INF721

2023/2

Aprendizado em Redes Neurais Profundas

A6: Backpropagation

Logística

Avisos

- Teste T2: Multilayer Perceptron na próxima aula!

Última aula

- Problemas linearmente não-separáveis
- Multilayer Perceptron (MLP)
- Forward Pass
- Funções de ativação

Plano de Aula

- Grafo computacional
- Gradiente da Regressão Logística
- Gradiente da MLP

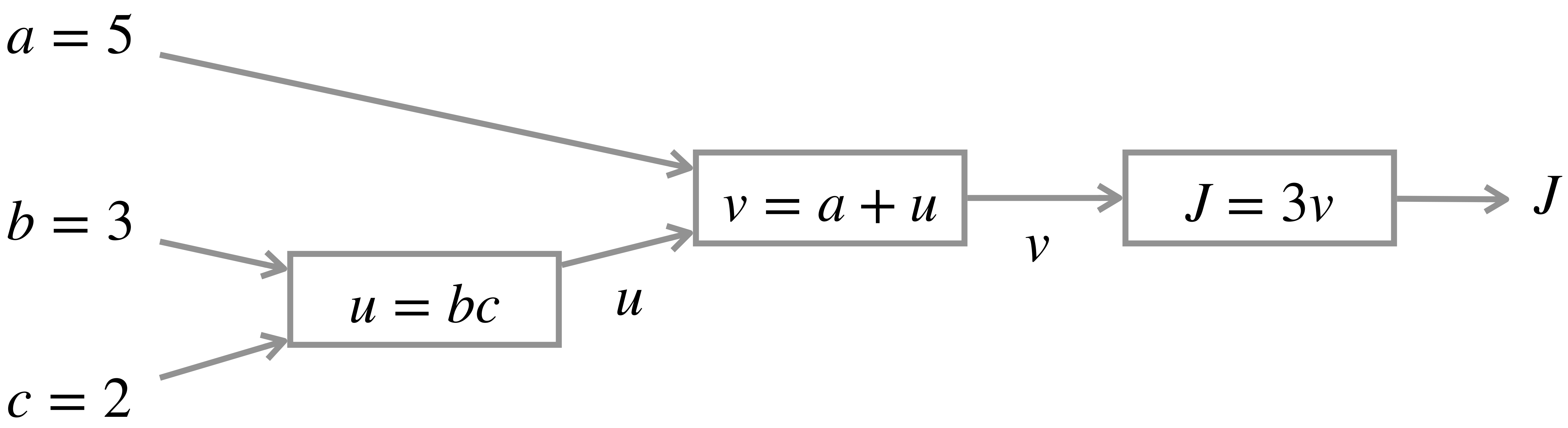
Grafo Computacional

Um grafo dirigido que descreve as expressões matemáticas de uma RNA passo a passo:

- Vértices representam operações
- Arestas representam entrada e saída

$$J(a, b, c) = 3(a + bc)$$

$$u = bc$$
$$v = a + u$$
$$J = 3V$$



Grafo Computacional e RNAs

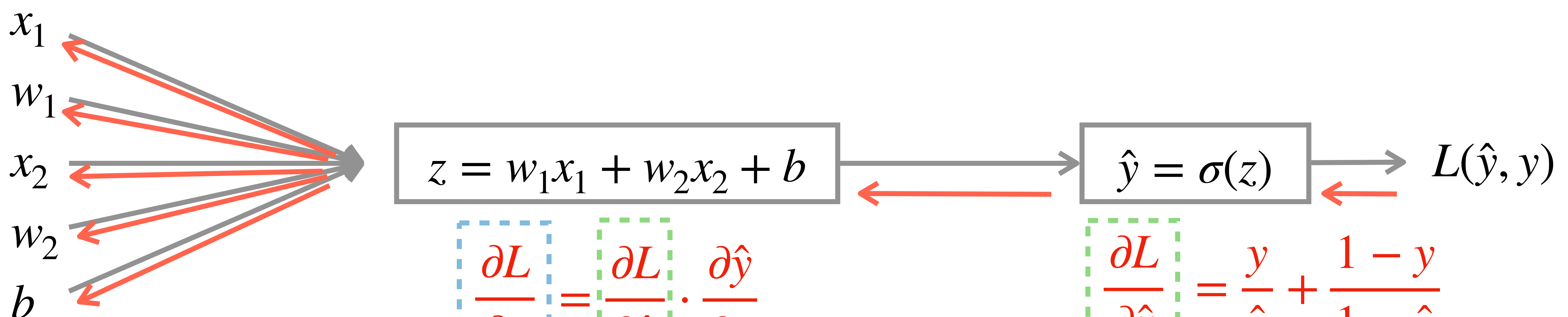
Grafos computacionais nos ajudam a calcular o gradiente de uma função de perda com relação aos pesos de uma RNA

Regressão Logística

$$z = \mathbf{w} \cdot \mathbf{x} + b$$

$$\hat{y} = h(\mathbf{x}) = \frac{1}{1 + e^{-z}}$$

$$L(\hat{y}, y) = -y \; log \; \hat{y} + (1 - y) \; log \; (1 - \hat{y}))$$



$$\frac{\partial L}{\partial z} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial z}$$

$$\frac{\partial L}{\partial \hat{y}} = \frac{y}{\hat{y}} + \frac{1 - y}{1 - \hat{y}}$$

$$= (\frac{y}{\hat{y}} + \frac{1 - y}{1 - \hat{y}}) \cdot \hat{y}(1 - \hat{y})$$

$$= \hat{y} - y$$

$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial z} \cdot \frac{\partial z}{\partial w_1}$$

$$= (\hat{y} - y) \cdot x_1$$

Regra da Cadeia!

Retropropagação (Backprop)

Calcular as derivadas parciais da função de perda com relação aos pesos $W^{[l]}$ e $\mathbf{b}^{[l]}$ para todas as camadas l de trás pra frente com a regra da cadeia.

MLP (1 camada escondidada)

$$\mathbf{z}^{[1]} = W^{[1]}\mathbf{x} + \mathbf{b}^{[1]} \qquad z^{[2]} = W^{[2]}\mathbf{a}^{[1]} + b^{[2]}$$

$$\mathbf{a}^{[1]} = g(\mathbf{z}^{[1]}) \qquad \hat{y} = \sigma(z^{[2]})$$

$$L(\hat{y}, y) = -y \log \hat{y} + (1-y) \log (1-\hat{y}))$$

$\mathbf{x}$, $W^{[1]}$, $\mathbf{b}^{[1]}$ → $\mathbf{z}^{[1]} = W^{[1]}\mathbf{x} + b^{[1]}$ → $\mathbf{a}^{[1]} = g(\mathbf{z}^{[1]})$ → (with $W^{[2]}$, $b^{[2]}$) $z^{[2]} = W^{[2]}\mathbf{a}^{[1]} + b^{[2]}$ → $\hat{y} = \sigma(z^{[2]})$ → $L(\hat{y}, y)$

$$\frac{\partial L}{\partial \mathbf{a}^{[1]}} = \frac{\partial L}{\partial z^{[2]}} \cdot \frac{\partial z^{[2]}}{\partial \mathbf{a}^{[1]}} = \frac{\partial L}{\partial z^{[2]}} \cdot W^{[2]}$$

$$\frac{\partial L}{\partial \mathbf{z}^{[1]}} = \frac{\partial L}{\partial \mathbf{a}^{[1]}} \cdot \frac{\partial \mathbf{a}^{[1]}}{\partial \mathbf{z}^{[1]}} = \frac{\partial L}{\partial z^{[2]}} \cdot W^{[2]} \times \frac{dg}{d\mathbf{z}^{[1]}} \cdot \mathbf{z}^{[1]}$$

$$\frac{\partial L}{\partial z^{[2]}} = \hat{y} - y$$

$$\frac{\partial L}{\partial \hat{y}} = \frac{y}{\hat{y}} + \frac{1-y}{1-\hat{y}}$$

$$\frac{\partial L}{\partial W^{[1]}} = \frac{\partial L}{\partial \mathbf{z}^{[1]}} \cdot \mathbf{x}^T$$

$$\frac{\partial L}{\partial W^{[1]}} = \frac{\partial L}{\partial \mathbf{z}^{[1]}}$$

$$\frac{\partial L}{\partial W^{[2]}} = \frac{\partial L}{\partial z^{[2]}} \cdot \frac{\partial z^{[2]}}{\partial W^{[2]}} = \frac{\partial L}{\partial z^{[2]}} \cdot {a^{[1]}}^T$$

$$\frac{\partial L}{\partial b^{[2]}} = \frac{\partial L}{\partial z^{[2]}} \cdot \frac{\partial z^{[2]}}{\partial b^{[2]}} = \frac{\partial L}{\partial z^{[2]}}$$

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Backward Pass

MLP (1 camada)

$$Z^{[1]} = W^{[1]}X + \mathbf{b}^{[1]}$$
$$A^{[1]} = \sigma(Z^{[1]})$$
$$Z^{[2]} = W^{[2]}\mathbf{a}^{[1]} + \mathbf{b}^{[2]}$$
$$\hat{Y} = \sigma(Z^{[2]})$$

Função de Perda

$$L(h) = -\frac{1}{n}\sum_{i=1}^{n}(y_i \, log \, \hat{y}_i + (1 - y_i) \, log \, (1 - \hat{y}_i))$$

Gradiente

$$dZ^{[2]} = \hat{Y} - Y$$
$$dW^{[2]} = \frac{1}{n} dZ^{[2]} \cdot A^{[1]^T}$$
$$db^{[2]} = \frac{1}{n}\sum_{i=1}^{n} dZ^{[2]}_{[:,i]}$$

$$dZ^{[1]} = W^{[2]^T} \cdot dZ^{[2]} \times \frac{dg}{dz^{[1]}} \cdot Z^{[1]}$$
$$dW^{[1]} = \frac{1}{n} dZ^{[1]} \cdot X^T$$
$$db^{[1]} = \frac{1}{n}\sum_{i=1}^{n} dZ^{[1]}_{[:,i]}$$

Inicialização de pesos na MLP

Em RNAs com pelo menos 1 camada escondidada (MLPs), temos que inicializar os pesos com valores aleatórios próximos de zero.

Se inicializarmos com zeros, os neurônios da camada escondida serão iguais!

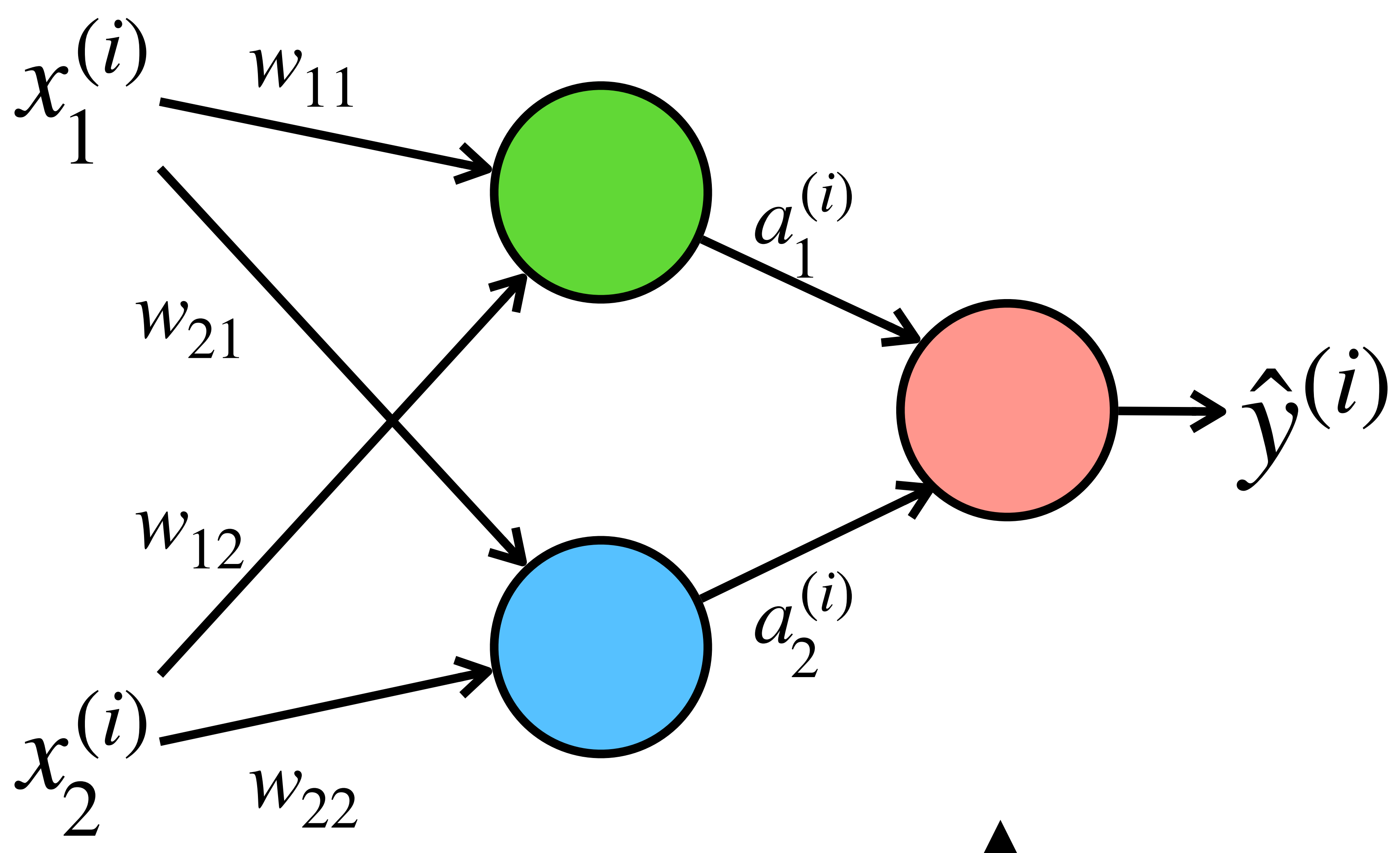
$$W^{[1]} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \quad b^{[1]} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$W^{[2]} = [0 \quad 0]$$

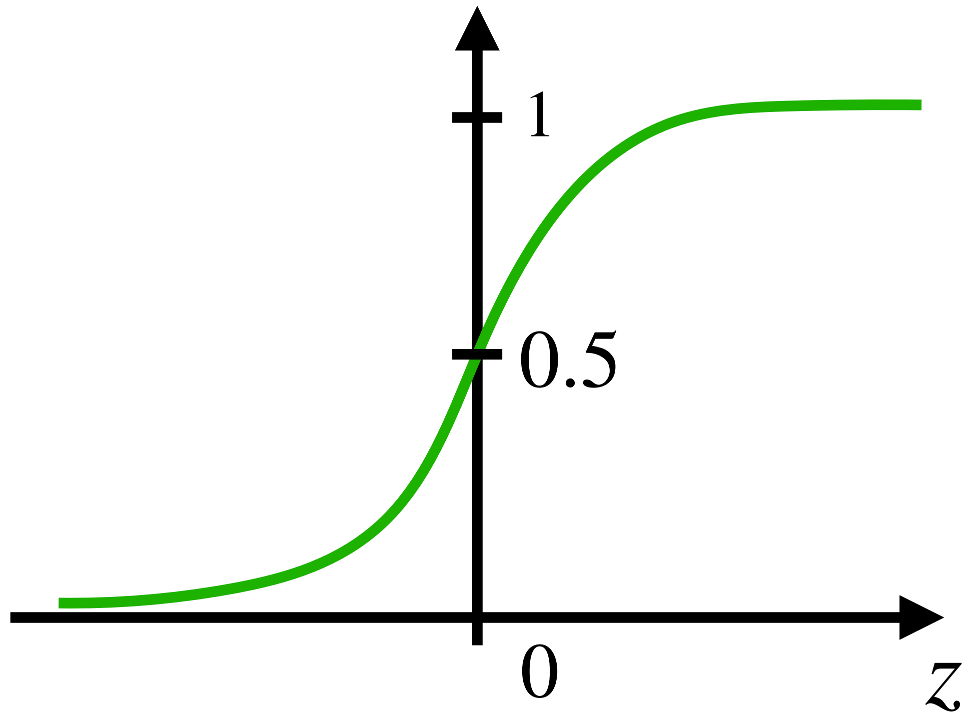
$$\downarrow$$

$$a_1^{(i)} = a_2^{(i)} \longrightarrow dZ_1^{[1]} = dZ_2^{[1]}$$

$$dW = \begin{bmatrix} u & u \\ u & u \end{bmatrix}$$



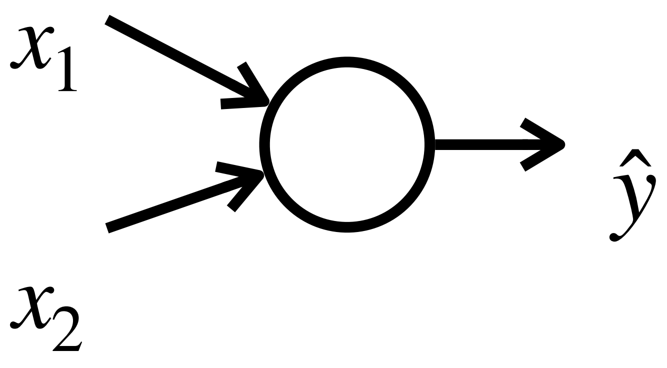
Ns regiões próximas de zero o gradiente é maior!



Redes Neurais Artificiais Profundas

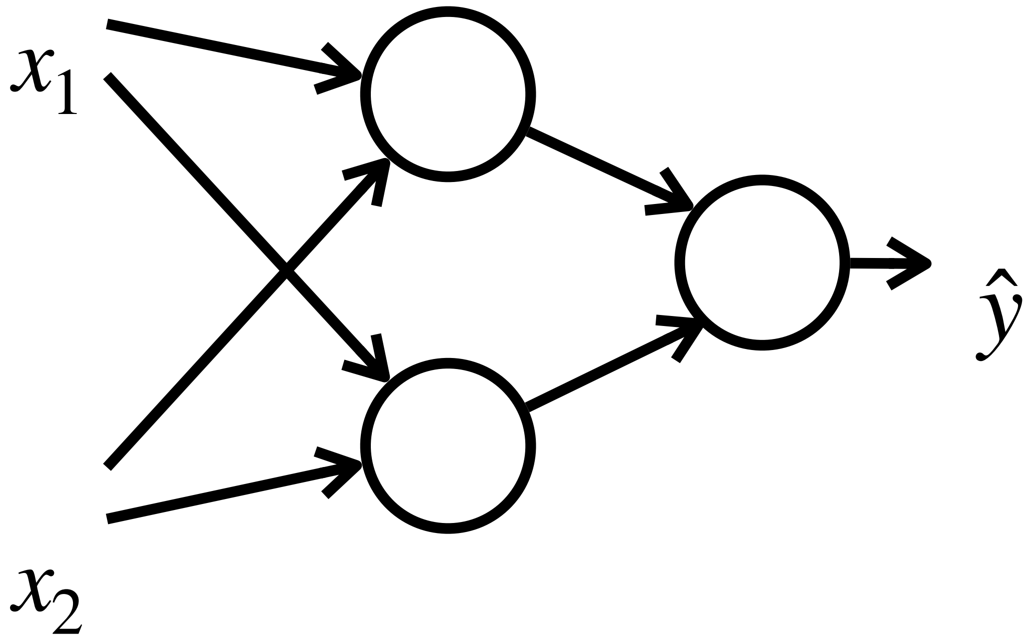
Regressão Logística

RNA de 1 camada (raza)



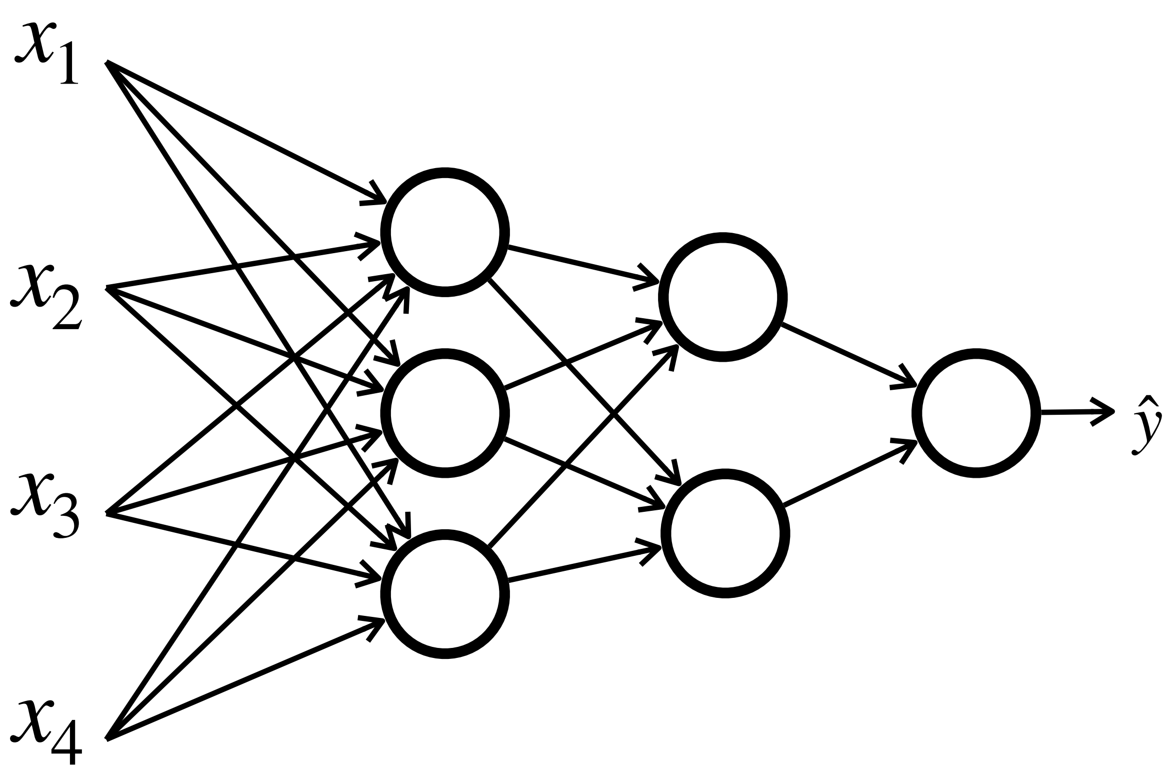
1 camada oculta

RNA de 2 camadas (raza)



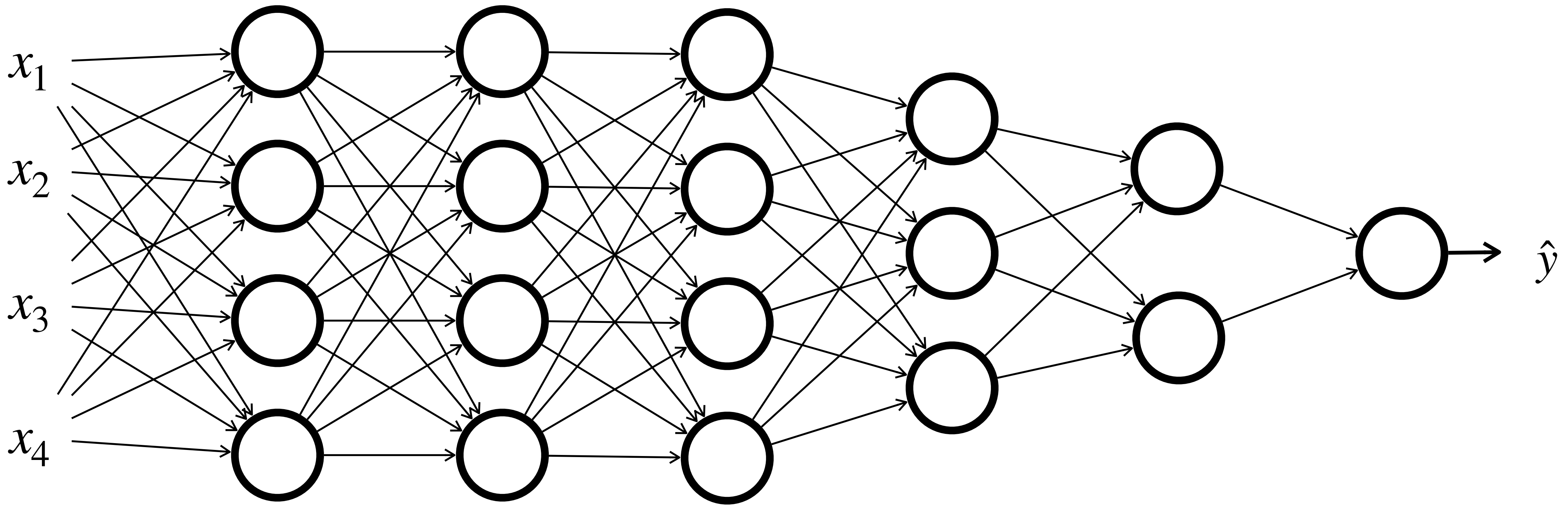
2 camadas ocultas

RNA de 3 camadas (raza)



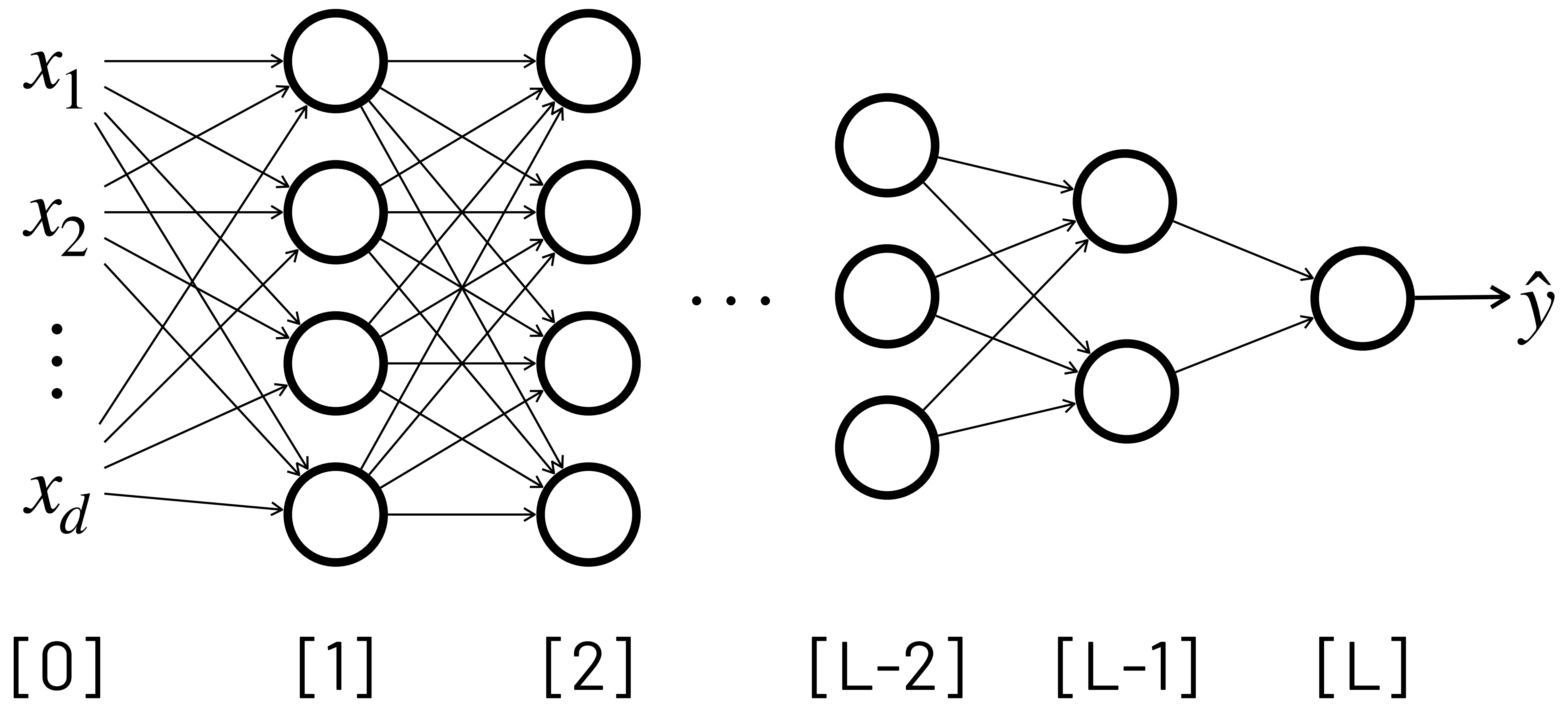
5 camadas ocultas

RNA de 6 camadas (profunda)



Redes Neurais Artificiais Profundas

RNA de L camadas



Para um exemplo $\mathbf{x}$:

$$\mathbf{z}^{[1]} = W^{[1]}\mathbf{x} + \mathbf{b}^{[1]}$$
$$\mathbf{a}^{[1]} = g(\mathbf{z}^{[1]})$$
$$\mathbf{z}^{[2]} = W^{[2]}\mathbf{a}^{[1]} + \mathbf{b}^{[2]}$$
$$\mathbf{a}^{[2]} = g(\mathbf{z}^{[2]})$$
$$\cdots$$
$$\mathbf{z}^{[L]} = W^{[L]}\mathbf{a}^{[L-1]} + b^{[L]}$$
$$\hat{y} = \sigma(\mathbf{z}^{[L]})$$

Regra geral:

$$\mathbf{z}^{[l]} = W^{[l]}\mathbf{a}^{[l-i]} + \mathbf{b}^{[l]}$$
$$\mathbf{a}^{[l]} = g(\mathbf{z}^{[l]})$$

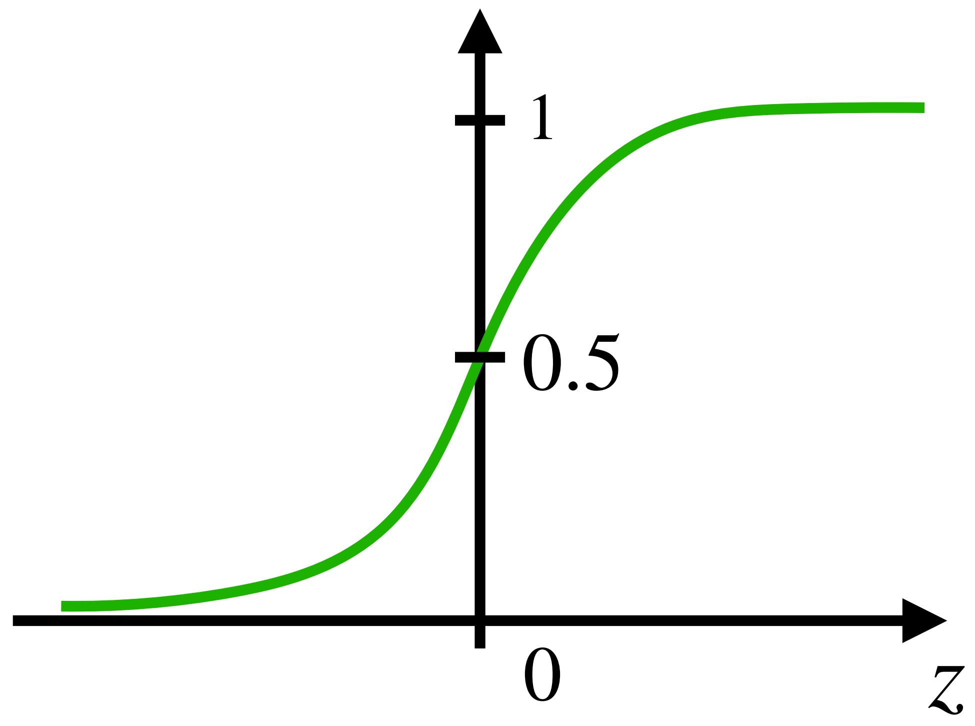
Vetorizado

$$Z^{[l]} = W^{[l]}A^{[l-1]} + \mathbf{b}^{[l]}$$
$$\mathbf{A}^{[l]} = g(Z^{[l]})$$

$$A^{[0]} = X$$
$$A^{[L]} = \hat{Y}$$

Funções de ativação na camada de saída

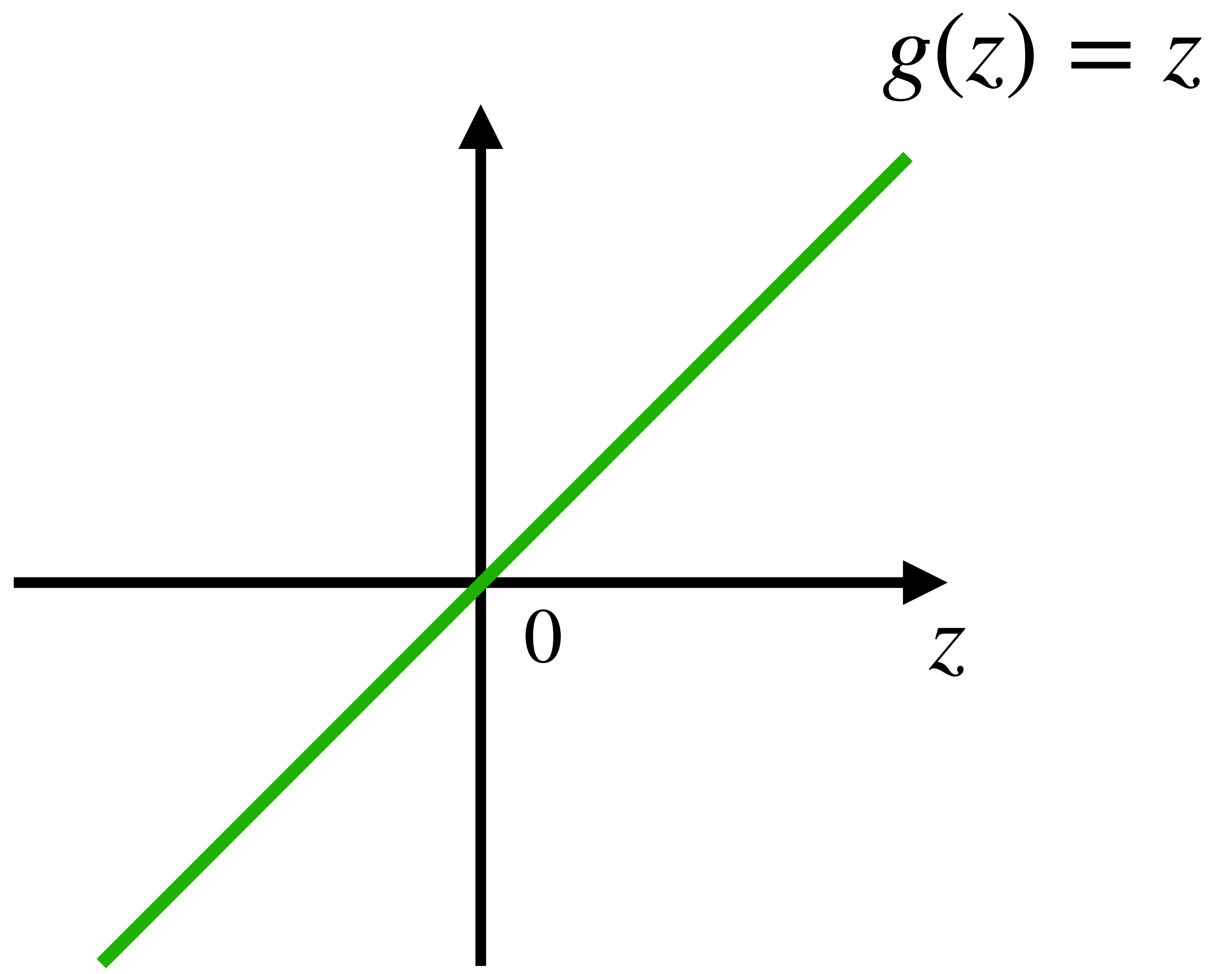
Logística (sigmoide)



$$g(z) = \frac{1}{(1 + e^{-z})}$$

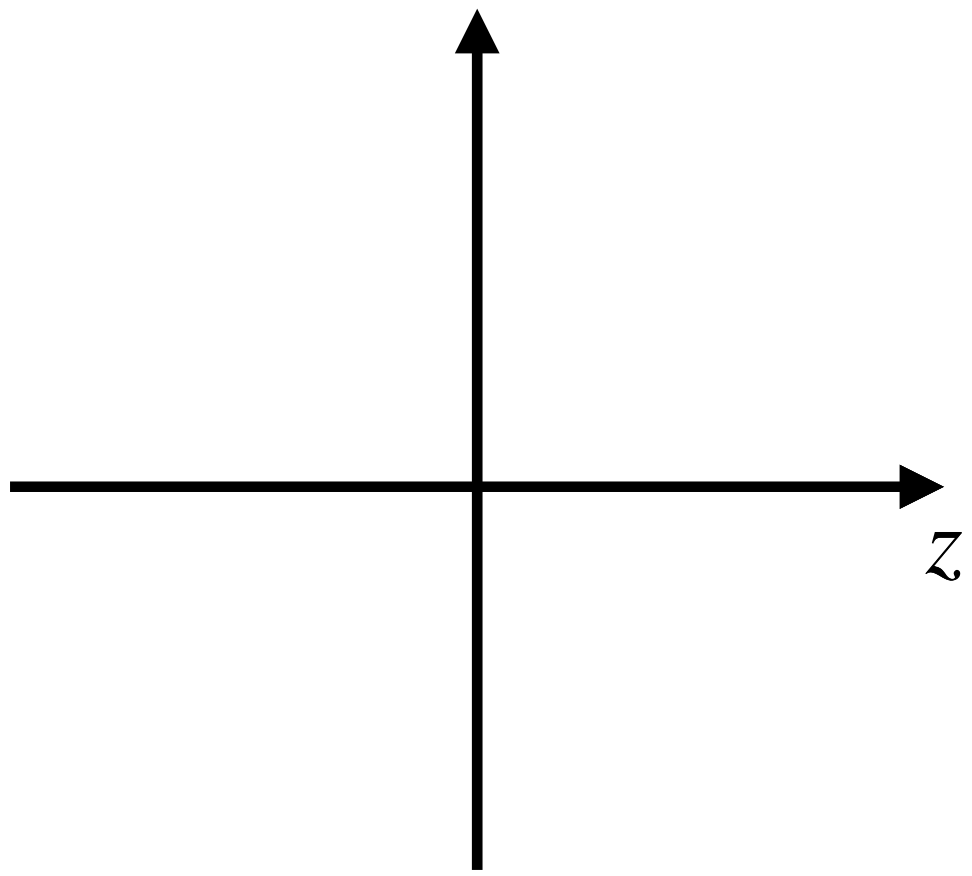
Classificação Binária

Linear



Regressão

?



Classificação Multiclasse

UFV

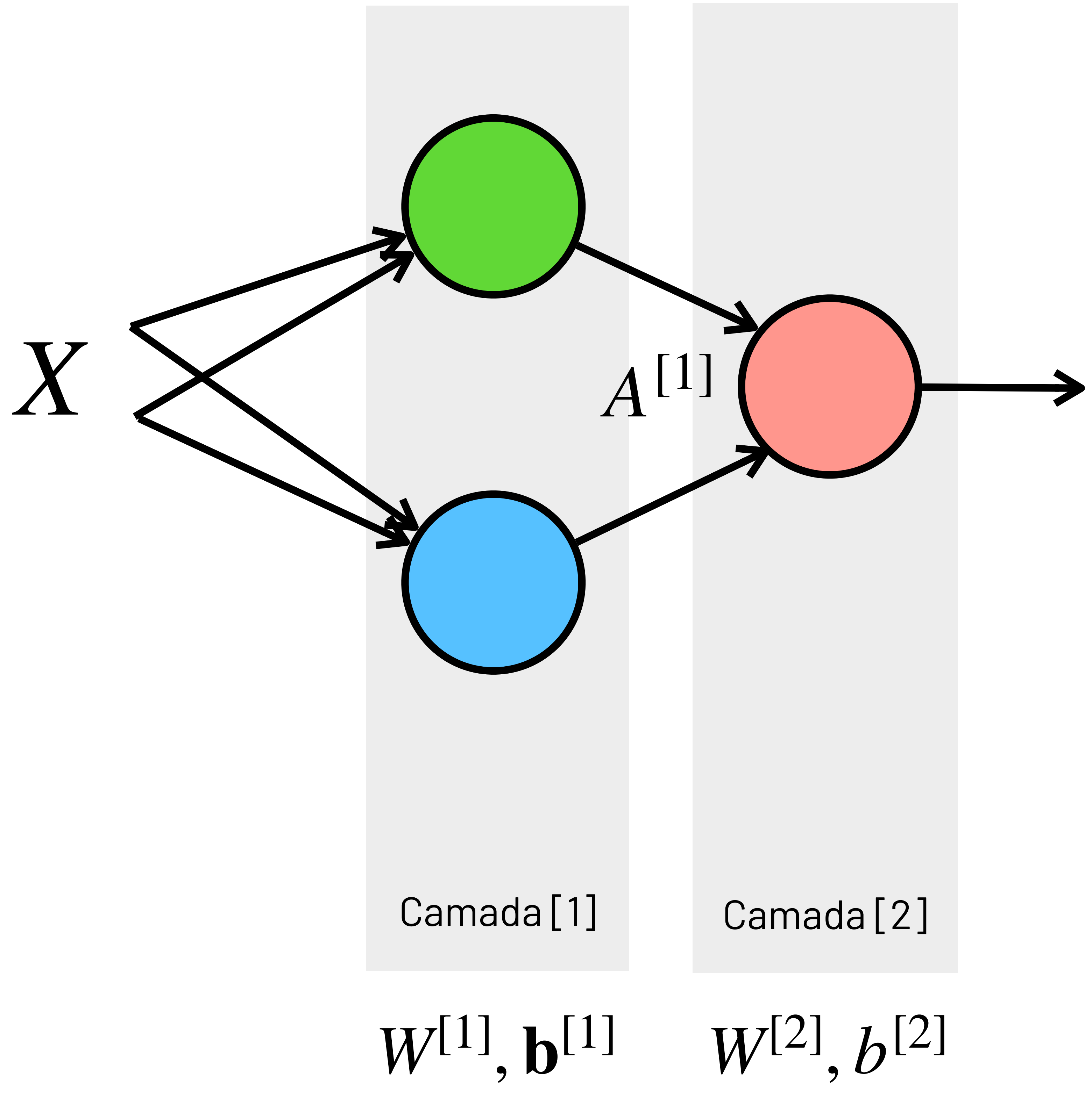
Função de ativação softmax para classificação multiclasse

Hipótese

$$Z^{[1]} = W^{[1]}X + \mathbf{b}^{[1]}$$
$$A^{[1]} = g(Z^{[1]})$$
$$Z^{[2]} = W^{[2]}\mathbf{a}^{[1]} + \mathbf{b}^{[2]}$$
$$\hat{Y} = softmax(Z^{[2]})$$

Softmax

$$g(z) = \frac{e^z}{\sum_{j=i}^{C} e_i^z}$$



$$Z = \begin{bmatrix} 5 \\ 2 \\ -1 \\ 3 \end{bmatrix} \quad e^z = \frac{\begin{bmatrix} e^5 \\ e^2 \\ e^{-1} \\ e^3 \end{bmatrix}}{\sum_{j=i}^{C} e_i^z = 176.3}$$

Probabilidades

$$\hat{y} = \begin{bmatrix} 0.842 \\ 0.042 \\ 0.002 \\ 0.114 \end{bmatrix} \begin{array}{l} \text{Classe 0} \\ \text{Classe 1} \\ \text{Classe 2} \\ \text{Classe 3} \end{array}$$

Próxima aula

A7: MLP em Numpy

Aula prática sobre implementação de redes neurais profundas com Numpy.