}^{(\ell)}} \cdot \left(\frac{\partial \mathrm{e}}{\partial \mathbf{s}^{(\ell)}}\right)^{\mathrm{T}}$$

a nivel de un enlace.

$$= \mathbf{x}^{(\ell-1)}(\boldsymbol{\delta}^{(\ell)})^{\mathrm{T}}$$

Backpropagation



Miremos esto:
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a nivel de un enlace.
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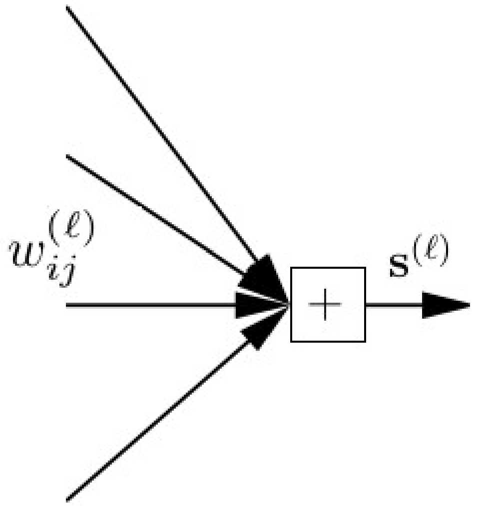
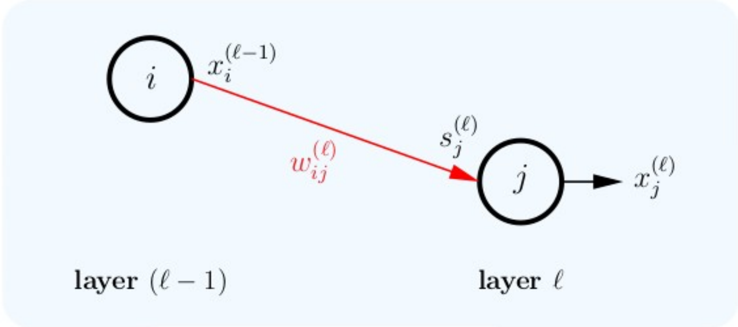
Tenemos:
$$\frac{\partial \mathrm{e}}{\partial\, w_{ij}^{(\ell)}} = \frac{\partial \mathbf{s}_j^{(\ell)}}{\partial w_{ij}^{(\ell)}} \cdot \frac{\partial \mathrm{e}}{\partial \mathbf{s}_j^{(\ell)}}$$

y sabemos que:
$$\mathbf{s}_j^{(\ell)} = \sum_{\alpha=0}^{d^{(\ell-1)}} w_{\alpha j}^{(\ell)} \mathbf{x}_\alpha^{(\ell-1)}$$



Backpropagation



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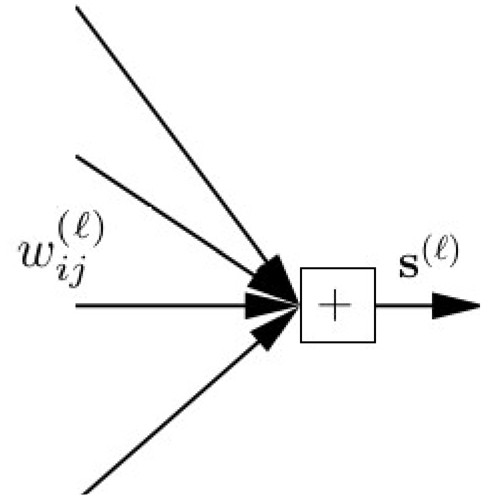
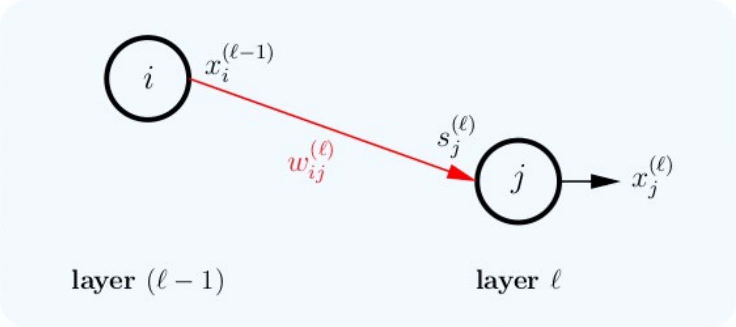


y sabemos que: $\mathbf{s}_j^{(\ell)} = \sum_{\alpha=0}^{d^{(\ell-1)}} w_{\alpha j}^{(\ell)} \mathbf{x}_\alpha^{(\ell-1)}$

por lo que al derivar con respecto a $w_{ij}^{(\ell)}$, queda: $\mathbf{x}_i^{(\ell-1)} \cdot \boldsymbol{\delta}_j^{(\ell)}$

Backpropagation



Miremos esto: $$\frac{\partial \mathrm{e}}{\partial \mathrm{W}^{(\ell)}} = \frac{\partial \mathbf{s}^{(\ell)}}{\partial \mathrm{W}^{(\ell)}} \cdot \left(\frac{\partial \mathrm{e}}{\partial \mathbf{s}^{(\ell)}}\right)^{\mathrm{T}}$$ a nivel de un enlace.

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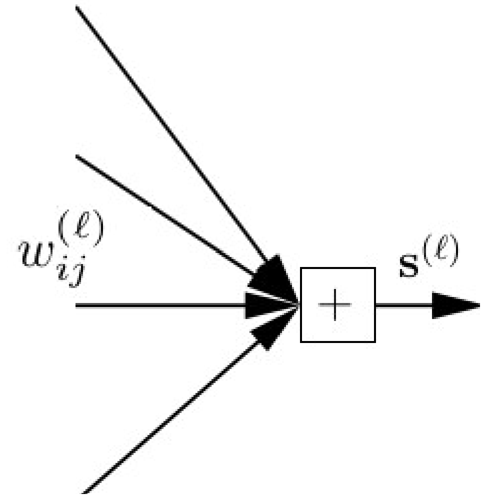


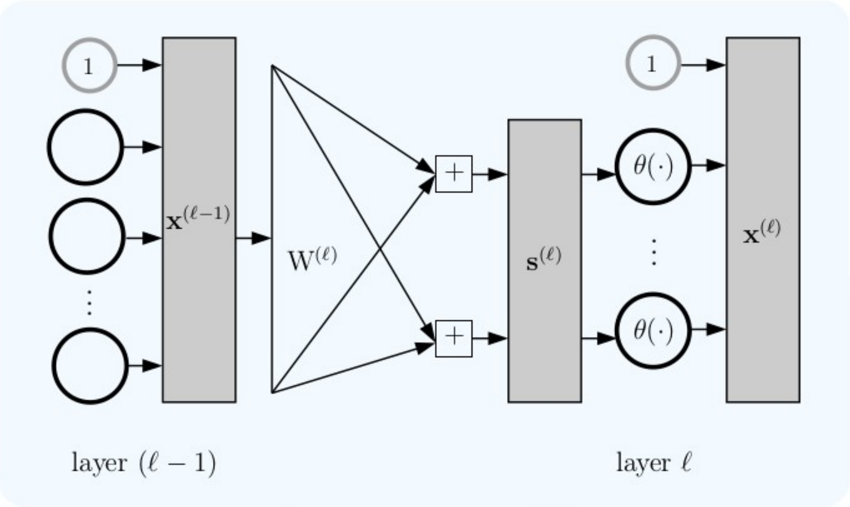
y sabemos que: $\mathbf{s}_j^{(\ell)} = \sum_{\alpha=0}^{d^{(\ell-1)}} w_{\alpha j}^{(\ell)} \mathbf{x}_\alpha^{(\ell-1)}$

por lo que al derivar con respecto a $w_{ij}^{(\ell)}$, queda: $\mathbf{x}_i^{(\ell-1)} \cdot \boldsymbol{\delta}_j^{(\ell)}$

Luego, haciendo lo mismo para cada parámetro, encontramos que: $$\frac{\partial \mathbf{s}^{(\ell)}}{\partial \mathrm{W}^{(\ell)}} = \mathbf{x}^{(\ell-1)} \quad \checkmark$$

Backpropagation

Ahora trabajaremos con: $$\boldsymbol{\delta}_j^{(\ell)} = \frac{\partial \mathrm{e}}{\partial \mathbf{s}_j^{(\ell)}}$$



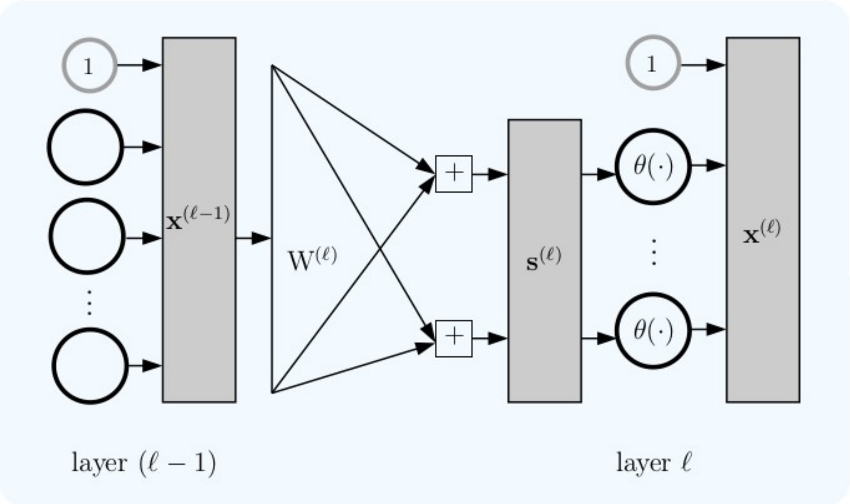
$$\frac{\partial \mathbf{s}^{(\ell)}}{\partial \mathrm{W}^{(\ell)}} = \mathbf{x}^{(\ell-1)} \quad ✓$$

Backpropagation

Ahora trabajaremos con: $$\boldsymbol{\delta}_j^{(\ell)} = \frac{\partial \mathrm{e}}{\partial \mathbf{s}_j^{(\ell)}}$$

Aplicamos regla de la cadena:

$$\frac{\partial \mathrm{e}}{\partial \mathbf{s}_j^{(\ell)}} = \frac{\partial \mathrm{e}}{\partial \mathbf{x}_j^{(\ell)}} \cdot \frac{\partial \mathbf{x}_j^{(\ell)}}{\partial \mathbf{s}_j^{(\ell)}}$$



$$\frac{\partial \mathbf{s}^{(\ell)}}{\partial \mathrm{W}^{(\ell)}} = \mathbf{x}^{(\ell-1)} \quad \checkmark$$

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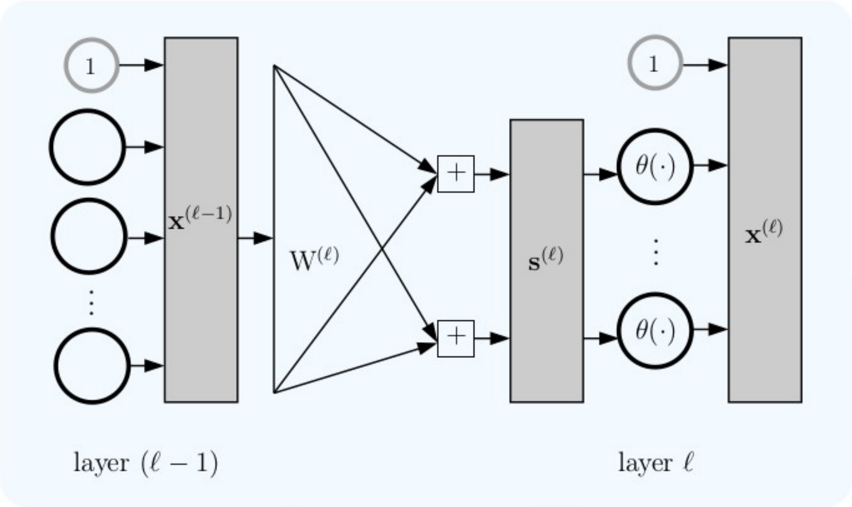

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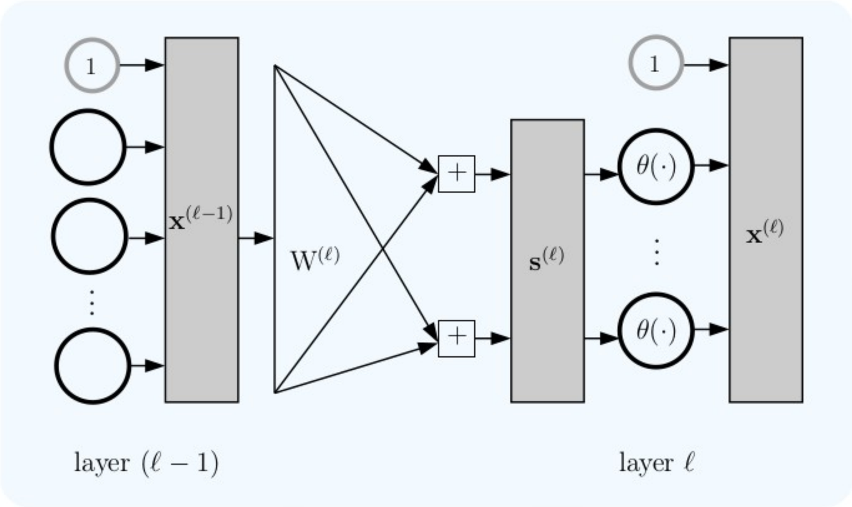
$$\frac{\partial \mathbf{s}^{(\ell)}}{\partial \mathrm{W}^{(\ell)}} = \mathbf{x}^{(\ell-1)} \quad \checkmark$$

$$= \frac{\partial \mathrm{e}}{\partial \mathbf{x}_j^{(\ell)}} \cdot \theta'\left(\mathbf{s}_j^{(\ell)}\right)$$

Derivada de la función de activación

Backpropagation

Ahora trabajaremos con: $$\boldsymbol{\delta}_j^{(\ell)} = \frac{\partial \mathrm{e}}{\partial \mathbf{s}_j^{(\ell)}}$$



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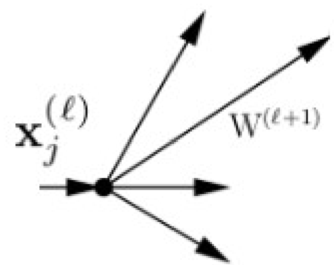
Derivada de la función de activación

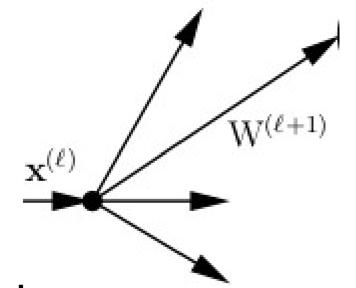
Ahora veamos que ocurre en:

$$\frac{\partial \mathrm{e}}{\partial \mathbf{x}_j^{(\ell)}}$$



Hay una multiplexión

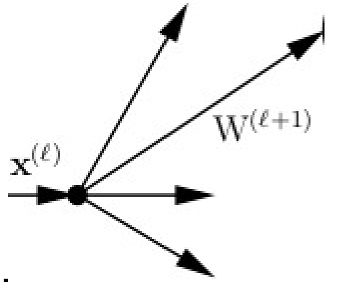
Backpropagation



Dado que una componente de $\mathbf{x}^{(\ell)}$ afecta a todas las componentes de $\mathbf{s}^{(\ell+1)}$, necesitamos sumar estas dependencias:

$$\frac{\partial \mathrm{e}}{\partial \mathbf{x}_j^{(\ell)}} = \sum_{k=1}^{d^{(\ell+1)}} \frac{\partial \mathbf{s}_k^{(\ell+1)}}{\partial \mathbf{x}_j^{(\ell)}} \cdot \frac{\partial \mathrm{e}}{\partial \mathbf{s}_k^{(\ell+1)}}$$

Backpropagation



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$$\frac{\partial \, \cancel{\mathbf{x}_j^{(\ell)}} \cdot w_{jk}^{(\ell+1)}}{\partial \mathbf{x}_j^{(\ell)}}$$

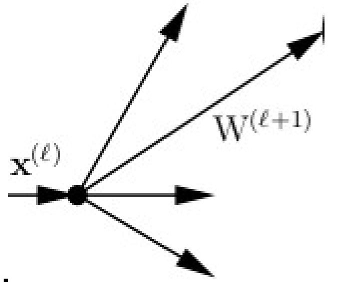
$$\frac{\partial \mathrm{e}}{\partial \mathbf{x}_j^{(\ell)}} = \sum_{k=1}^{d^{(\ell+1)}} \frac{\partial \mathbf{s}_k^{(\ell+1)}}{\partial \mathbf{x}_j^{(\ell)}} \cdot \frac{\partial \mathrm{e}}{\partial \mathbf{s}_k^{(\ell+1)}}$$

$$= \sum_{k=1}^{d^{(\ell+1)}} w_{jk}^{(\ell+1)} \boldsymbol{\delta}_k^{(\ell+1)}.$$

Sabemos que:

$$\frac{\partial \mathbf{s}^{(\ell)}}{\partial \mathrm{W}^{(\ell)}} = \mathbf{x}^{(\ell-1)}$$

Backpropagation



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Sabemos que:

$$\frac{\partial \mathbf{s}^{(\ell)}}{\partial \mathrm{W}^{(\ell)}} = \mathbf{x}^{(\ell-1)}$$

Luego:

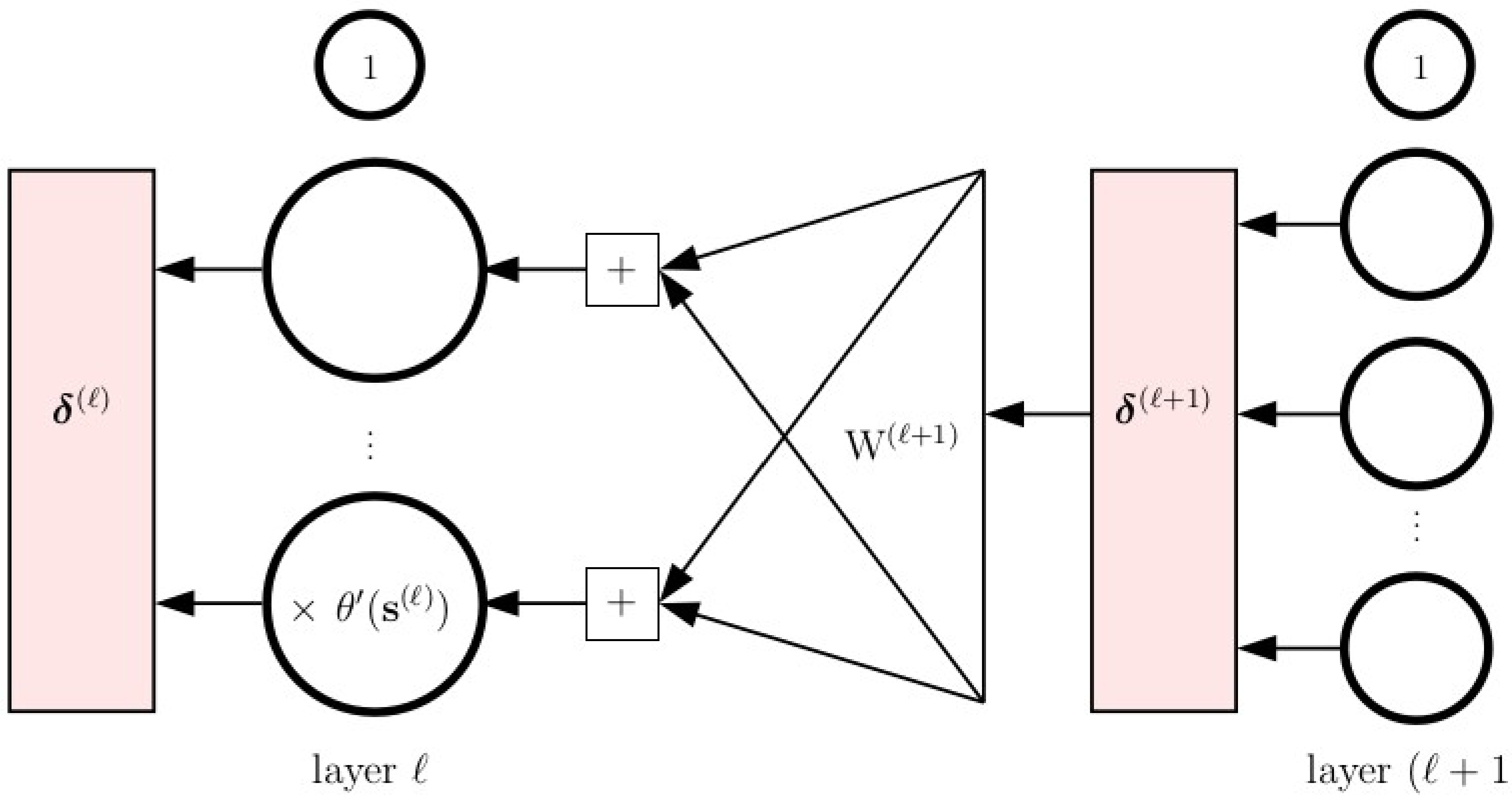
$$\frac{\partial \mathrm{e}}{\partial \mathbf{s}_j^{(\ell)}} = \frac{\partial \mathrm{e}}{\partial \mathbf{x}_j^{(\ell)}} \cdot \frac{\partial \mathbf{x}_j^{(\ell)}}{\partial \mathbf{s}_j^{(\ell)}}$$

$$\boldsymbol{\delta}_j^{(\ell)} = \theta'(\mathbf{s}_j^{(\ell)}) \sum_{k=1}^{d^{(\ell+1)}} w_{jk}^{(\ell+1)} \boldsymbol{\delta}_k^{(\ell+1)}$$

Backpropagation

$$\tanh'(\mathbf{s}^{(\ell)}) = \mathbf{1} - \tanh^2(\mathbf{s}^{(\ell)})$$

$$\boldsymbol{\delta}_j^{(\ell)} = \theta'(\mathbf{s}_j^{(\ell)}) \sum_{k=1}^{d^{(\ell+1)}} w_{jk}^{(\ell+1)} \boldsymbol{\delta}_k^{(\ell+1)}$$



$$\boldsymbol{\delta}^{(1)} \longleftarrow \boldsymbol{\delta}^{(2)} \cdots \longleftarrow \boldsymbol{\delta}^{(L-1)} \longleftarrow \boldsymbol{\delta}^{(L)}$$

Backpropagation

$$\boldsymbol{\delta}_j^{(\ell)} = \theta'(\mathbf{s}_j^{(\ell)}) \sum_{k=1}^{d^{(\ell+1)}} w_{jk}^{(\ell+1)} \boldsymbol{\delta}_k^{(\ell+1)}$$

Backpropagation de sensibilidad:

$$\boldsymbol{\delta}^{(1)} \longleftarrow \boldsymbol{\delta}^{(2)} \cdots \longleftarrow \boldsymbol{\delta}^{(L-1)} \longleftarrow \boldsymbol{\delta}^{(L)}$$

Nos falta calcular $\boldsymbol{\delta}^{(L)}$.

Backpropagation

$$\boldsymbol{\delta}_j^{(\ell)} = \theta'(\mathbf{s}_j^{(\ell)}) \sum_{k=1}^{d^{(\ell+1)}} w_{jk}^{(\ell+1)} \boldsymbol{\delta}_k^{(\ell+1)}$$

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Nos falta calcular $\boldsymbol{\delta}^{(L)}$.

Sabemos que: $\mathrm{e} = (\mathbf{x}^{(L)} - y)^2 = (\theta(\mathbf{s}^{(L)}) - y)^2$

Backpropagation

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Nos falta calcular $\boldsymbol{\delta}^{(L)}$.

Sabemos que: $\mathrm{e} = \underline{(\mathbf{x}^{(L)} - y)^2} = (\theta(\mathbf{s}^{(L)}) - y)^2$

Luego:

$$\begin{aligned} \boldsymbol{\delta}^{(L)} &= \frac{\partial \mathrm{e}}{\partial \mathbf{s}^{(L)}} \\ &= \frac{\partial}{\partial \mathbf{s}^{(L)}} (\mathbf{x}^{(L)} - y)^2 \end{aligned}$$

Backpropagation

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Backpropagation de sensibilidad:

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Sabemos que: $\mathrm{e} = \underline{(\mathbf{x}^{(L)} - y)^2} = (\theta(\underline{\mathbf{s}^{(L)})} - y)^2$

Luego:

$$\begin{aligned} \boldsymbol{\delta}^{(L)} &= \frac{\partial \mathrm{e}}{\partial \mathbf{s}^{(L)}} \\ &= \frac{\partial}{\partial \mathbf{s}^{(L)}} (\mathbf{x}^{(L)} - y)^2 \\ &= 2(\mathbf{x}^{(L)} - y) \frac{\partial \mathbf{x}^{(L)}}{\partial \mathbf{s}^{(L)}} \\ &= 2(\mathbf{x}^{(L)} - y)\underline{\theta'(\mathbf{s}^{(L)})}. \end{aligned}$$

Esto es 0 si la red acierta

$$\begin{aligned} \tanh'(\mathbf{s}^{(\ell)}) &= \mathbf{1} - \tanh^2(\mathbf{s}^{(\ell)}) \\ &= 1 - (x^{(L)})^2 \end{aligned}$$

Backpropagation

Backpropagation

$$\delta^{(L)} \leftarrow 2(x^{(L)} - y) \cdot \theta'(s^{(L)})$$

for $\ell = L-1$ to 1 **do**

Compute $\theta'(\mathbf{s}^{(\ell)}) = \left[1 - \mathbf{x}^{(\ell)} \otimes \mathbf{x}^{(\ell)}\right]_1^{d^{(\ell)}}$

$$\boldsymbol{\delta}^{(\ell)} \leftarrow \theta'(\mathbf{s}^{(\ell)}) \otimes \left[\mathrm{W}^{(\ell+1)}\boldsymbol{\delta}^{(\ell+1)}\right]_1^{d^{(\ell)}}$$

end for

Backpropagation nos permite obtener la cadena de sensibilidades:

$$\boldsymbol{\delta}^{(1)} \longleftarrow \boldsymbol{\delta}^{(2)} \ \dots \ \longleftarrow \boldsymbol{\delta}^{(L-1)} \longleftarrow \boldsymbol{\delta}^{(L)}$$

Backpropagation

Recordar que: $$\frac{\partial \mathrm{e}}{\partial \mathrm{W}^{(\ell)}} = \frac{\partial \mathbf{s}^{(\ell)}}{\partial \mathrm{W}^{(\ell)}} \cdot \left(\frac{\partial \mathrm{e}}{\partial \mathbf{s}^{(\ell)}} \right)^{\mathrm{T}} = \mathbf{x}^{(\ell-1)}(\boldsymbol{\delta}^{(\ell)})^{\mathrm{T}}$$

Luego, podemos calcular los gradientes para aplicar GD:

Algorithm to Compute $E_{\text{in}}(\mathbf{w})$ and $\mathbf{g} = \nabla E_{\text{in}}(\mathbf{w})$:
Input: weights $\mathbf{w} = \{\mathrm{W}^{(1)}, \ldots, \mathrm{W}^{(L)}\}$; data $\mathcal{D}$.
Output: error $E_{\text{in}}(\mathbf{w})$ and gradient $\mathbf{g} = \{\mathrm{G}^{(1)}, \ldots, \mathrm{G}^{(L)}\}$.

```
Initialize: E_in = 0; for ℓ = 1, ..., L, G^(ℓ) = 0 · W^(ℓ) .
for Each data point x_n (n = 1, ..., N) do
    Compute x^(ℓ) for ℓ = 0, ..., L.   [forward propagation]
    Compute δ^(ℓ) for ℓ = 1, ..., L.   [backpropagation]
    for ℓ = 1, ..., L do
        G^(ℓ)(x_n) = [x^(ℓ-1) (δ^(ℓ))^T]
        G^(ℓ) ← G^(ℓ) + (1/N) G^(ℓ)(x_n).
    end for
end for
```

Backpropagation

Recordar que:

$$\frac{\partial \mathrm{e}}{\partial \mathrm{W}^{(\ell)}} = \frac{\partial \mathbf{s}^{(\ell)}}{\partial \mathrm{W}^{(\ell)}} \cdot \left(\frac{\partial \mathrm{e}}{\partial \mathbf{s}^{(\ell)}}\right)^{\mathrm{T}}$$

Luego, podemos calcular los gradientes para aplicar GD:

$$= \mathbf{x}^{(\ell-1)}(\boldsymbol{\delta}^{(\ell)})^{\mathrm{T}}$$

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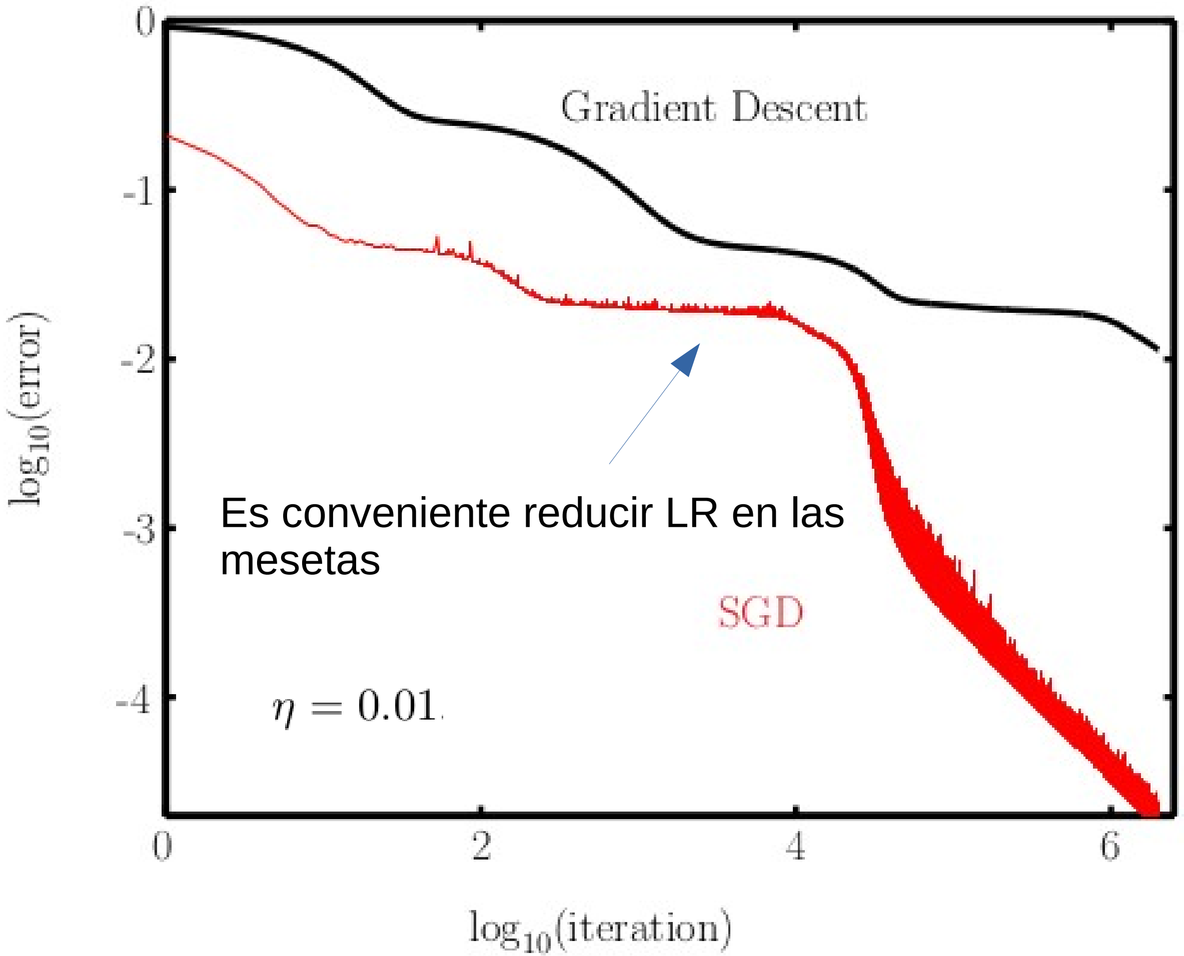
Input: weights $\mathbf{w} = \{\mathrm{W}^{(1)}, \ldots, \mathrm{W}^{(L)}\}$; data $\mathcal{D}$.
Output: error $E_{\text{in}}(\mathbf{w})$ and gradient $\mathbf{g} = \{\mathrm{G}^{(1)}, \ldots, \mathrm{G}^{(L)}\}$.

Initialize: $E_{\text{in}} = 0$; for $\ell = 1, \ldots, L$, $\mathrm{G}^{(\ell)} = 0 \cdot \mathrm{W}^{(\ell)}$.
for Each data point $\mathbf{x}_n$ $(n = 1, \ldots, N)$ **do**
  Compute $\mathbf{x}^{(\ell)}$ for $\ell = 0, \ldots, L$. [forward propagation]
  Compute $\boldsymbol{\delta}^{(\ell)}$ for $\ell = 1, \ldots, L$. [backpropagation]
  for $\ell = 1, \ldots, L$ **do**
    $\mathrm{G}^{(\ell)}(\mathbf{x}_n) = [\mathbf{x}^{(\ell-1)}(\boldsymbol{\delta}^{(\ell)})^{\mathrm{T}}]$
    $\mathrm{G}^{(\ell)} \leftarrow \mathrm{G}^{(\ell)} + \frac{1}{N}\mathrm{G}^{(\ell)}(\mathbf{x}_n)$.
  end for
end for

$$E_{\text{in}} \leftarrow E_{\text{in}} + \tfrac{1}{N}(\mathbf{x}_n^{(L)} - y_n)^2.$$

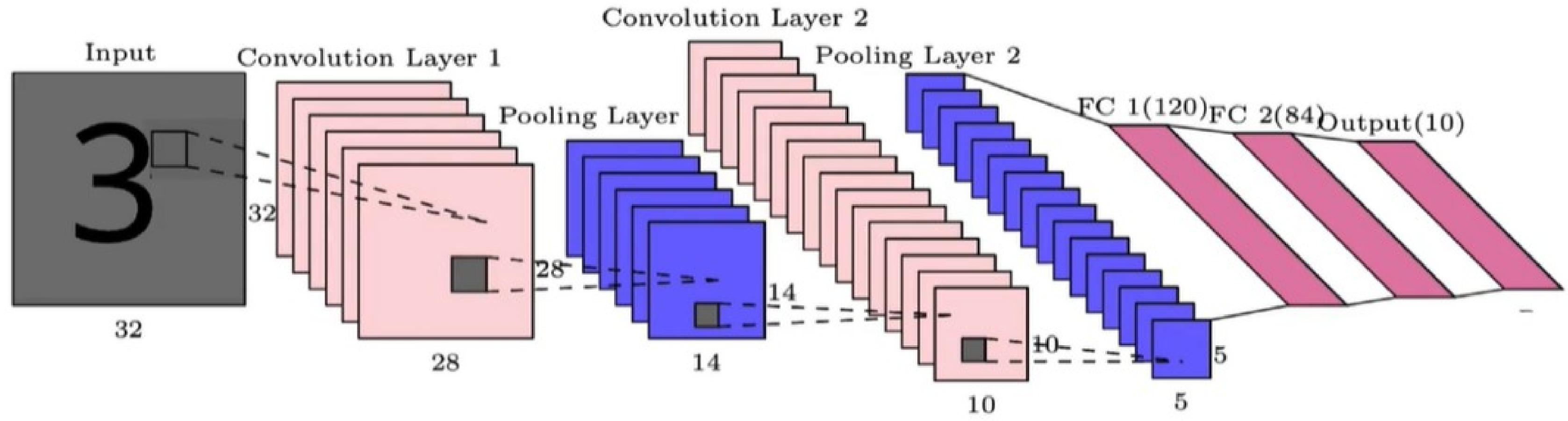
Backpropagation

GD para redes feed-forward: $\mathrm{W}^{(\ell)} = \mathrm{W}^{(\ell)} - \eta \mathrm{G}^{(\ell)}(\mathbf{x}_n).$



Digits

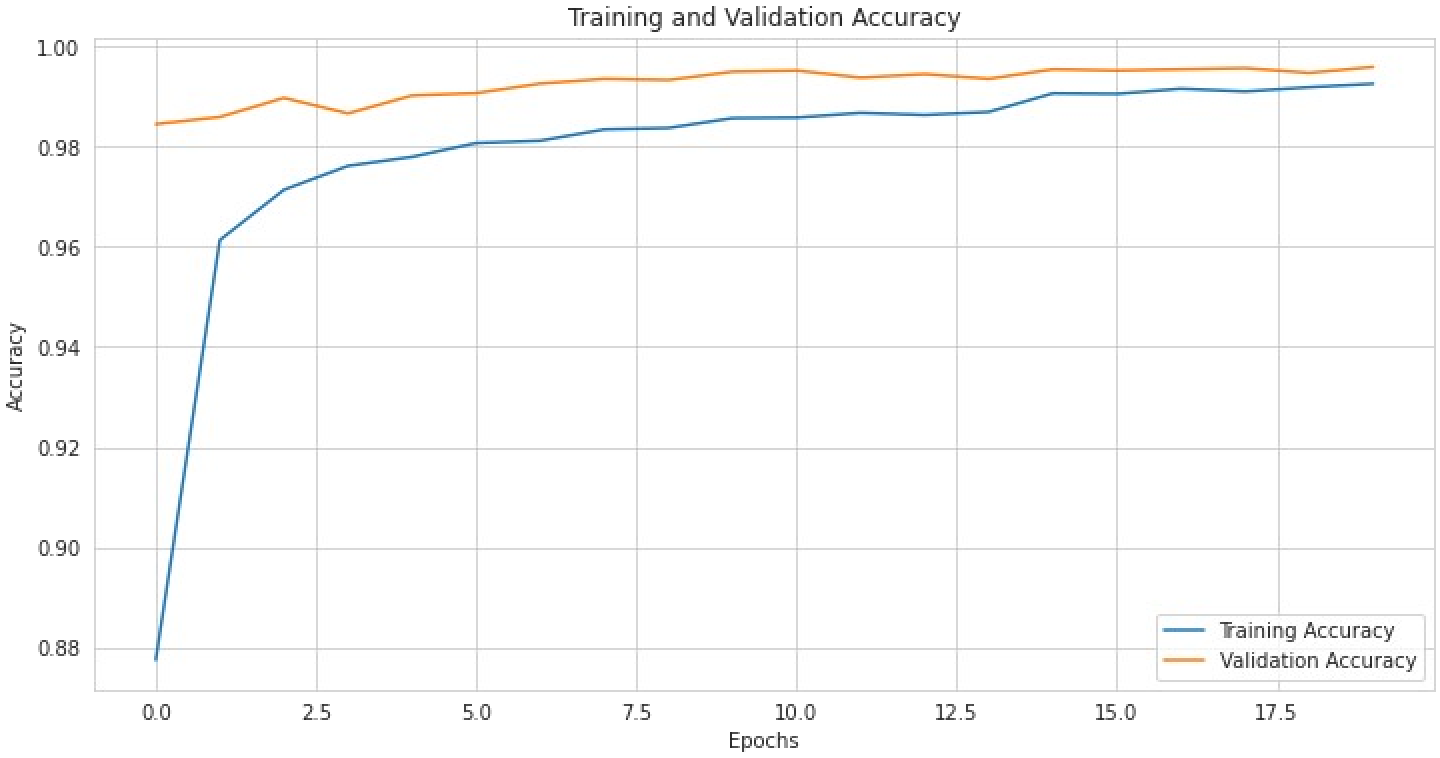
Las redes neuronales son útiles para trabajar sobre datos raw



En este caso, la red trabaja directamente sobre la imagen. Usa dos operadores (filtro convolucional y pooling) para extraer patches desde la entrada.

Al final, usa capas densas y colapsa a una softmax.

Si la red aprende, debiera existir un gap pequeño entre accuracy de validación y training (idem para pérdida)

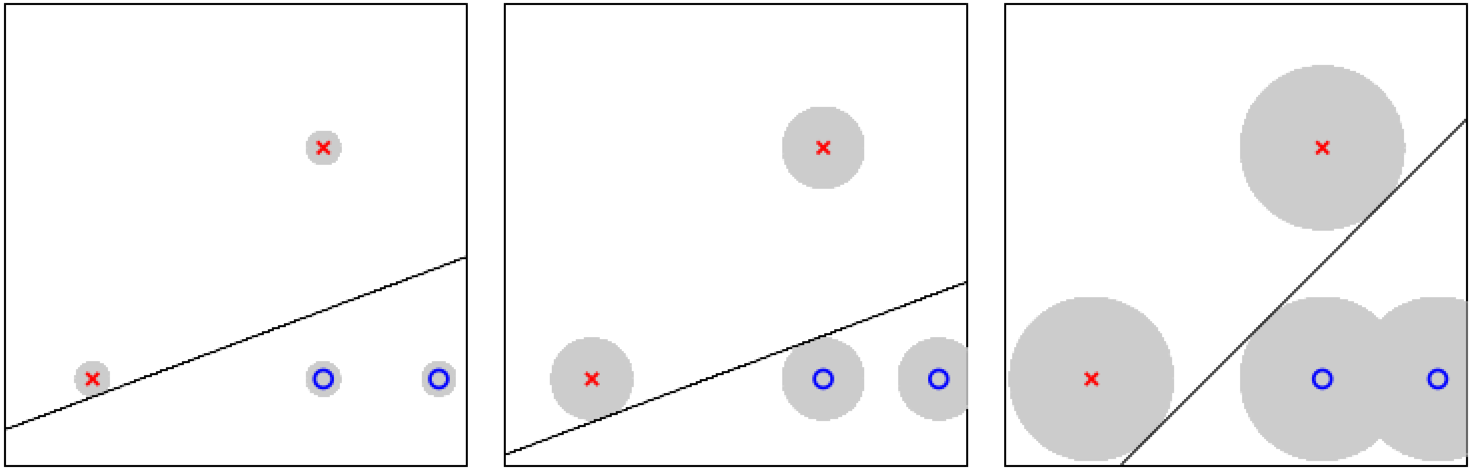


- SUPPORT VECTOR MACHINES -

Separadores y datos ruidosos

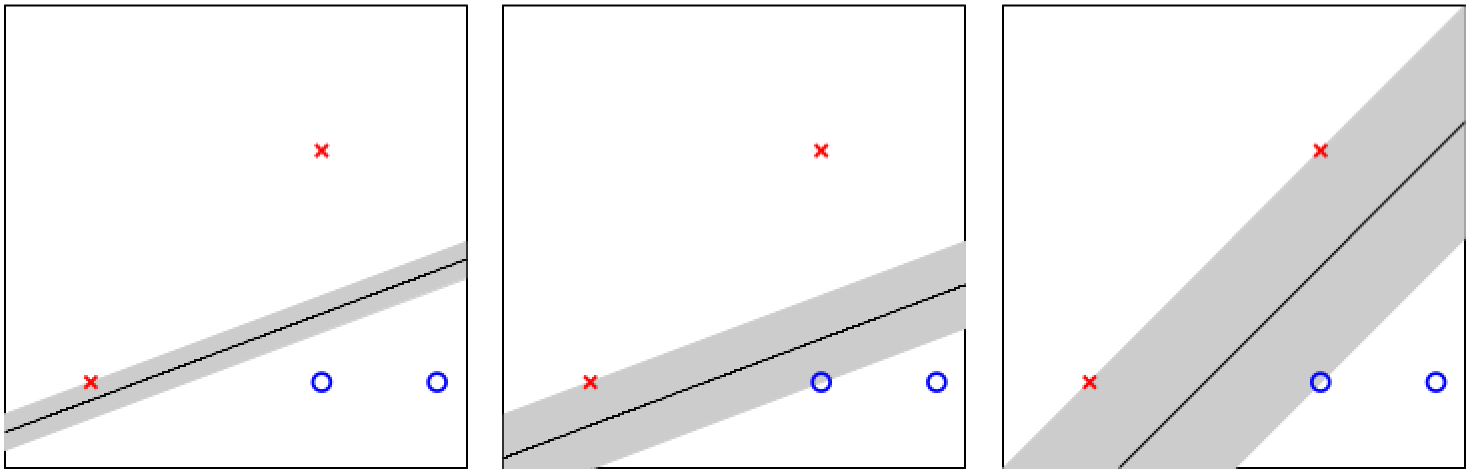
- Los datos pueden ser ruidosos (ruido de medición).
- Nuestros modelos debieran ser robustos a datos ruidosos.

<u>Idea</u>: La robustez al ruido tiene relación con considerar un margen de error para las mediciones.



Separadores y datos ruidosos

Una idea análoga a márgenes para datos consiste en trabajar con **hiperplanos gruesos**, agregando un margen al separador.



Separadores y datos ruidosos

Para trabajar con un hiperlano grueso, podemos usar el sesgo de una manera ingeniosa.

<u>Hiperplano estrecho</u>

$$\mathbf{x} \in \{1\} \times \mathbb{R}^d; \;\; \mathbf{w} \in \mathbb{R}^{d+1}$$

$$\mathbf{x} = \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_d \end{bmatrix}; \quad \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \end{bmatrix}.$$

$$\text{signal} = \mathbf{w}^{\mathrm{T}}\mathbf{x}$$

El sesgo se codifica como una dimensión más

Red neuronal

<u>Hiperplano grueso</u>

$$\mathbf{x} \in \mathbb{R}^d; \;\; b \in \mathbb{R}, \;\; \mathbf{w} \in \mathbb{R}^d$$

$$\text{bias } b$$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}; \quad \mathbf{w} = \begin{bmatrix} w_1 \\ \vdots \\ w_d \end{bmatrix}.$$

$$\text{signal} = \mathbf{w}^{\mathrm{T}}\mathbf{x} + b$$

El sesgo aditivo interviene en el espacio de representación

SVM

Separadores y datos ruidosos

Hiperplano grueso

$$\mathbf{x} \in \mathbb{R}^d;\ b \in \mathbb{R},\ \mathbf{w} \in \mathbb{R}^d$$

bias b

$$\mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}; \quad \mathbf{w} = \begin{bmatrix} w_1 \\ \vdots \\ w_d \end{bmatrix}.$$

$$\text{signal} = \mathbf{w}^{\mathrm{T}}\mathbf{x} + b$$

sesgo