CS4641 Spring 2025

Neural Networks: Backpropagation

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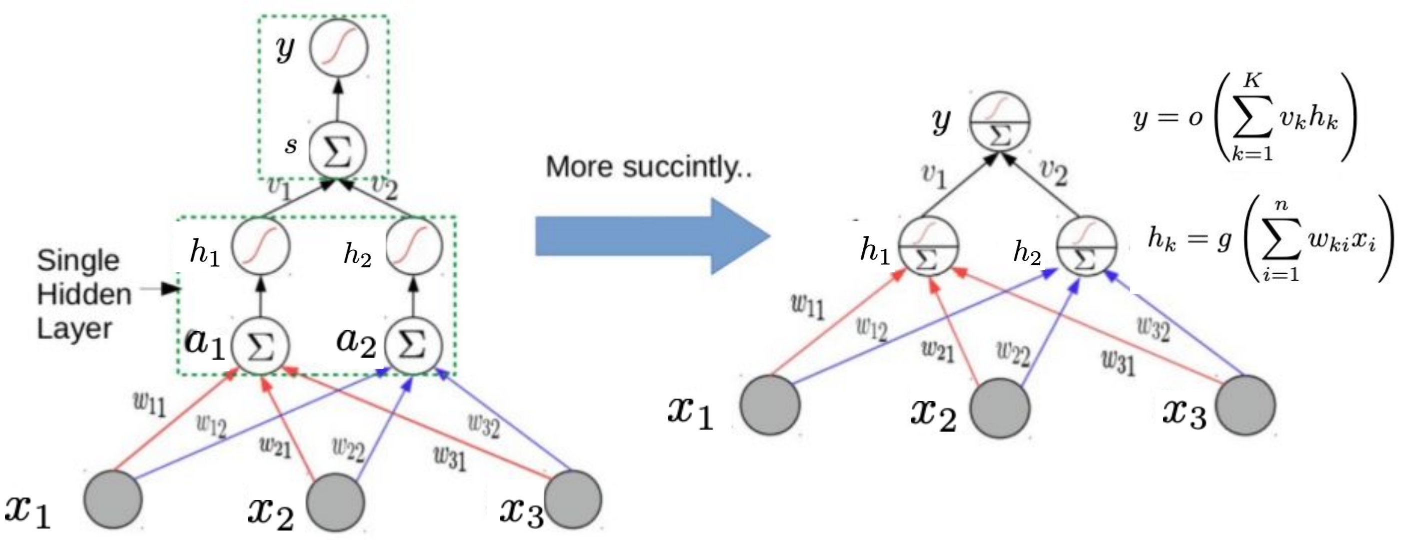
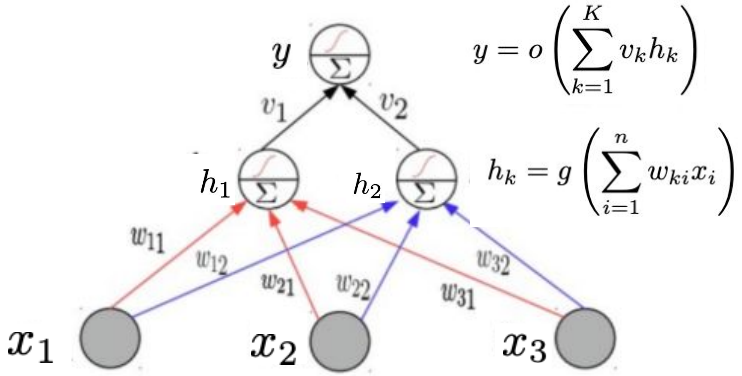
Neural Network Revisit



Vector Formation

$$W = \begin{bmatrix} w_{11} & w_{21} & w_{31} \\ w_{12} & w_{22} & w_{32} \end{bmatrix}$$

$$x = [x_1, x_2, x_3]^\top$$



Vector Formation

$$h = [h_1, h_2]^\top = g(Wx)$$

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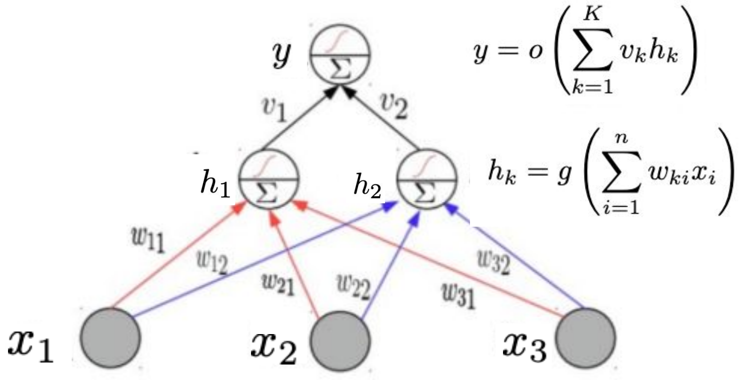

Vector Formation

$$y = o(Vh)$$

$$V = [v_1, v_2]$$

$$h = [h_1, h_2]^\top = g(Wx)$$

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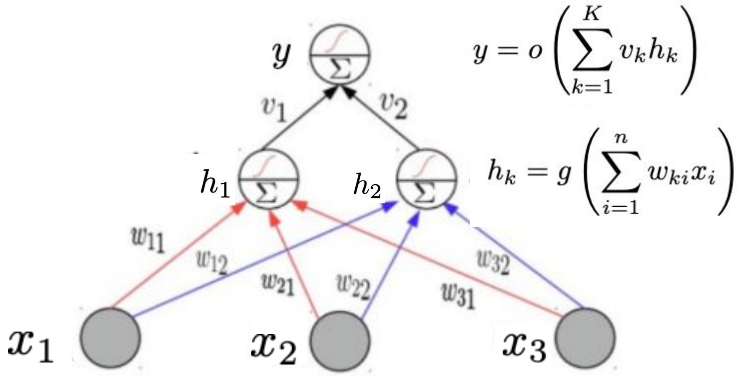

Vector Formation

$$y = o(Vg(Wx))$$

$$V = [v_1, v_2]$$

$$h = [h_1, h_2]^\top = g(Wx)$$

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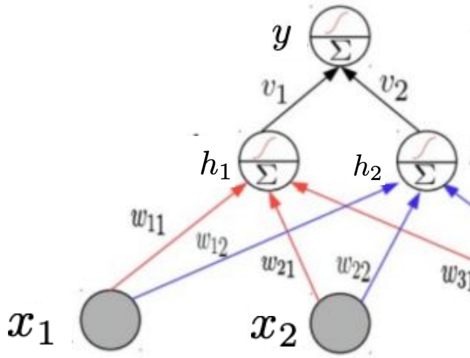
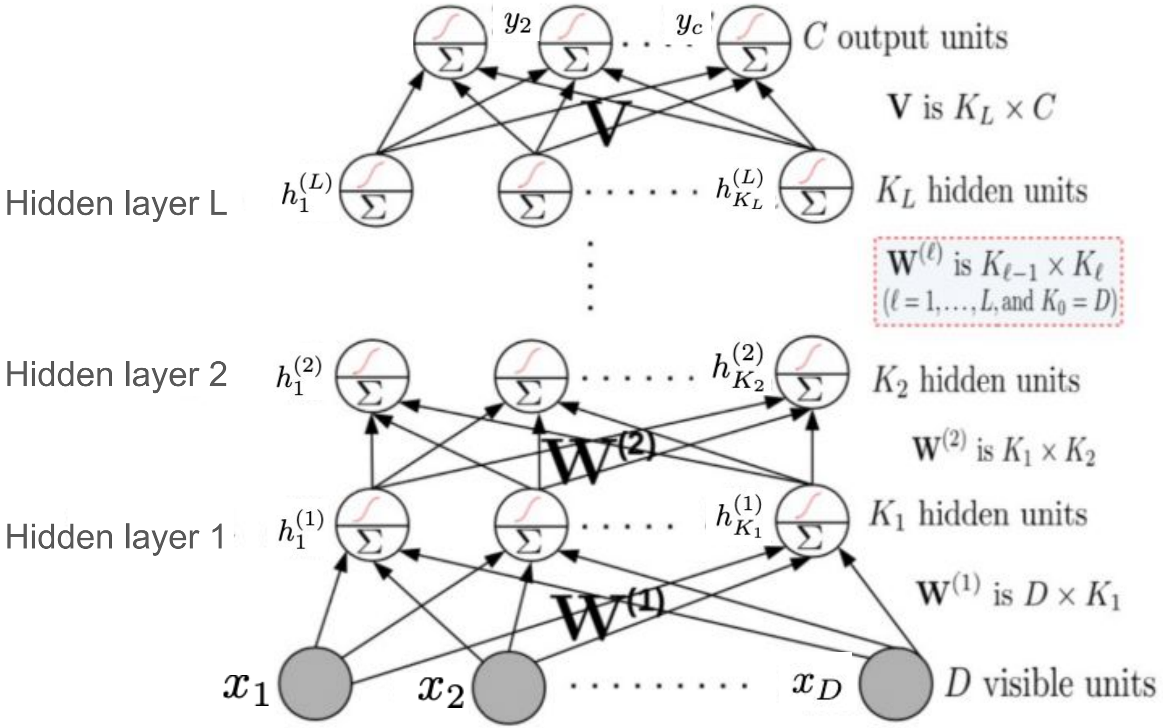


$$y = o\left(\sum_{k=1}^{K} v_k h_k\right)$$

$$h_k = g\left(\sum_{i=1}^{n} w_{ki} x_i\right)$$

Multi-Layer Perception

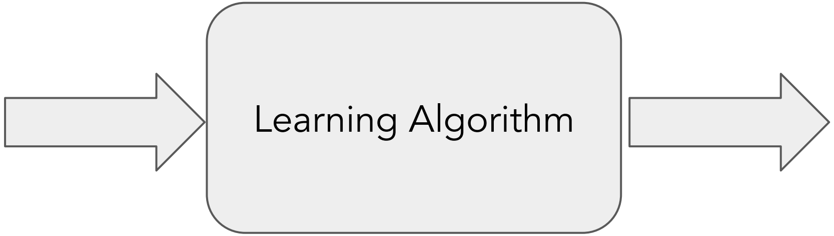
$$y = f_L(W_L f_{L-1}(W_{L-1} \ldots f_1(W_1 x))$$



Regression Algorithms

Training Data

$\{x^i, y^i\}_{i=1}^m$



Predictor

$f : X \rightarrow Y$

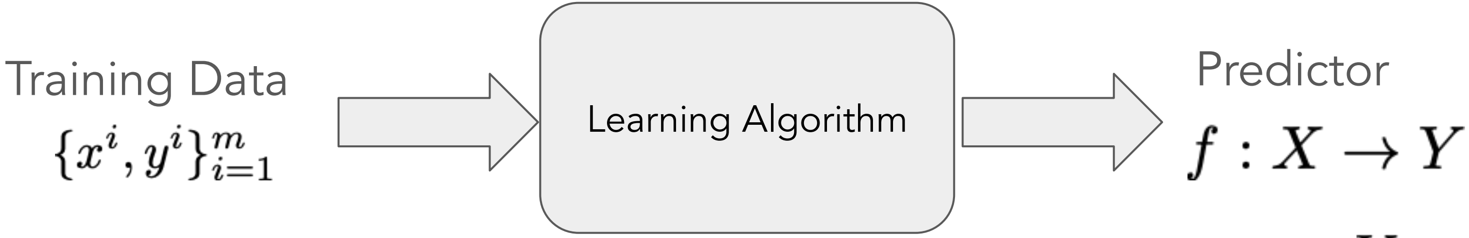
$Y \in \mathbb{R}$

Linear Regression Pipeline

1. Build probabilistic models:
   Gaussian Distribution + Neural Network
2. Derive loss function: MLE and MAP
3. Select optimizer: (Stochastic) GD

$$y = o(V g(W x))$$

Binary Classification Algorithms



Binary Classification $Y \in \{0, 1\}$

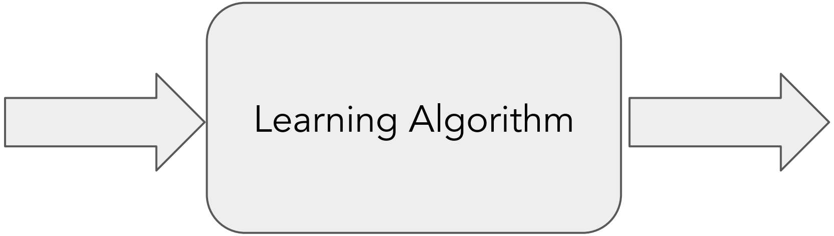
Binary Logistic Regression Pipeline

1. Build probabilistic models:
   Bernoulli Distribution + Neural Network $y = o(Vg(Wx))$
2. Derive loss function: MLE and MAP
3. Select optimizer: (Stochastic) Gradient Descent

Multiclass Logistic Regression Algorithms

Training Data

$\{x^i, y^i\}_{i=1}^m$



Classifier

$f : X \to Y$

Multiclass Classification $Y \in \{0, 1, \ldots, k\}$

Multiclass Logistic Regression Pipeline

1. Build probabilistic models:
   Categorical Distribution + Neural Network $y = o(Vg(Wx))$
2. Derive loss function: MLE and MAP
3. Select optimizer: (Stochastic) Gradient Descent

Select Optimizer

$$\ell(x^i, y^i, \theta) = (o(Vg(Wx^i)) - y^i)^2$$

$$L(\theta) = \sum_{i=1}^{m} \ell(x^i, y^i, \theta) + \lambda\Omega(\theta)$$

$$\theta = [V, W]$$

Select Optimizer

$$\ell(x^i, y^i, \theta) = (o(Vg(Wx^i)) - y^i)^2$$

$$L(\theta) = \sum_{i=1}^{m} \ell(x^i, y^i, \theta) + \lambda\Omega(\theta)$$

$$\theta = [V, W]$$

$$\ell(x^i, y^i, \theta) = -y^i \log \sigma(o(Vg(Wx^i))) \\ -(1 - y^i) \log(1 - \sigma(o(V_j g(Wx^i))))$$

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$$\ell(x^i, y^i, \theta) = -\sum_{j=1}^{k} y^i \log \frac{\exp(o(V_j g(Wx^i)))}{\sum_{c=1}^{k} \exp(o(V_c g(Wx^i)))}$$

Select Optimizer

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- (Stochastic) Gradient Descent

(Stochastic) Gradient Descent

- Initialize parameter θ^0
- Sample $\{x^i, y^i\}_{i=1}^{B}$
- Do $$\theta^{t+1} \leftarrow \theta^t - \eta \sum_{i=1}^{B} \nabla_\theta \ell(x^i, y^i, \theta^t) - (\lambda \nabla \Omega(\theta^t))$$

Chain Rule

- A composite function is the combination of two functions: a function that takes as input the output of another function

$$h(\theta) = g(f(\theta))$$

$$\text{E.g, } f(\theta) = 2\theta + 1,\ g(\theta) = \theta^4,\ h(\theta) = (2\theta+1)^4$$

Let's call $u = f(\theta)$ the output of the inner function $\rightarrow h(\theta) = g(u)$

$$h' = \frac{dh}{d\theta} = \frac{dh}{du}\frac{du}{d\theta}$$

$$\frac{dh}{du} = 4(2\theta+1)^3 \qquad \frac{du}{d\theta} = 2 \qquad h' = 8(2\theta+1)^3$$

Derivative of outer part of *h(θ)* Derivative of inner part of *h(θ)*

Chain Rule

$$h(\theta) = g(f(\theta))$$
$$u = f(\theta)$$

where $\theta \in \mathbb{R}^m, \mathbf{u} \in \mathbb{R}^n$

$h : \mathbb{R}^m \to \mathbb{R}$

$f : \mathbb{R}^m \to \mathbb{R}^n$ Vector function

$g : \mathbb{R}^n \to \mathbb{R}$

The inner vector function f maps m inputs to n outputs, while the outer function g receives n inputs to produce one output, h.

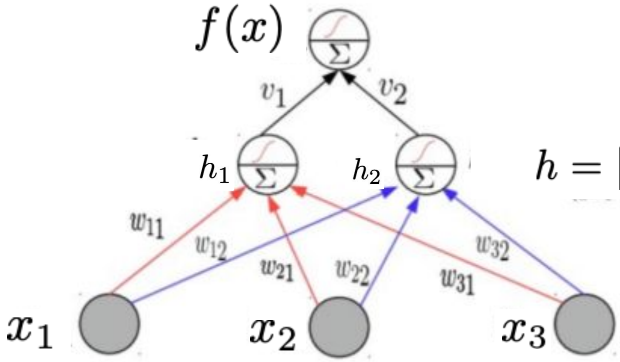
The chain rule allows to compute the variation (i.e., the partial derivative) of the function w.r.t. each component of the multivariate input → Gradient vector of $h(\theta)$

$$\frac{\partial h}{\partial \theta_i} = \frac{\partial h}{\partial u_1}\frac{\partial u_1}{\partial \theta_i} + \frac{\partial h}{\partial u_2}\frac{\partial u_2}{\partial \theta_i} + \cdots + \frac{\partial h}{\partial u_n}\frac{\partial u_n}{\partial \theta_i} = \sum_{j=1}^{n} \frac{\partial h}{\partial u_j}\frac{\partial u_j}{\partial \theta_i} \qquad i = 1, \ldots, m$$

$$\nabla h(\theta) = \left(\frac{\partial h}{\partial \theta_1}, \frac{\partial h}{\partial \theta_2}, \ldots, \frac{\partial h}{\partial \theta_m}\right)^T$$

Backpropagation: Chain Rule on Neural Network

$$\ell(x^i, y^i, \theta) = (f(x^i, V, W) - y^i)^2$$



$$h = [h_1, h_2]^\top = g(Wx)$$

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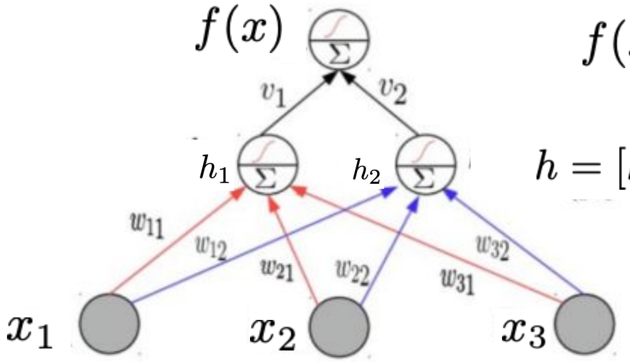

$$f(x) = o(Vh)$$

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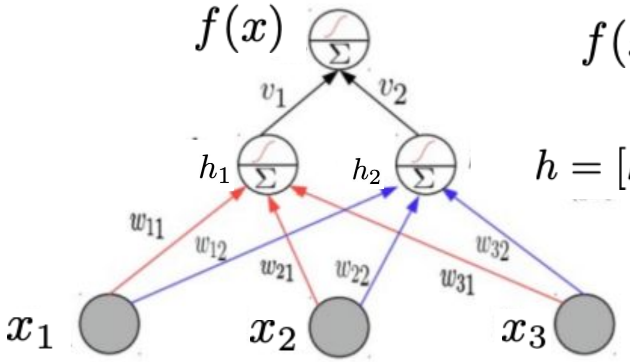
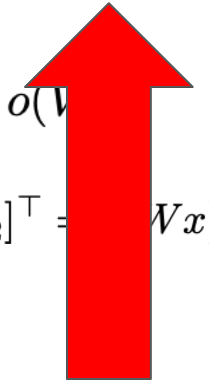


$f(x) = o(V$

$h = [h_1, h_2]^\top =$ $Wx)$

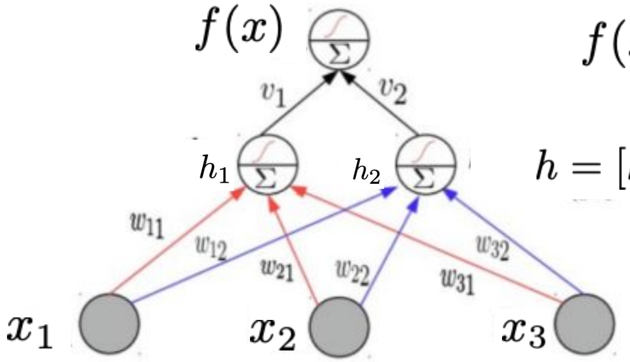


Forward Pass

Backpropagation: Chain Rule on Neural Network

$$\ell(x^i, y^i, \theta) = (f(x^i, V, W) - y^i)^2$$

$$\nabla_\theta \ell(x^i, y^i, \theta)$$



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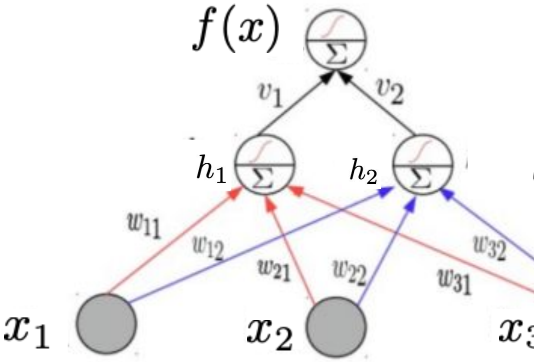
$$\nabla_\theta \ell(x^i, y^i, \theta) = \left[\frac{\partial \ell(x^i, y^i, \theta)}{\partial V}, \frac{\partial \ell(x^i, y^i, \theta)}{\partial W}\right]$$

$$\frac{\partial \ell(x^i, y^i, \theta)}{\partial V} = \frac{\partial \ell(x^i, y^i, \theta)}{\partial f} \frac{\partial f}{\partial V}$$



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Backpropagation: Chain Rule on Neural Network

$$\ell(x^i, y^i, \theta) = (f(x^i, \color{red}{V, W}) - y^i)^2$$

$$\frac{\partial \ell(x^i, y^i, \theta)}{\partial V} = \frac{\partial \ell(x^i, y^i, \theta)}{\partial f} \frac{\partial f}{\partial V}$$

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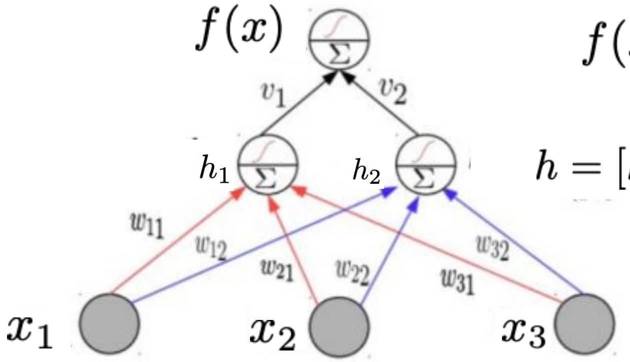

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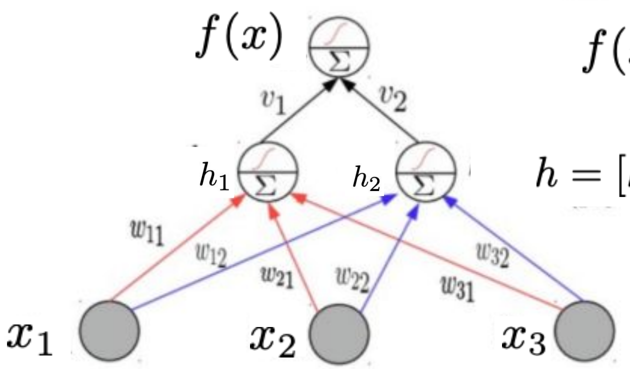

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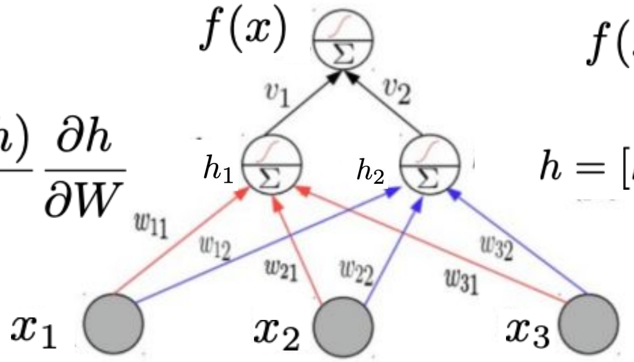
$$\frac{\partial \ell(x^i, y^i, \theta)}{\partial W} = \frac{\partial \ell(x^i, y^i, \theta)}{\partial f} \frac{\partial f}{\partial W}$$

$$\frac{\partial f}{\partial W} = \frac{\partial o(Vh)}{\partial h} \frac{\partial h}{\partial W}$$



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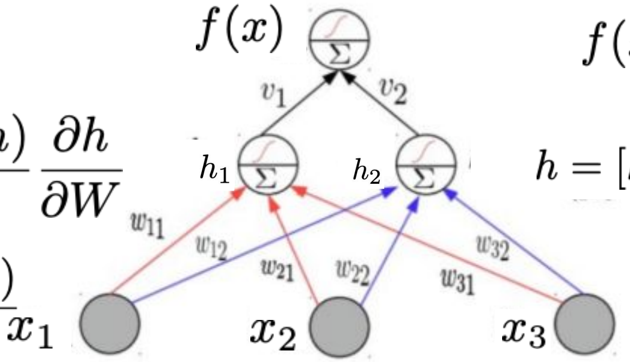

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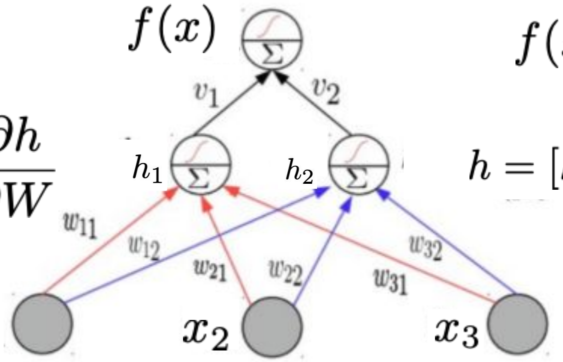

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Backpropagation: Chain Rule on Neural Network

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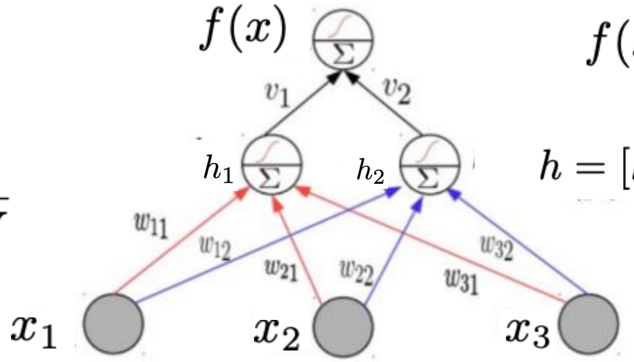

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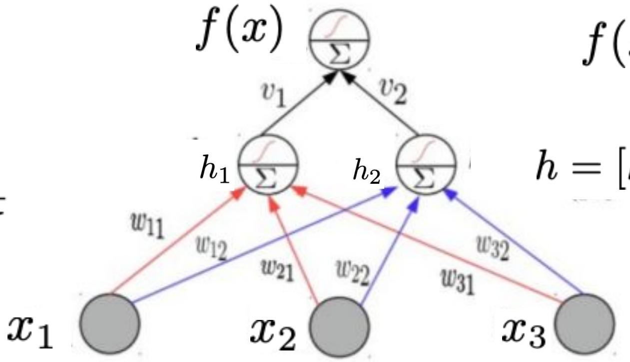

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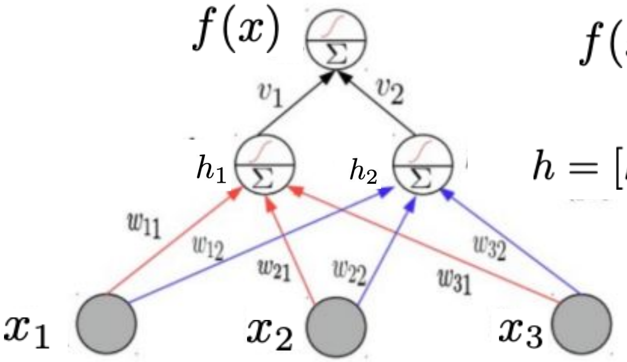

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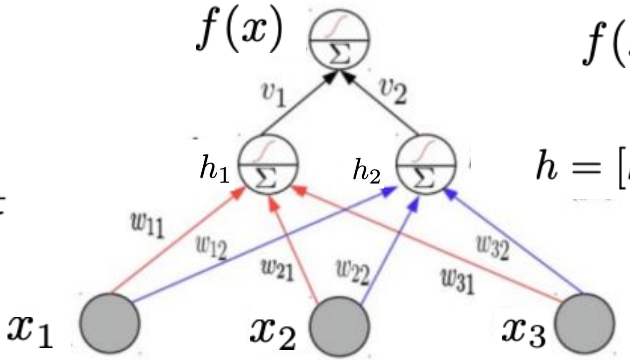

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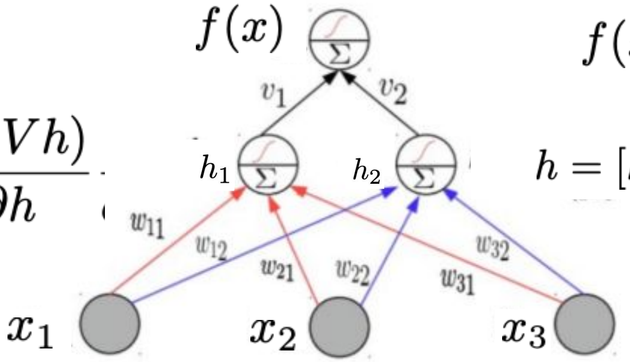

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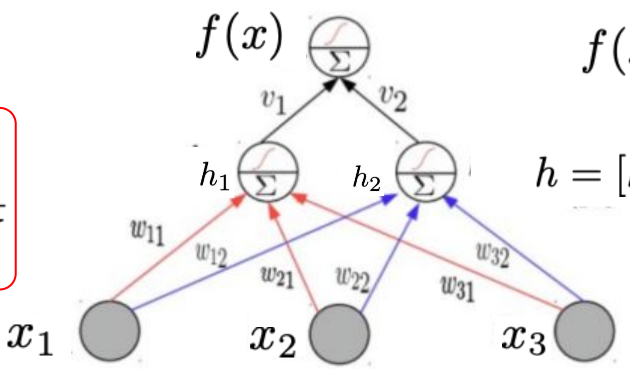

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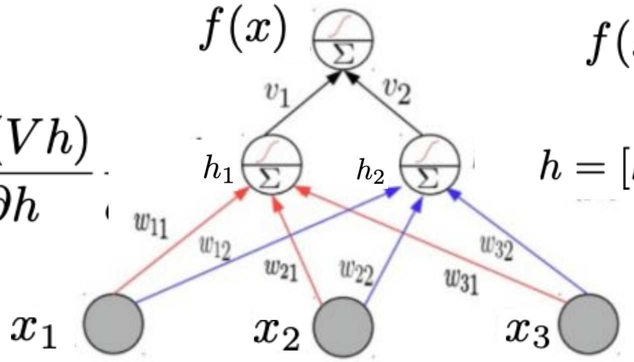

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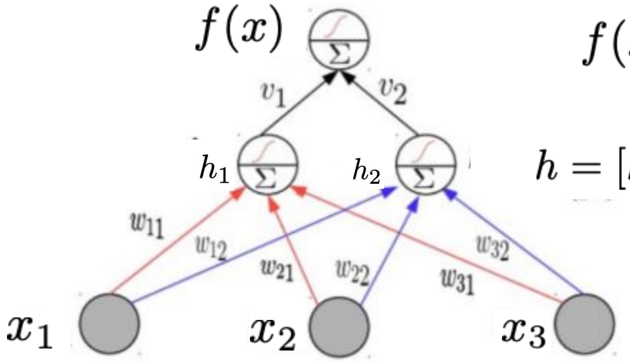

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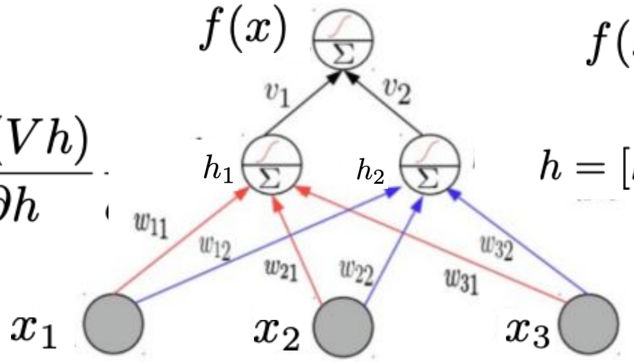
$$\frac{\partial \ell(x^i, y^i, \theta)}{\partial f}$$

$$\frac{\partial o(Vh)}{\partial V} \quad \frac{\partial o(Vh)}{\partial h}$$



$$f(x) = o(Vh)$$

$$h = [h_1, h_2]^\top = g(Wx)$$

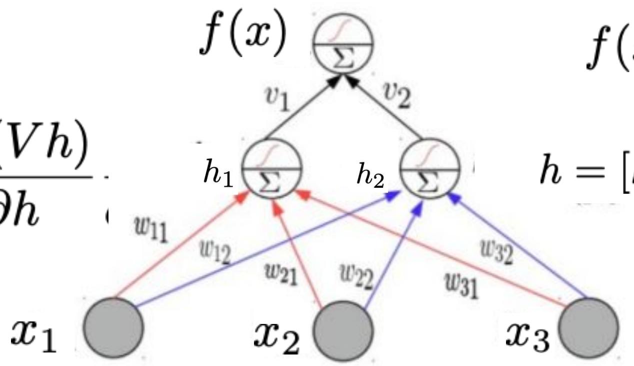
Backpropagation: Chain Rule on Neural Network

$$\ell(x^i, y^i, \theta) = (f(x^i, V, W) - y^i)^2$$

$$\frac{\partial \ell(x^i, y^i, \theta)}{\partial f}$$

$$\frac{\partial o(Vh)}{\partial V} \quad \frac{\partial o(Vh)}{\partial h}$$

$$\frac{\partial h}{\partial W}$$



$$f(x) = o(Vh)$$

$$h = [h_1, h_2]^\top = g(Wx)$$

Backpropagation: Chain Rule on Neural Network

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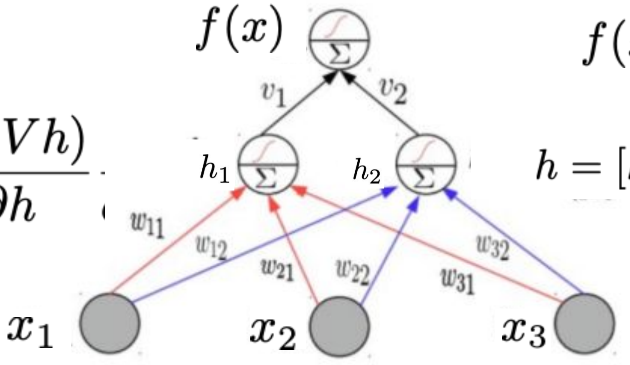
$$\frac{\partial o(Vh)}{\partial V} \quad \frac{\partial o(Vh)}{\partial h}$$

$$\frac{\partial h}{\partial W}$$



$$f(x) = o(Vh)$$

$$h = [h_1, h_2]^\top = g(Wx)$$

Backward Pass

(Stochastic) Gradient Descent

- Initialize parameter θ^0
- Sample $\{x^i, y^i\}_{i=1}^{B}$
- Do $$\theta^{t+1} \leftarrow \theta^t - \eta \sum_{i=1}^{B} \nabla_\theta \ell(x^i, y^i, \theta^t) - (\lambda \nabla \Omega(\theta^t))$$

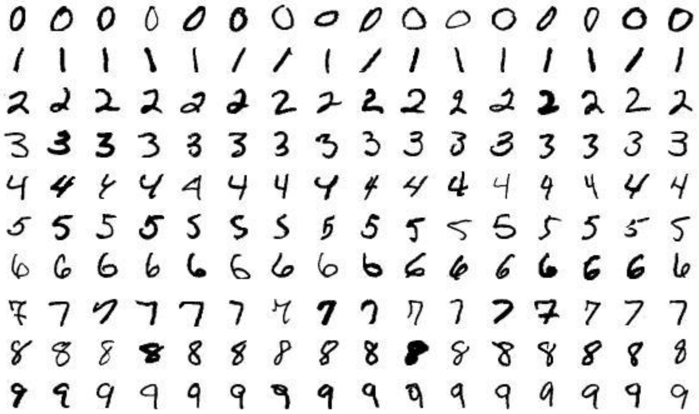
Auto-differentiation Packages

PyTorch

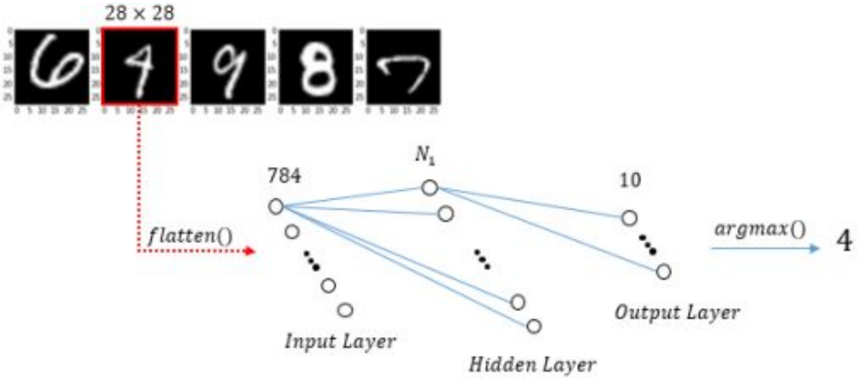
JAX

Tensorflow

MLP example: MNIST



MNIST hand-written character recognition



- 60,000 images
- 28x28 pixels = 784
- Grayscale, from 0 to 255 → Converted to [0,1]

PyTorch

```
#@title Define model class

class Net(nn.Module):
  def __init__(self, input_size, hidden_size, num_classes):
    super(Net,self).__init__()
    self.fc1 = nn.Linear(input_size, hidden_size)
    self.relu = nn.ReLU()
    self.fc2 = nn.Linear(hidden_size, num_classes)

  def forward(self,x):
    out = self.fc1(x)
    out = self.relu(out)
    out = self.fc2(out)
    return out
```

```
#@title Define loss-function & optimizer

loss_function = nn.CrossEntropyLoss()
optimizer = torch.optim.Adam( net.parameters(), lr=lr)
```

PyTorch

```
#@title Training the model

for epoch in range(num_epochs):
  for i ,(images,labels) in enumerate(train_gen):
    images = Variable(images.view(-1,28*28)).cuda()
    labels = Variable(labels).cuda()

    optimizer.zero_grad()
    outputs = net(images)
    loss = loss_function(outputs, labels)
    loss.backward()
    optimizer.step()
```

Q&A