Chapter 5

# Deep feedforward networks

Neural networks and deep learning

# Chain rule of differentiation

Let $x, y, J \in \boldsymbol{R}$ be one-dimensional variables and

$$y = f(x)$$
$$J = g(y)$$

Chain rule of differentiation states that:

$$\frac{\partial J}{\partial x} = \frac{\partial J}{\partial y}\frac{\partial y}{\partial x}$$

$$\nabla_x J = \left(\frac{\partial y}{\partial x}\right) \nabla_y J$$

$$\begin{tikzcd} \nabla_x J & \nabla_y J & \\ x \arrow[r, "f"] & y \arrow[r, "g"] & J \end{tikzcd}$$

Note the transfer of gradient of $J$ from $y$ to $x$.

# Chain rule in multidimensions

$$\begin{tikzcd}
\nabla_{x} J & \nabla_{y} J & \\
x \arrow[r, "f"] & y \arrow[r, "g"] & J
\end{tikzcd}$$

$\boldsymbol{x} = (x_1, x_2, \cdots x_n) \in \boldsymbol{R}^n, \;\; \boldsymbol{y} = (y_1, y_2, \cdots y_K) \in \boldsymbol{R}^K, \; J \in \boldsymbol{R}$, and

$$\boldsymbol{y} = f(\boldsymbol{x})$$
$$J = g(\boldsymbol{y})$$

Then, the chain rule of differentiation states that:

$$\nabla_{\boldsymbol{x}} J = \left(\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}}\right)^T \nabla_{\boldsymbol{y}} J$$

The matrix $\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}}$ is known as the **Jacobian** of the function $f$ where $\boldsymbol{y} = f(\boldsymbol{x})$.

# Chain rule in multidimensions

$$\nabla_{\boldsymbol{x}} J = \left(\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}}\right)^T \nabla_{\boldsymbol{y}} J$$

where

$$\nabla_{\boldsymbol{x}} J = \frac{\partial J}{\partial \boldsymbol{x}} = \begin{pmatrix} \frac{\partial J}{\partial x_1} \\ \frac{\partial J}{\partial x_2} \\ \vdots \\ \frac{\partial J}{\partial x_n} \end{pmatrix} \text{ and } \nabla_{\boldsymbol{y}} J = \frac{\partial J}{\partial \boldsymbol{y}} = \begin{pmatrix} \frac{\partial J}{\partial y_1} \\ \frac{\partial J}{\partial y_2} \\ \vdots \\ \frac{\partial J}{\partial y_K} \end{pmatrix},$$

$$\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}} = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \cdots & \frac{\partial y_2}{\partial x_n} \\ \vdots & \vdots & \cdots & \vdots \\ \frac{\partial y_K}{\partial x_1} & \frac{\partial y_K}{\partial x_2} & \cdots & \frac{\partial y_K}{\partial x_n} \end{pmatrix}$$

Note that differentiation of a scalar by a vector results in a vector and differentiation of a vector by a vector results in a matrix.

# Example 1

Let $\boldsymbol{x} = (x_1, x_2, x_3) \in \boldsymbol{R}^3$, $\boldsymbol{y} = (y_1, y_2) \in \boldsymbol{R}^2$, and $\boldsymbol{y} = f(\boldsymbol{x})$ where $f$ is given by

$$y_1 = 5 - 2x_1 + 3x_3$$
$$y_2 = x_1 + 5{x_2}^2 + {x_3}^3 - 1$$

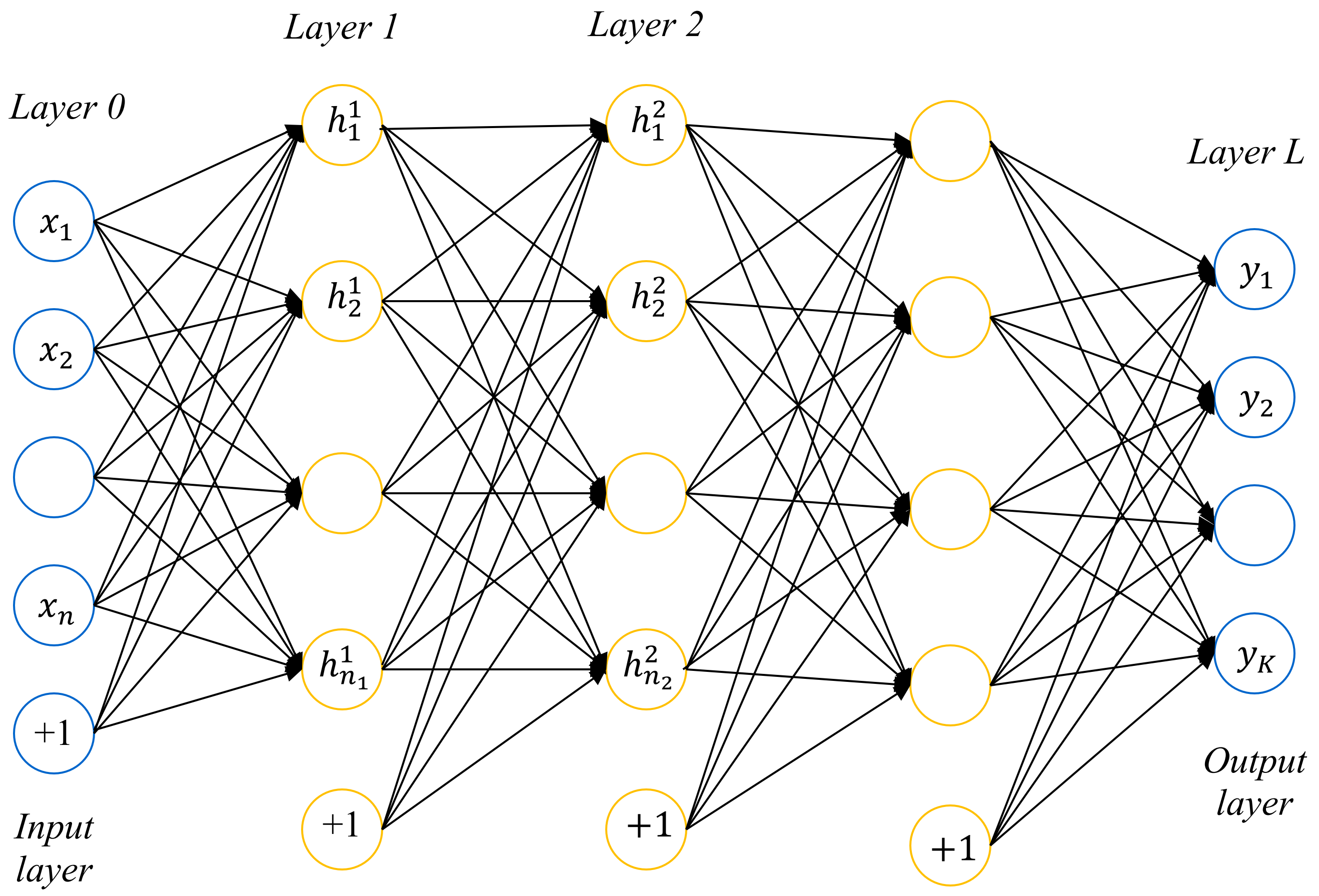
Find the Jacobian of $f$.

$$\frac{\partial y_1}{\partial x_1} = -2, \qquad \frac{\partial y_1}{\partial x_2} = 0, \qquad \frac{\partial y_1}{\partial x_3} = 3$$
$$\frac{\partial y_2}{\partial x_1} = 1, \qquad \frac{\partial y_2}{\partial x_2} = 10x_2, \qquad \frac{\partial y_2}{\partial x_3} = 3{x_3}^2$$

Jacobian:

$$\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}} = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \frac{\partial y_1}{\partial x_3} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \frac{\partial y_2}{\partial x_3} \end{pmatrix} = \begin{pmatrix} -2 & 0 & 3 \\ 1 & 10x_2 & 3{x_3}^2 \end{pmatrix}$$

# Deep feedforward networks (FFN)



$L$+1 layer network

## Deep feedforward networks (FFN)

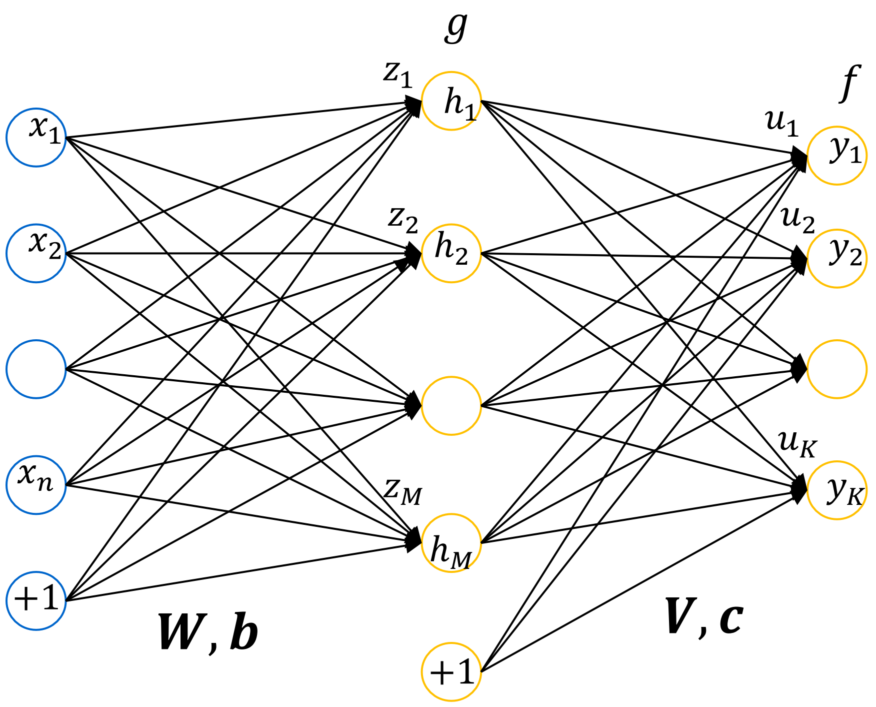
**Feedforward networks (FFN)** consists of several layers  of neurons where activations propagate from input layer to output layer. The layers between the input and output layers are referred to as **hidden layers**.

The number of layers is referred to as the **depth** of the feedforward network. When a network has many hidden layers of neurons, feedforward networks are referred to as **deep neural networks (DNN)**.  Learning in deep neural networks is referred to as **deep learning**.  The number of neurons in a layer is referred to as the **width** of that layer.

The hidden layers are usually composed of perceptrons (sigmoidal units) or ReLU units and the output layer is  usually

- A linear neuron layer for regression
- A softmax layer for classification

# Three-layer FFN



Input $\boldsymbol{x} = (x_1 \quad x_2 \quad \cdots \quad x_n)^T$
Hidden-layer output $\boldsymbol{h} = (h_1 \quad h_2 \quad \cdots \quad h_M)^T$
Output $\boldsymbol{y} = (y_1 \quad y_2 \quad \cdots \quad y_K)^T$

$\boldsymbol{W}, \boldsymbol{b}$ – weight and bias of hidden layer
$\boldsymbol{V}, \boldsymbol{c}$ – weight and bias of output layer

# Forward propagation of activations: single pattern

Consider an input pattern $(\boldsymbol{x}, \boldsymbol{d})$ to 3-layer FFN:

$$\begin{tikzcd}
\boldsymbol{x} \arrow[r, "\boldsymbol{W}, \boldsymbol{b}"] & \boldsymbol{z} \arrow[r, "g"] & \boldsymbol{h} \arrow[r, "\boldsymbol{V}, \boldsymbol{c}"] & \boldsymbol{u} \arrow[r, "f"] & \boldsymbol{y} \arrow[r] & J & \boldsymbol{d} \arrow[l]
\end{tikzcd}$$

Synaptic input $\boldsymbol{z}$ to hidden layer:

$$\boldsymbol{z} = \boldsymbol{W}^T \boldsymbol{x} + \boldsymbol{b}$$

Output $\boldsymbol{h}$ of hidden layer:

$$\boldsymbol{h} = g(\boldsymbol{z})$$

$g$ is hidden layer activation function.

Synaptic input $\boldsymbol{u}$ to output layer:

$$\boldsymbol{u} = \boldsymbol{V}^T \boldsymbol{h} + \boldsymbol{c}$$

Output $\boldsymbol{y}$ of output layer:

$$\boldsymbol{y} = f(\boldsymbol{u})$$

# Backpropagation of gradients

$$\begin{tikzcd}
 & \nabla_{\boldsymbol{z}} J & & \nabla_{\boldsymbol{h}} J & & \nabla_{\boldsymbol{u}} J & & & & & \\
\boldsymbol{x} \arrow[rr, "\boldsymbol{W}, \boldsymbol{b}"] & & \boldsymbol{z} \arrow[rr, "g"] & & \boldsymbol{h} \arrow[rr, "\boldsymbol{V}, \boldsymbol{c}"] & & \boldsymbol{u} \arrow[rr, "f"] & & \boldsymbol{y} \arrow[r] & J & \boldsymbol{d} \arrow[l]
\end{tikzcd}$$

Since the targets appear at the output, the error gradient at the output layer is $\nabla_{\boldsymbol{u}} J$ is known. Therefore output weights and bias, $\boldsymbol{V}, \boldsymbol{c}$ , can be learnt.

Key to learning deep neural network is to propagate the output gradient back to other layers to learn their weights and biases.

# Derivatives

$$\boldsymbol{u} = \boldsymbol{V}^T\boldsymbol{h} + \boldsymbol{c}$$

Consider $k$th neuron at the output layer:
weight vector $\boldsymbol{v}_k = (v_{k1} \quad v_{k2} \quad \cdots \quad v_{kM})^T$ and bias $c_k$.

The synaptic input $u_k$ due to $\boldsymbol{h}$ is given by

$$u_k = \boldsymbol{v}_k{}^T\boldsymbol{h} + c_k = v_{k1}h_1 + v_{k2}h_2 + \cdots + v_{kM}h_M + c_k$$

$$\frac{\partial u_k}{\partial h_j} = v_{kj} \qquad for\ all\ j = 1,2, \dots K$$

Therefore

$$\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{h}} = \begin{pmatrix} \frac{\partial u_1}{\partial h_1} & \frac{\partial u_1}{\partial h_2} & \cdots & \frac{\partial u_1}{\partial h_M} \\ \frac{\partial u_2}{\partial h_1} & \frac{\partial u_2}{\partial h_2} & \cdots & \frac{\partial u_2}{\partial h_M} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial u_K}{\partial h_1} & \frac{\partial u_K}{\partial h_2} & \cdots & \frac{\partial u_K}{\partial h_K} \end{pmatrix} = \begin{pmatrix} v_{11} & v_{12} & \cdots & v_{1M} \\ v_{21} & v_{22} & \cdots & v_{2M} \\ \vdots & \vdots & \vdots & \vdots \\ v_{K1} & v_{K2} & \cdots & v_{KM} \end{pmatrix} = \boldsymbol{V}^T$$

That is,

$$\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{h}} = \boldsymbol{V}^T$$

# Derivatives

$$\boldsymbol{y} = f(\boldsymbol{u})$$

Considering $k$th neuron:

$$y_k = f(u_k)$$

$$\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{u}} = \begin{pmatrix} \frac{\partial y_1}{\partial u_1} & \frac{\partial y_1}{\partial u_2} & \cdots & \frac{\partial y_1}{\partial u_K} \\ \frac{\partial y_2}{\partial u_1} & \frac{\partial y_2}{\partial u_2} & \cdots & \frac{\partial y_2}{\partial u_K} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial y_K}{\partial u_1} & \frac{\partial y_K}{\partial u_2} & \cdots & \frac{\partial y_K}{\partial u_K} \end{pmatrix} = \begin{pmatrix} f'(u_1) & 0 & \cdots & 0 \\ 0 & f'(u_2) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & f'(u_K) \end{pmatrix} = diag\left(f'(\boldsymbol{u})\right)$$

That is,

$$\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{u}} = diag\left(f'(\boldsymbol{u})\right)$$

where $diag\left(f'(\boldsymbol{u})\right)$ is a diagonal matrix composed of derivatives corresponding to individual components of $\boldsymbol{u}$ in the diagonal.

# Derivatives

$$\begin{tikzcd} & \nabla_{\boldsymbol{z}} J & \nabla_{\boldsymbol{h}} J & \nabla_{\boldsymbol{u}} J & & & \\ \boldsymbol{x} \arrow[r, "\boldsymbol{W},\boldsymbol{b}"] & \boldsymbol{z} \arrow[r, "g"] & \boldsymbol{h} \arrow[r, "\boldsymbol{V},\boldsymbol{c}"] & \boldsymbol{u} \arrow[r, "f"] & \boldsymbol{y} \arrow[r] & J & \boldsymbol{d} \arrow[l] \end{tikzcd}$$

$$\boldsymbol{u} = \boldsymbol{V}^T \boldsymbol{h} + \boldsymbol{c}$$

$$\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{h}} = \boldsymbol{V}^T$$

$$\boldsymbol{h} = g(\boldsymbol{z})$$

$$\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} = diag\left(g'(\boldsymbol{z})\right)$$

# Back-propagation of gradients: single pattern

$$\begin{tikzcd}
 & \nabla_{\boldsymbol{z}} J & \nabla_{\boldsymbol{h}} J & \nabla_{\boldsymbol{u}} J & & & \\
\boldsymbol{x} \arrow[r, "\boldsymbol{W}{,}\, \boldsymbol{b}"] & \boldsymbol{z} \arrow[r, "g"] & \boldsymbol{h} \arrow[r, "\boldsymbol{V}{,}\, \boldsymbol{c}"] & \boldsymbol{u} \arrow[r, "f"] & \boldsymbol{y} \arrow[r] & J & \boldsymbol{d} \arrow[l]
\end{tikzcd}$$

Considering output layer,

$$\nabla_{\boldsymbol{u}} J = \begin{cases} -(\boldsymbol{d} - \boldsymbol{y}) & \text{for a linear layer} \\ -\left(1(\boldsymbol{k} = d) - f(\boldsymbol{u})\right) & \text{for a softmax layer} \end{cases}$$

From chain rule of differentiation,

$$\nabla_{\boldsymbol{h}} J = \left(\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{h}}\right)^T \nabla_{\boldsymbol{u}} J = \boldsymbol{V} \nabla_{\boldsymbol{u}} J$$

$$\nabla_{\boldsymbol{z}} J = \left(\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}}\right)^T \nabla_{\boldsymbol{h}} J = diag\left(g'(\boldsymbol{z})\right) \boldsymbol{V} \nabla_{\boldsymbol{u}} J = \boldsymbol{V} \nabla_{\boldsymbol{u}} J \cdot g'(\boldsymbol{z}) \qquad \text{(A)}$$

## Proof

For a vector $\boldsymbol{x}$ :

$$diag\big(f'(\boldsymbol{u})\big)\boldsymbol{x} = \begin{pmatrix} f'(u_1) & 0 & \cdots & 0 \\ 0 & f'(u_2) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & f'(u_K) \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_K \end{pmatrix} = \begin{pmatrix} f'(u_1)x_1 \\ f'(u_2)x_2 \\ \vdots \\ f'(u_K)x_K \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_K \end{pmatrix} \cdot \begin{pmatrix} f'(u_1) \\ f'(u_2) \\ \vdots \\ f'(u_K) \end{pmatrix}$$

That is:

$$diag\big(f'(\boldsymbol{u})\big)\boldsymbol{x} = \boldsymbol{x} \cdot f'(\boldsymbol{u}) = f'(\boldsymbol{u}) \cdot \boldsymbol{x}$$

## Back-propagation of gradients: single pattern

From (A);

$$\nabla_{\boldsymbol{z}} J = \boldsymbol{V} \nabla_{\boldsymbol{u}} J \cdot g'(\boldsymbol{z})$$

That is, gradients at hidden layer can be derived from gradients at output layer. The gradients at output layer are multiplied by $\boldsymbol{V}$ and back-propagated to hidden layer.

Note that hidden-layer activations are multiplied by $\boldsymbol{V}^T$ (Note $\boldsymbol{u} = \boldsymbol{V}^T\boldsymbol{h} + \boldsymbol{c}$) in forward propagation and in back-propagation, the gradients are multiplied by $\boldsymbol{V}$.

This leads to the **back-propagation** (backprop) algorithm.

# SGD of three-layer FFN

Output layer:

$$\nabla_{\boldsymbol{u}} J = \begin{cases} -(\boldsymbol{d} - \boldsymbol{y}) & \text{for linear layer} \\ -\left(1(\boldsymbol{k} = d) - f(\boldsymbol{u})\right) & \text{for softmax layer} \end{cases}$$

Hidden layer:

$$\nabla_{\boldsymbol{z}} J = \boldsymbol{V} \nabla_{\boldsymbol{u}} J \cdot g'(\boldsymbol{z})$$

# SGD for a three-layer FFN

```
Given a training dataset $\{(\boldsymbol{x}, \boldsymbol{d})\}$
Set learning parameter α
Initialize $\boldsymbol{W}, \boldsymbol{b}, \boldsymbol{V}, \boldsymbol{c}$
Repeat until convergence:
        For every pattern $(\boldsymbol{x}, \boldsymbol{d})$:
                $\boldsymbol{z} = \boldsymbol{W}^T \boldsymbol{x} + \boldsymbol{b}$
                $\boldsymbol{h} = g(\boldsymbol{z})$
                $\boldsymbol{u} = \boldsymbol{V}^T \boldsymbol{h} + \boldsymbol{c}$
                $\boldsymbol{y} = f(\boldsymbol{u})$

                $\nabla_{\boldsymbol{u}} J = \begin{cases} -(\boldsymbol{d} - \boldsymbol{y}) \\ -\big(1(\boldsymbol{k} = d) - f(\boldsymbol{u})\big) \end{cases}$
                $\nabla_{\boldsymbol{z}} J = \boldsymbol{V} \nabla_{\boldsymbol{u}} J \cdot g'(\boldsymbol{z})$

                $\boldsymbol{V} \leftarrow \boldsymbol{V} - \alpha \boldsymbol{h} (\nabla_{\boldsymbol{u}} J)^T$
                $\boldsymbol{c} \leftarrow \boldsymbol{c} - \alpha \nabla_{\boldsymbol{u}} J$
                $\boldsymbol{W} \leftarrow \boldsymbol{W} - \alpha \boldsymbol{x} (\nabla_{\boldsymbol{z}} J)^T$
                $\boldsymbol{b} \leftarrow \boldsymbol{b} - \alpha \nabla_{\boldsymbol{z}} J$
```

Forward propagation

Backward propagation

# Forward propagation of activations: batch of patterns

Computational graph of 3-layer FFN for a batch of patterns $(\boldsymbol{X}, \boldsymbol{D})$:

$$\begin{tikzcd}
\boldsymbol{X} \arrow[r, "\boldsymbol{W}, \boldsymbol{b}"] & \boldsymbol{Z} \arrow[r, "g"] & \boldsymbol{H} \arrow[r, "\boldsymbol{V}, \boldsymbol{c}"] & \boldsymbol{U} \arrow[r, "f"] & \boldsymbol{Y} \arrow[r] & J & \boldsymbol{D} \arrow[l]
\end{tikzcd}$$

Synaptic input $\boldsymbol{Z}$ to hidden layer:

$$\boldsymbol{Z} = \boldsymbol{X}\boldsymbol{W} + \boldsymbol{B}$$

Output $\boldsymbol{H}$ of the hidden layer:

$$\boldsymbol{H} = g(\boldsymbol{Z})$$

Synaptic input $\boldsymbol{U}$ to output layer:

$$\boldsymbol{U} = \boldsymbol{H}\boldsymbol{V} + \boldsymbol{C}$$

Output $\boldsymbol{Y}$ of the output layer:

$$\boldsymbol{Y} = f(\boldsymbol{U})$$

# Back-propagation of gradients: batch of patterns

$$\begin{tikzcd}
 & \nabla_Z J & & & \nabla_U J & & & \\
\boldsymbol{X} \arrow[r, "\boldsymbol{W},\boldsymbol{b}"] & \boldsymbol{Z} \arrow[r, "g"] & \boldsymbol{H} \arrow[r, "\boldsymbol{V},\boldsymbol{c}"] & \boldsymbol{U} \arrow[r, "f"] & \boldsymbol{Y} \arrow[r] & J & \boldsymbol{D} \arrow[l]
\end{tikzcd}$$

$$\nabla_U J = \begin{cases} -(\boldsymbol{D} - \boldsymbol{Y}) & \text{for linear layer} \\ -(\boldsymbol{K} - f(\boldsymbol{U})) & \text{for softmax layer} \end{cases}$$

$$\nabla_{\boldsymbol{Z}} J = \begin{pmatrix} (\nabla_{\boldsymbol{z}_1} J)^T \\ (\nabla_{\boldsymbol{z}_2} J)^T \\ \vdots \\ (\nabla_{\boldsymbol{z}_P} J)^T \end{pmatrix} = \begin{pmatrix} \left(\boldsymbol{V}\nabla_{\boldsymbol{u}_1} J \cdot g'(\boldsymbol{z}_1)\right)^T \\ \left(\boldsymbol{V}\nabla_{\boldsymbol{u}_2} J \cdot g'(\boldsymbol{z}_2)\right)^T \\ \vdots \\ \left(\boldsymbol{V}\nabla_{\boldsymbol{u}_P} J \cdot g'(\boldsymbol{z}_P)\right)^T \end{pmatrix}$$

Substituting from (A)

# Back-propagation of gradients: batch of patterns

$$\nabla_{\boldsymbol{Z}} J = \begin{pmatrix} \left(\nabla_{\boldsymbol{u}_1} J\right)^T \boldsymbol{V}^T \cdot \left(g'(\boldsymbol{z}_1)\right)^T \\ \left(\nabla_{\boldsymbol{u}_2} J\right)^T \boldsymbol{V}^T \cdot \left(g'(\boldsymbol{z}_2)\right)^T \\ \vdots \\ \left(\nabla_{\boldsymbol{u}_P} J\right)^T \boldsymbol{V}^T \cdot \left(g'(\boldsymbol{z}_P)\right)^T \end{pmatrix}$$

$$(XY)^T = Y^T X^T$$

$$= \begin{pmatrix} \left(\nabla_{\boldsymbol{u}_1} J\right)^T \\ \left(\nabla_{\boldsymbol{u}_2} J\right)^T \\ \vdots \\ \left(\nabla_{\boldsymbol{u}_P} J\right)^T \end{pmatrix} \boldsymbol{V}^T \cdot \begin{pmatrix} \left(g'(\boldsymbol{z}_1)\right)^T \\ \left(g'(\boldsymbol{z}_2)\right)^T \\ \vdots \\ \left(g'(\boldsymbol{z}_P)\right)^T \end{pmatrix}$$

$$= (\nabla_{\boldsymbol{U}} J)\boldsymbol{V}^T \cdot g'(\boldsymbol{Z})$$

$$\nabla_{\boldsymbol{Z}} \boldsymbol{J} = (\nabla_{\boldsymbol{U}} J)\boldsymbol{V}^T \cdot g'(\boldsymbol{Z})$$

# GD of three-layer FFN

Output layer:

$$\nabla_{\boldsymbol{U}} J = \begin{cases} -(\boldsymbol{D} - \boldsymbol{Y}) & \text{for linear layer} \\ -\big(\boldsymbol{K} - f(\boldsymbol{U})\big) & \text{for softmax layer} \end{cases}$$

Hidden layer:

$$\nabla_{\boldsymbol{Z}} J = (\nabla_{\boldsymbol{U}} J)\boldsymbol{V}^T \cdot g'(\boldsymbol{Z})$$

# GD for a three-layer FFN

Given a training dataset $(\boldsymbol{X}, \boldsymbol{D})$
Set learning parameter α
Initialize $\boldsymbol{W}$, $\boldsymbol{b}$, $\boldsymbol{V}$, $\boldsymbol{c}$
Repeat until convergence:

$$\boldsymbol{Z} = \boldsymbol{X}\boldsymbol{W} + \boldsymbol{B}$$
$$\boldsymbol{H} = g(\boldsymbol{Z})$$
$$\boldsymbol{U} = \boldsymbol{H}\boldsymbol{V} + \boldsymbol{C}$$
$$\boldsymbol{Y} = f(\boldsymbol{U})$$

Forward propagation

$$\nabla_{\boldsymbol{U}} J = \begin{cases} -(\boldsymbol{D} - \boldsymbol{Y}) \\ -\left(\boldsymbol{K} - f(\boldsymbol{U})\right) \end{cases}$$
$$\nabla_{\boldsymbol{Z}} J = (\nabla_{\boldsymbol{U}} J)\boldsymbol{V}^T \cdot g'(\boldsymbol{Z})$$

Backward propagation

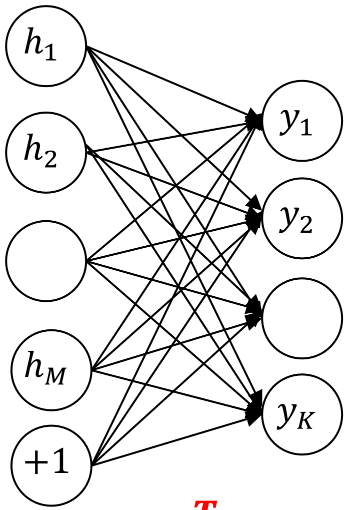
$$\boldsymbol{V} \leftarrow \boldsymbol{V} - \alpha \boldsymbol{H}^T \nabla_{\boldsymbol{U}} J$$
$$\boldsymbol{c} \leftarrow \boldsymbol{c} - \alpha (\nabla_{\boldsymbol{U}} J)^T \boldsymbol{1}_P$$
$$\boldsymbol{W} \leftarrow \boldsymbol{W} - \alpha \boldsymbol{X}^T \nabla_{\boldsymbol{Z}} J$$
$$\boldsymbol{b} \leftarrow \boldsymbol{b} - \alpha (\nabla_{\boldsymbol{Z}} J)^T \boldsymbol{1}_P$$

# Learning in three-layer FFN

| GD | SGD |
|---|---|
| $(\boldsymbol{X}, \boldsymbol{D})$ | $(\boldsymbol{x}, \boldsymbol{d})$ |
| $\boldsymbol{Z} = \boldsymbol{X}\boldsymbol{W} + \boldsymbol{B}$ | $\boldsymbol{z} = \boldsymbol{W}^T\boldsymbol{x} + \boldsymbol{b}$ |
| $\boldsymbol{H} = g(\boldsymbol{Z})$ | $\boldsymbol{h} = g(\boldsymbol{z})$ |
| $\boldsymbol{U} = \boldsymbol{H}\boldsymbol{V} + \boldsymbol{C}$ | $\boldsymbol{u} = \boldsymbol{V}^T\boldsymbol{h} + \boldsymbol{c}$ |
| $\boldsymbol{Y} = f(\boldsymbol{U})$ | $\boldsymbol{y} = f(\boldsymbol{u})$ |
| | |
| $\nabla_{\boldsymbol{U}} J = \begin{cases} -(\boldsymbol{D} - \boldsymbol{Y}) \\ -\big(\boldsymbol{K} - f(\boldsymbol{U})\big) \end{cases}$ | $\nabla_{\boldsymbol{u}} J = \begin{cases} -(\boldsymbol{d} - \boldsymbol{y}) \\ \big(1(\boldsymbol{k} = d) - f(\boldsymbol{u})\big) \end{cases}$ |
| $\nabla_{\boldsymbol{Z}} J = (\nabla_{\boldsymbol{U}} J)\boldsymbol{V}^T \cdot g'(\boldsymbol{Z})$ | $\nabla_{\boldsymbol{z}} J = \boldsymbol{V}\nabla_{\boldsymbol{u}} J \cdot g'(\boldsymbol{z})$ |
| | |
| $\boldsymbol{W} \leftarrow \boldsymbol{W} - \alpha\boldsymbol{X}^T\ \nabla_{\boldsymbol{Z}} J$ | $\boldsymbol{W} \leftarrow \boldsymbol{W} - \alpha\boldsymbol{x}(\nabla_{\boldsymbol{z}} J)^T$ |
| $\boldsymbol{b} \leftarrow \boldsymbol{b} - \alpha(\nabla_{\boldsymbol{Z}} J)^T\boldsymbol{1}_P$ | $\boldsymbol{b} \leftarrow \boldsymbol{b} - \alpha\nabla_{\boldsymbol{z}} J$ |
| $\boldsymbol{V} \leftarrow \boldsymbol{V} - \alpha\boldsymbol{H}^T\ \nabla_{\boldsymbol{U}} J$ | $\boldsymbol{V} \leftarrow \boldsymbol{V} - \alpha\boldsymbol{h}(\nabla_{\boldsymbol{u}} J)^T$ |
| $\boldsymbol{c} \leftarrow \boldsymbol{c} - \alpha(\nabla_{\boldsymbol{U}} J)^T\boldsymbol{1}_P$ | $\boldsymbol{c} \leftarrow \boldsymbol{c} - \alpha\nabla_{\boldsymbol{u}} J$ |

# Back-propagation

$$\boldsymbol{H} \xrightarrow{\boldsymbol{V}} \boldsymbol{U} = \boldsymbol{H}\boldsymbol{V} + \boldsymbol{C}$$



$$\nabla_{\boldsymbol{Z}}\boldsymbol{J} = (\nabla_{\boldsymbol{U}}J)\boldsymbol{V}^T \cdot g'(\boldsymbol{Z}) \xleftarrow{\boldsymbol{V}^T} \nabla_{\boldsymbol{U}}J$$

The error gradient can be seen as propagating from the output layer to the hidden layer and so learning in feedforward networks is known as the *back-propagation* algorithm

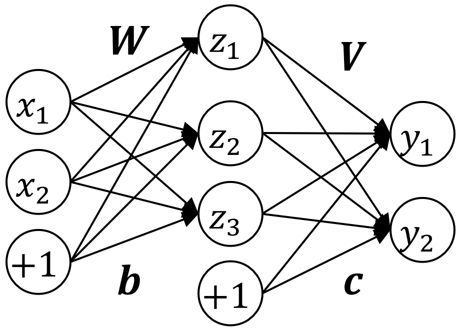
# Example 2

Design a three-layer FFN, using gradient descent to perform the following mapping. Use a learning factor = 0.05 and three perceptrons in the hidden-layer.

| Inputs $\boldsymbol{x} = (x_1, x_2)$ | Targets $\boldsymbol{d} = (d_1, d_2)$ |
|---|---|
| $(0.77, 0.02)$ | $(0.44, -0.42)$ |
| $(0.63, 0.75)$ | $(0.84, 0.43)$ |
| $(0.50, 0.22)$ | $(0.09, -0.72)$ |
| $(0.20, 0.76)$ | $(-0.25, 0.35)$ |
| $(0.17, 0.09)$ | $(-0.12\ \ -0.13)$ |
| $(0.69, 0.95)$ | $(0.24, 0.03)$ |
| $(0.00\ , 0.51)$ | $(0.30, 0.20)$ |
| $(0.81, 0.61)$ | $(0.61,0.04)$ |

# Example 2

$$\boldsymbol{X} = \begin{pmatrix} 0.77 & 0.02 \\ 0.63 & 0.75 \\ 0.50 & 0.22 \\ 0.20 & 0.76 \\ 0.17 & 0.09 \\ 0.69 & 0.95 \\ 0.00 & 0.51 \\ 0.81 & 0.61 \end{pmatrix} \text{ and } \boldsymbol{D} = \begin{pmatrix} 0.44 & -0.42 \\ 0.84 & 0.43 \\ 0.09 & -0.72 \\ -0.25 & 0.35 \\ -0.12 & -0.13 \\ 0.24 & 0.03 \\ 0.30 & 0.20 \\ 0.61 & 0.04 \end{pmatrix}$$



Output layer is a linear neuron layer

Hidden layer is a sigmoidal layer

Initialized (weights using a uniform distribution):

$$\boldsymbol{W} = \begin{pmatrix} -3.97 & 1.10 & 0.42 \\ 2.79 & -2.64 & 3.13 \end{pmatrix}, \boldsymbol{b} = \begin{pmatrix} 0.0 \\ 0.0 \\ 0.0 \end{pmatrix}, \boldsymbol{V} = \begin{pmatrix} 3.58 & -1.58 \\ -3.58 & -1.75 \\ -3.38 & 2.88 \end{pmatrix}, \mathbf{c} = \begin{pmatrix} 0.0 \\ 0.0 \end{pmatrix}$$

# Example 2

**Epoch 1:**

$$\boldsymbol{Z} = \boldsymbol{X}\boldsymbol{W} + \boldsymbol{B} = \begin{pmatrix} 0.77 & 0.02 \\ 0.63 & 0.75 \\ 0.50 & 0.22 \\ 0.20 & 0.76 \\ 0.17 & 0.09 \\ 0.69 & 0.95 \\ 0.00 & 0.51 \\ 0.81 & 0.61 \end{pmatrix} \begin{pmatrix} -3.97 & 1.10 & 0.42 \\ 2.79 & -2.64 & 3.13 \end{pmatrix} + \begin{pmatrix} 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \end{pmatrix} = \begin{pmatrix} -3.00 & 0.8 & 0.39 \\ -0.42 & -1.27 & 2.61 \\ -1.35 & -0.04 & 0.91 \\ 1.34 & -1.79 & 2.46 \\ -0.42 & -0.05 & 0.35 \\ -0.05 & -1.76 & 3.27 \\ 1.42 & -1.34 & 1.60 \\ -1.51 & -0.72 & 2.25 \end{pmatrix}$$

$$\boldsymbol{H} = g(\boldsymbol{Z}) = \frac{1}{1 + e^{-\boldsymbol{z}}} = \begin{pmatrix} 0.05 & 0.69 & 0.60 \\ 0.40 & 0.22 & 0.93 \\ 0.21 & 0.49 & 0.71 \\ 0.79 & 0.14 & 0.92 \\ 0.40 & 0.49 & 0.59 \\ 0.49 & 0.15 & 0.96 \\ 0.80 & 0.21 & 0.83 \\ 0.18 & 0.33 & 0.91 \end{pmatrix}$$

# Example 2

$$\boldsymbol{Y} = \boldsymbol{H}V + \boldsymbol{C} = \begin{pmatrix} 0.05 & 0.69 & 0.60 \\ 0.40 & 0.22 & 0.93 \\ 0.21 & 0.49 & 0.71 \\ 0.79 & 0.14 & 0.92 \\ 0.40 & 0.49 & 0.59 \\ 0.49 & 0.15 & 0.96 \\ 0.80 & 0.21 & 0.83 \\ 0.18 & 0.33 & 0.91 \end{pmatrix} \begin{pmatrix} 2.38 & -4.2 \\ 1.17 & 2.18 \\ -0.01 & -2.41 \end{pmatrix} + \begin{pmatrix} 0.0 & 0.0 \\ 0.0 & 0.0 \\ 0.0 & 0.0 \\ 0.0 & 0.0 \\ 0.0 & 0.0 \\ 0.0 & 0.0 \\ 0.0 & 0.0 \\ 0.0 & 0.0 \end{pmatrix} = \begin{pmatrix} -4.32 & 0.44 \\ -2.52 & 1.67 \\ -3.43 & 0.87 \\ -0.79 & 1.15 \\ -2.32 & 0.21 \\ -2.04 & 1.75 \\ -0.67 & 0.76 \\ -3.59 & 1.75 \end{pmatrix}$$

$$\nabla_U J = -(\boldsymbol{D} - \boldsymbol{Y}) = -\left( \begin{pmatrix} 0.44 & -0.42 \\ 0.84 & 0.43 \\ 0.09 & -0.72 \\ -0.25 & 0.35 \\ -0.12 & -0.13 \\ 0.24 & 0.03 \\ 0.30 & 0.20 \\ 0.61 & 0.04 \end{pmatrix} - \begin{pmatrix} -4.32 & 0.44 \\ -2.52 & 1.67 \\ -3.43 & 0.87 \\ -0.79 & 1.15 \\ -2.32 & 0.21 \\ -2.04 & 1.75 \\ -0.67 & 0.76 \\ -3.59 & 1.75 \end{pmatrix} \right) = \begin{pmatrix} -4.76 & 0.85 \\ -3.35 & 1.24 \\ -3.52 & 1.59 \\ -0.54 & 0.80 \\ -2.20 & 0.34 \\ -2.28 & 1.72 \\ -0.98 & 0.56 \\ -4.20 & 1.70 \end{pmatrix}$$

# Example 2

$$g'(\boldsymbol{Z}) = \boldsymbol{H} \cdot (\boldsymbol{1} - \boldsymbol{H}) = \begin{pmatrix} 0.04 & 0.21 & 0.24 \\ 0.24 & 0.17 & 0.06 \\ 0.16 & 0.25 & 0.20 \\ 0.16 & 0.12 & 0.07 \\ 0.24 & 0.25 & 0.24 \\ 0.25 & 0.13 & 0.04 \\ 0.16 & 0.16 & 0.14 \\ 0.15 & 0.22 & 0.09 \end{pmatrix}$$

$$\nabla_{\boldsymbol{Z}} J = (\nabla_{\boldsymbol{U}} J)\boldsymbol{V}^T \cdot g'(\boldsymbol{Z})$$

$$= \begin{pmatrix} -4.76 & 0.85 \\ -3.35 & 1.24 \\ -3.52 & 1.59 \\ -0.54 & 0.80 \\ -2.20 & 0.34 \\ -2.28 & 1.72 \\ -0.98 & 0.56 \\ -4.20 & 1.70 \end{pmatrix} \begin{pmatrix} 3.58 & -1.58 \\ -3.58 & -1.75 \\ -3.38 & 2.88 \end{pmatrix}^T \cdot \begin{pmatrix} 0.04 & 0.21 & 0.24 \\ 0.24 & 0.17 & 0.06 \\ 0.16 & 0.25 & 0.20 \\ 0.16 & 0.12 & 0.07 \\ 0.24 & 0.25 & 0.24 \\ 0.25 & 0.13 & 0.04 \\ 0.16 & 0.16 & 0.14 \\ 0.15 & 0.22 & 0.09 \end{pmatrix}$$

# Example 2

Hidden layer:

$$\nabla_{\boldsymbol{V}} J = \boldsymbol{H}^T \nabla_{\boldsymbol{U}} J = \begin{pmatrix} -6.23 & 3.22 \\ -8.81 & 2.85 \\ -17.07 & 7.40 \end{pmatrix}$$

$$\nabla_{\boldsymbol{c}} J = (\nabla_{\boldsymbol{U}} J)^T \mathbf{1}_P = \begin{pmatrix} -21.83 \\ 8.81 \end{pmatrix}$$

Output layer:

$$\nabla_{\boldsymbol{W}} J = \boldsymbol{X}^T \nabla_{\boldsymbol{Z}} J = \begin{pmatrix} -8.43 & 7.81 & 7.79 \\ -8.21 & 4.56 & 3.76 \end{pmatrix}$$

$$\nabla_{\boldsymbol{b}} J = (\nabla_{\boldsymbol{Z}} J)^T \mathbf{1}_P = \begin{pmatrix} -15.22 \\ 13.11 \\ 13.92 \end{pmatrix}$$

## Example 2

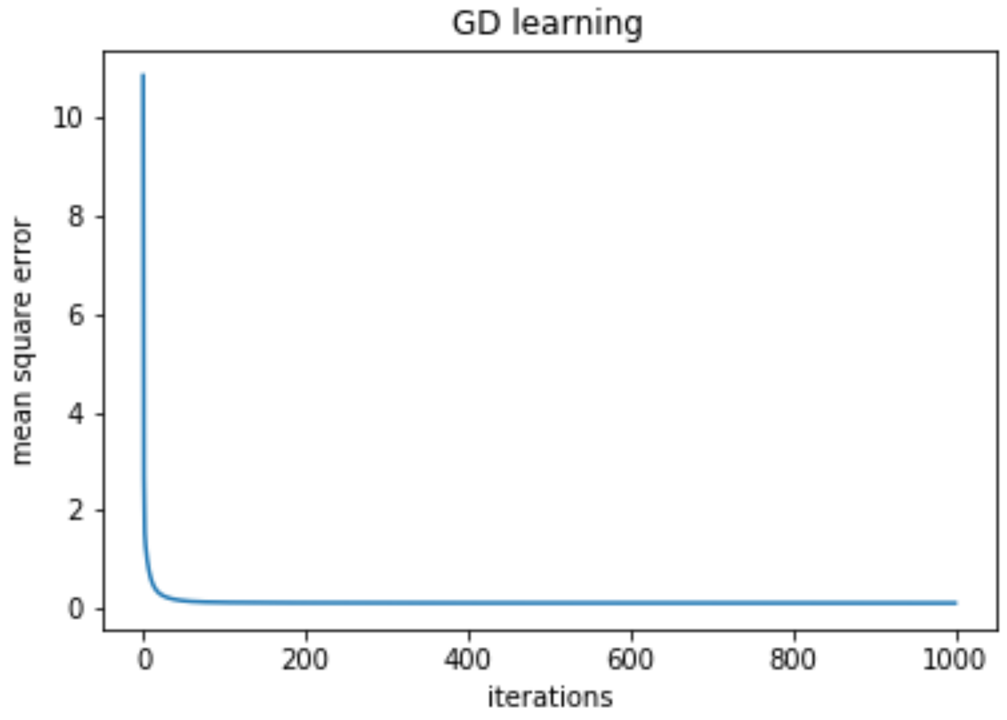
$$\boldsymbol{V} \leftarrow \boldsymbol{V} - \alpha \nabla_{\boldsymbol{V}} J = \begin{pmatrix} 3.89 & -1.74 \\ -3.14 & -1.89 \\ -2.53 & 2.51 \end{pmatrix}$$

$$\boldsymbol{c} \leftarrow \boldsymbol{c} - \alpha \nabla_{\boldsymbol{c}} J = \begin{pmatrix} 1.09 \\ -0.44 \end{pmatrix}$$

$$\boldsymbol{W} \leftarrow \boldsymbol{W} - \alpha \nabla_{\boldsymbol{W}} J = \begin{pmatrix} -3.55 & 0.72 & 0.03 \\ 3.21 & -2.87 & 2.94 \end{pmatrix}$$

$$\boldsymbol{b} \leftarrow \boldsymbol{b} - \alpha \nabla_{\boldsymbol{b}} J = \begin{pmatrix} 0.76 \\ -0.66 \\ -0.70 \end{pmatrix}$$

# Example 2


GD learning
mean square error
iterations
0
2
4
6
8
10
0
200
400
600
800
1000

## Example 2

After 1,000 epochs,

m. s. e = 0.107

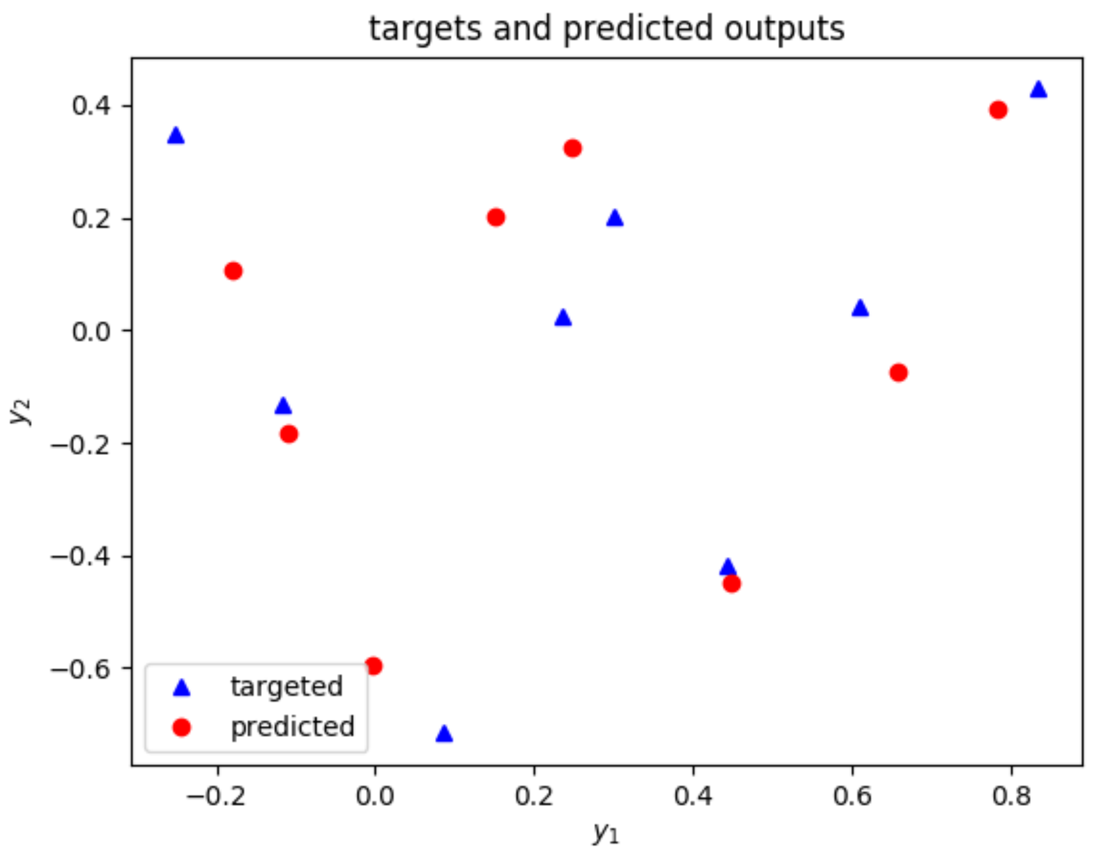
$$\boldsymbol{W} = \begin{pmatrix} -2.04 & -0.52 & -1.88 \\ 3.55 & -2.6 & 2.43 \end{pmatrix}$$

$$\boldsymbol{b} = \begin{pmatrix} 0.22 \\ -0.93 \\ 0.15 \end{pmatrix}$$

$$\boldsymbol{V} = \begin{pmatrix} 2.14 & -1.14 \\ -2.93 & -1.78 \\ 3.59 & 2.28 \end{pmatrix}$$

$$\boldsymbol{c} = \begin{pmatrix} 1.25 \\ -0.43 \end{pmatrix}$$

## Example 2



After 20,000 iterations

## The universal approximation theorem

Kolmogorov Theorem:

Given any function $\phi: I^n \rightarrow \boldsymbol{R}^K$ where $I$ is the closed unit interval [0,1], an arbitrary function $\phi$ can be implemented exactly by a multilayer perceptron (MLP) network with one hidden layer, $n$ input nodes, $2n+1$ hidden layer neurons and $K$ output layer neurons.

The theorem does not refer to learning algorithms or the amount of training data needed for the universal approximation. Recent researches find that due to the limited amount of training data and limitations of learning algorithms, deeper neural networks and a large set of training data are required in order to learn an arbitrary complex function.

## Normalization of inputs

If inputs have similar variations, better approximation of inputs or prediction of outputs is achieved. Mainly, there are two approaches to normalization of inputs.

Suppose $i$th input $x_i \in [x_{i,min}, x_{i,max}]$ and has a mean $\mu_i$ and a standard deviation $\sigma_i$.

If $\tilde{x}_i$ denotes the normalized input.

1. Scale the inputs such that $x_i \in [0, 1]$ :

$$\tilde{x}_i = \frac{x_i - x_{i,min}}{x_{i,max} - x_{i,min}}$$

2. Normalize the input to have standard normal distributions $x_i \sim N(0,1)$:

$$\tilde{x}_i = \frac{x_i - \mu_i}{\sigma_i}$$

## Output-layer activation function

Sigmoid activation function:

If output $y \in [y_{min}, y_{max}]$, the output-layer activation function:

$$f(u) = \frac{a}{1+e^{-u}} + b$$

where $a = y_{max} - y_{min}$

$b = y_{min}$

Linear activation function:

The convergence is usually improved if each output is normalized to have zero mean and unit standard deviation: $y_k \sim N(0,1)$

$$\tilde{y}_k = \frac{y_k - \mu_k}{\sigma_k}$$

## Boston housing dataset

https://www.cs.toronto.edu/~delve/data/boston/bostonDetail.html

**14 variables**

CRIM - per capita crime rate by town
ZN - proportion of residential land zoned for lots over 25,000 sq.ft.
INDUS - proportion of non-retail business acres per town.
CHAS - Charles River dummy variable (1 if tract bounds river; 0 otherwise)
NOX - nitric oxides concentration (parts per 10 million)
RM - average number of rooms per dwelling
AGE - proportion of owner-occupied units built prior to 1940
DIS - weighted distances to five Boston employment centres
RAD - index of accessibility to radial highways
TAX - full-value property-tax rate per $10,000
PTRATIO - pupil-teacher ratio by town
B - 1000(Bk - 0.63)^2 where Bk is the proportion of blacks by town
LSTAT - % lower status of the population
MEDV - Median value of owner-occupied homes in $1000's

506 data points
Try to predict MEDV by using other 13 variables

## Example 3: Predicting housing prices in Boston

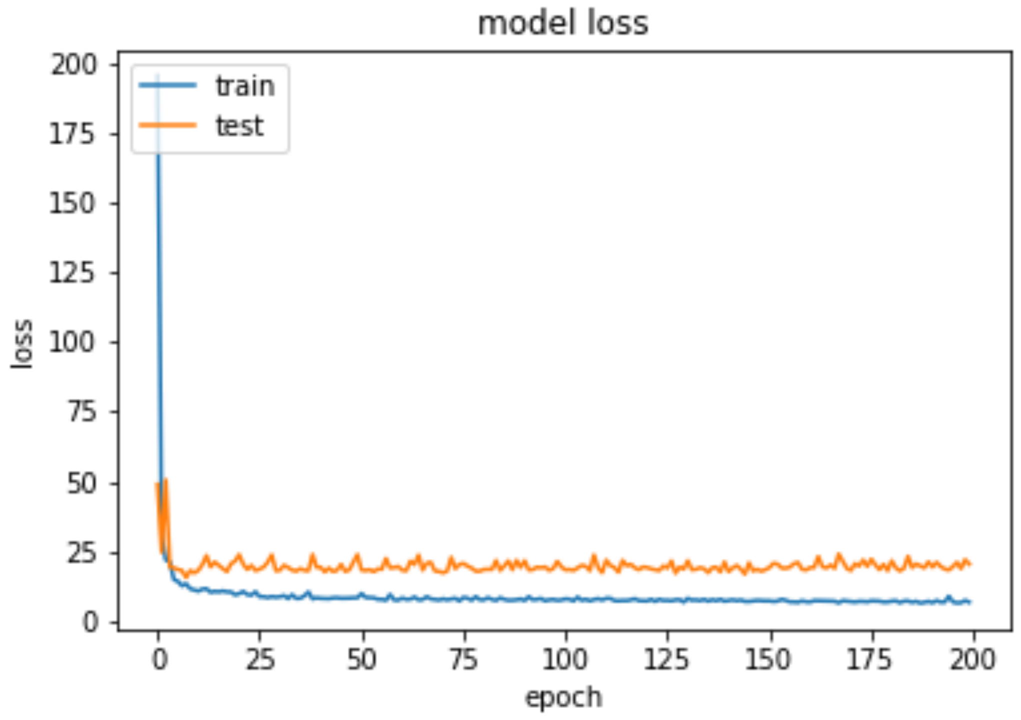
404 training samples, 102 testing samples
Thirteen input variables, One output variable

We use FFN with one hidden layer with 10 neuron
Network size: [13, 10, 1]

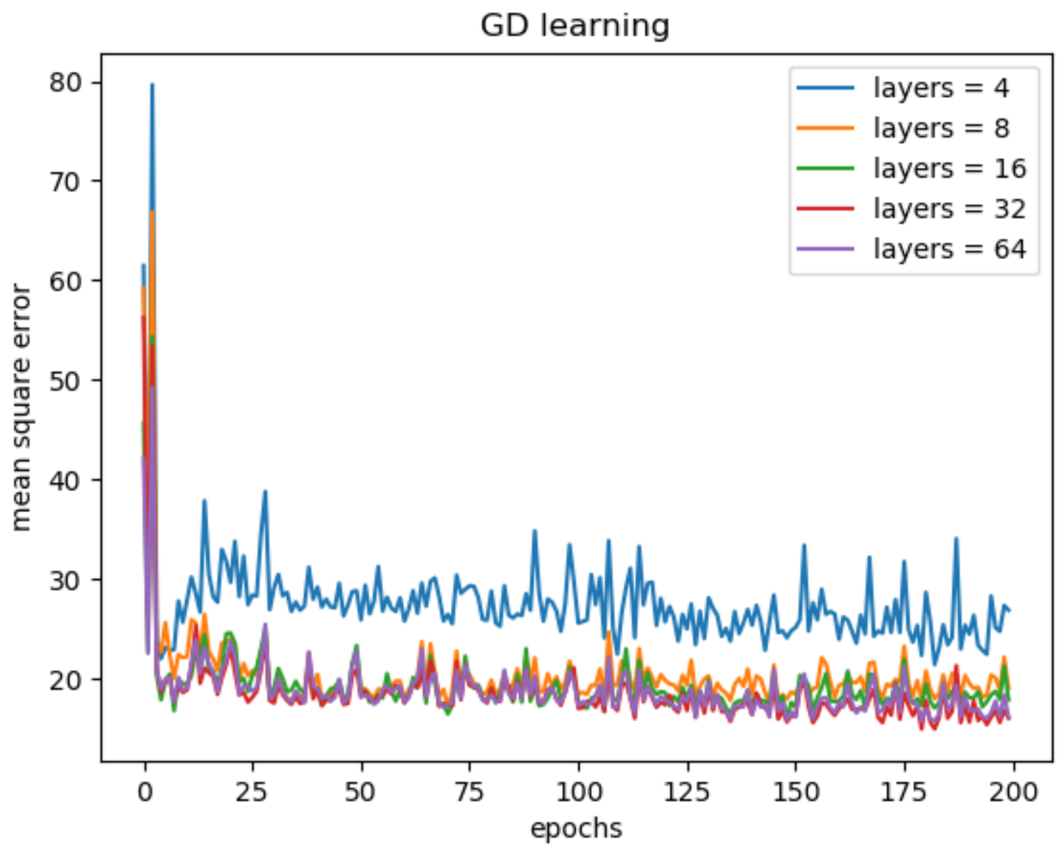
```
from tensorflow.keras import Sequential
from tensorflow.keras.layers import Dense

model = Sequential([
   Dense(10, activation='relu'),
   Dense(1, activation='linear')
])
```

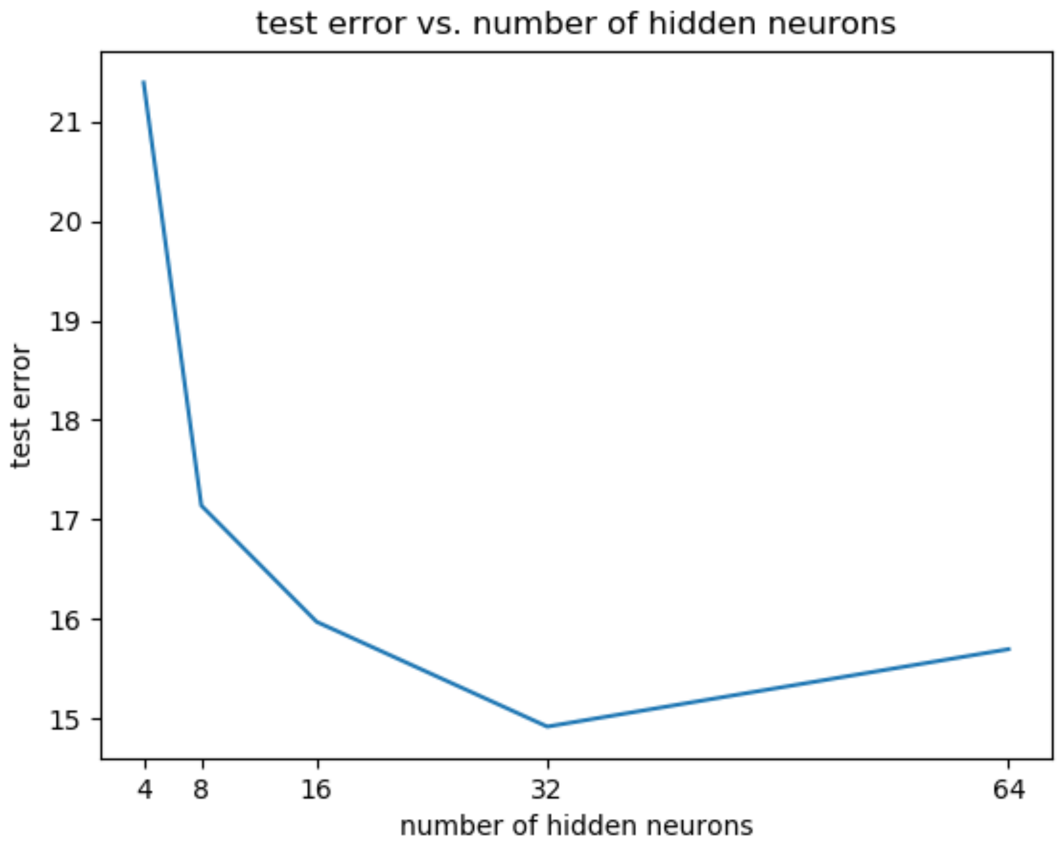
## Example 3


model loss
train
test
loss
epoch
200
175
150
125
100
75
50
25
0
0
25
50
75
100
125
150
175
200

## Example 3: Number of hidden neurons



## Example 3



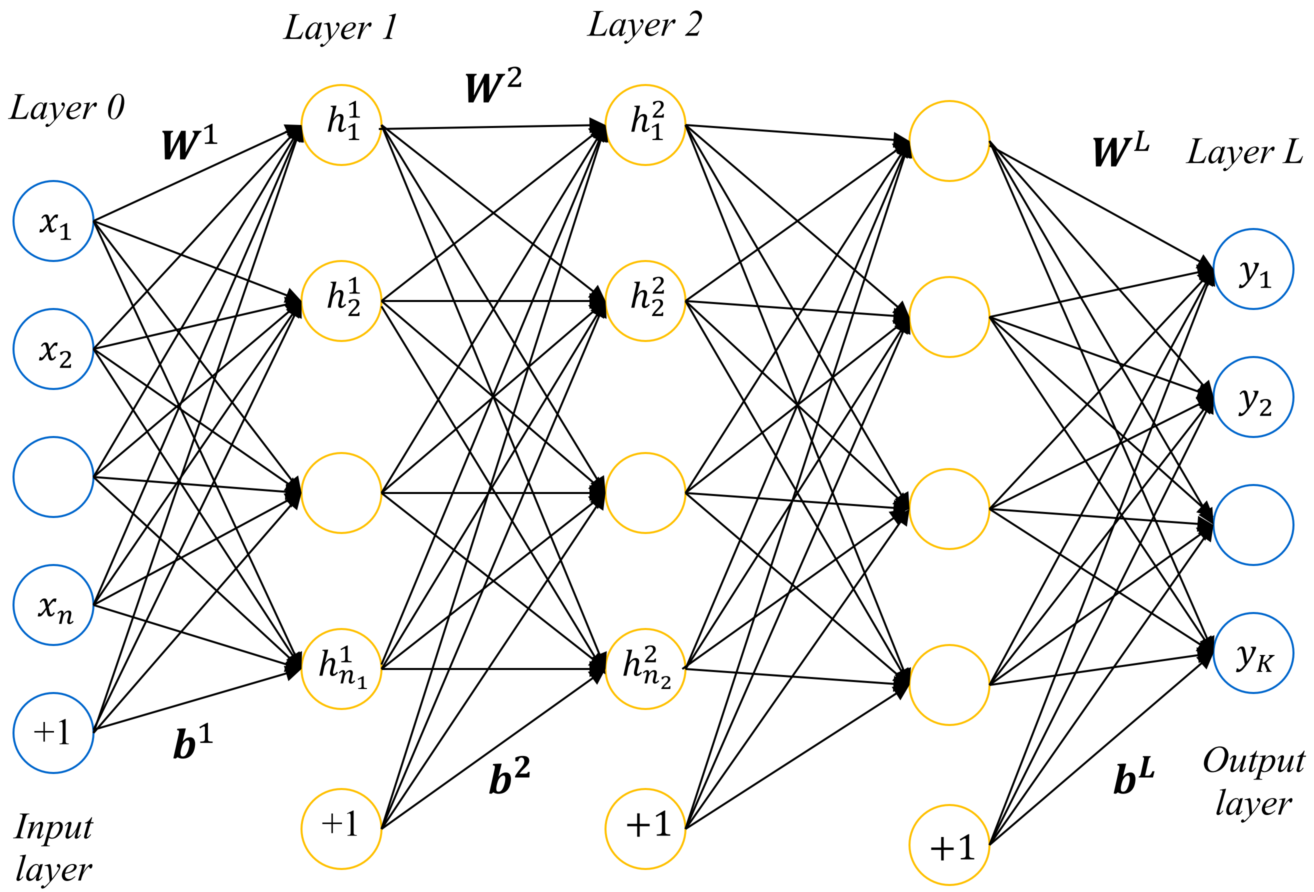
Optimum number of hidden neurons 32

## Width: the number of hidden neurons

The number of parameters of the network increases with the number of hidden units. Therefore, the network attempts to remember the training patterns with increasing number of parameters. In other words, the network aims at minimizing the training error at the expense of its generalization ability on unseen data.

As the number of hidden units increases, the test error decreases initially but tends to increase at some point. The optimal number of hidden units is often determined empirically (that is, by trial and error).

# Deep neural networks (DNN)



Depth = $L + 1$

# DNN

Input layer $l = 0$:
Width = $n$
Input $\boldsymbol{x}, \boldsymbol{X}$

Hidden layers $l = 1, 2, \cdots L - 1$
Width: $n_l$
Weight matrix $\boldsymbol{W}^l$, bias vector $\boldsymbol{b}^l$
Synaptic input $\boldsymbol{u}^l, \boldsymbol{U}^l$
Activation function $f^l$
Output $\boldsymbol{h}^l, \boldsymbol{H}^l$

Output layer $l = L$
Width: $K$
Synaptic input $\boldsymbol{u}^L, \boldsymbol{U}^L$
Activation function $f^L$
Output $\boldsymbol{y}, \boldsymbol{Y}$
Desired output $\boldsymbol{d}, \boldsymbol{D}$

# Forward propagation of activation in DNN: single pattern

```
Input $(\boldsymbol{x}, \boldsymbol{d})$
$\boldsymbol{u}^1 = \boldsymbol{W}^{1^T} \boldsymbol{x} + \boldsymbol{b}^1$
For layers $l = 1, 2, \cdots, L-1$:
        $\boldsymbol{h}^l = f^l(\boldsymbol{u}^l)$
        $\boldsymbol{u}^{l+1} = \boldsymbol{W}^{l+1^T} \boldsymbol{h}^l + \boldsymbol{b}^{l+1}$
$\boldsymbol{y} = f^L(\boldsymbol{u}^L)$
```

# Back-propagation of gradients in DNN: single pattern

if $l = L$:

$$\nabla_{\boldsymbol{u}^l} J = \begin{cases} -(\boldsymbol{d} - \boldsymbol{y}) & \text{for linear layer} \\ -\left(1(\boldsymbol{k} = d) - f^L(\boldsymbol{u}^L)\right) & \text{for softmax layer} \end{cases}$$

else:

$$\nabla_{\boldsymbol{u}^l} J = \boldsymbol{W}^{l+1}\left(\nabla_{\boldsymbol{u}^{l+1}} J\right) \cdot f^{l'}\left(\boldsymbol{u}^l\right) \qquad \text{from (A)}$$

$$\nabla_{\boldsymbol{W}^l} J = \boldsymbol{h}^{l-1}\left(\nabla_{\boldsymbol{u}^l} J\right)^T$$

$$\nabla_{\boldsymbol{b}^l} J = \nabla_{\boldsymbol{u}^l} J$$

# Stochastic backpropagation for DNN

```
For layers $l = L, L-1, \cdots, 2$:
    If $l = L$:
        $\nabla_{\boldsymbol{u}^l} J = \begin{cases} -(\boldsymbol{d} - \boldsymbol{y}) \\ -\left(1(\boldsymbol{k} = d) - f^L(\boldsymbol{u}^L)\right) \end{cases}$
    Else:
        $\nabla_{\boldsymbol{u}^l} J = \left(\boldsymbol{W}^{l+1} \nabla_{\boldsymbol{u}^{l+1}} J\right) \cdot f^{l\prime}(\boldsymbol{u}^l)$

    $\nabla_{\boldsymbol{W}^l} J = \boldsymbol{h}^{l-1} \left(\nabla_{\boldsymbol{u}^l} J\right)^T$
    $\nabla_{\boldsymbol{b}^l} J = \nabla_{\boldsymbol{u}^l} J$

$\nabla_{\boldsymbol{u}^1} J = (\boldsymbol{W}^2 \nabla_{\boldsymbol{u}^2} J) \cdot f^{1\prime}(\boldsymbol{u}^1)$
$\nabla_{\boldsymbol{W}^1} J = \boldsymbol{x} (\nabla_{\boldsymbol{u}^1} J)^T$
$\nabla_{\boldsymbol{b}^1} J = \nabla_{\boldsymbol{u}^1} J$
```

# Forward propagation of activation in DNN: batch of patterns

```
Input $(\boldsymbol{X}, \boldsymbol{D})$
$\boldsymbol{U}^1 = \boldsymbol{X}\boldsymbol{W}^1 + \boldsymbol{B}^1$
For layers $l = 1, 2, \cdots, L-1$:
        $\boldsymbol{H}^l = f^l(\boldsymbol{U}^l)$
        $\boldsymbol{U}^{l+1} = \boldsymbol{H}^l\boldsymbol{W}^{l+1} + \boldsymbol{B}^{l+1}$
$\boldsymbol{Y} = f^L(\boldsymbol{U}^L)$
```

# Back-propagation of gradients in DNN: batch of patterns

If $l = L$:

$$\nabla_{\boldsymbol{U}^l} J = \begin{cases} -(\boldsymbol{D} - \boldsymbol{Y}) \\ -\left(\boldsymbol{K} - f^L(\boldsymbol{U}^L)\right) \end{cases}$$

Else:

$$\nabla_{\boldsymbol{U}^l} J = \left(\nabla_{\boldsymbol{U}^{l+1}} J\right) \boldsymbol{W}^{l+1^T} \cdot f^{l'}\left(\boldsymbol{U}^l\right)$$

$$\nabla_{\boldsymbol{W}^l} J = \boldsymbol{H}^{l-1^T}\left(\nabla_{\boldsymbol{U}^l} J\right)$$

$$\nabla_{\boldsymbol{b}^l} J = \left(\nabla_{\boldsymbol{U}^l} J\right)^T \boldsymbol{1}_P$$

# Back-propagation for DNN

```
For layers $l = L, L-1, \cdots, 2$:
    If $l = L$:
        $\nabla_{\boldsymbol{U}^l} J = \begin{cases} -(\boldsymbol{D} - \boldsymbol{Y}) \\ -\left(\boldsymbol{K} - f^L(\boldsymbol{U}^L)\right) \end{cases}$
    Else:
        $\nabla_{\boldsymbol{U}^l} J = \left(\nabla_{\boldsymbol{U}^{l+1}} J\right) {\boldsymbol{W}^{l+1}}^T \cdot {f^l}'(\boldsymbol{U}^l)$

    $\nabla_{\boldsymbol{W}^l} J = {\boldsymbol{H}^{l-1}}^T \left(\nabla_{\boldsymbol{U}^l} J\right)$
    $\nabla_{\boldsymbol{b}^l} J = \left(\nabla_{\boldsymbol{U}^l} J\right)^T \mathbf{1}_P$
```

$$\nabla_{\boldsymbol{U}^1} J = (\nabla_{\boldsymbol{U}^2} J) {\boldsymbol{W}^2}^T \cdot {f^1}'(\boldsymbol{U}^1)$$
$$\nabla_{\boldsymbol{W}^1} J = \boldsymbol{X}^T (\nabla_{\boldsymbol{U}^1} J)$$
$$\nabla_{\boldsymbol{b}^1} J = (\nabla_{\boldsymbol{U}^1} J)^T \mathbf{1}_P$$

# Example 4

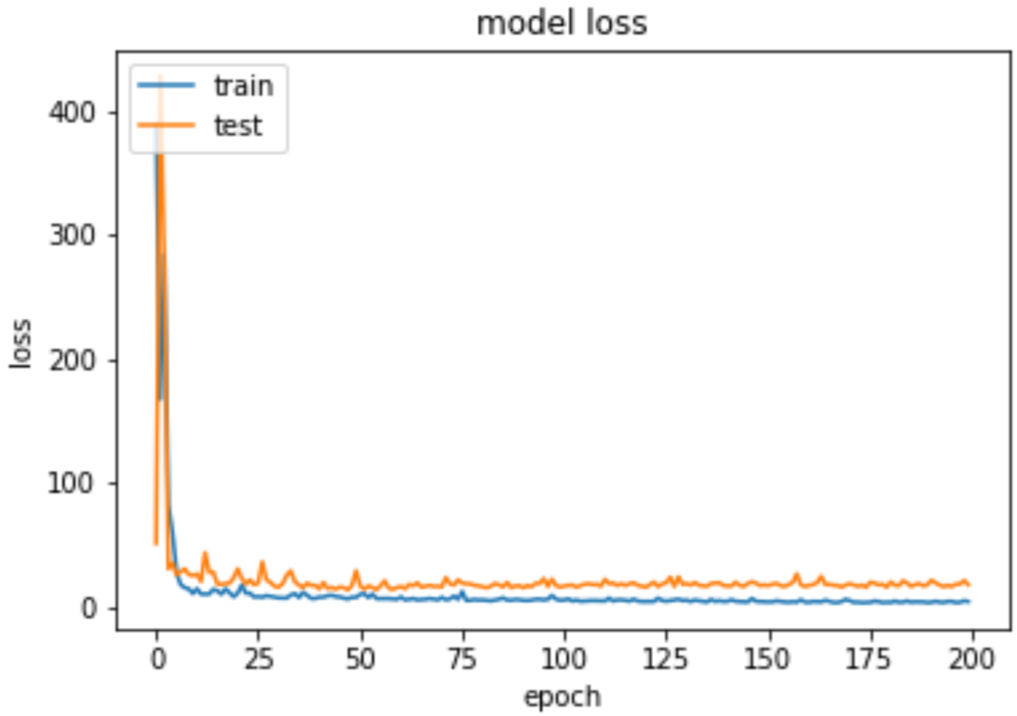
Boston housing data:
https://www.cs.toronto.edu/~delve/data/boston/bostonDetail.html

Predicting housing price from other 13 variables

DNN with two hidden layers:
[13, 10, 5, 1]

```
model = Sequential([
   Dense(10, activation='relu'),
   Dense(5, activation='relu'),
   Dense(1, activation='linear’)])
```

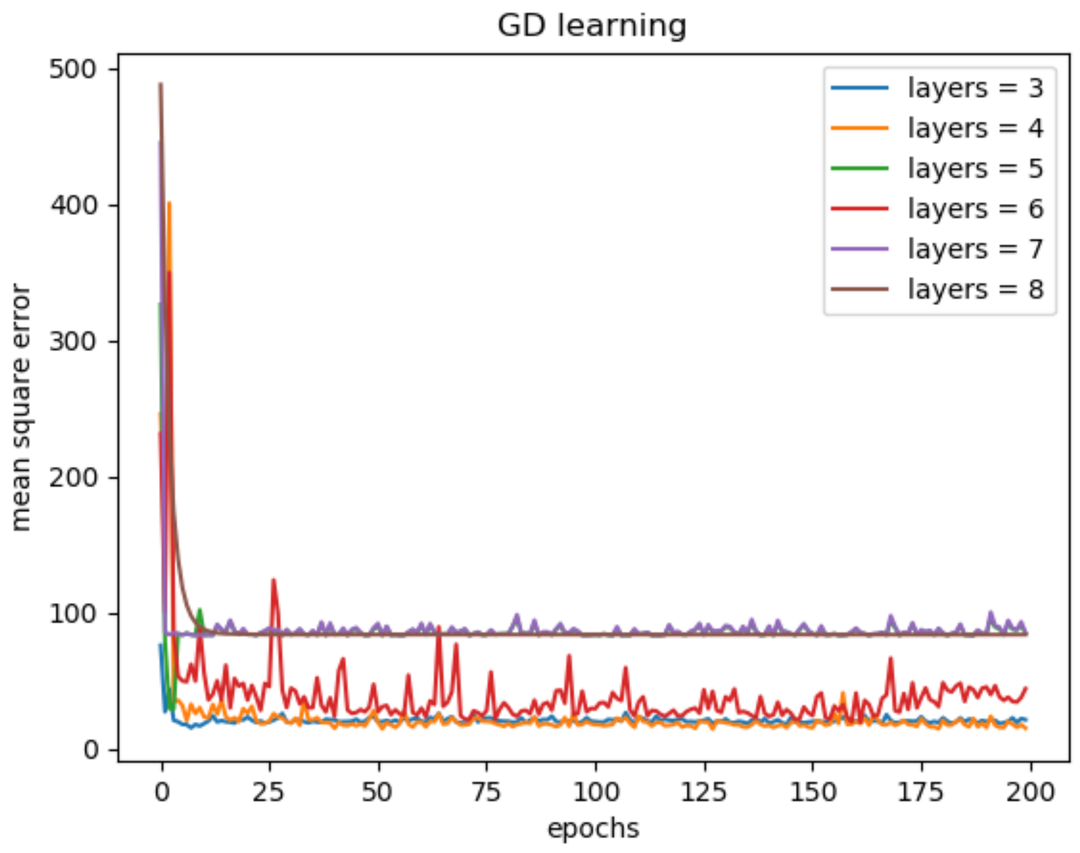
# Example 4


model loss
train
test
loss
epoch
0
100
200
300
400
0
25
50
75
100
125
150
175
200

## Example 4: Varying the number of layers

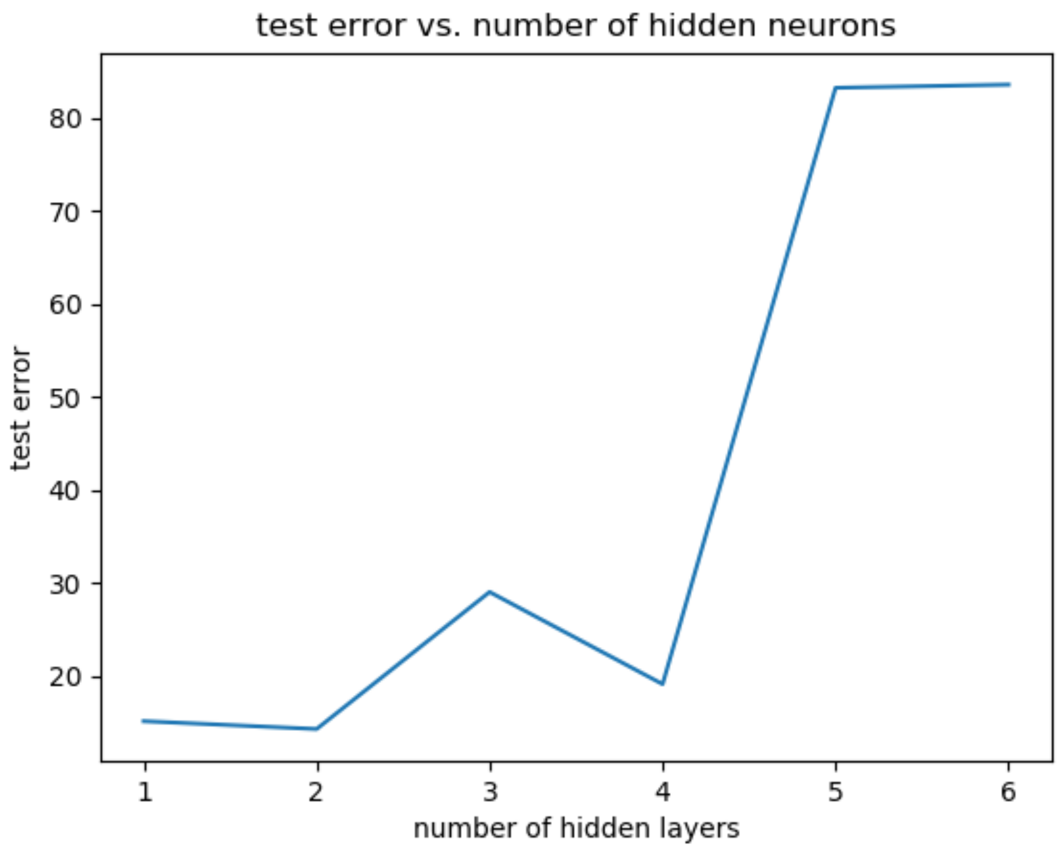
Architectures:
One hidden layer: [13, 5, 1]
Two hidden layers: [13, 5, 5, 1]
Three hidden layers: [13, 5, 5, 5, 1]
Four hidden layers: [13, 5, 5, 5, 5, 1]
Five hidden layers: [13, 5, 5, 5, 5, 5, 1]

# Example 4



GD learning
mean square error
epochs
0
100
200
300
400
500
0
25
50
75
100
125
150
175
200
layers = 3
layers = 4
layers = 5
layers = 6
layers = 7
layers = 8

# Example 4



Optimum number of hidden layers = 2

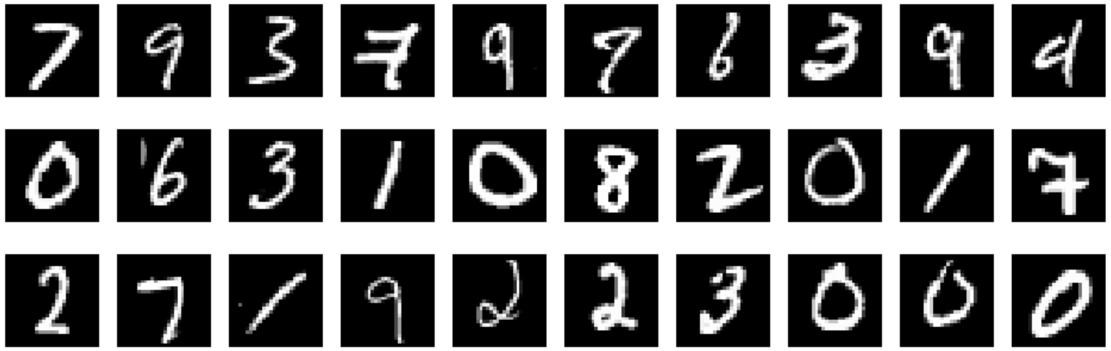
## Depth: number of hidden layers

The deep networks extract features at different levels of complexity for regression or classification. However, the depth or the number of layers that you can have for the networks depend on the number of training patterns available. The deep networks have more parameters (weights and biases) to learn, so need more data to train. Deep networks can learn complex mapping accurately if sufficient training data is available.

The optimal number of layers is determined usually through experiments. The optimal architecture minimizes the error (training, test, and validation).

## MNIST images

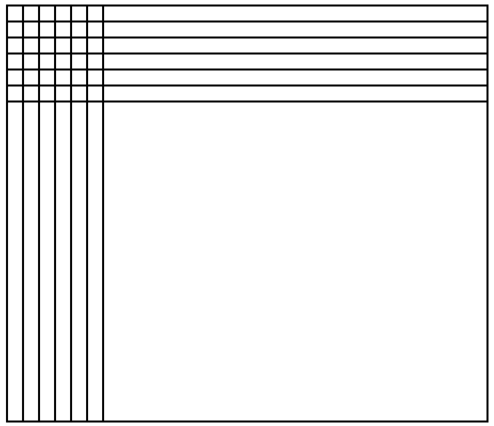
The MNIST database of gray level images of handwritten digits:
http://yann.lecun.com/exdb/mnist/



Each image is 28x28 size.
Intensities are in the range [0, 255].

Training set: 60,000
Test set: 10,000

# MNIST images



An image is divided into rows and columns and defined by its pixels.

Size of the image = rows x columns  pixels

Pixels of grey-level image are assigned intensity values: For example, integer values between 0 and 255 assigned as intensities (grey-values) for pixels with 0 representing 'black' and 255 representing 'white'.

Color images has three color channels: red, green, and blue. A pixel in a color image is a vector (r, g, b) denoting intensity in red, green, and blue channels.

## Example 5: Classification of MNIST images

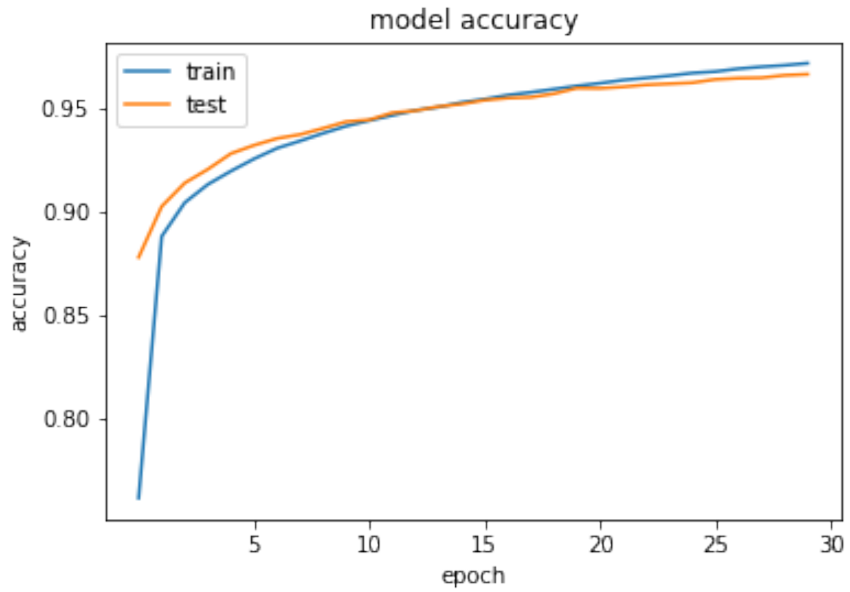
No of inputs $n = 28 \times 28 = 784$
Inputs were normalized to $[0.0, \quad 1.0]$

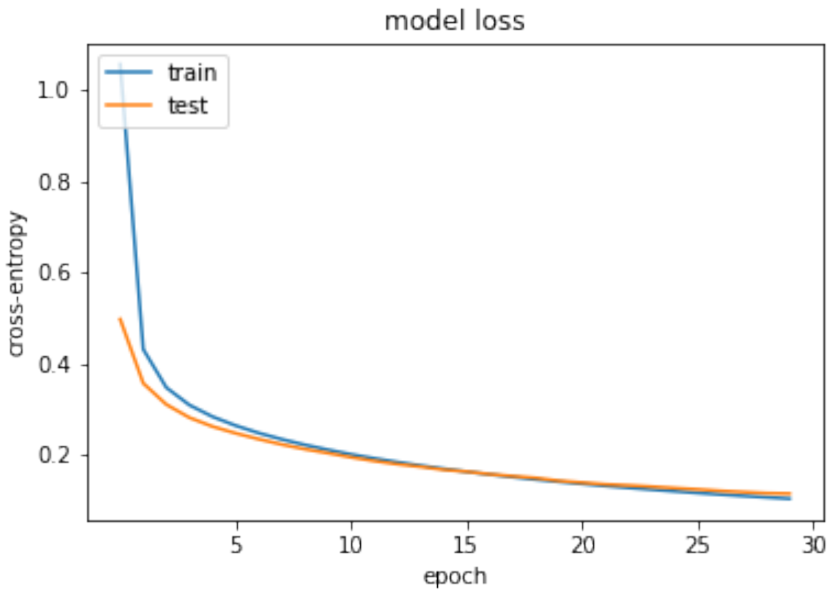
Use a 4-layer FFN
- Hidden-layer-1 is a sigmoid layer
- Hidden-layer-2 is sigmoid layer
- Output-layer is a softmax layer

Input-layer size $n = 784$
Hidden-layer-1 size $n_1 = 625$
Hidden-layer-2 size $n_2 = 100$
Output-layer size $K = 10$

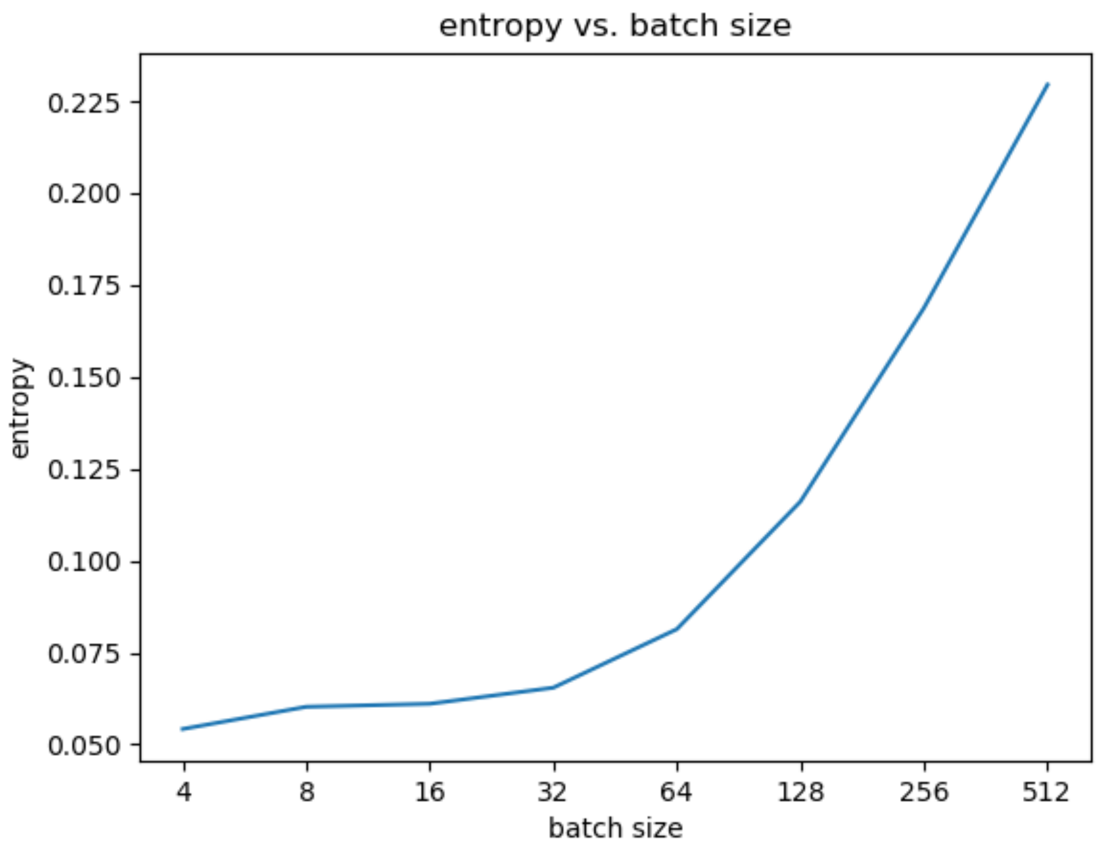
Training:
Batch size = 64
Learning rate $\alpha = 0.01$

## Example 5

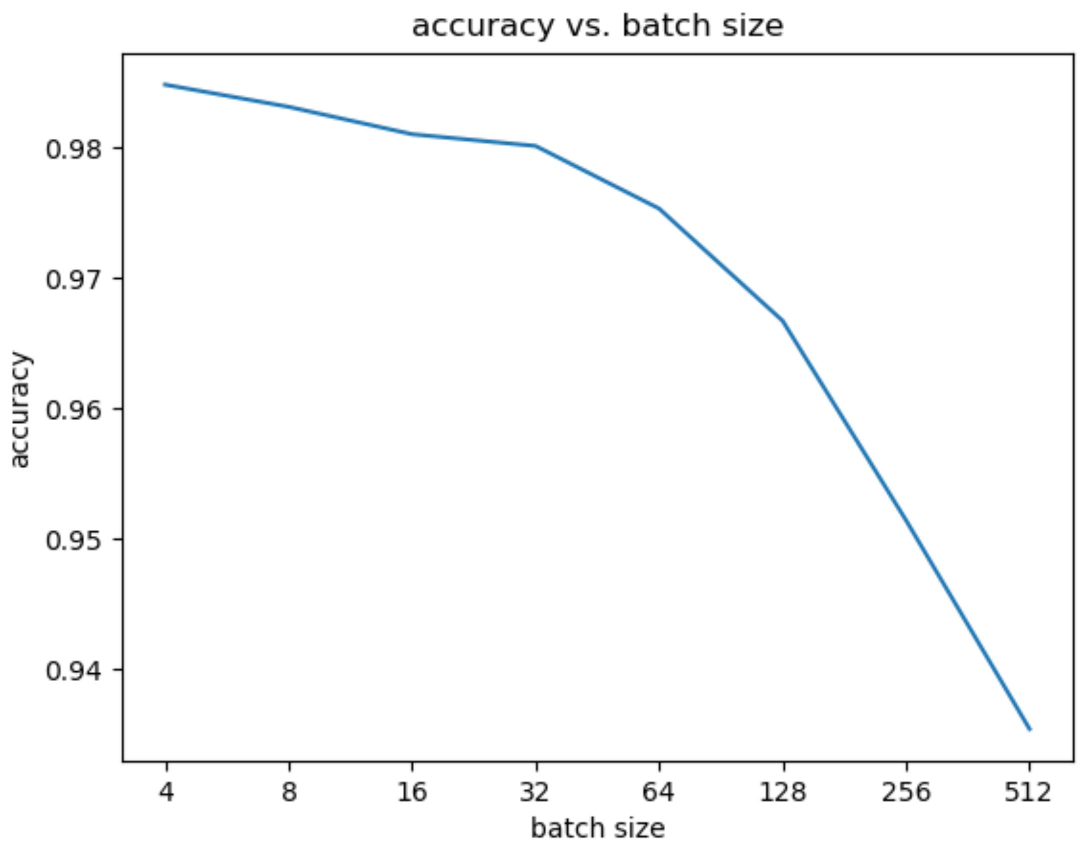

model accuracy
train
test
accuracy
0.80
0.85
0.90
0.95
epoch
5
10
15
20
25
30


model loss
train
test
cross-entropy
0.2
0.4
0.6
0.8
1.0
epoch
5
10
15
20
25
30

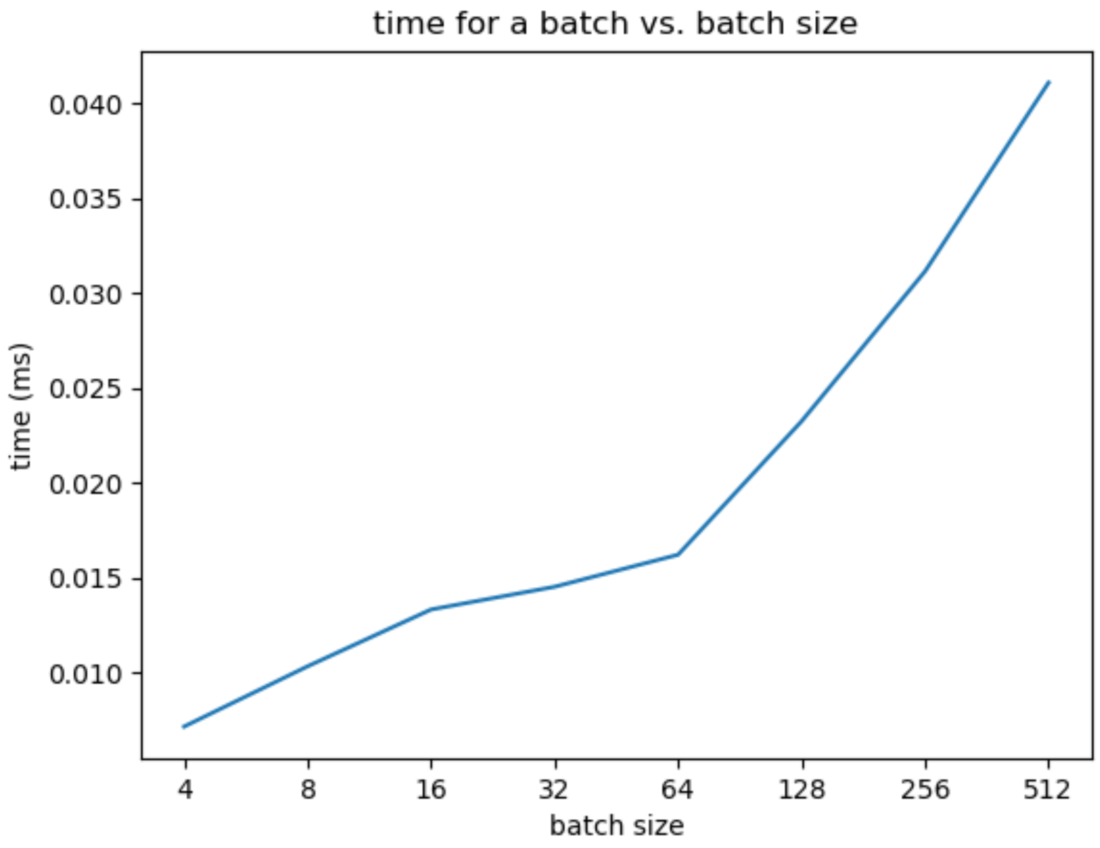
## Example 5b: effect of batch size



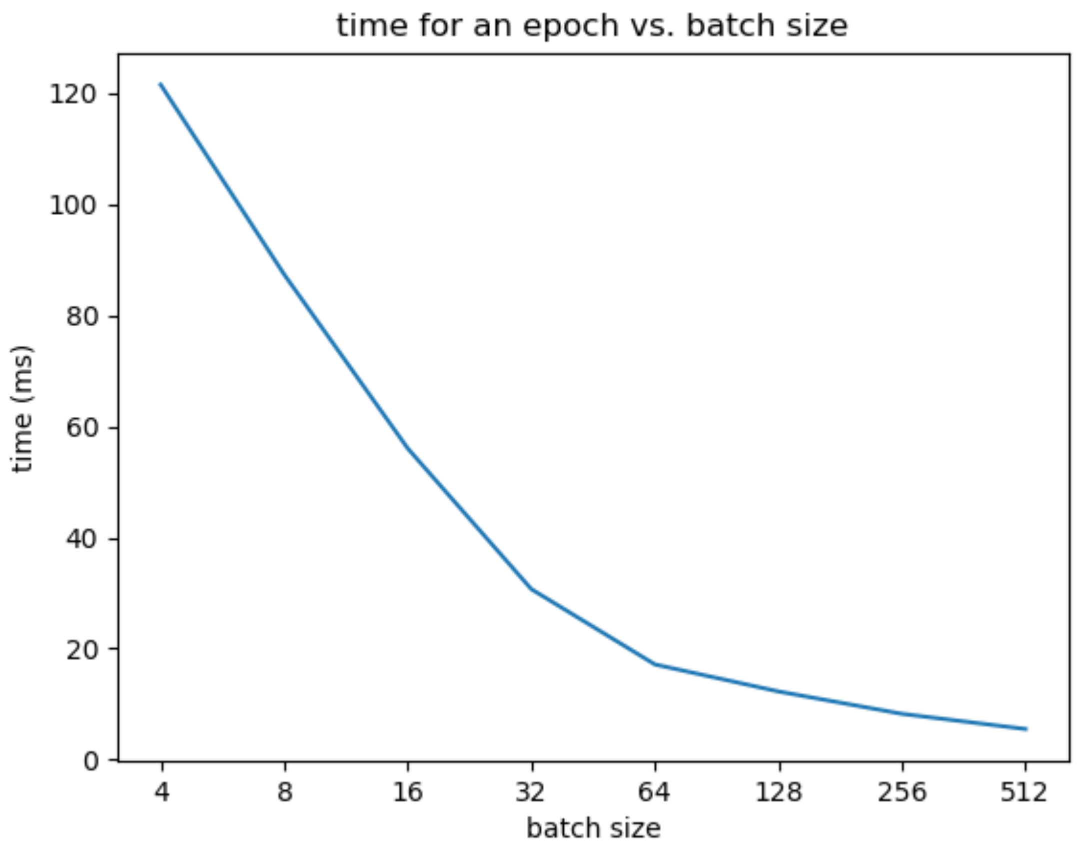
## Example 5b: effect of batch size



## Example 5b: effect of batch size



## Example 5b: effect of batch size



## Mini-batch SGD

In practice, gradient descent is performed on *mini-batch* updates of gradients within a *batch* or *block* of data of size $B$. In mini-batch SGD, the data is divided into blocks and the gradients are evaluated on each block in an epoch.

$B = 1$: stochastic (online) gradient descent
$B = P$ (size of training data): (batch) gradient descent
$1 < B < P \rightarrow$ mini-batch stochastic gradient descent

When $B$ increases, more add-multiply operations per second, taking advantages of parallelism and matrix computations. On the other hand, as $B$ increases, the number of computations per update (of weights, biases) increases.

Therefore, the curve of the time for weight update against batch size usually take a U-shape curve.  There exists an optimal value of $B$ – that depends on the sizes of the caches as well.

## Batch size for mini-batch SGD

For SGD, it is desirable to randomly sample the patterns from training data in each epoch. In order to efficiently sample blocks, the training patterns are shuffled at the beginning of every training epoch and then blocks are sequentially fetched from memory.

Typical batch sizes: 16, 32, 64, 128, and 256.

The batch size is dependent on the size of caches of CPU and GPUs.

## Summary

- Chain rule for backpropagation of gradients: $\nabla_{\boldsymbol{x}} J = \left(\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}}\right)^{T} \nabla_{\boldsymbol{y}} J$
- FFN with one hidden layer (Shallow FFN)
- Backpropagation for FFN with one hidden layer:

$$\nabla_{\boldsymbol{Z}} J = (\nabla_{\boldsymbol{U}} J)\boldsymbol{V}^{T} \cdot g'(\boldsymbol{Z})$$

- Backpropagation learning for deep FFN (DNN)
- Training deep neural networks (GD and SGD):
  - Forward propagation of activation
  - Backpropagation of gradients
  - Updating weights

- Parameters to be decided: depth, width, and batch size