



"The Bitter Lesson"



Rich Sutton 强化学习之父

The biggest lesson that can be read from 70 years of AI research is that general methods that **leverage computation** are ultimately the most effective, and by a large margin

We want AI agents that can **discover like we can**, not which contain what we have discovered. Building in our discoveries only makes it harder to see how the discovering process can be done.

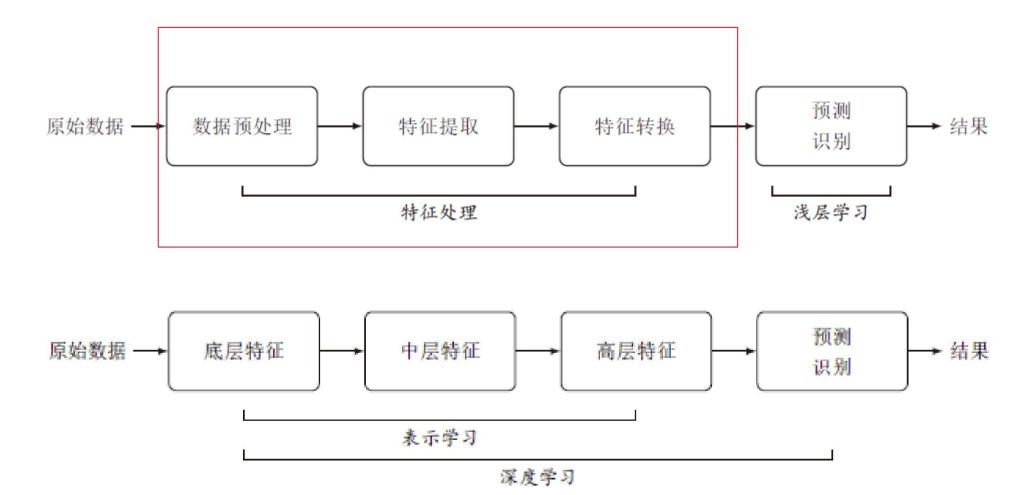
- AI 研究人员常常试图在自身智能体中构建知识,
- 从短期看,这通常是有帮助的,能够令研究人员满意,
- 但从长远看,这会令研究人员停滞不前,甚至抑制进一步发展,
- 突破性进展最终可能会通过一种相反的方法——基于以大规模计算为基础的搜索和学习



回顾: 特征工程问题

□ 模型

在实际应用中,特征往往比分类器更重要



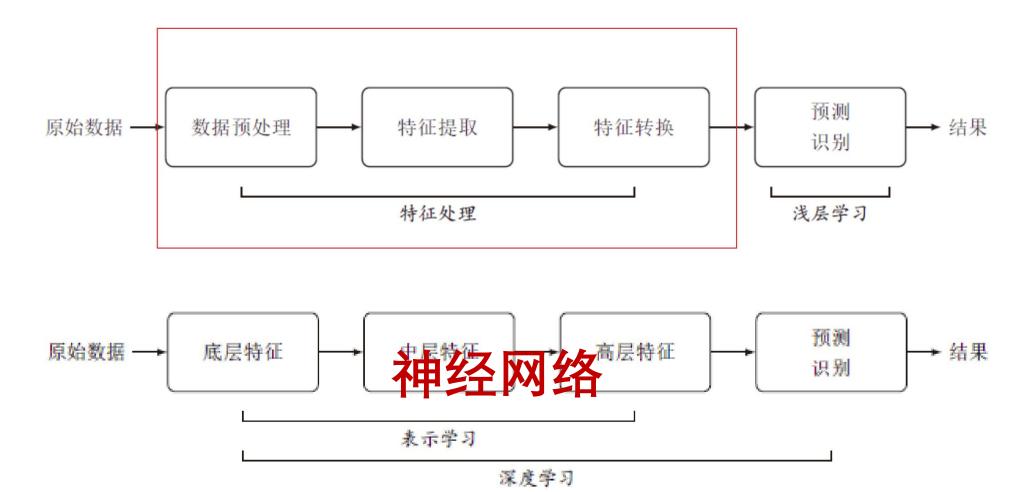
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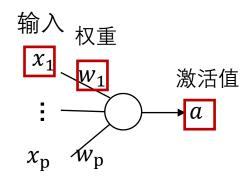
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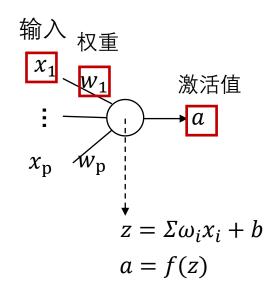


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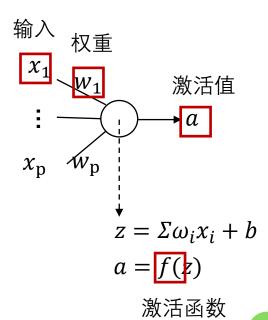


- □ 神经网络的基本概念
- □ 循环神经网络
- □ 卷积神经网络

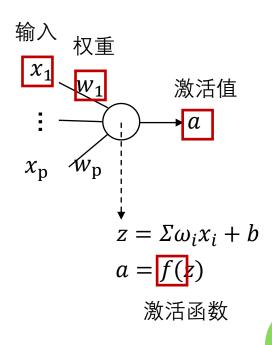




一个神经元是一个多元、复合函数



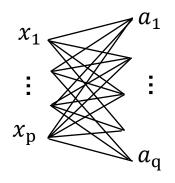
根据万能逼近定理,一个包含至少一层隐 含层和非线性激活函数的神经网络可以逼 近任何连续函数



激活函数	函数	导数
Logistic 函数	$f(x) = \frac{1}{1 + \exp(-x)}$	f'(x) = f(x)(1 - f(x))
Tanh 函数	$f(x) = \frac{\exp(x) - \exp(-x)}{\exp(x) + \exp(-x)}$	$f'(x) = 1 - f(x)^2$
ReLU 函数	$f(x) = \max(0, x)$	f'(x) = I(x > 0)
ELU函数	$f(x) = \max(0, x) + \min(0, \gamma(\exp(x) - 1))$	$f'(x) = I(x > 0) + I(x \le 0) \cdot \gamma \exp(x)$
SoftPlus 函数	$f(x) = \log(1 + \exp(x))$	$f'(x) = \frac{1}{1 + \exp(-x)}$

- •ReLU**及其变体**:由于其**计算效率高**且在许多情况下性能良好, ReLU通常是隐藏层的首选。它有**助于缓解梯度消失问题**,特别适 用于深层网络。
- •Tanh: 当数据中心化(均值为0)时, Tanh函数是一个好的选择, 因为它的输出范围是-1到1, 这有助于数据的平滑传递。
- •Sigmoid: 尽管在隐藏层较少使用,但在需要输出概率或进行精细控制时(例如在某些类型的循环神经网络中),仍然可以考虑 Sigmoid函数。

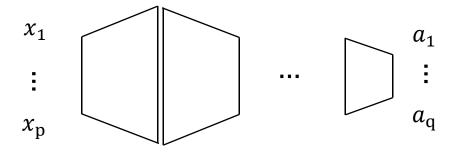
神经层



$$\boldsymbol{a} = f(\boldsymbol{W}\boldsymbol{x} + b)$$

- · 一个神经层包含**多个**神经元
- 每个神经元**输入都是相同**的,但激活方式不一样
- 一个神经层是一个多元向量函数

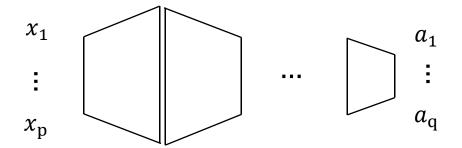




浅层神经网络

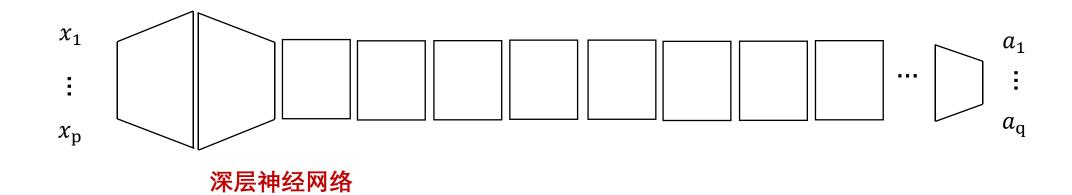
- · 将神层堆叠起来
- 输入输出维度要的对齐



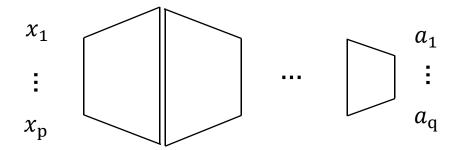


- 将神层堆叠起来
- 输入输出维度要的对齐
- 神经网络可以一直加深

浅层神经网络

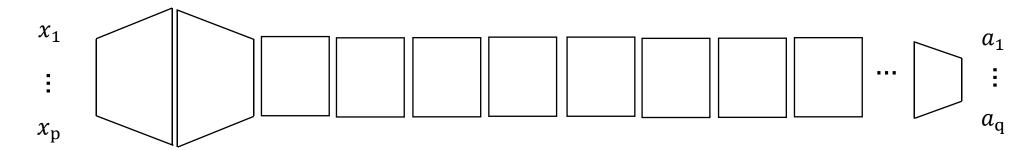






- 将神层堆叠起来
- 输入输出维度要的对齐
- 神经网络可以一直加深

浅层神经网络



深层神经网络

大语言模型是一个深度神经网络模型。比如LLaMa2 70B网络层数为80



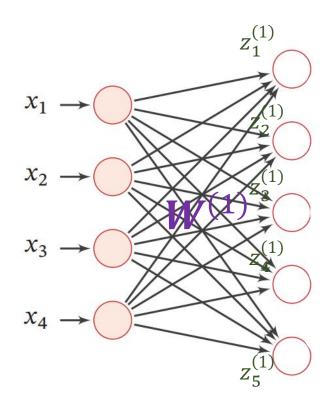
$$x_1 \rightarrow \bigcirc$$

$$x_2 \rightarrow$$

$$x_3 \rightarrow$$

$$x_4 \rightarrow$$



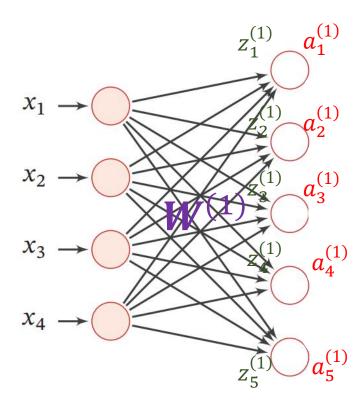


$$a^0(i.e., x) \rightarrow z^1$$

线性变换

$$z^{l+1} = W^l a^l + b^l$$



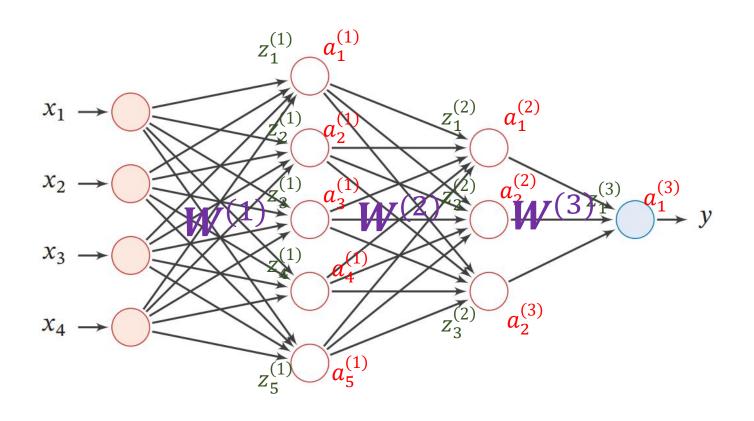


$$a^0(i.e., x) \rightarrow z^1 \rightarrow a^1$$

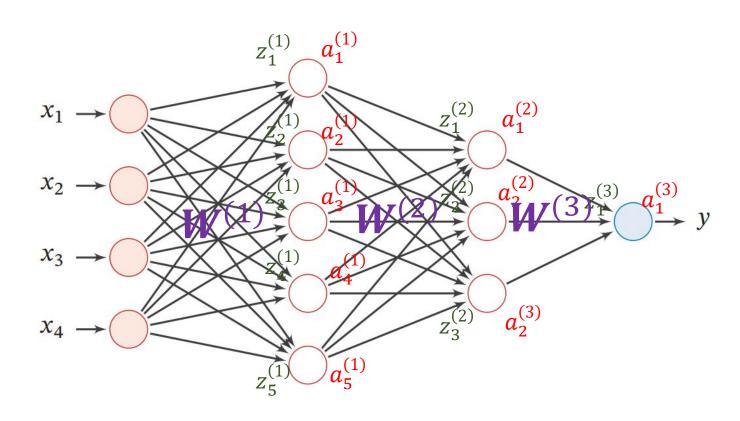
非线性变换

$$a^l = f(z^l)$$





$$a^0(i.e., x) \rightarrow z^1 \rightarrow a^1 \rightarrow z^2 \rightarrow a^2... \rightarrow z^L \rightarrow a^L$$
 多次正向传播



超参数

L: 层数

n^l:神经元数目

 f^l 激活函数

学习参数

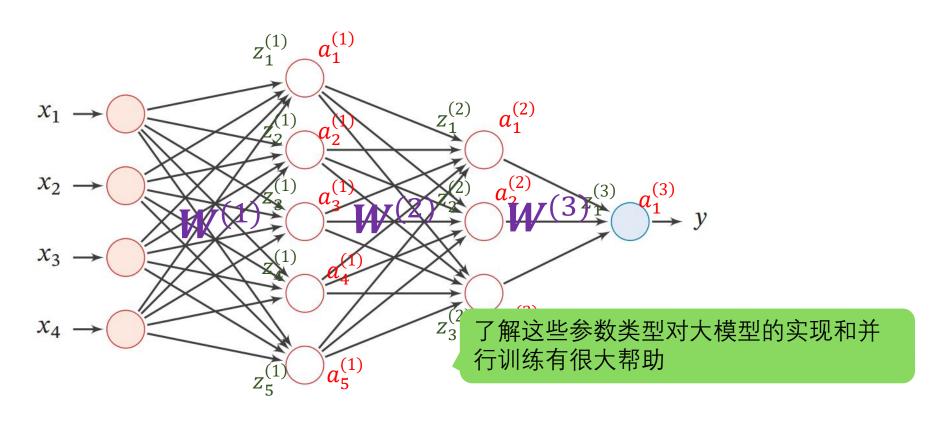
W^l:连接权重

b^l:l层偏置

状态量

 z^l : l层神经元状态

 a^l : l层神经元激活



超参数

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- □ 数据: (x_i, y_i)
- \Box 模型: $\{y = h(x|w,b), w,b\}$
- □ 优化准则:
 - 损失函数: $\mathcal{L}(\mathbf{y}, \hat{\mathbf{y}}) = -\mathbf{y}^{\mathsf{T}} \log \hat{\mathbf{y}},$
 - 经验损失函数
 - $L(y_i, h(x_i|w,b)) + \lambda ||w||^2 = L(y_i, a^L(x_i))$

- □ 数据: (x_i, y_i)
- □ 模型: $\{y = h(x|w,b), w,b\}$
- □ 优化准则:
 - 损失函数: $\mathcal{L}(\mathbf{y}, \hat{\mathbf{y}}) = -\mathbf{y}^{\mathsf{T}} \log \hat{\mathbf{y}},$
 - 经验损失函数: $\mathcal{R}(\mathbf{W}, \mathbf{b}) = \frac{1}{N} \sum_{n=1}^{N} \mathcal{L}(\mathbf{y}^{(n)}, \hat{\mathbf{y}}^{(n)})$

$$\mathbf{W}^{(l)} \leftarrow \mathbf{W}^{(l)} - \alpha \frac{\partial \mathcal{R}(\mathbf{W}, \mathbf{b})}{\partial \mathbf{W}^{(l)}}$$

$$= \boldsymbol{W}^{(l)} - \alpha \left(\frac{1}{N} \sum_{n=1}^{N} \left(\frac{\partial \mathcal{L}(\boldsymbol{y}^{(n)}, \hat{\boldsymbol{y}}^{(n)})}{\partial \boldsymbol{W}^{(l)}} \right) + \lambda \boldsymbol{W}^{(l)} \right),$$

$$\boldsymbol{b}^{(l)} \leftarrow \boldsymbol{b}^{(l)} - \alpha \frac{\partial \mathcal{R}(\boldsymbol{W}, \boldsymbol{b})}{\partial \boldsymbol{b}^{(l)}}$$

$$= \boldsymbol{b}^{(l)} - \alpha \left(\frac{1}{N} \sum_{n=1}^{N} \frac{\partial \mathcal{L}(\boldsymbol{y}^{(n)}, \hat{\boldsymbol{y}}^{(n)})}{\partial \boldsymbol{b}^{(l)}} \right),$$

梯度下降法更新参数

- □ 数据: (x_i, y_i)
- □ 模型: $\{y = h(x|w,b), w,b\}$
- □ 优化准则:
 - 损失函数: $\mathcal{L}(\mathbf{y}, \hat{\mathbf{y}}) = -\mathbf{y}^{\mathsf{T}} \log \hat{\mathbf{y}}$,
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$$\frac{\partial \mathcal{R}(\mathbf{W}, \mathbf{b})}{\partial \mathbf{W}^{(l)}}$$

$$\boldsymbol{b}^{(l)} \leftarrow \boldsymbol{b}^{(l)} - \alpha \frac{\partial \mathcal{R}(\boldsymbol{W}, \boldsymbol{b})}{\partial \boldsymbol{b}^{(l)}}$$

$$= \boldsymbol{b}^{(l)} - \alpha \left(\frac{1}{N} \sum_{n=1}^{N} \frac{\partial \mathcal{L}(\boldsymbol{y}^{(n)}, \hat{\boldsymbol{y}}^{(n)})}{\partial \boldsymbol{b}^{(l)}} \right),$$

偏导数求解

参数更新
$$\mathbf{w}^{(l)} = \frac{\partial \mathcal{L}(\mathbf{y}, \hat{\mathbf{y}})}{\partial w_{ij}^{(l)}} = \frac{\partial \mathbf{z}^{(l)}}{\partial w_{ij}^{(l)}} \frac{\partial \mathcal{L}(\mathbf{y}, \hat{\mathbf{y}})}{\partial \mathbf{z}^{(l)}},$$

$$\mathbf{b}^{(l)} = \frac{\partial \mathcal{L}(\mathbf{y}, \hat{\mathbf{y}})}{\partial \mathbf{b}^{(l)}} = \frac{\partial \mathcal{L}(\mathbf{y}, \hat{\mathbf{y}})}{\partial \mathbf{b}^{(l)}} \frac{\partial \mathcal{L}(\mathbf{y}, \hat{\mathbf{y}})}{\partial \mathbf{z}^{(l)}}.$$

$$\frac{\partial \mathcal{L}(\mathbf{y}, \hat{\mathbf{y}})}{\partial \mathbf{b}^{(l)}} \frac{\partial \mathcal{L}(\mathbf{y}, \hat{\mathbf{y}})}{\partial \mathbf{z}^{(l)}}.$$

链式法则 (Chain Rule)

若
$$z = f(y)$$
 $y = g(x)$ 则:

$$x \to y \to z$$

$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$$

若
$$z = f(x,y), x = g(t), y = h(t)$$
 则:

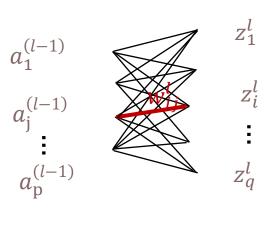
$$t \xrightarrow{x} z \qquad \frac{dz}{dt} = \frac{dz}{dy}\frac{dy}{dt} + \frac{dz}{dx}\frac{dx}{dt}$$

参与计算的路径都会 获得梯度



- (1) 先正向思考因变量是怎么由自变量计算出来的
- (2) 参与计算的才有资格拿到梯度

$$\begin{split} \frac{\partial \boldsymbol{z}^{(l)}}{\partial w_{ij}^{(l)}} &= \left[\frac{\partial z_{1}^{(l)}}{\partial w_{ij}^{(l)}}, \cdots, \frac{\partial z_{i}^{(l)}}{\partial w_{ij}^{(l)}}, \cdots, \frac{\partial z_{M_{l}}^{(l)}}{\partial w_{ij}^{(l)}}\right] \\ &= \left[0, \cdots, \frac{\partial (\boldsymbol{w}_{i:}^{(l)} \boldsymbol{a}^{(l-1)} + b_{i}^{(l)})}{\partial w_{ij}^{(l)}}, \cdots, 0\right] \\ &= \left[0, \cdots, a_{j}^{(l-1)}, \cdots, 0\right] \\ &\triangleq \mathbb{I}_{i}(a_{j}^{(l-1)}) \quad \in \mathbb{R}^{1 \times M_{l}}, \end{split}$$



计算
$$\frac{\partial z^{(l)}}{\partial b^{(l)}}$$

$$\frac{\partial \boldsymbol{z}^{(l)}}{\partial \boldsymbol{b}^{(l)}} = \boldsymbol{I}_{M_l} \quad \in \mathbb{R}^{M_l \times M_l}$$

为 $M_l \times M_l$ 的单位矩阵

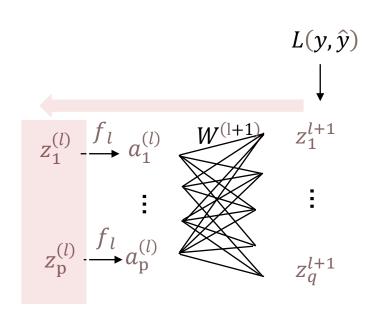
计算
$$\frac{\partial \mathcal{L}(y, \hat{y})}{\partial z^{(l)}}$$

$$\delta^{(l)} \triangleq \frac{\partial \mathcal{L}(\boldsymbol{y}, \hat{\boldsymbol{y}})}{\partial \boldsymbol{z}^{(l)}}$$

$$= \underbrace{\frac{\partial \boldsymbol{a}^{(l)}}{\partial \boldsymbol{z}^{(l)}} \cdot \frac{\partial \boldsymbol{z}^{(l+1)}}{\partial \boldsymbol{a}^{(l)}} \cdot \frac{\partial \mathcal{L}(\boldsymbol{y}, \hat{\boldsymbol{y}})}{\partial \boldsymbol{z}^{(l+1)}}}_{\boldsymbol{z}^{(l+1)}}$$

$$= \underbrace{\operatorname{diag}(f_l'(\boldsymbol{z}^{(l)})) \cdot (\boldsymbol{W}^{(l+1)})^{\mathsf{T}} \cdot \delta^{(l+1)}}_{\boldsymbol{z}^{(l+1)}}$$

$$= f_l'(\boldsymbol{z}^{(l)}) \odot \left((\boldsymbol{W}^{(l+1)})^{\mathsf{T}} \delta^{(l+1)} \right) \in \mathbb{R}^{M_l}$$



参数更新



反向传播算法

算法 4.1 使用反向传播算法的随机梯度下降训练过程

输入: 训练集 $\mathcal{D} = \{(x^{(n)}, y^{(n)})\}_{n=1}^{N}$, 验证集 \mathcal{V} , 学习率 α , 正则化系数 λ , 网络层数 L, 神经元数量 M_{l} , $1 \leq l \leq L$.

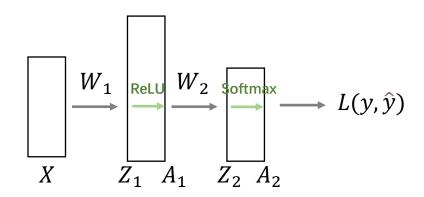
1 随机初始化 W,b;

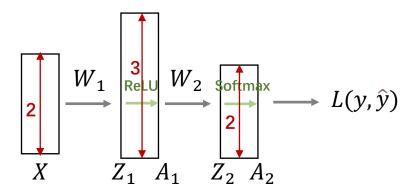
```
2 repeat
            对训练集\mathcal{D}中的样本随机重排序;
 3
           for n = 1 \cdots N do
                   从训练集\mathcal{D}中选取样本(\mathbf{x}^{(n)}, \mathbf{y}^{(n)});
 5
                   前馈计算每一层的净输入\mathbf{z}^{(l)}和激活值\mathbf{a}^{(l)},直到最后一层;
                   反向传播计算每一层的误差\delta^{(l)};
                                                                                                               // 公式 (4.63)
                   // 计算每一层参数的导数
                                 \frac{\partial \mathcal{L}(\mathbf{y}^{(n)}, \hat{\mathbf{y}}^{(n)})}{\partial \mathbf{w}^{(l)}} = \delta^{(l)}(\boldsymbol{a}^{(l-1)})^{\mathsf{T}};
                                                                                                                // 公式 (4.68)
 8
                                \frac{\partial \mathcal{L}(\mathbf{y}^{(n)}, \mathbf{\hat{y}}^{(n)})}{\partial \mathcal{L}(\mathbf{y}^{(n)}, \mathbf{\hat{y}}^{(n)})} = \delta^{(l)};
                                                                                                               // 公式 (4.69)
                   // 更新参数
                   \boldsymbol{W}^{(l)} \leftarrow \boldsymbol{W}^{(l)} - \alpha(\delta^{(l)}(\boldsymbol{a}^{(l-1)})^{\mathsf{T}} + \lambda \boldsymbol{W}^{(l)});
10
                  \mathbf{b}^{(l)} \leftarrow \mathbf{b}^{(l)} - \alpha \delta^{(l)};
11
            end
12
13 until 神经网络模型在验证集 V上的错误率不再下降;
     输出: W, b
```

- □ 假设我们要构建一个简单的**前馈神 经网络**,用于解决**二分类**问题
 - 输入层: 2个特征
 - 隐藏层: 1个,使用3个神经元, 激活函数为ReLU
 - 输出层: **2**个神经元(对应于两个类别),激活函数为softmax
 - 交叉熵做损失函数
 - 两个训练样本
 - □ [0.1, 0.2] -> [1,0]
 - □ [0.3, 0.4] -> [0,1]

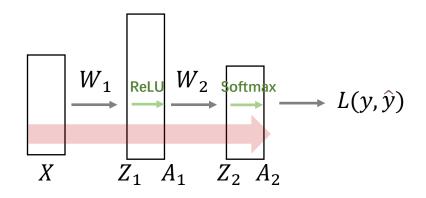


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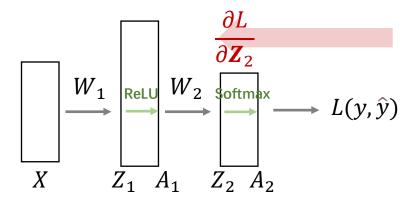
```
import numpy as np
# 初始化参数
np.random.seed(42) # 确保每次运行结果一致
input_size = 2 # 輸入层节点数
hidden_size = 3 # 隐藏层节点数
output_size = 2 # 輸出层节点数
learning rate = 0.1 # 学习率
# 随机初始化权重和偏置
W1 = np.random.randn(input_size, hidden_size)
b1 = np.zeros(hidden_size)
W2 = np.random.randn(hidden_size, output_size)
b2 = np.zeros(output_size)
# ReLU激活函数及其导数
def relu(x):
   return np.maximum(0, x)
def relu_derivative(x):
   return (x > 0).astype(float)
# Softmax函数
def softmax(x):
   exp_x = np.exp(x - np.max(x, axis=1, keepdims=True))
   return exp_x / np.sum(exp_x, axis=1, keepdims=True)
# 交叉熵损失及其导数
def cross_entropy_loss(y_pred, y_true):
   m = y_true.shape[0]
   return -np.sum(y_true * np.log(y_pred)) / m
def delta_cross_entropy_softmax(y_pred, y_true):
   return y_pred - y_true
```



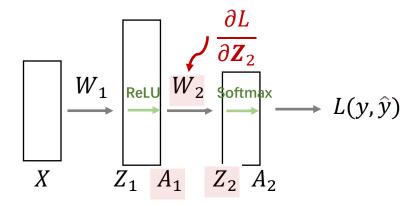
```
# 前向传播

def forward_propagation(X):
    Z1 = X.dot(W1) + b1
    A1 = relu(Z1)
    Z2 = A1.dot(W2) + b2
    A2 = softmax(Z2)
    return Z1, A1, Z2, A2
```

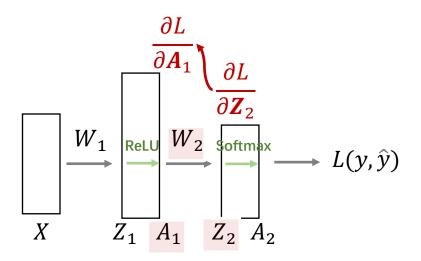
真实实现中要时刻留心矩阵的维度



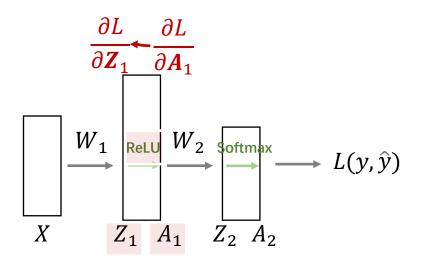
```
# 反向传播
def backward_propagation(X, Y, Z1, A1, Z2, A2):
   m = X.shape[0]
   dZ2 = delta_cross_entropy_softmax(A2, Y)
   dW2 = (1/m) * np.dot(A1.T, dZ2)
   db2 = (1/m) * np.sum(dZ2, axis=0)
   dA1 = np.dot(dZ2, W2.T)
   dZ1 = dA1 * relu derivative(Z1)
   dW1 = (1/m) * np.dot(X.T, dZ1)
   db1 = (1/m) * np.sum(dZ1, axis=0)
   return dW1, db1, dW2, db2
# 更新参数
def update_parameters(dW1, db1, dW2, db2):
   global W1, b1, W2, b2
   W1 -= learning_rate * dW1
   b1 -= learning_rate * db1
   W2 -= learning_rate * dW2
   b2 -= learning_rate * db2
```



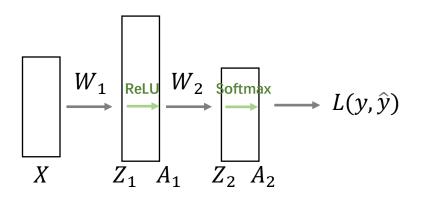
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    return dW1, db1, dW2, db2
# 更新参数
def update_parameters(dW1, db1, dW2, db2):
    global W1, b1, W2, b2
   W1 -= learning_rate * dW1
   b1 -= learning_rate * db1
   W2 -= learning_rate * dW2
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```



```
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    dZ2 = delta_cross_entropy_softmax(A2, Y)
    dW2 = (1/m) * np.dot(A1.T, dZ2)
    db2 = (1/m) * np.sum(dZ2, axis=0)
   dA1 = np.dot(dZ2, W2.T)
    dZ1 = dA1 * relu derivative(Z1)
    dW1 = (1/m) * np.dot(X.T, dZ1)
    db1 = (1/m) * np.sum(dZ1, axis=0)
    return dW1, db1, dW2, db2
# 更新参数
def update_parameters(dW1, db1, dW2, db2):
    global W1, b1, W2, b2
   W1 -= learning_rate * dW1
    b1 -= learning_rate * db1
   W2 -= learning_rate * dW2
    b2 -= learning_rate * db2
```



```
# 反向传播
def backward_propagation(X, Y, Z1, A1, Z2, A2):
    m = X.shape[0]
    dZ2 = delta_cross_entropy_softmax(A2, Y)
    dW2 = (1/m) * np.dot(A1.T, dZ2)
    db2 = (1/m) * np.sum(dZ2, axis=0)
    dA1 = np.dot(dZ2, W2.T)
    dZ1 = dA1 * relu derivative(Z1)
    dW1 = (1/m) * np.dot(X.T, dZ1)
    db1 = (1/m) * np.sum(dZ1, axis=0)
    return dW1, db1, dW2, db2
# 更新参数
def update_parameters(dW1, db1, dW2, db2):
    global W1, b1, W2, b2
   W1 -= learning_rate * dW1
    b1 -= learning_rate * db1
   W2 -= learning_rate * dW2
    b2 -= learning_rate * db2
```



```
# 示例输入和标签
X = np.array([[0.1, 0.2], [0.3, 0.4]]) # 2个样本
Y = np.array([[1, 0], [0, 1]]) # 对应的one-hot标签

# 执行一次前向传播
Z1, A1, Z2, A2 = forward_propagation(X)

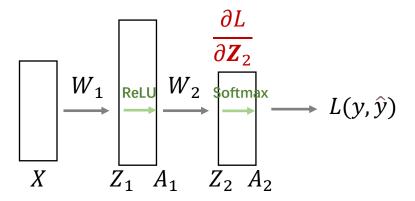
# 计算损失
loss = cross_entropy_loss(A2, Y)

# 执行一次反向传播
dW1, db1, dW2, db2 = backward_propagation(X, Y, Z1, A1, Z2, A2)

# 更新参数
update_parameters(dW1, db1, dW2, db2)
```



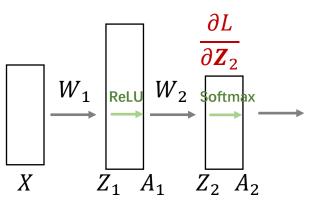
深层网络: 计算开销大

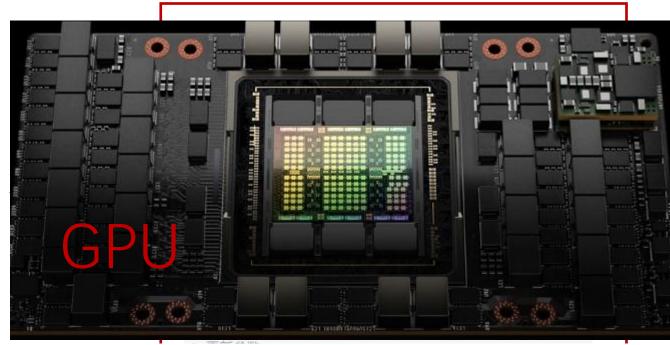


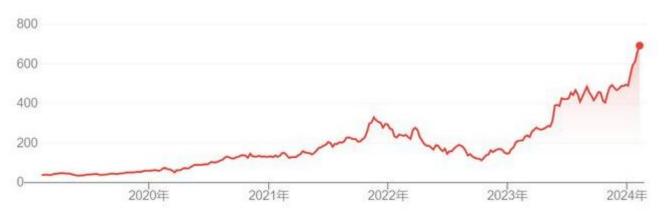
```
# 前向传播
def forward_propagation(X):
   Z1 = X.dot(W1) + b1
   A1 = relu(Z1)
                                  如果是100层呢?
   Z2 = A1.dot(W2) + b2
   A2 = softmax(Z2)
   return Z1, A1, Z2, A2
# 反向传播
def backward_propagation(X, Y, Z1, A1, Z2, A2):
    m = X.shape[0]
   dZ2 = delta_cross_entropy_softmax(A2, Y)
   dW2 = (1/m) * np.dot(A1.T, dZ2)
   db2 = (1/m) * np.sum(dZ2, axis=0)
   dA1 = np.dot(dZ2, W2.T)
   dZ1 = dA1 * relu_derivative(Z1)
   dW1 = (1/m) * np.dot(X.T, dZ1)
   db1 = (1/m) * np.sum(dZ1, axis=0)
   return dW1, db1, dW2, db2
```



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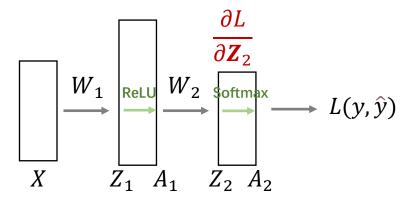








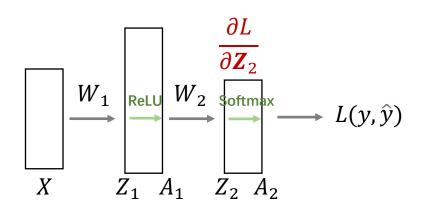
深层网络: 反向传播求导很繁琐



```
# 反向传播
def backward_propagation(X, Y, Z1, A1, Z2, A2):
   m = X.shape[0]
   dZ2 = delta cross entropy softmax(A2, Y)
   dW2 = (1/m) * np.dot(A1.T, dZ2)
   db2 = (1/m) * np.sum(dZ2, axis=0)
   dA1 = np.dot(dZ2, W2.T)
   dZ1 = dA1 * relu derivative(Z1)
   dW1 = (1/m) * np.dot(X.T, dZ1)
   db1 = (1/m) * np.sum(dZ1, axis=0)
   return dW1, db1, dW2, db2
# 更新参数
def update_parameters(dW1, db1, dW2, db2):
   global W1, b1, W2, b2
   W1 -= learning_rate * dW1
   b1 -= learning_rate * db1
   W2 -= learning_rate * dW2
   b2 -= learning_rate * db2
```



深层网络: 反向传播求导很繁琐



















从特征工程 到 结构工程

□ 神经网络避免了繁琐的**手工设计特征**过程,但需要**人工设计网络结构**



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- □ 不同网络结构往往包含了**不同的结构先验** (inductive bias)
- □ 不同的**任务、模态**可能需要不同结构的网络



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- □ 常见网络架构
 - 循环神经网络
 - 卷积神经网络
 - 递归神经网络
 - 图神经网络