### EECS 545: Machine Learning

# Lecture 11. Neural Networks and Deep Learning

Honglak Lee 02/17/2025



# Logistics

- · HW3 is due 02/25/25
  - We highly recommend you start ASAP.

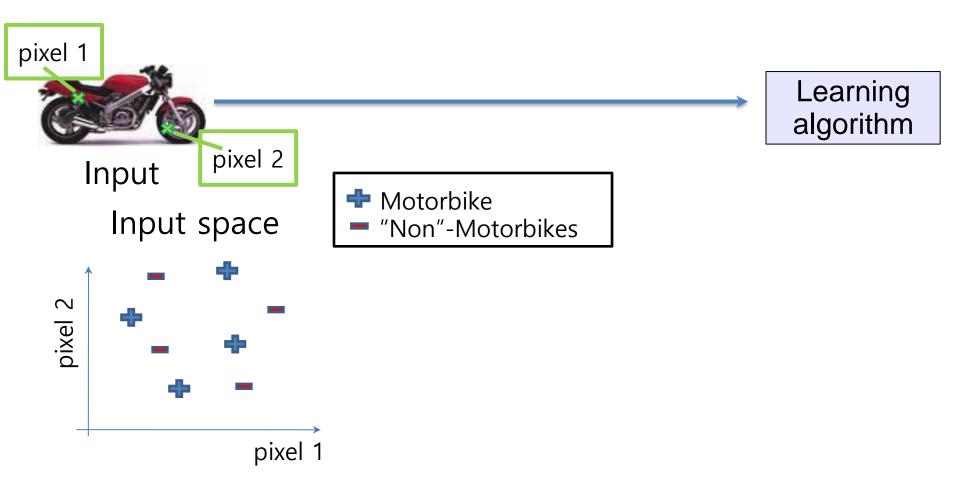
## Representing Data

 The success of machine learning applications relies on having a good representation of the data.

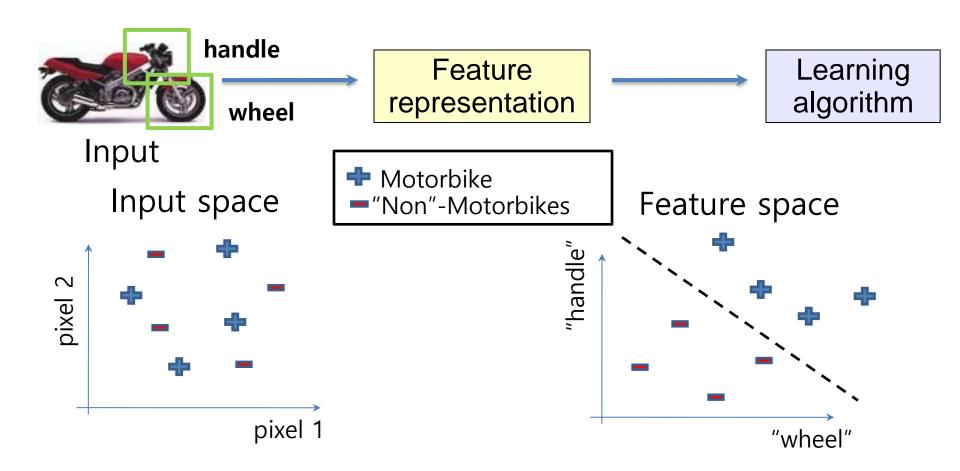
 Machine learning practitioners put lots of efforts in "feature engineering".

 How can we develop good representations automatically?

# Feature representations



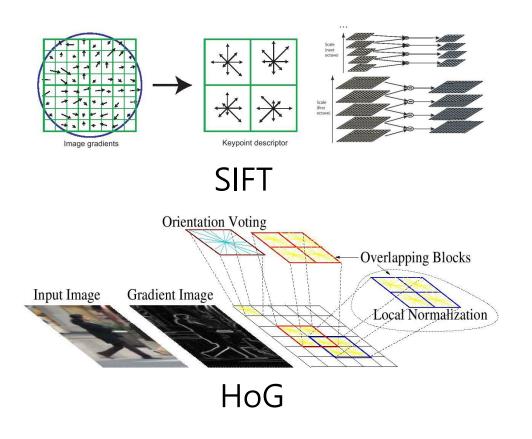
# Feature representations

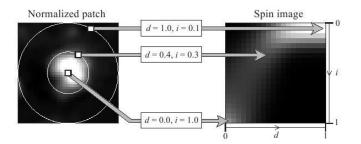


# How is computer perception done?

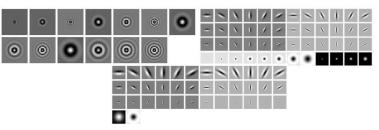
State-of-the-art: "hand-crafting" Feature representation Learning Input data algorithm Low-level **Image** Object Detection vision features or Classification (SIFT, HOG, etc.)

## **Computer Vision Features**





Spin image



**Textons** 

# Issues with hand-crafted Features (in Computer Vision, Speech Recognition, etc.)

- Need expert knowledge
- Requires time-consuming hand-tuning
- (Arguably) a key limiting factor in advancing the state-of-the-art

# Learning Feature Representations

- Key idea of Deep Learning:
  - Learn <u>multiple levels</u> of representation of increasing complexity/abstraction.
  - The representations can be learned in both supervised and/or unsupervised settings.
  - These features can be used for downstream tasks.

## Example: Learning Feature Hierarchy

Feature representation

**Pixels** 

 Efficiently learn useful attributes (features) from unlabeled and labeled data

3rd layer Input data "Objects" 2nd layer "Object parts" 1st layer "Edges" Fill in representation gap in machine learning

# Taxonomy of machine learning methods **Supervised**

- Support Vector Machine
- Logistic Regression
- Perceptron
- Shallow
  - Denoising Autoencoder
  - Restricted Boltzmann machine\*
  - Sparse coding\*

- Deep Neural Network
- Convolutional Neural Network\*
- Recurrent Neural Network\*
- Variational Autoencoder\*
  - Generative Adversarial Network
  - Transformers\*
  - Diffusion Models\*

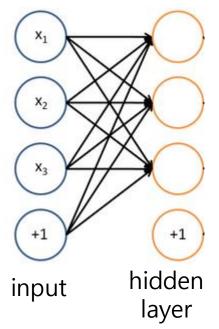
Unsupervised

Network, Deep Boltzmann machines\*
\* both supervised and unsupervised versions exist

Deep

#### Neural network

- Neural network: similar to running several logistic regressions at the same time
- If we feed a vector of inputs through a bunch of logistic regression functions, then we get a vector of outputs

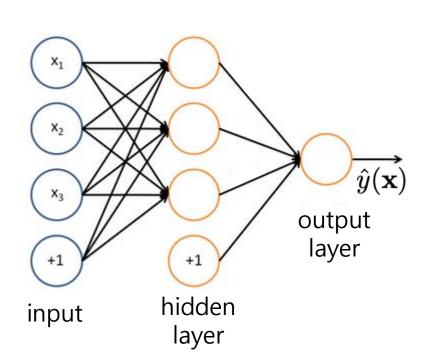


But we don't have to decide ahead of time what variables these logistic regressions are trying to predict!

Slide Credit: Yoshua Bengio

#### Neural network

... which we can feed into another logistic regression function



and it is the training criterion that will decide what those intermediate binary target variables should be, so as to make a good job of predicting the targets for the next layer, etc.

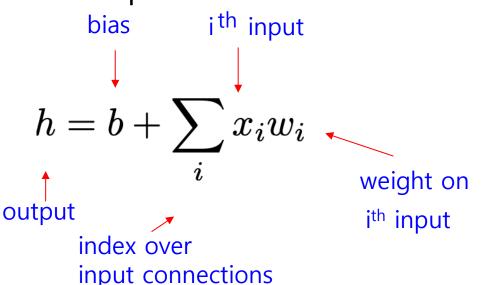
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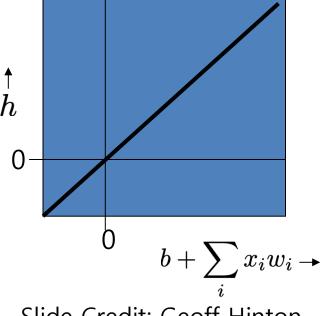
## Types of Neurons: Linear Neurons

- These are simple but limited in terms of representation power
  - e.g., composition of linear layers is still a linear function

- If we can make them learn we may get insight into more

complicated neurons.





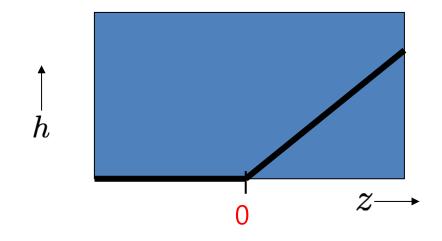
Slide Credit: Geoff Hinton

### Rectified Linear (linear threshold) Neurons

- They compute a linear weighted sum of their inputs.
- The output is a non-linear function of the total input.

$$z = b + \sum_{i} x_i w_i$$

$$h = \begin{cases} z & \text{if } z > 0 \\ 0 & \text{otherwise} \end{cases}$$



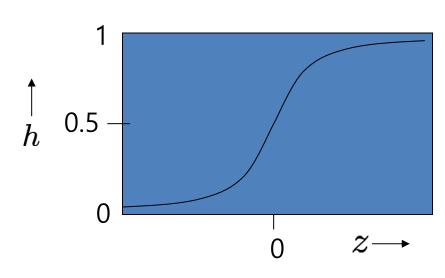
Slide Credit: Geoff Hinton

## Sigmoid (logistic) neurons

- These give a real-valued output that is a smooth and bounded function of their total input.
  - They have nice derivatives which make learning easy

$$z = b + \sum_{i} x_i w_i$$

$$h = \frac{e^z}{1 + e^z} = \frac{1}{1 + e^{-z}}$$



Slide Credit: Geoff Hinton

#### Tanh neurons

- These give a real-valued output that is a smooth and bounded function of their total input. Output range: (-1, 1)
  - larger gradient than Sigmoid

$$z = b + \sum_i x_i w_i$$

$$h = \tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$

$$h = \tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$
Note: tanh and sigmoid is equivalent after shifting and scaling!
$$\sigma(z) = \frac{1}{2} + \frac{1}{2} \tanh\left(\frac{z}{2}\right) \quad \text{or} \quad \tanh(z) = 2\sigma(2z) - 1$$

#### Softmax neurons

- These give a real-valued output that is a smooth and bounded function of their total input.
  - The outputs sum up to 1 (useful for classification problems)
  - They have nice derivatives which make learning easy

$$z_k = b^k + \sum_i x_i w_i^k$$

 $\mathbf{w}^k$  is the weight vector for the k-th output  $b^k$  is the bias for the k-th output

$$h_j = \frac{e^{z_j}}{\sum_k e^{z_k}}$$

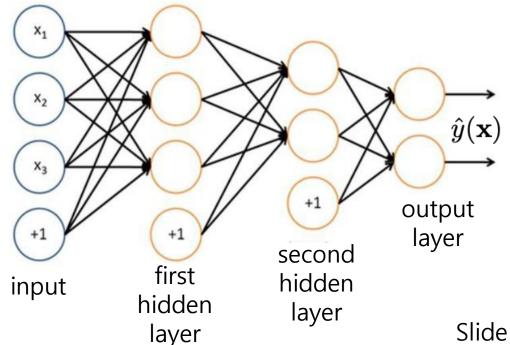
Recall:

This softmax function is a generalization of logistic (sigmoid) function.

Slide Credit: Geoff Hinton

## Multilayer neural networks

- We can construct a multilayer neural network by defining the network connectivity and (nonlinear or linear) activation functions.
  - Sigmoid nonlinearity for hidden layers
  - Softmax for the output layer



Slide Credit: Yoshua Bengio

### **Training Neural Network**

#### Repeat until convergence

```
(\mathbf{x}, \mathbf{y}) : Sample an example (or a mini-batch) from data
```

 $\hat{\mathbf{y}} \leftarrow f(\mathbf{x}; \theta)$ : Forward propagation

Compute  $\mathcal{L}(\mathbf{y}, \hat{\mathbf{y}})$ 

 $\nabla_{\theta} \mathcal{L}$ : Backward propagation

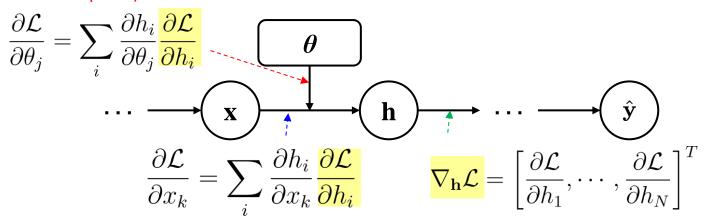
 $\theta \leftarrow \theta - \alpha \nabla_{\theta} \mathcal{L}$ : Update weights using (stochastic) gradient descent

### Overview of backpropagation

- Recall: Deep Neural Network represents a complex function with nested, composite functions (represented by layer-wise operation and nonlinearity, etc.)
- Q. How can we compute the gradient of the complex function?
- A. Backpropagation:
  - Computing gradient via chain rule for compositional function
  - The chain rule can be expressed as a local computation
  - Think about it as a computational graph

- Denote  $\mathbf{x}\in\mathbb{R}^D, \mathbf{h}\in\mathbb{R}^N, \theta\in\mathbb{R}^M$  as the input, output and parameter of a layer.
- It is non-trivial to derive the gradient of loss w.r.t. parameters in intermediate layers, but we can derive a recursion rule for the gradient.

"gradient w.r.t. parameters" (to be used for SGD update)

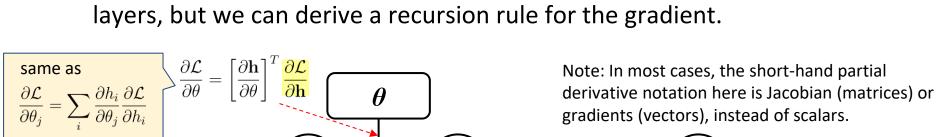


"gradient w.r.t. input" (to be propagated to lower layers in backprop recursion)

"gradient w.r.t. hidden layer above" (given)

## Backpropagation: vectorized formula

- Denote  $\mathbf{x} \in \mathbb{R}^D, \mathbf{h} \in \mathbb{R}^N, \theta \in \mathbb{R}^M$  as the input, output and parameters
- It is non-trivial to derive the gradient of loss w.r.t. parameters in intermediate layers, but we can derive a recursion rule for the gradient.



$$\frac{\partial \mathcal{L}}{\partial x_k} = \sum_i \frac{\partial h_i}{\partial x_k} \frac{\partial \mathcal{L}}{\partial h_i}$$
Note:  $\frac{\partial \mathcal{L}}{\partial \mathbf{h}} = \nabla_{\mathbf{h}} \mathcal{L}$ : N x 1 vector (gradient vector)  $\frac{\partial \mathbf{h}}{\partial \theta} = \nabla_{\theta} \mathbf{h}$ : N

Simplified notation: this denotes a vector or matrix, not a scalar, and the meaning should be clear from the context.

$$\frac{\partial \mathbf{h}}{\partial \theta} = \nabla_{\theta} \mathbf{h}$$
: N x N matrix (Jacobian matrix); i.e.  $\begin{bmatrix} \partial \mathbf{h} \end{bmatrix}_{i,j} = \frac{\partial \theta_j}{\partial \theta_j}$ 

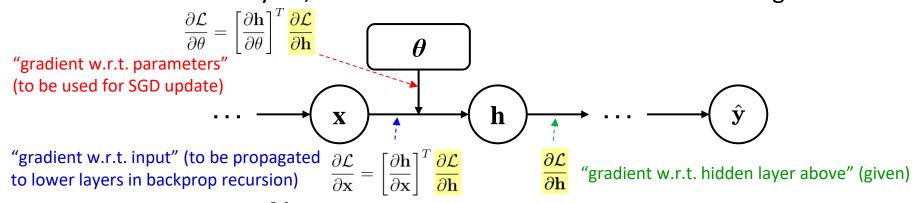
$$\frac{\partial \mathcal{L}}{\partial \theta} = \nabla_{\theta} \mathcal{L} : \text{M x 1 vector (gradient vector)} \qquad \frac{\partial \mathbf{h}}{\partial \mathbf{x}} = \nabla_{\mathbf{x}} \mathbf{h} : \text{N x D matrix (Jacobian matrix); i.e. } \begin{bmatrix} \frac{\partial \mathbf{h}}{\partial \mathbf{x}} \end{bmatrix}_{i,j} = \frac{\partial h_i}{\partial x_j}$$

$$\frac{\partial \mathbf{h}}{\partial \theta} = \nabla_{\theta} \mathbf{h}$$
: N x M matrix (Jacobian matrix); i.e.  $\left[\frac{\partial \mathbf{h}}{\partial \theta}\right]_{i,j} = \frac{\partial h_i}{\partial \theta_j}$ 

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}} = \nabla_{\mathbf{x}} \mathcal{L}$$
: D x 1 vector (gradient vector)

$$\left[\frac{\partial \mathbf{x}}{\partial \mathbf{x}}\right]_{i,j} = \frac{\partial \mathcal{H}}{\partial x_j}$$

- Denote x, h,  $\theta$  is the input, output and parameter of a layer.
- It is non-trivial to derive the gradient of loss w.r.t. parameters in intermediate layers, but we can derive a recursion rule for the gradient.



• Assuming that  $\frac{\partial \mathcal{L}}{\partial h}$  is given, use the **chain rule** to compute the gradients.



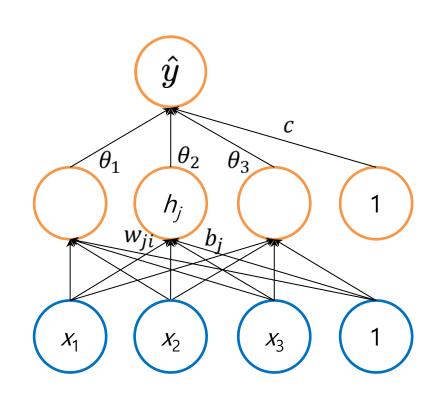
Repeat recursion backwards (until reaching the bottom layers).

# Backpropagation: Examples (NN with 1-hidden layer for regression)

# **Forward Propagation**

- Example: a network with 1 hidden layer
  - Input: X
  - Output:  $\hat{y}$
  - Target: y
  - Loss function: square error  $(\hat{y}-y)^2$

Hidden layer 
$$h_j = f(\sum_i w_{ji} x_i + b_j)$$
 Output  $\hat{y} = \sum_j \theta_j h_j + c$ 

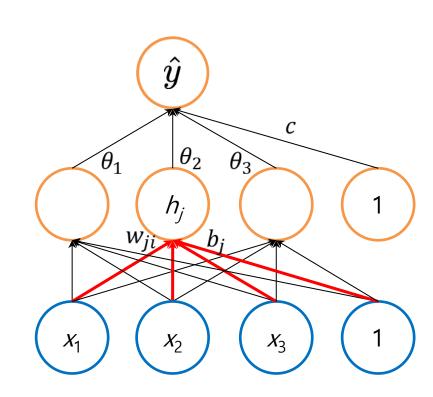


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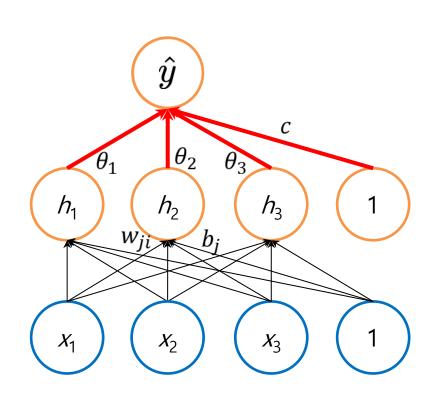


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Hidden layer 
$$h_j = f(\sum_i w_{ji} x_i + b_j)$$

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$$\hat{y} = \sum_j \theta_j h_j + c$$



$$h_j = f(\sum_i w_{ji}x_i + b_j), \forall j$$
$$\hat{y} = \sum_j \theta_j h_j + c$$

- Goal: Compute gradient w.r.t. parameters  $\{W,\,b,\,\theta,\,c\}$   $\mathcal{L}=(\hat{y}-y)^2$
- Main idea: Apply a chin rule recursively!

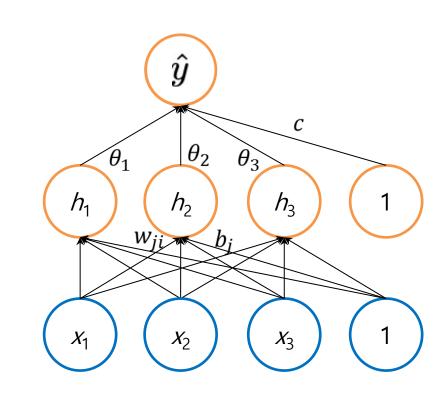
$$\frac{\partial \mathcal{L}}{\partial \hat{y}} = 2(\hat{y} - y)$$

$$\frac{\partial \mathcal{L}}{\partial \theta_{j}} = \frac{\partial \hat{y}}{\partial \theta_{j}} \frac{\partial \mathcal{L}}{\partial \hat{y}} = h_{j} \frac{\partial \mathcal{L}}{\partial \hat{y}}$$

$$\frac{\partial \mathcal{L}}{\partial h_{j}} = \frac{\partial \hat{y}}{\partial h_{j}} \frac{\partial \mathcal{L}}{\partial \hat{y}} = \theta_{j} \frac{\partial \mathcal{L}}{\partial \hat{y}}$$

$$\frac{\partial \mathcal{L}}{\partial w_{ji}} = \frac{\partial h_{j}}{\partial w_{ji}} \frac{\partial \mathcal{L}}{\partial h_{j}} = f'x_{i} \frac{\partial \mathcal{L}}{\partial h_{j}}$$

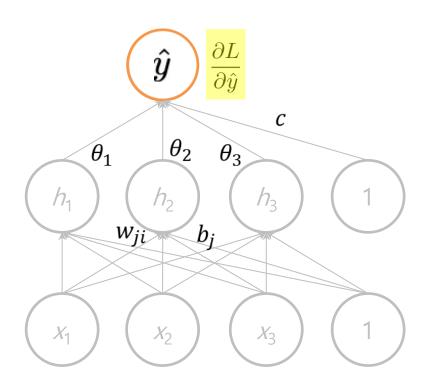
$$\text{where } f' = f'(\sum_{i} w_{ji}x_{i} + b_{j})$$



$$h_j = f(\sum_i w_{ji}x_i + b_j), \forall j$$
  $\hat{y} = \sum_j \theta_j h_j + c$ 

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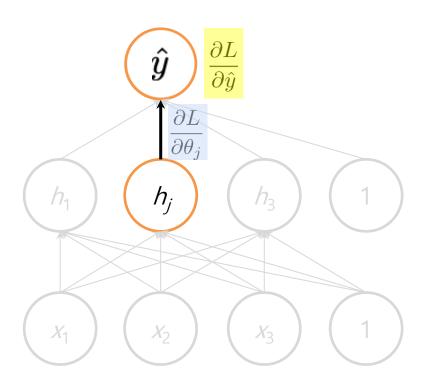
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$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \hat{y}} &= 2(\hat{y} - y) \\
\frac{\partial \mathcal{L}}{\partial \theta_j} &= \frac{\partial \hat{y}}{\partial \theta_j} \frac{\partial \mathcal{L}}{\partial \hat{y}} = h_j \frac{\partial \mathcal{L}}{\partial \hat{y}}
\end{aligned}$$



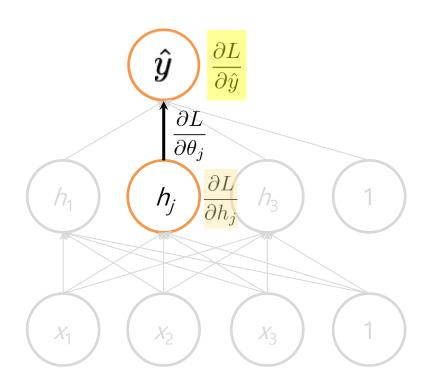
$$h_j = f(\sum_i w_{ji}x_i + b_j), \forall j$$
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- Goal: Compute gradient w.r.t. parameters  $\{W, b, \theta, c\}$   $\mathcal{L} = (\hat{y} y)^2$
- Main idea: Apply a chin rule recursively!

$$\frac{\partial \mathcal{L}}{\partial \hat{y}} = 2(\hat{y} - y)$$

$$\frac{\partial \mathcal{L}}{\partial \theta_{j}} = \frac{\partial \hat{y}}{\partial \theta_{j}} \frac{\partial \mathcal{L}}{\partial \hat{y}} = h_{j} \frac{\partial \mathcal{L}}{\partial \hat{y}}$$

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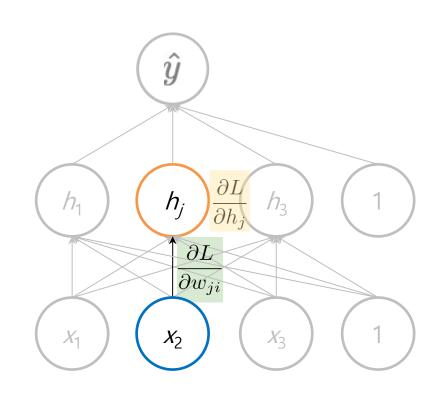
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# Backpropagation: examples (NN with 2-hidden layer for regression)

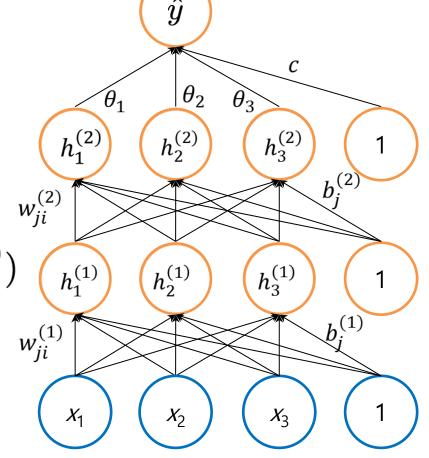
# Multilayer neural network

#### Example: a network with 2 hidden layers

- Input: X
- Output:  $\hat{y}$
- Target: y
- · argett (

- Loss function: square error 
$$(\hat{y}-y)^2$$
 First hidden  $h_j^{(1)}=f(\sum_i w_{ji}^{(1)}x_i+b_j^{(1)})$  layer

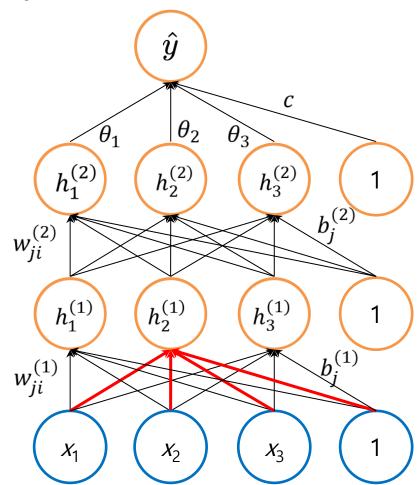
Second hidden  $h_j^{(2)}=f(\sum_i w_{ji}^{(2)}h_i^{(1)}+b_j^{(2)})$  layer  $\hat{y}=\sum_i \theta_j h_j^{(2)}+c$  Output



# Multilayer neural network

- Example: a network with 2 hidden layers
  - Input: X
  - Output:  $\hat{y}$
  - Target: y
  - Loss function: square error  $(\hat{y} y)^2$

 $\underset{\text{layer}}{\operatorname{First}} h_j^{(1)} = f(\sum_i w_{ji}^{(1)} x_i + b_j^{(1)})$ 



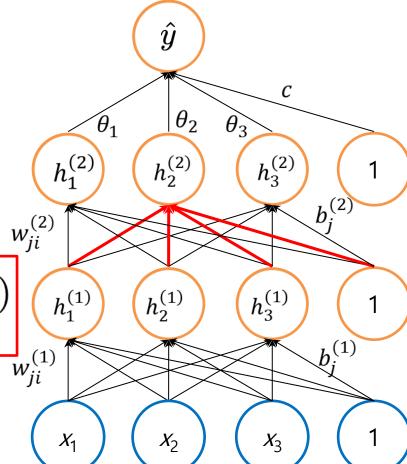
## Multilayer neural network

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Second 
$$h_j^{(2)} = f(\sum_i w_{ji}^{(2)} h_i^{(1)} + b_j^{(2)})$$
 layer



## Multilayer neural network

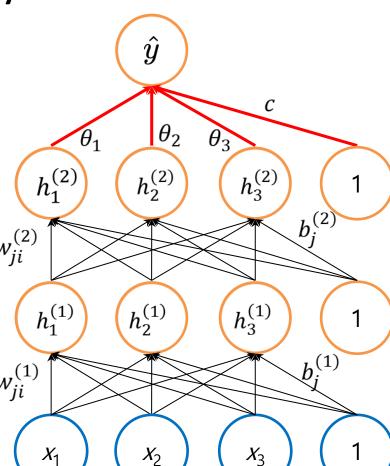
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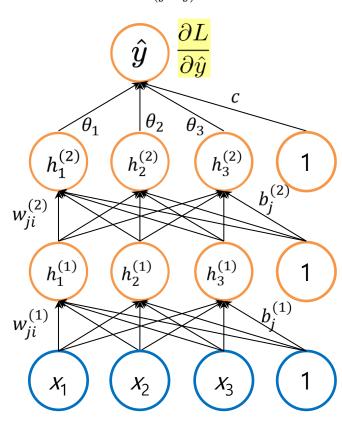
Output 
$$\hat{y} = \sum_j heta_j h_j^{(2)} + c$$



**Backpropagation**: Compute gradient w.r.t. parameters  $\{W^{(1)}, W^{(2)}, b^{(1)}, b^{(2)}, \theta, c\}$ 

$$\frac{\frac{\partial \mathcal{L}}{\partial \hat{y}}}{\partial \hat{y}} = 2(\hat{y} - y)$$

$$h_{j}^{(1)} = f(\sum_{i} w_{ji}^{(1)} x_{i} + b_{j}^{(1)}), \forall j$$
 $h_{j}^{(2)} = f(\sum_{i} w_{ji}^{(2)} h_{i}^{(1)} + b_{j}^{(2)}), \forall j$ 
 $\hat{y} = \sum_{j} \theta_{j} h_{j}^{(2)} + c$ 
 $\mathcal{L} = (\hat{y} - y)^{2}$ 

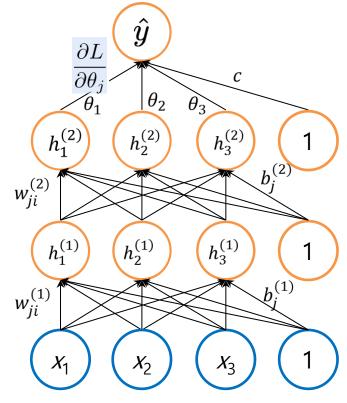


**Backpropagation**: Compute gradient w.r.t. parameters  $\{W^{(1)}, W^{(2)}, b^{(1)}, b^{(2)}, \theta, c\}$ 

$$\frac{\frac{\partial \mathcal{L}}{\partial \hat{y}}}{\frac{\partial \mathcal{L}}{\partial \theta_{j}}} = 2(\hat{y} - y)$$

$$\frac{\partial \mathcal{L}}{\partial \theta_{j}} = \frac{\partial \hat{y}}{\partial \theta_{j}} \frac{\partial \mathcal{L}}{\partial \hat{y}} = h_{j}^{(2)} \frac{\partial \mathcal{L}}{\partial \hat{y}}$$

$$h_j^{(1)} = f(\sum_i w_{ji}^{(1)} x_i + b_j^{(1)}), \forall j$$
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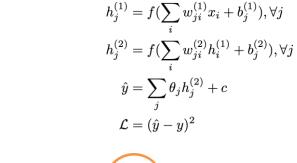


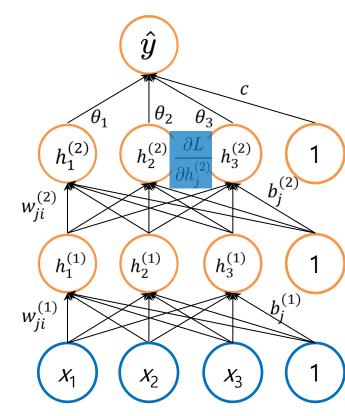
**Backpropagation**: Compute gradient w.r.t. parameters  $\{W^{(1)}, W^{(2)}, b^{(1)}, b^{(2)}, \theta, c\}$ 

$$\frac{\frac{\partial \mathcal{L}}{\partial \hat{y}}}{\frac{\partial \mathcal{L}}{\partial \theta_{j}}} = 2(\hat{y} - y)$$

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**Backpropagation**: Compute gradient w.r.t. parameters 
$$\{W^{(1)}, W^{(2)}, b^{(1)}, b^{(2)}, \theta, c\}$$

$$\frac{\partial \mathcal{L}}{\partial \hat{y}} = 2(\hat{y} - y)$$

$$\frac{\partial \mathcal{L}}{\partial \hat{y}} = \frac{\partial \hat{y}}{\partial y} \frac{\partial \mathcal{L}}{\partial y} - \frac{\partial \hat{y}}{\partial y} \frac{\partial \hat{y}}{\partial y} - \frac{\partial$$

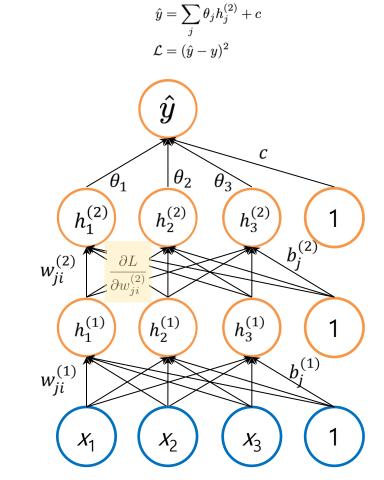
$$\frac{\partial \mathcal{L}}{\partial \theta_{j}} = \frac{\partial \hat{y}}{\partial \theta_{j}} \frac{\partial \mathcal{L}}{\partial \hat{y}} = h_{j}^{(2)} \frac{\partial \mathcal{L}}{\partial \hat{y}}$$

$$\frac{\partial \mathcal{L}}{\partial h_{j}^{(2)}} = \frac{\partial \hat{y}}{\partial h_{j}^{(2)}} \frac{\partial \mathcal{L}}{\partial \hat{y}} = \theta_{j} \frac{\partial \mathcal{L}}{\partial \hat{y}}$$

$$\frac{\partial \mathcal{L}}{\partial h_{j}^{(2)}} = \frac{\partial h_{j}^{(2)}}{\partial h_{j}^{(2)}} \frac{\partial \mathcal{L}}{\partial \hat{y}} = f'(z^{(2)})h^{(1)} \frac{\partial \mathcal{L}}{\partial \mathcal{L}}$$

$$\frac{\partial \mathcal{L}}{\partial h_{j}^{(2)}} = \frac{\partial \hat{y}}{\partial h_{j}^{(2)}} \frac{\partial \mathcal{L}}{\partial \hat{y}} = \theta_{j} \frac{\partial \mathcal{L}}{\partial \hat{y}}$$

$$\frac{\partial \mathcal{L}}{\partial w_{ji}^{(2)}} = \frac{\partial h_{j}^{(2)}}{\partial w_{ji}^{(2)}} \frac{\partial \mathcal{L}}{\partial h_{j}^{(2)}} = f'(z_{j}^{(2)}) h_{i}^{(1)} \frac{\partial \mathcal{L}}{\partial h_{j}^{(2)}}$$



**Backpropagation**: Compute gradient w.r.t. parameters 
$$\{W^{(1)}, W^{(2)}, b^{(1)}, b^{(2)}, \theta, c\}$$

$$\frac{\partial \mathcal{L}}{\partial \hat{y}} = 2(\hat{y} - y)$$

$$\frac{\partial \mathcal{L}}{\partial \theta_j} = \frac{\partial \hat{y}}{\partial \theta_j} \frac{\partial \mathcal{L}}{\partial \hat{y}} = h_j^{(2)} \frac{\partial \mathcal{L}}{\partial \hat{y}}$$

$$\hat{y} = \sum_j \theta_j h_j^{(2)} + c$$

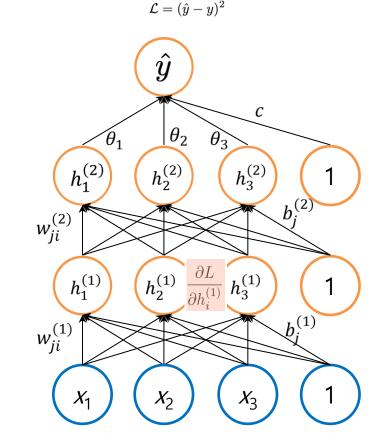
$$\frac{\partial \mathcal{L}}{\partial \theta_{j}} = \frac{\partial g}{\partial \theta_{j}} \frac{\partial \mathcal{L}}{\partial \hat{y}} = h_{j}^{(2)} \frac{\partial \mathcal{L}}{\partial \hat{y}}$$

$$\frac{\partial \mathcal{L}}{\partial h_{j}^{(2)}} = \frac{\partial \hat{y}}{\partial h_{j}^{(2)}} \frac{\partial \mathcal{L}}{\partial \hat{y}} = \theta_{j} \frac{\partial \mathcal{L}}{\partial \hat{y}}$$

$$\frac{\partial \mathcal{L}}{\partial w_{ji}^{(2)}} = \frac{\partial h_{j}^{(2)}}{\partial w_{ji}^{(2)}} \frac{\partial \mathcal{L}}{\partial h_{j}^{(2)}} = f'(z_{j}^{(2)}) h_{i}^{(1)} \frac{\partial \mathcal{L}}{\partial h_{j}^{(2)}}$$

$$\frac{\partial \mathcal{L}}{\partial w_{ji}^{(2)}} = \frac{\partial v_j}{\partial w_{ji}^{(2)}} \frac{\partial \mathcal{L}}{\partial h_j^{(2)}} = f'(z_j^{(2)}) h_i^{(1)} \frac{\partial \mathcal{L}}{\partial h_j^{(2)}}$$

$$\frac{\partial \mathcal{L}}{\partial h_i^{(1)}} = \sum_j \frac{\partial h_j^{(2)}}{\partial h_i^{(1)}} \frac{\partial \mathcal{L}}{\partial h_j^{(2)}} = \sum_j f'(z_j^{(2)}) w_{ji}^{(2)} \frac{\partial \mathcal{L}}{\partial h_j^{(2)}}$$



**Backpropagation**: Compute gradient w.r.t. parameters 
$$\{W^{(1)}, W^{(2)}, b^{(1)}, b^{(2)}, \theta, c\}$$

$$\frac{\partial \mathcal{L}}{\partial \hat{y}} = 2(\hat{y} - y)$$

$$\frac{\partial \mathcal{L}}{\partial \theta_{j}} = \frac{\partial \hat{y}}{\partial \theta_{j}} \frac{\partial \mathcal{L}}{\partial \hat{y}} = h_{j}^{(2)} \frac{\partial \mathcal{L}}{\partial \hat{y}}$$

$$\frac{\partial \mathcal{L}}{\partial h_{j}^{(2)}} = \frac{\partial \hat{y}}{\partial h_{j}^{(2)}} \frac{\partial \mathcal{L}}{\partial \hat{y}} = \theta_{j} \frac{\partial \mathcal{L}}{\partial \hat{y}}$$

$$\frac{\partial \mathcal{L}}{\partial h_{j}^{(2)}} = \frac{\partial \hat{y}}{\partial h_{j}^{(2)}} \frac{\partial \mathcal{L}}{\partial \hat{y}} = \theta_{j} \frac{\partial \mathcal{L}}{\partial \hat{y}}$$

$$\hat{y} = \sum_{j} \theta_{j} h_{j}^{(2)} + c$$

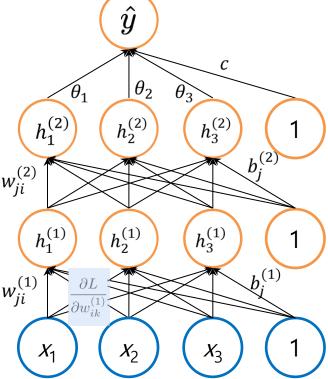
$$\hat{y}$$

 $\frac{\partial \mathcal{L}}{\partial w_{ji}^{(2)}} = \frac{\partial h_j^{(2)}}{\partial w_{ji}^{(2)}} \frac{\partial \mathcal{L}}{\partial h_i^{(2)}} = f'(z_j^{(2)}) h_i^{(1)} \frac{\partial \mathcal{L}}{\partial h_i^{(2)}}$  $\frac{\partial \mathcal{L}}{\partial h_i^{(1)}} = \sum_i \frac{\partial h_j^{(2)}}{\partial h_i^{(1)}} \frac{\partial \mathcal{L}}{\partial h_i^{(2)}} = \sum_i f'(z_j^{(2)}) w_{ji}^{(2)} \frac{\partial \mathcal{L}}{\partial h_i^{(2)}}$ 

 $w_{ji}^{(2)}$ 

$$\frac{\partial \mathcal{L}}{\partial w_{ik}^{(1)}} = \frac{\partial h_i^{(1)}}{\partial w_{ik}^{(1)}} \frac{\partial \mathcal{L}}{\partial h_i^{(1)}} = f'(z_i^{(1)}) x_k \frac{\partial \mathcal{L}}{\partial h_i^{(1)}}$$
where  $z_j^{(2)} = \sum_i h_i^{(1)} w_{ji}^{(2)} + b_j^{(2)}$ 

$$z_i^{(1)} = \sum_k x_k w_{ik}^{(1)} + b_i^{(1)}$$



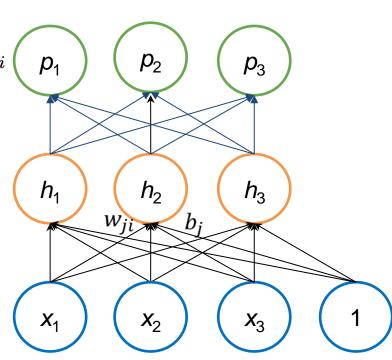
## Backpropagation: examples (NN with 1-hidden layer for classification)

### **Forward Propagation**

- Example: a network with 1 hidden layer
  - Input: x
  - Output: P
  - Target: y (one-hot vector)
  - Loss function: cross entropy  $\sum_i y_i \log p_i$  (

$$\begin{array}{ll} \text{Hidden} & h_j = f(\sum_i w_{ji} x_i + b_j) \\ \text{layer} & \end{array}$$

Output 
$$p_i = \frac{e^{h_i}}{\sum_k e^{h_k}}$$

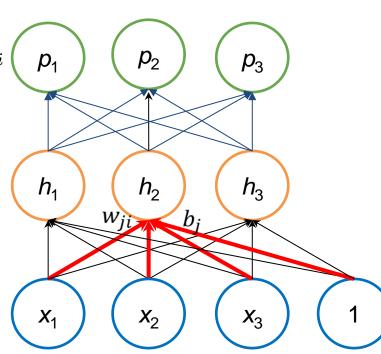


### **Forward Propagation**

- Example: a network with 1 hidden layer
  - Input: x
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  - Loss function: cross entropy  $\sum_i y_i \log p_i$  (

Hidden 
$$h_j = f(\sum_i w_{ji}x_i + b_j)$$
 layer

Output 
$$p_i = \frac{e^{n_i}}{\sum_k e^{h_k}}$$

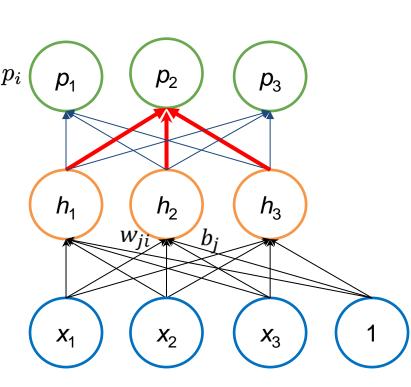


### **Forward Propagation**

- Example: a network with 1 hidden layer
  - Input: x
  - Output: P
  - Target: y (one-hot vector)
  - Loss function: cross entropy  $-\sum y_i \log p_i$  (

$$\begin{array}{ll} \text{Hidden} & h_j = f(\sum_i w_{ji} x_i + b_j) \\ \text{layer} & \end{array}$$

Output 
$$p_i = rac{e^{h_i}}{\sum_k e^{h_k}}$$



### Backpropagation

- Example: a network with 1 hidden layer
  - Goal: Compute Gradients w.r.t parameters  $\{W, b\}$
  - Main Idea: Apply Chain Rule recursively

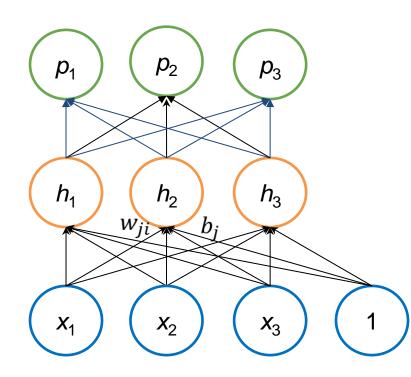
$$\mathcal{L} = -\sum_{i} y_{i} \log p_{i} = -\sum_{i} y_{i} \log \frac{e^{h_{i}}}{\sum_{k} e^{h_{k}}}$$

$$= -\sum_{i} y_{i} h_{i} + (\sum_{i} y_{i}) \log(\sum_{k} e^{h_{k}})$$

$$= \log(\sum_{k} e^{h_{k}}) - \sum_{k} y_{k} h_{k}$$

$$\frac{\partial \mathcal{L}}{\partial h_{j}} = \frac{e^{h_{j}}}{\sum_{k} e^{h_{k}}} - y_{j} = p_{j} - y_{j}$$

$$\frac{\partial \mathcal{L}}{\partial w_{ji}} = \frac{\partial h_{j}}{\partial w_{ji}} \frac{\partial \mathcal{L}}{\partial h_{j}} = f' x_{i} \frac{\partial \mathcal{L}}{\partial h_{j}}$$
where  $f' = f'(\sum_{i} w_{ji} x_{i} + b_{j})$ 



### Backpropagation

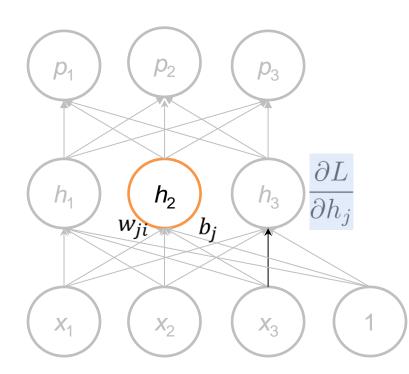
- Example: a network with 1 hidden layer
  - Goal: Compute Gradients w.r.t parameters  $\{W, b\}$
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$$\mathcal{L} = -\sum_{i} y_{i} \log p_{i} = -\sum_{i} y_{i} \log \frac{e^{h_{i}}}{\sum_{k} e^{h_{k}}}$$

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$$= \log(\sum_{k} e^{h_{k}}) - \sum_{k} y_{k} h_{k}$$

$$\frac{\partial \mathcal{L}}{\partial h_{j}} = \frac{e^{h_{j}}}{\sum_{k} e^{h_{k}}} - y_{j} = p_{j} - y_{j}$$



### Backpropagation

- Example: a network with 1 hidden layer
  - Goal: Compute Gradients w.r.t parameters  $\{W, b\}$
  - Main Idea: Apply Chain Rule recursively

$$\mathcal{L} = -\sum_{i} y_{i} \log p_{i} = -\sum_{i} y_{i} \log \frac{e^{h_{i}}}{\sum_{k} e^{h_{k}}}$$

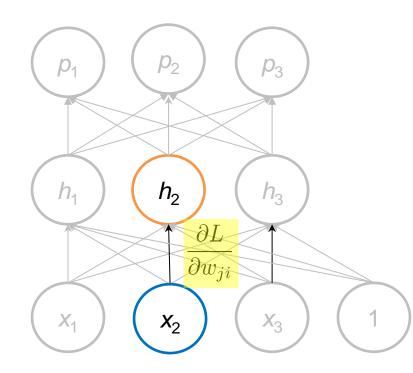
$$= -\sum_{i} y_{i} h_{i} + (\sum_{i} y_{i}) \log(\sum_{k} e^{h_{k}})$$

$$= \log(\sum_{k} e^{h_{k}}) - \sum_{k} y_{k} h_{k}$$

$$\frac{\partial \mathcal{L}}{\partial h_{j}} = \frac{e^{h_{j}}}{\sum_{k} e^{h_{k}}} - y_{j} = p_{j} - y_{j}$$

$$\frac{\partial \mathcal{L}}{\partial w_{ji}} = \frac{\partial h_{j}}{\partial w_{ji}} \frac{\partial \mathcal{L}}{\partial h_{j}} = f'x_{i} \frac{\partial \mathcal{L}}{\partial h_{j}}$$

$$\text{where } f' = f'(\sum_{i} w_{ji}x_{i} + b_{j})$$

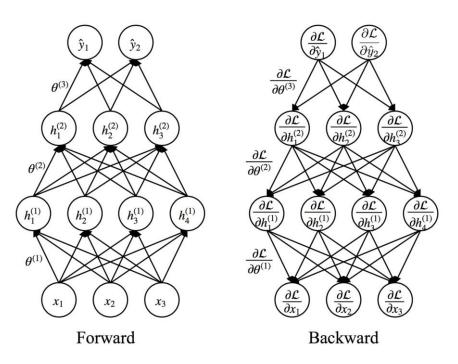


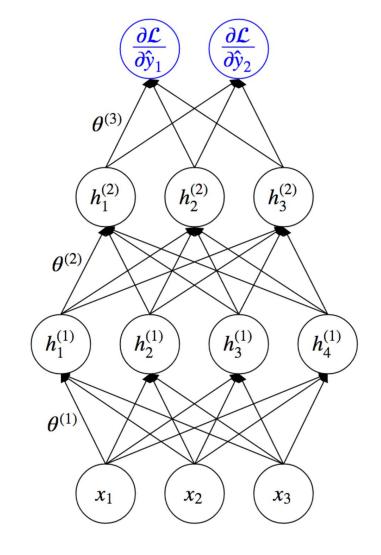
### Deep Neural Networks

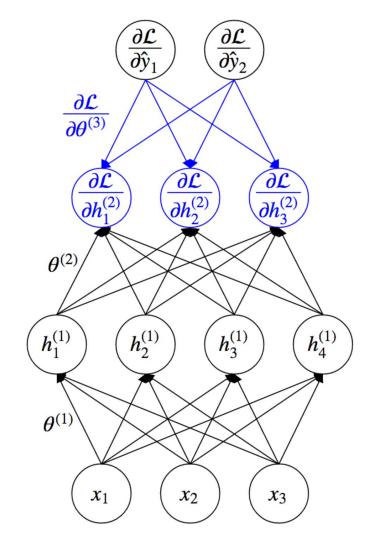
 Construction is straightforward: recursively stacking the blocks of layers

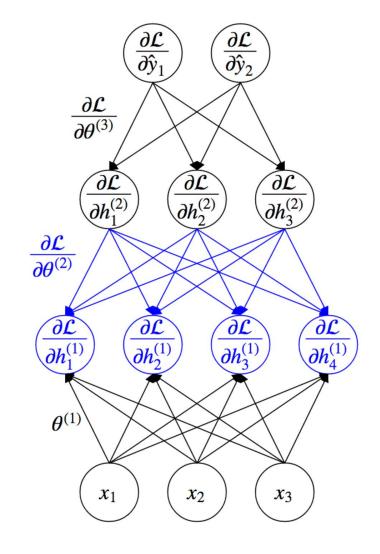
- Computing gradient is straightforward (via back propagation)
  - For general formula, see Bishop's book.

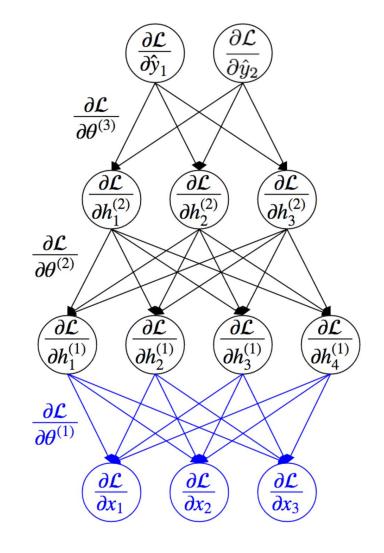
- Computing gradient via chain rule for compositional function
- The chain rule can be expressed as a local computation
- Think of it as a computational graph











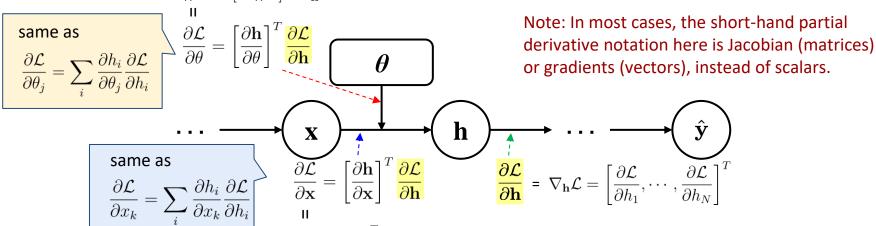
### Back-Propagation Algorithm: Recap

- Compute  $\nabla_y \mathcal{L} = \left[ \frac{\partial \mathcal{L}}{\partial y_1}, \cdots, \frac{\partial \mathcal{L}}{\partial y_n} \right]^T$  directly from the loss function.
- For each layer (from top to bottom) with output  $\mathbf{h}$ , input  $\mathbf{x}$ , and weights  $\mathbf{W}$ ,
  - O Assuming that  $\nabla_{\mathbf{h}} \mathcal{L}$  is given, compute gradients using the **chain rule** as:

$$\left[ 
abla_{\mathbf{W}} \mathcal{L} = \left[ 
abla_{\mathbf{W}} \mathbf{h} \right]^T 
abla_{\mathbf{h}} \mathcal{L} \qquad 
abla_{\mathbf{x}} \mathcal{L} = \left[ 
abla_{\mathbf{x}} \mathbf{h} \right]^T 
abla_{\mathbf{h}} \mathcal{L}$$

"gradient w.r.t. parameters"

(to be used for SGD update)  $\nabla_{\mathbf{W}} \mathcal{L} = \left[ \nabla_{\mathbf{W}} \mathbf{h} \right]^T \nabla_{\mathbf{h}} \mathcal{L}$ 



 $abla_{\mathbf{x}}\mathcal{L} = \left[
abla_{\mathbf{x}}\mathbf{h}
ight]^T
abla_{\mathbf{h}}\mathcal{L}$ 

"gradient w.r.t. input" (to be propagated to lower layers in backprop recursion)

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"gradient w.r.t. hidden layer above" (given)

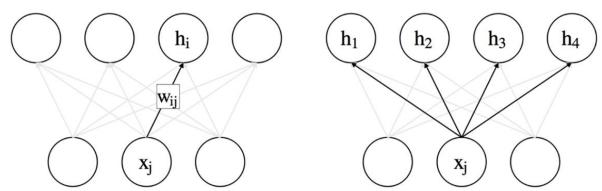
#### Practice: Linear

- Forward:  $h_i = \sum_j w_{ij} x_j + b_i \Longleftrightarrow \mathbf{h} = \mathbf{W}\mathbf{x} + \mathbf{b}$
- Gradient w.r.t parameters

$$\frac{\partial \mathcal{L}}{\partial w_{ij}} = \frac{\partial \mathcal{L}}{\partial h_i} \frac{\partial h_i}{\partial w_{ij}} = \frac{\partial \mathcal{L}}{\partial h_i} x_j \Longleftrightarrow \nabla_{\mathbf{W}} \mathcal{L} = \nabla_{\mathbf{h}} \mathcal{L} \mathbf{x}^{\top}$$

• Gradient w.r.t inputs

$$\frac{\partial \mathcal{L}}{\partial x_{i}} = \sum_{i} \frac{\partial \mathcal{L}}{\partial h_{i}} \frac{\partial h_{i}}{\partial x_{j}} = \sum_{i} \frac{\partial \mathcal{L}}{\partial h_{i}} w_{ij} \Longleftrightarrow \nabla_{\mathbf{x}} \mathcal{L} = \mathbf{W}^{\top} \nabla_{\mathbf{h}} \mathcal{L}$$



column major notation. However, PyTorch / NumPy typically uses row major notation (i.e., vectors are represented as row vectors by default). Please also see the note in the questions in HW3 and HW4, which uses row major notation.

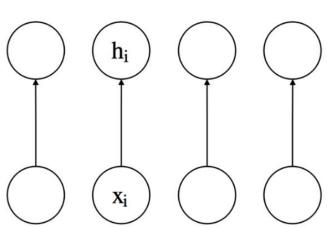
Note 2: In HW3 and HW4, we will ask you to do additional vectorization for backpropagation using multiple input examples (i.e., input/output of a layer can be represented as matrix, not a vector)

### Practice: Non-Linear Activation (Sigmoid)

- Forward:  $h_i = \sigma(x_i) = \frac{1}{1 + \exp(-x_i)} \Longleftrightarrow \mathbf{h} = \sigma(\mathbf{x})$
- Gradient w.r.t inputs

$$\frac{\partial \mathcal{L}}{\partial x_i} = \frac{\partial \mathcal{L}}{\partial h_i} \frac{\partial h_i}{\partial x_i} = \frac{\partial \mathcal{L}}{\partial h_i} \sigma(x_i) (1 - \sigma(x_i)) = \frac{\partial \mathcal{L}}{\partial h_i} h_i (1 - h_i)$$

$$\nabla_{\mathbf{x}} \mathcal{L} = \nabla_{\mathbf{h}} \mathcal{L} \odot \mathbf{h} \odot (1 - \mathbf{h})$$



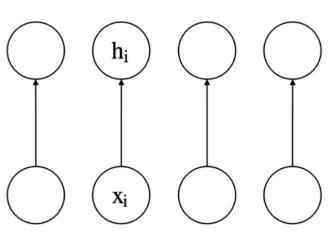
### Practice: Non-Linear Activation (tanh)

• Forward: 
$$h_i = \tanh(x_i) = \frac{\exp(x_i) - \exp(-x_i)}{\exp(x_i) + \exp(-x_i)} \iff \mathbf{h} = \tanh(\mathbf{x})$$

• Gradient w.r.t inputs

$$\frac{\partial \mathcal{L}}{\partial x_i} = \frac{\partial \mathcal{L}}{\partial h_i} \frac{\partial h_i}{\partial x_i} = \frac{\partial \mathcal{L}}{\partial h_i} (1 - \tanh^2(x_i)) = \frac{\partial \mathcal{L}}{\partial h_i} (1 - h_i^2)$$

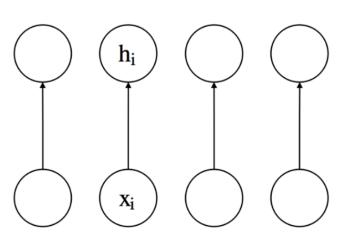
$$\nabla_{\mathbf{x}} \mathcal{L} = \nabla_{\mathbf{h}} \mathcal{L} \odot (1 - \mathbf{h} \odot \mathbf{h})$$



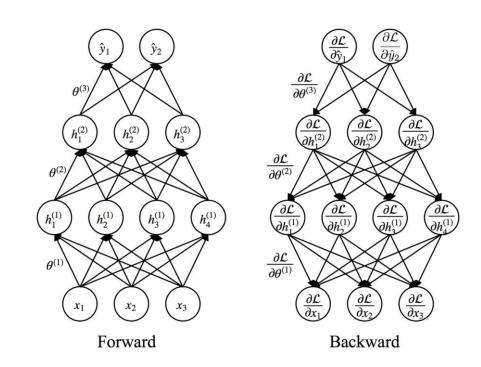
### Practice: Non-Linear Activation (ReLU)

- Forward:  $h_i = \text{ReLU}(x_i) = \max(x_i, 0) \iff \mathbf{h} = \text{ReLU}(\mathbf{x})$
- Gradient w.r.t inputs

$$\frac{\partial \mathcal{L}}{\partial x_i} = \frac{\partial \mathcal{L}}{\partial h_i} \frac{\partial h_i}{\partial x_i} = \begin{cases} \frac{\partial \mathcal{L}}{\partial h_i} & x_i > 0 \\ 0 & x_i < 0 \end{cases}$$



- Computing gradient via chain rule for compositional function
- The chain rule can be expressed as a local computation
- Think of it as a computational graph



## **Problems with Back Propagation**

- Gradient is progressively getting more diluted
  - Below top few layers, correction signals can be significantly reduced

- Easy to get stuck in local minima
  - Especially since they start out far from 'good' regions (i.e., random initialization)

### **Back Propagation & Amount of Data**

- Typically requires lots of labeled data
- Given limited amounts of labeled data, training via backpropagation does not work well
  - Deep networks trained with backpropagation (without any sort of unsupervised pretraining) sometimes perform worse than shallow networks – Overfitting
- However, when there is a large amount of labeled data, backpropagation works surprisingly well.
  - Example of success: Convolutional Neural Networks trained from ImageNet classification (~1M labeled images from 1000 classes)

#### Any feedback (about lecture, slide, homework, project, etc.)?

(via anonymous google form: <a href="https://forms.gle/fpYmiBtG9Me5qbP37">https://forms.gle/fpYmiBtG9Me5qbP37</a>)



Change Log of lecture slides: <a href="https://docs.google.com/document/d/e/2PACX-1vSSIHJjklypK7rKFSR1-5GYXyBCEW8UPtpSfCR9AR6M1l7K9ZQEmxfFwaWaW7kLDxusthsF8WlCyZJ-/pub">https://docs.google.com/document/d/e/2PACX-1vSSIHJjklypK7rKFSR1-5GYXyBCEW8UPtpSfCR9AR6M1l7K9ZQEmxfFwaWaW7kLDxusthsF8WlCyZJ-/pub</a>