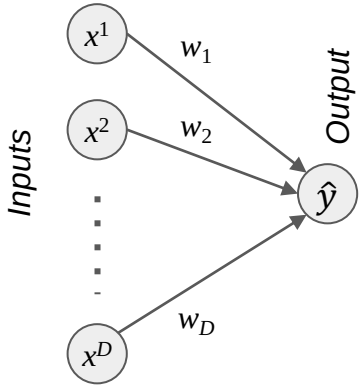
#Code

Artificial Intelligence and Machine Learning (AIML)

2023–24

- **Last lecture**:
  - Neural networks
    - Single-layer perceptron concept (“neuron unit”)



activation function (nonlinear, differentiable)

$$\hat{y} = f(w_1 x^1 + w_2 x^2 + \cdots + w_D x^D)$$

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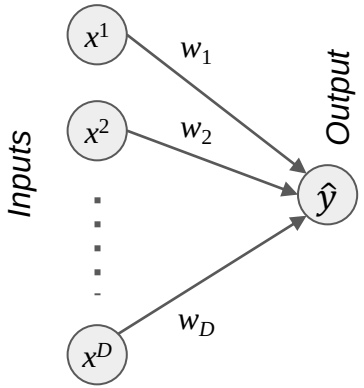

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$$\hat{y} = f(w^T x)$$

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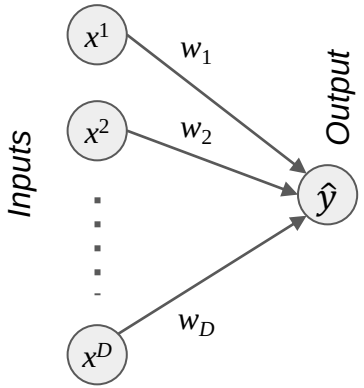

activation function (nonlinear, differentiable)

$$\hat{y} = f(w_1 x^1 + w_2 x^2 + \cdots + w_D x^D)$$

$$\hat{y} = f(w^T x) \qquad w^T = [w_1 \quad w_2 \quad \cdots \quad w_D], \; x = \begin{bmatrix} x^1 \\ x^2 \\ \vdots \\ x^D \end{bmatrix}$$

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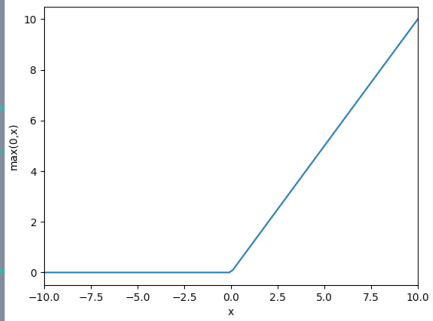
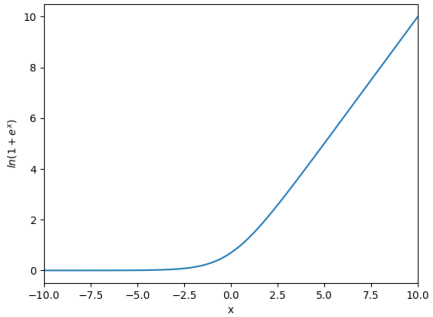
    - Activation functions

ReLU
$(\max(0, x))$

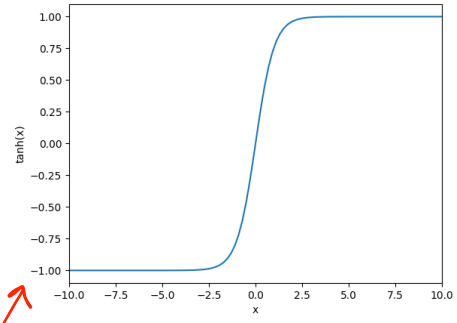


Softplus
$(ln(1 + e^x))$



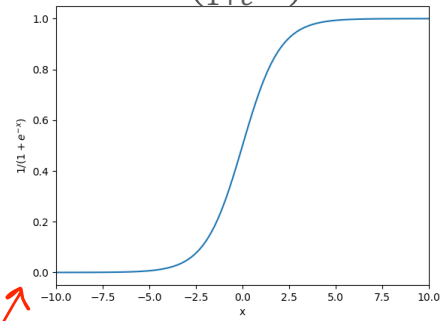
-1 ~ 1

Hyperbolic Tangent
$(\tanh(x))$

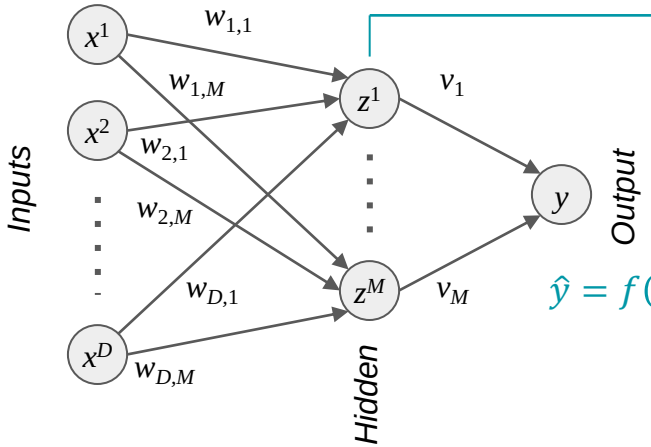


0 ~ 1

Logistic
$\left(\frac{1}{1+e^{-x}}\right)$



- **Neural networks**
  - Single-layer perceptron concept (“neuron unit”)
  - Activation functions
  - Perceptron extensions

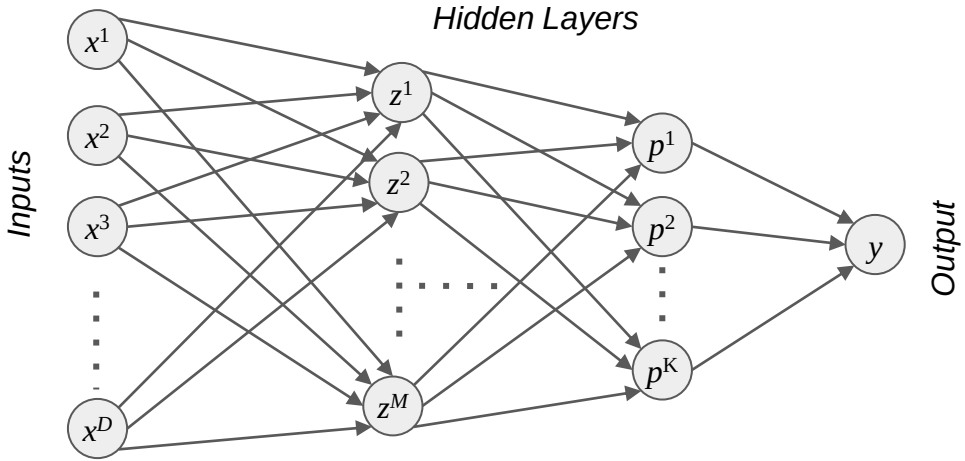


$$z^1 = f\left(w_{1,1}x^1 + w_{2,1}x^2 + \cdots + w_{D,1}x^D\right)$$
$$\vdots$$
$$z^M = f\left(w_{1,M}x^1 + w_{2,M}x^2 + \cdots + w_{D,M}x^D\right)$$

$$\hat{y} = f(v_1 z^1 + v_2 z^2 + \cdots + v_M z^M)$$

[matrix notation]
$$z = f(W^T x)$$

- **Neural Networks**
  - Single-layer perceptron concept (“neuron unit”)
  - Activation functions
  - Perceptron extensions and deep learning



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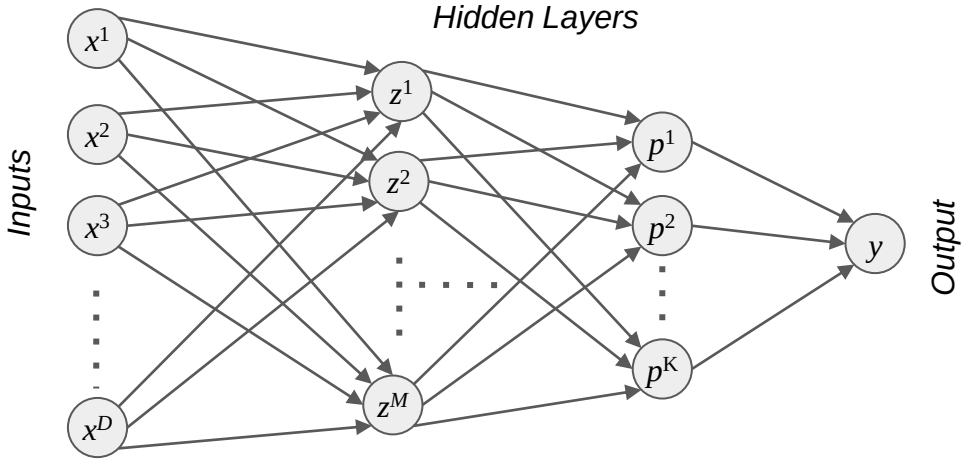
Neural networks

- Single-layer perceptron concept (“neuron unit”)
- Activation functions
- Perceptron extensions and deep learning



Fully Connected Network:

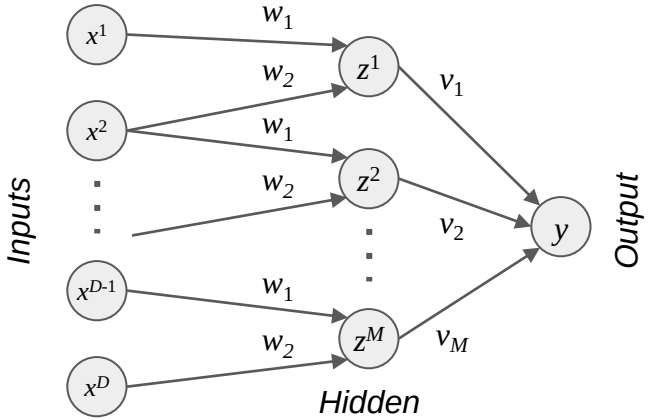
Input → Hidden Layer 1: $D \times M$ weights

HL1 → HL 2: $M \times K$ weights

⋮

Hidden Layer N: $K \times 1$ weights

- **Neural networks**
  - Single-layer perceptron concept (“neuron unit”)
  - Activation functions
  - Perceptron extensions and deep learning
    - Weights problem & weight sharing (CNN)



$$z^1 = \max(0, w^T[x^1\ x^2]^T)$$

$$z^2 = \max(0, w^T[x^2\ x^3]^T)$$

$$\dots$$

$$z^M = \max(0, w^T[x^{D-1}\ x^D]^T)$$

$$y = \max(0, v^T z)$$

- **Neural networks**
  - Single-layer perceptron concept (“neuron unit”)
  - Activation functions
  - Perceptron extensions and deep learning
    - Weights problem & weight sharing (CNN)

- **Next:**

  How to train deep neural networks

Training ML algorithms

#Code

TRAINING:
Iterative procedure for minimization of an error function, with adjustments to the weights being made at each step.

STAGE 1:
Evaluate derivatives of the error function wrt the weights

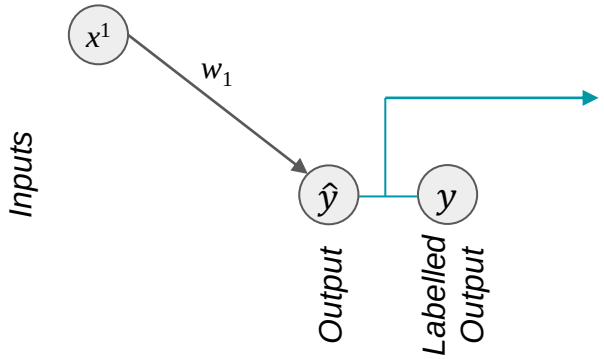
with respect to

STAGE 2:
Use derivatives to compute adjustments to be made to the weights

(e.g., gradient descent)

Training a single layer linear perceptron using gradient descent

#Code



Error Function

Sum of Squares:

$$F(w) = \sum_{i=1}^{N} (w_1 x_i^1 - y_i)^2$$

Weight update:

Model:

$$f(w, x) = \hat{y} = w_1 x^1$$

Training a single layer linear perceptron using gradient descent

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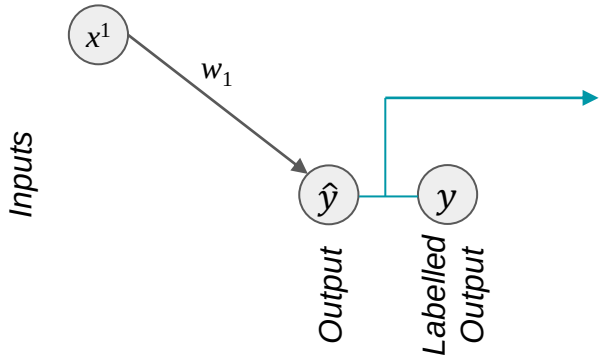

Error Function

Sum of Squares:

$$F(w) = \sum_{i=1}^{N} (w_1 x_i^1 - y_i)^2$$

Weight update:

$$w_{n+1} = w_n - \alpha F_w(w_n)$$

Model:

$$f(w, x) = \hat{y} = w_1 x^1$$

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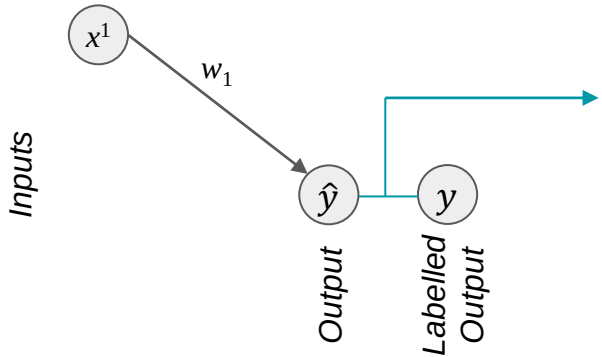
Training a single layer linear perceptron using gradient descent

Weight update: $w_{n+1} = w_n - \alpha F_w(w_n)$



Error Function

Sum of Squares:

$$F(w) = \sum_{i=1}^{N} (w_1 x_i^1 - y_i)^2$$

Derivative

$$F_w(w) = \frac{dF}{dw_1}$$

Sum of Squares:

$$F_w(w) = 2\sum_{i=1}^{N} (w_1 x_i^1 - y_i) x_i^1$$

Model:

$$f(w, x) = \hat{y} = w_1 x^1$$

Training a single layer linear perceptron using gradient descent

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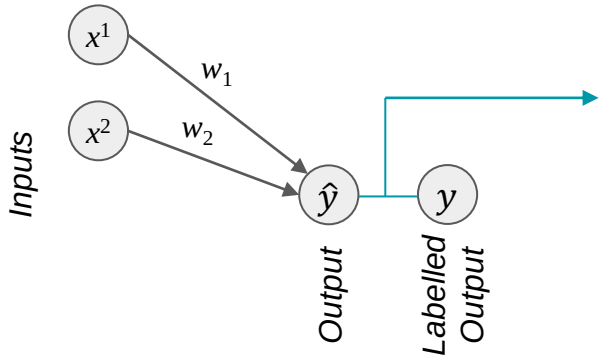
Weight update: $w_{n+1} = w_n - \alpha F_w(w_n)$



Error Function

Sum of Squares:

$$F(w) = \sum_{i=1}^{N} \left((w_1 x_i^1 + w_2 x_i^2) - y_i\right)^2$$

Gradient

$$F_w(w) = \begin{bmatrix} \frac{\partial F}{\partial w_1} \\ \frac{\partial F}{\partial w_2} \end{bmatrix}$$

Sum of Squares:

$$F_w(w) = 2\sum_{i=1}^{N} ((w_1 x_i^1 + w_2 x_i^2) - y_i) \begin{bmatrix} x_i^1 \\ x_i^2 \end{bmatrix}$$

Model:

$$f(w, x) = \hat{y} = w_1 x^1 + w_2 x^2$$

AIML

Training a single layer linear perceptron using gradient descent

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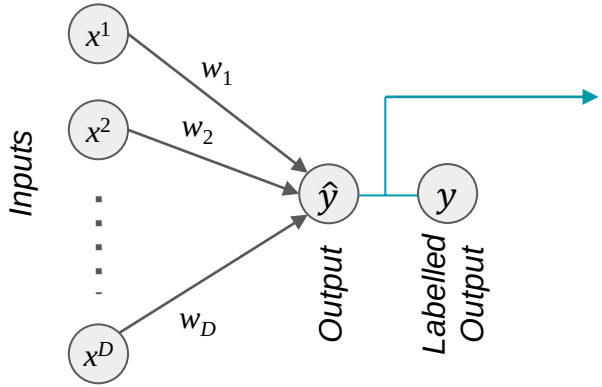

Model:

$$f(w,x) = \hat{y} = w_1 x^1 + w_2 x^2 + \cdots + w_D x^D$$

(vector notation) $f(w,x) = \hat{y} = w^T x$

Error Function

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Neural networks: training by gradient descent

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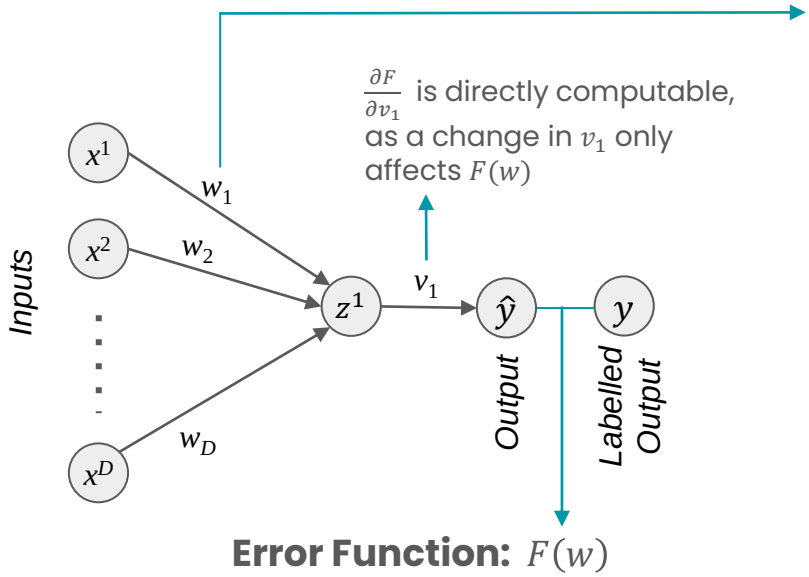

We need $\frac{\partial F}{\partial w_1}$

A change in w_1 will affect the output of z^1: $\frac{\partial z^1}{\partial w_1}$

The change in z^1 induced by w_1 will change the predicted output: $\frac{\partial F}{\partial z^1}$

w1引起的z1的变化将会改变预测结果

The total change in the output due to a change in w_1 will then be:

$$\frac{\partial F}{\partial w_1} = \frac{\partial F}{\partial z^1}\frac{\partial z^1}{\partial w_1}$$ (chain rule)

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Chain rule of Calculus

(**Gill**, Section 5.4)

- Provides a means of differentiating nested functions.
- Given two functions, $f(x)$ and $g(x)$, and the nested form

$$h = f\big(g(x)\big)$$

we need to account for the actual order of the nesting relationship to correctly differentiate h:

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$$h = f\big(g(x)\big)$$

we need to account for the actual order of the nesting relationship to correctly differentiate h:

$$\frac{dh}{dx} = \frac{d}{dx} f\big(g(x)\big) = f'\big(g(x)\big)g'(x)$$

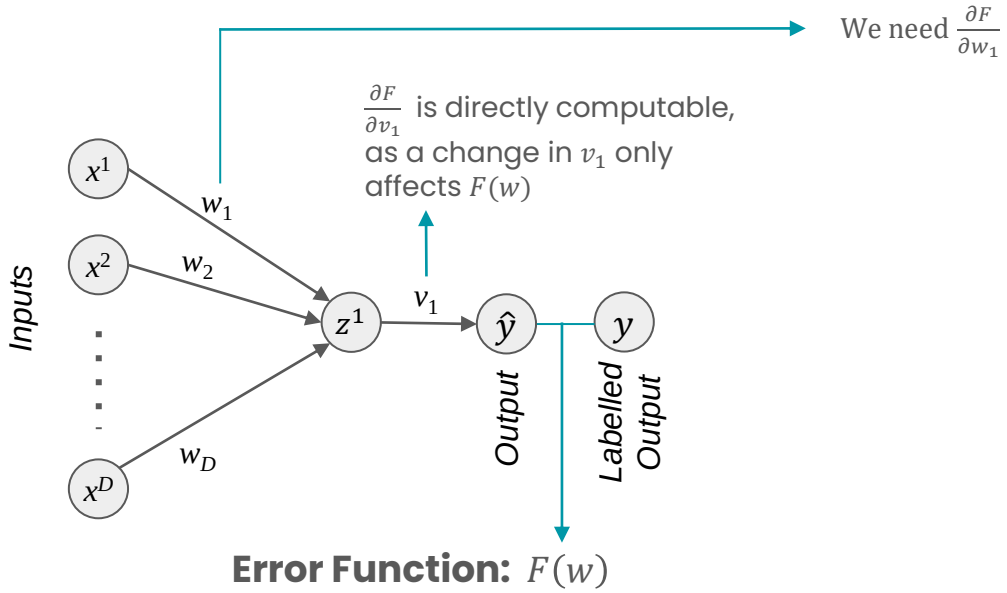
where $f'(x)$ is shorthand for $\frac{df(x)}{dx}$.

Neural networks: Training using gradient descent

#Code

- Gradient Descent Approach

$$w_{n+1} = w_n - \alpha F_w(w_n)$$



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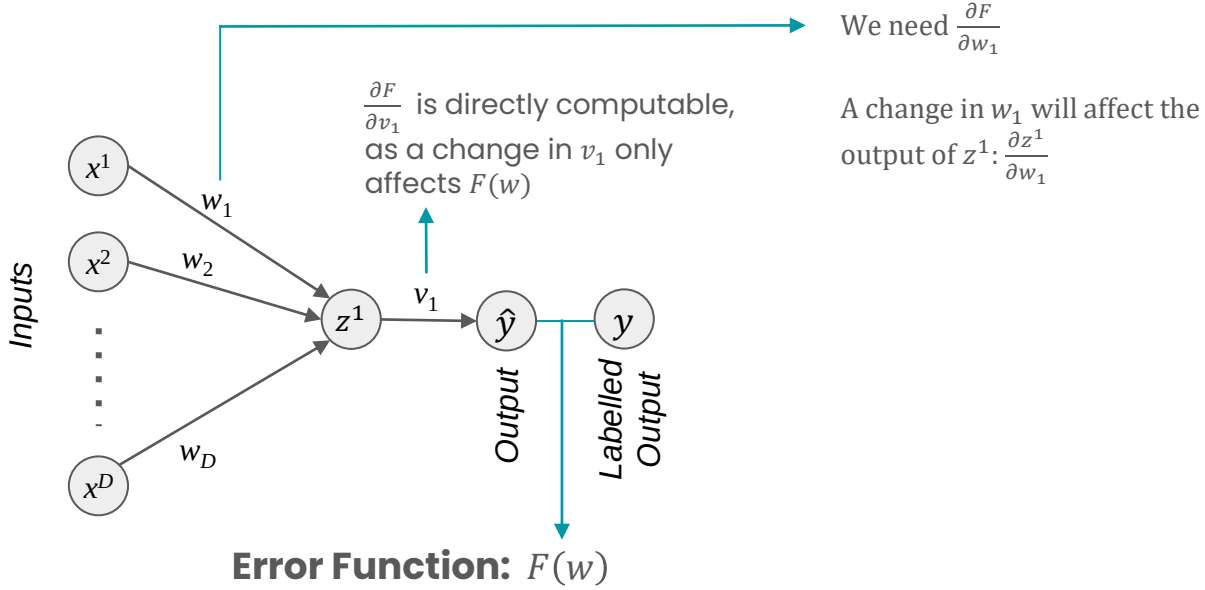

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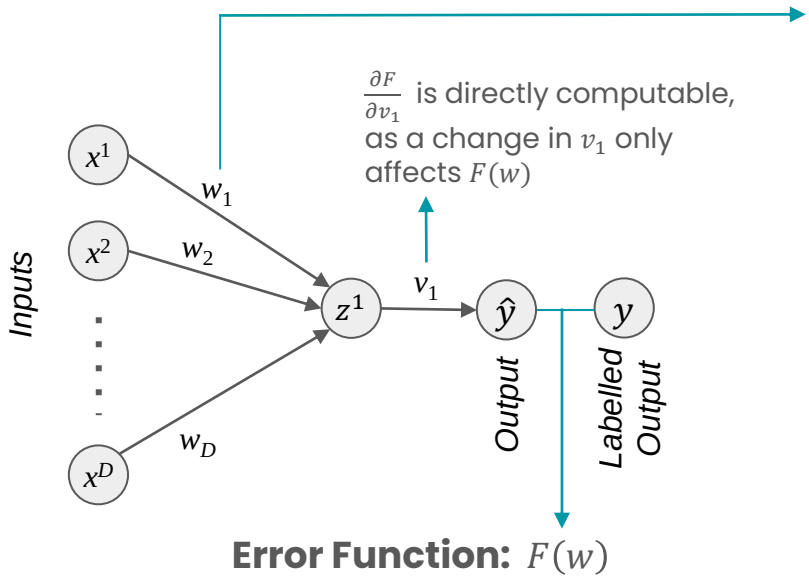

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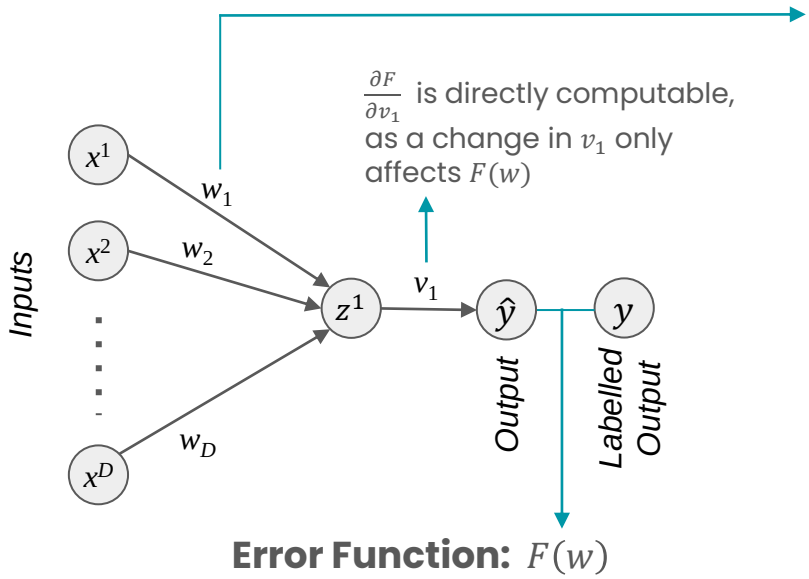

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Gradient

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Neural networks: Training using gradient descent

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- Gradient Descent Approach

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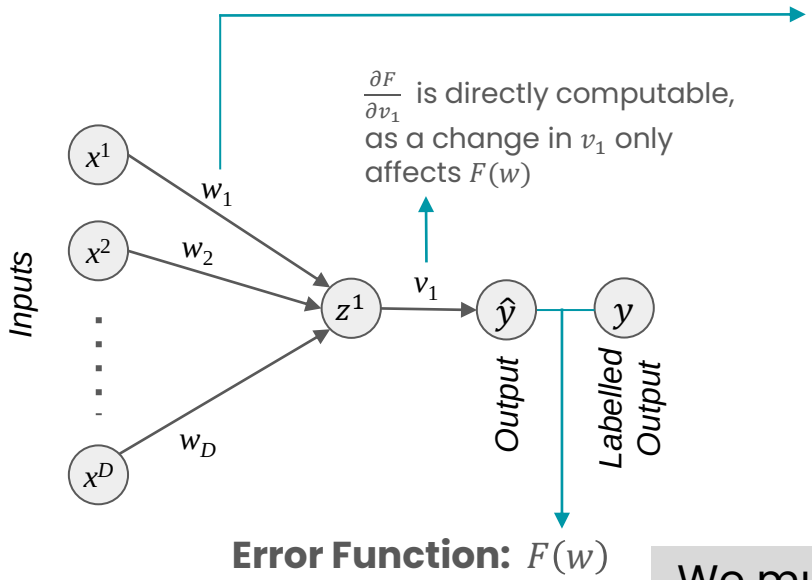

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We must **propagate gradients** from the output error $F(w)$, all the way through each layer

Training deep networks

#Code

TRAINING:
Iterative procedure for minimization of an error function, with adjustments to the weights being made at each step.

STAGE 1:
Evaluate derivatives of the error function wrt the weights

Analytical gradient expressions quickly become intractable

STAGE 2:
Use derivatives to compute adjustments to be made to the weights

Training deep networks

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TRAINING:
Iterative procedure for minimization of an error function, with adjustments to the weights being made at each step.

STAGE 1:
Evaluate derivatives of the error function wrt the weights

Analytical gradient expressions quickly become intractable

More sophisticated gradient calculation methods:
backpropagation and **automatic differentiation** (**AD**)

STAGE 2:
Use derivatives to compute adjustments to be made to the weights

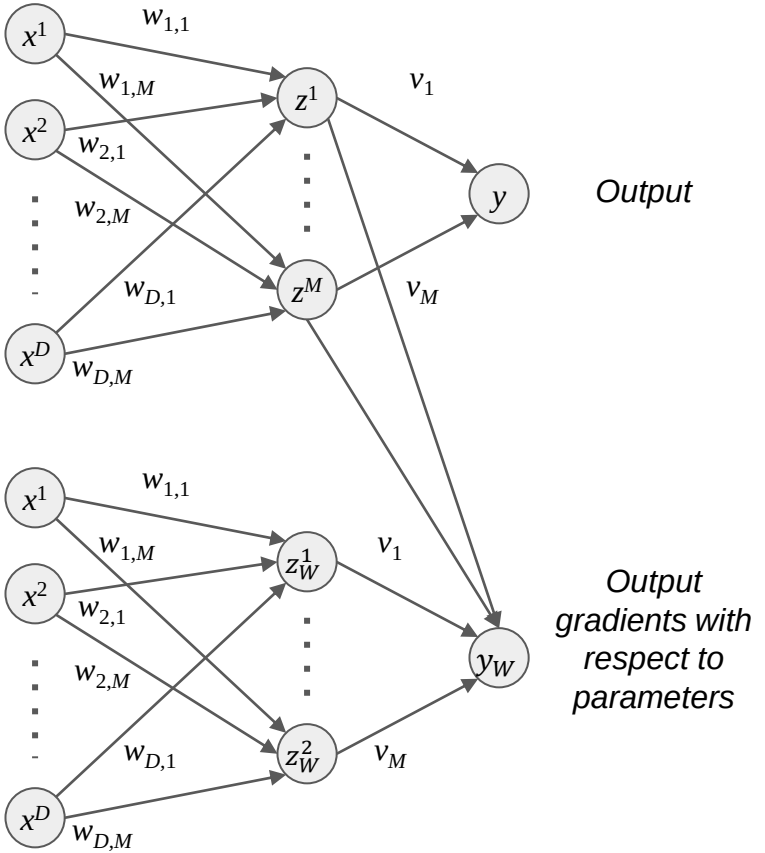
(e.g., gradient descent)

#Code

Automatic differentiation

- "**meta-programming**" approach to gradient calculation

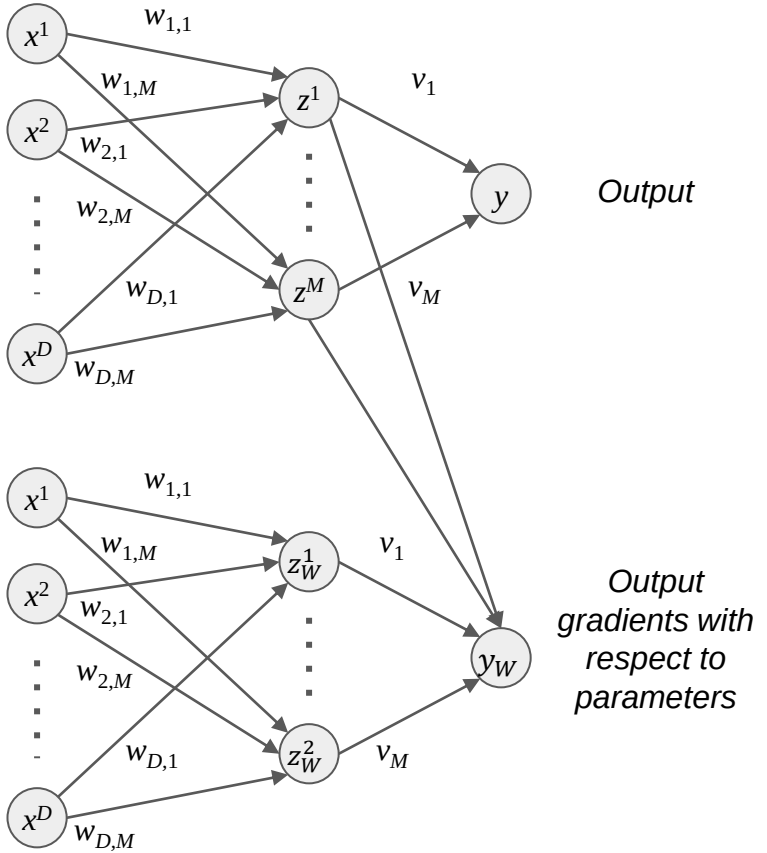
- Obtains the gradients of the output simultaneous with the output of the network



#Code

Automatic differentiation

- "**meta-programming**" approach to gradient calculation
- Obtains the gradients of the output simultaneous with the output of the network
- Software packages such as PyTorch, JAX largely avoid the need for any hand-computed gradients in this way



Algebra of dual numbers

- Dual numbers are an easy way to handle chained computations and automate calculations for AD

- Keeps track of current computation's value u and its derivative u' as a pair:

$$(u, u')$$

Algebra of dual numbers

#Code

- Dual numbers are an easy way to handle chained computations and automate calculations for AD

- Keeps track of current computation's value u and its derivative u' as a pair:

$$(u, u')$$

- In dual number form, the general chain rule is,

$$f((u, u')) = (f(u), f'(u)u')$$

- Most forms of computational operations used in ML, are special cases of this rule

Algebra of dual numbers

#Code

Computations which commonly occur in deep learning, in dual number form

- **Addition**: $f(u, v) = u + v$

Example: Suppose $u = 2x^1$ and $v = x^1 + x^2$.

For $x^1 = 3, x^2 = 4$, we want to compute

1. $z = u + v$

2. $\frac{dz}{dx^1}$

Algebra of dual numbers

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For $x^1 = 3, x^2 = 4$, we want to compute

1. $z = u + v$

$$u = 2 \times 3 = 6$$
$$v = 3 + 4 = 7$$
$$z = 6 + 7$$

2. $\frac{dz}{dx^1} = \frac{d}{dx^1}(u + v) = \frac{du}{dx^1} + \frac{dv}{dx^1} = 2 + 1 = 3$

Algebra of dual numbers

#Code

Computations which commonly occur in deep learning, in dual number form

- **Addition**: $f(u, v) = u + v$

$$(u, u') + (v, v') = (u + v, u' + v')$$

Example: Suppose $u = 2x^1$ and $v = x^1 + x^2$.

For $x^1 = 3, x^2 = 4$, we want to compute

1. $z = u + v$

$$u = 2 \times 3 = 6$$
$$v = 3 + 4 = 7$$
$$z = 6 + 7$$

2. $\frac{dz}{dx^1} = \frac{d}{dx^1}(u + v) = \frac{du}{dx^1} + \frac{dv}{dx^1} = 2 + 1 = 3$

AIML

#Code

Algebra of dual numbers

Computations which commonly occur in deep learning, in dual number form

- **Multiplication**: $f(u, v) = uv$

Example: Suppose $u = 2x^1$ and $v = x^1 + x^2$.

For $x^1 = 3, x^2 = 4$, we want to compute

1. $z = uv$

2. $\frac{dz}{dx^1}$

Algebra of dual numbers

#Code

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$$u = 2 \times 3 = 6$$
$$v = 3 + 4 = 7$$
$$z = 6 \times 7 = 42$$

2. $\frac{dz}{dx^1} = \frac{d}{dx^1}(uv) = \frac{du}{dx^1}v + u\frac{dv}{dx^1} = 2 \times 7 + 6 \times 1 = 20$

Algebra of dual numbers

#Code

Computations which commonly occur in deep learning, in dual number form

- **Multiplication**: $f(u, v) = uv$

$$(u, u') \times (v, v') = (uv, u'v + uv')$$

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Algebra of dual numbers

#Code

Computations which commonly occur in deep learning, in dual number form

- **Addition**: $(u, u') + (v, v') = (u + v, u' + v')$
- **Multiplication**: $(u, u') \times (v, v') = (uv, u'v + uv')$
- **ReLU activation**: $\text{relu}((u, u')) = (\max(0, u), u'\mathbb{I}[u \geq 0])$
- **Constants** $f(u) = c$

$$f((u, u')) = (c, 0)$$

Here is an example of a chained calculation carried out using dual numbers. Given the constants $y = 3$ and $z = -1$ and variable $x = 2$, compute $u(x, y, z) = \max(yz, y + 2x)$ and its derivative, $u_x(x, y, z)$. Applying the rules above successively (and using additional symbols for intermediate computational results),

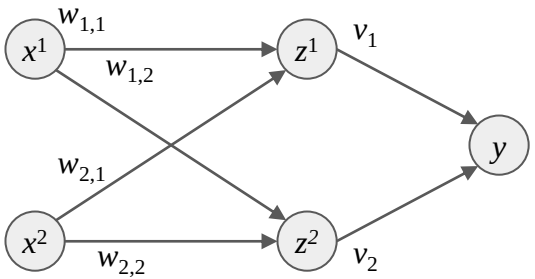
u_x: derivative of u with respect to x

$$
\begin{aligned}
\bar{x} &= (2, 1) \\
\bar{y} &= (3, 0) \\
\bar{z} &= (-1, 0) \\
\text{let} \quad c &= (2, 0) \\
c\bar{x} &= (2, 0) \times (2, 1) = (4, 2) \\
r_1 &= \bar{y} \times \bar{z} = (3, 0) \times (-1, 0) = (-3, 0) \\
r_2 &= \bar{y} + c\bar{x} = (3, 0) + (4, 2) = (7, 2) \\
\bar{u} &= \max((-3, 0), (7, 2)) = (7, 2),
\end{aligned}
\tag{14.7}
$$

therefore $u(x, y, z) = 7$ and $u_x(x, y, z) = 2$. While it is, of course, always possible to find the symbolic derivative of the function $u(x, y, z)$, AD enables entirely 'mechanical' calculational steps which lends itself to software implementation.

Automatic differentiation in action

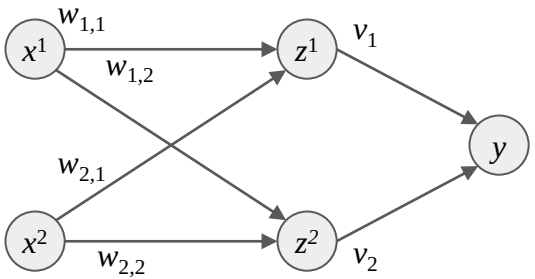
#Code



$z^1 = \text{relu}(w_{1,1}x^1 + w_{2,1}x^2)$

Automatic differentiation in action

#Code

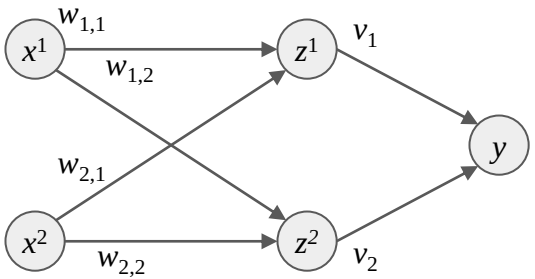


$z^1 = \text{relu}(w_{1,1}x^1 + w_{2,1}x^2)$

$w_{1,1} \rightarrow (w_{1,1}, 1), w_{2,1} \rightarrow (w_{2,1}, 0), x^1 \rightarrow (x^1, 0), x^2 \rightarrow (x^2, 0)$

Automatic differentiation in action

#Code



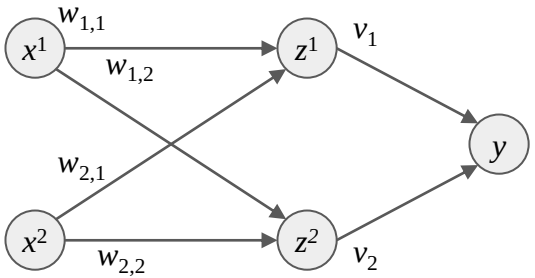
$z^1 = \text{relu}(w_{1,1}x^1 + w_{2,1}x^2)$

$= \text{relu}((w_{1,1}, 1) \times (x^1, 0) + (w_{2,1}, 0) \times (x^2, 0))$

$w_{1,1} \rightarrow (w_{1,1}, 1), w_{2,1} \rightarrow (w_{2,1}, 0), x^1 \rightarrow (x^1, 0), x^2 \rightarrow (x^2, 0)$

Automatic differentiation in action

#Code



$z^1 = \text{relu}(w_{1,1}x^1 + w_{2,1}x^2)$

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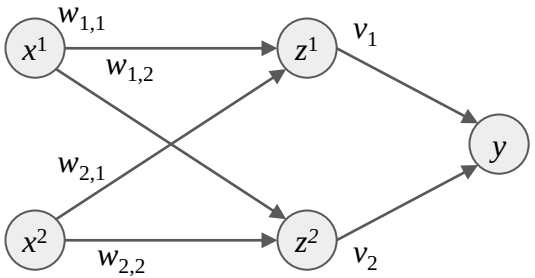
$= \text{relu}((w_{1,1}x^1, x^1) + (w_{2,1}x^2, 0))$

$w_{1,1} \rightarrow (w_{1,1}, 1), w_{2,1} \rightarrow (w_{2,1}, 0), x^1 \rightarrow (x^1, 0), x^2 \rightarrow (x^2, 0)$

$(u, u') \times (v, v') = (uv, u'v + v'u)$

Automatic differentiation in action

#Code



$$z^1 = \text{relu}(w_{1,1}x^1 + w_{2,1}x^2)$$

$$= \text{relu}((w_{1,1}, 1) \times (x^1, 0) + (w_{2,1}, 0) \times (x^2, 0))$$

$$= \text{relu}((w_{1,1}x^1, x^1) + (w_{2,1}x^2, 0))$$

$$= \text{relu}((w_{1,1}x^1 + w_{2,1}x^2, x^1))$$

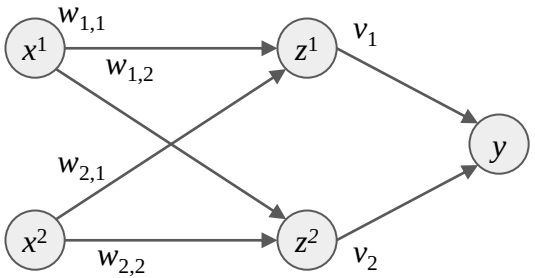
$w_{1,1} \to (w_{1,1}, 1), w_{2,1} \to (w_{2,1}, 0), x^1 \to (x^1, 0), x^2 \to (x^2, 0)$

$(u, u') \times (v, v') = (uv, u'v + v'u)$

$(u, u') + (v, v') = (u + v, u' + v')$

Automatic differentiation in action

#Code



derivate with respect to w_1,1

$z^1 = \text{relu}(w_{1,1}x^1 + w_{2,1}x^2)$

$w_{1,1} \to (w_{1,1}, 1), w_{2,1} \to (w_{2,1}, 0), x^1 \to (x^1, 0), x^2 \to (x^2, 0)$

$= \text{relu}((w_{1,1}, 1) \times (x^1, 0) + (w_{2,1}, 0) \times (x^2, 0))$ $\quad (u, u') \times (v, v') = (uv, u'v + v'u)$

$= \text{relu}((w_{1,1}x^1, x^1) + (w_{2,1}x^2, 0))$ $\quad (u, u') + (v, v') = (u + v, u' + v')$

$= \text{relu}((w_{1,1}x^1 + w_{2,1}x^2, x^1))$ $\quad \text{relu}((u, u')) = (\max(0, u), u' 1[u \geq 0])$

$= (\max(0, w_{1,1}x^1 + w_{2,1}x^2), x^1 1[w_{1,1}x^1 + w_{2,1}x^2])$

#Code

To recap

- We learned one approach of finding the optimal set of weights for a neural network (i.e., **train the network**)
  - Analytical gradient expressions quickly become intractable
  - Automatic differentiation computes derivatives in a single forward pass
    - We learned the *forward mode* version of AD; there is also *reverse* mode
- **Next**: Probability and probabilistic AI

Further Reading

- **PRML**, Section 5.3
- **R&N**, Section 18.7
- **H&T**, Section 11.4, Section 11.7