EECS 545: Machine Learning

Lecture 11. Neural Networks and Deep Learning

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02/14/2022

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?

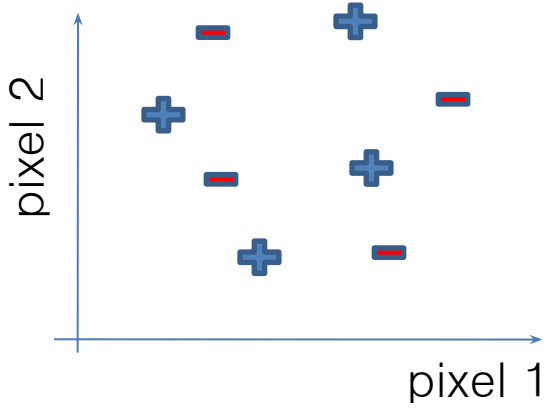
Feature representations

Input

Learning algorithm

Input space

Motorbike
"Non"–Motorbikes



Feature representations

handle

wheel

Input

Feature representation

Learning algorithm

Input space

pixel 2

pixel 1

Motorbike

"Non"-Motorbikes

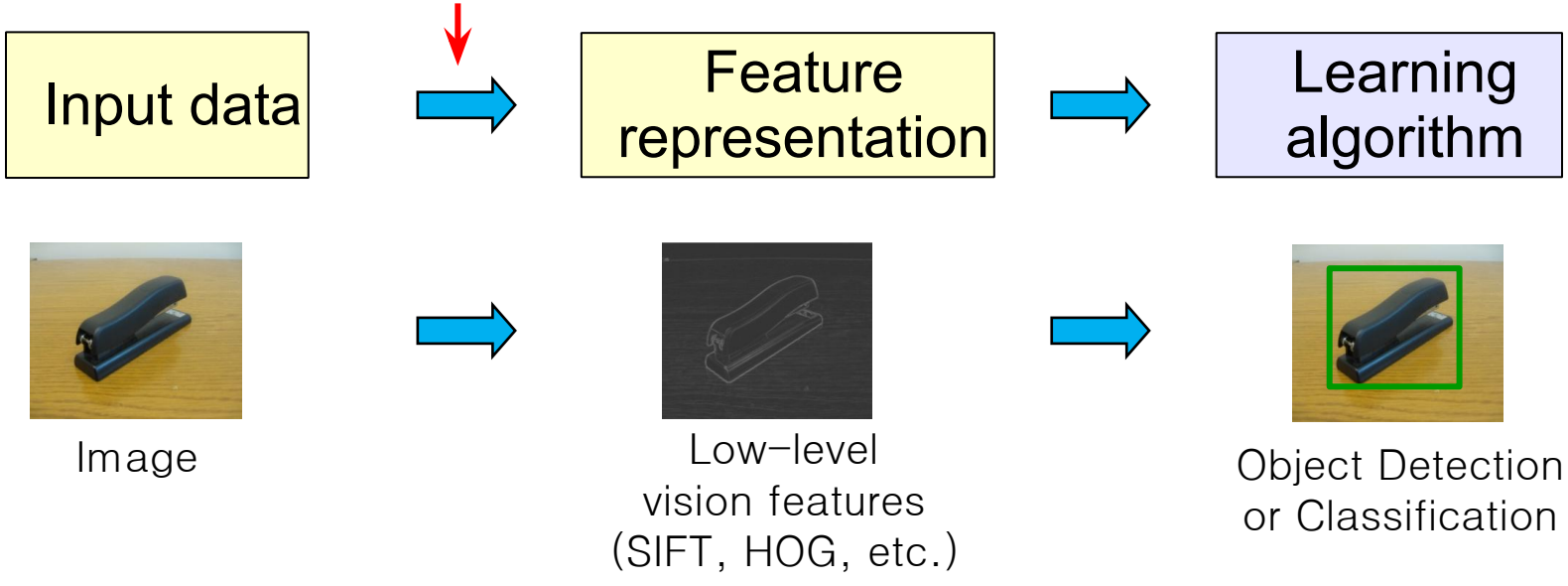
Feature space

"handle"

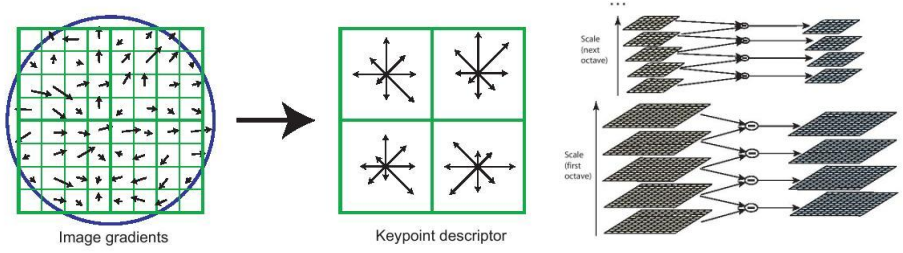
"wheel"

How is computer perception done?

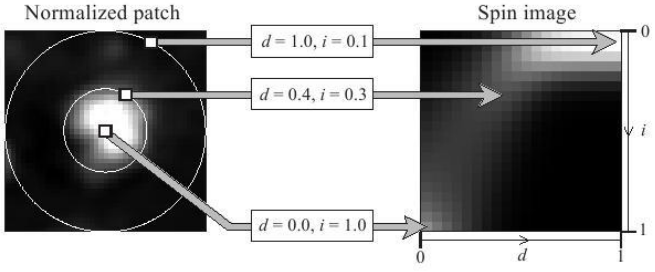
State-of-the-art:
"hand-crafting"



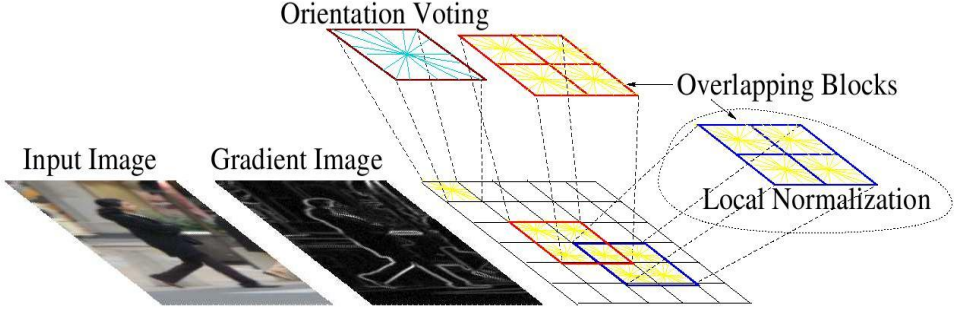
Computer Vision Features



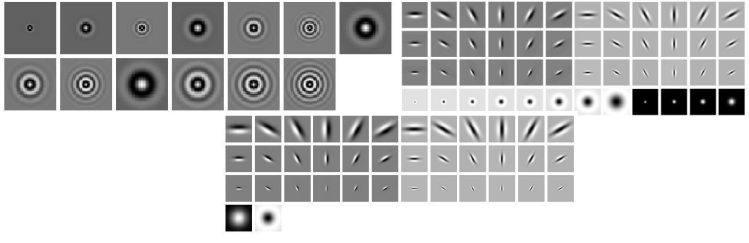
SIFT



Spin image



HoG



Textons

Issues with hand-crafted Computer Vision Features

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

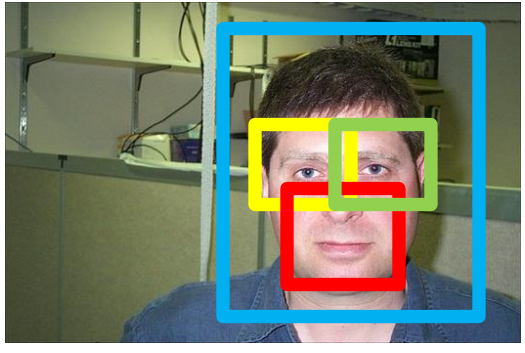
Learning Feature Representations

- Key idea of **Deep Learning**:
  - Learn multiple levels 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.

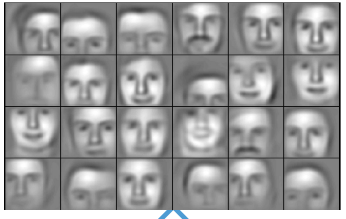
Example: Learning Feature Hierarchy

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

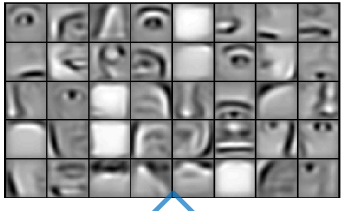
Input data



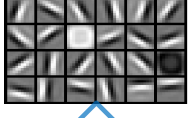
Feature representation



3rd layer
"Objects"



2nd layer
"Object parts"



1st layer
"Edges"

Pixels

2. **Fill in representation gap** in machine learning

Taxonomy of machine learning methods

Supervised

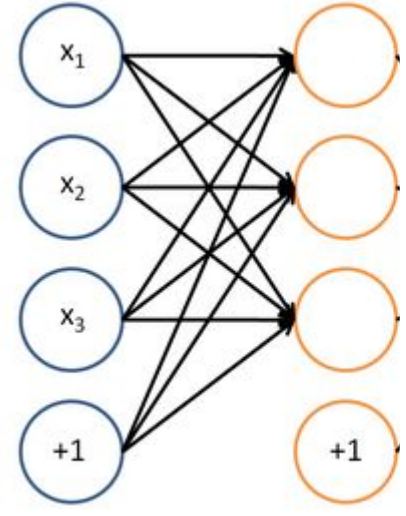
Shallow	**Deep**
• Support Vector Machine • Logistic Regression • Perceptron	• Deep Neural Network • Convolutional Neural Network • Recurrent Neural Network
• Denoising Autoencoder • Restricted Boltzmann machine* • Sparse coding*	• Variational Autoencoder • Generative Adversarial Network • Deep Belief Network* • Deep Boltzmann machine*

Unsupervised

* supervised version exists

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

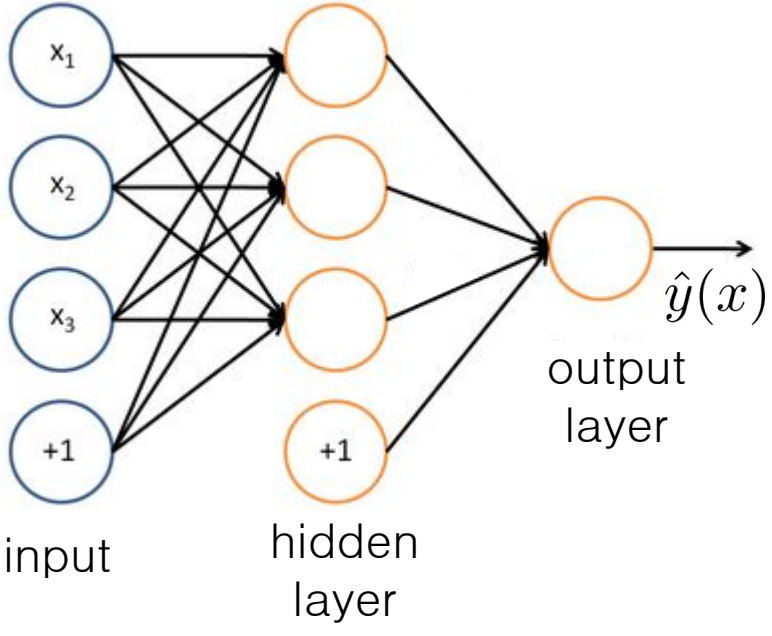


But we don't have to decide ahead of time what variables these logistic regressions are trying to predict!

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.

Slide Credit: Yoshua Bengio

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.

bias

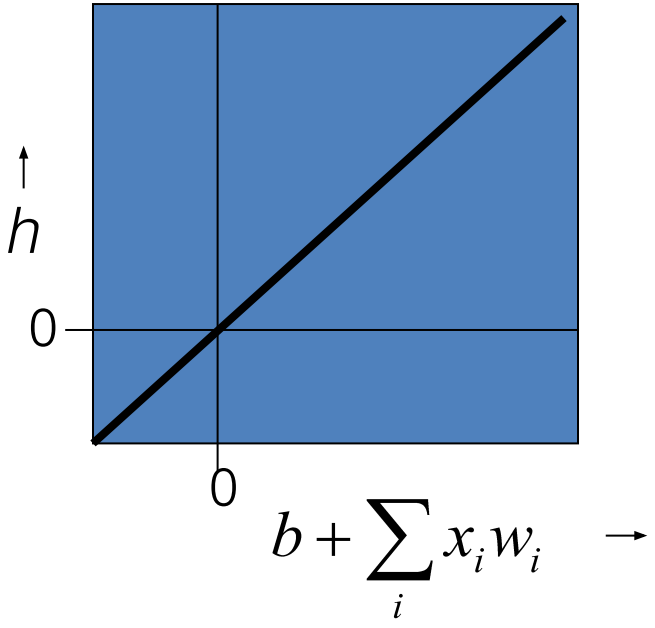
i^{th} input

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

output

index over input connections

weight on i^{th} input



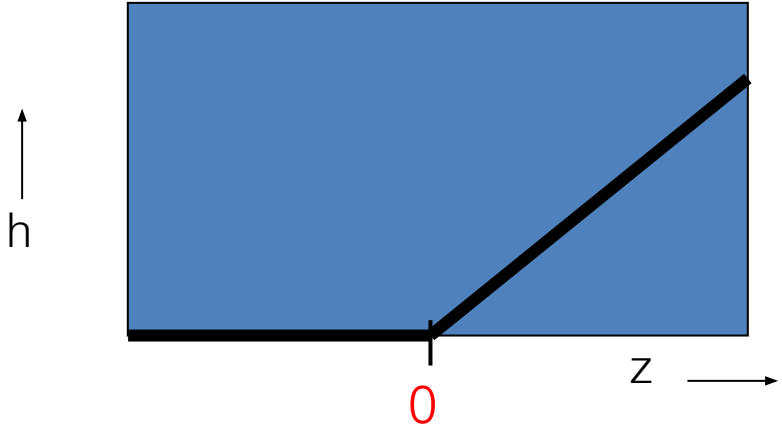
Slide Credit: Geoff Hinton

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.

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

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



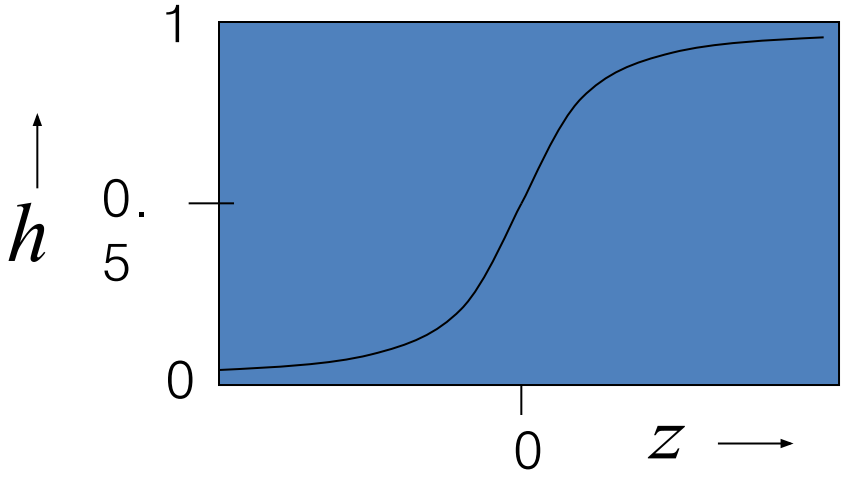
Slide Credit: Geoff Hinton

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

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

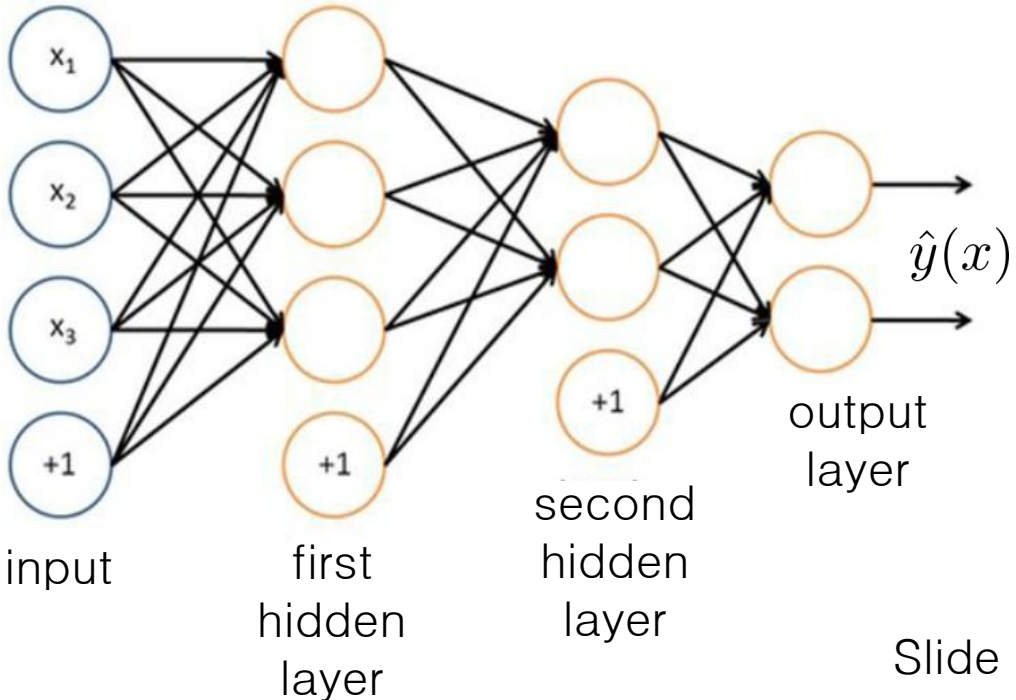
$$h_j = \frac{e^{z_j}}{\sum_k e^{z_k}}$$

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
  - $(\mathbf{x}, \mathbf{y}) \leftarrow$ Sample an example (or a mini-batch) from data
  - $\hat{\mathbf{y}} \leftarrow f(\mathbf{x}; \theta)$ Forward propagation
  - Compute $\mathcal{L}(\mathbf{y}, \hat{\mathbf{y}})$
  - $\nabla_\theta \mathcal{L} \leftarrow$ Backward propagation
  - Update weights using (stochastic) gradient descent
    - $\theta \leftarrow \theta - \alpha \nabla_\theta \mathcal{L}$

Slide credit: Junhyuk Oh, Jacob Abernethy

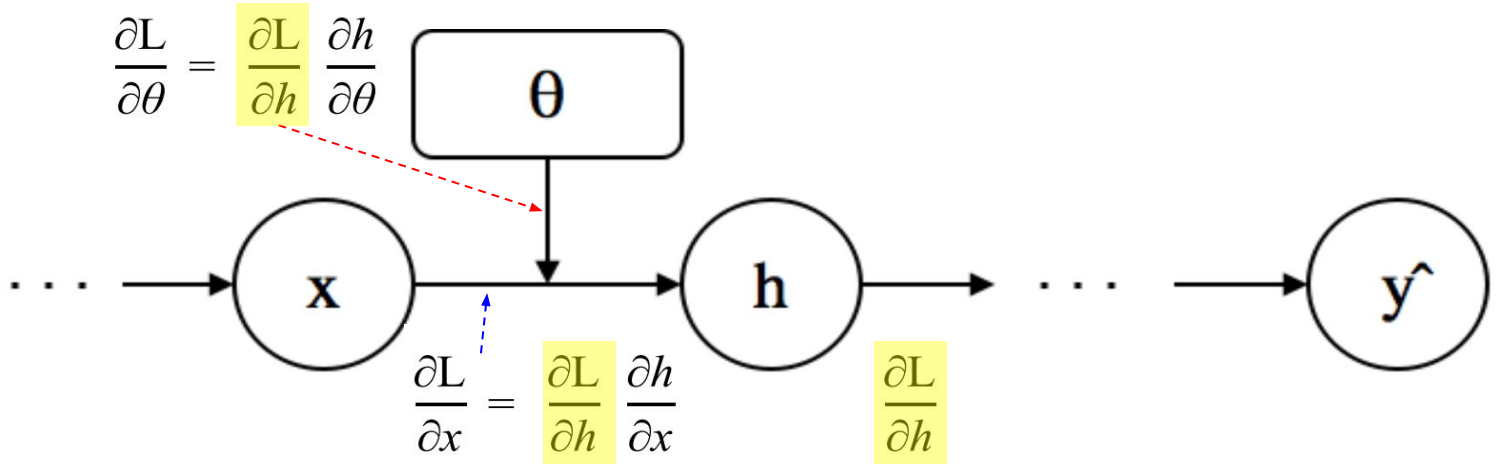
Overview of backpropagation

- Recall: Deep Neural Network represents a complex function with nested, composite functions (represented by layer-wise operation and nonlinearity, etc.)

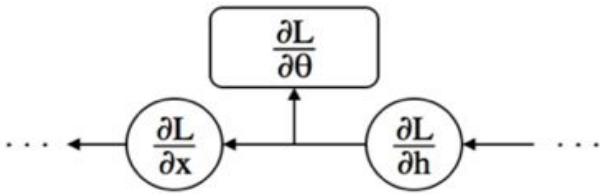
- Q. How can we compute the gradient of the complex function?
- A. Backpropagation:
  - Computing gradient via **chain rule** for compositional function
  - The chain rule can be expressed as a **local computation**
  - Think about it as a **computational graph**

Backpropagation

- Denote x, h, θ 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



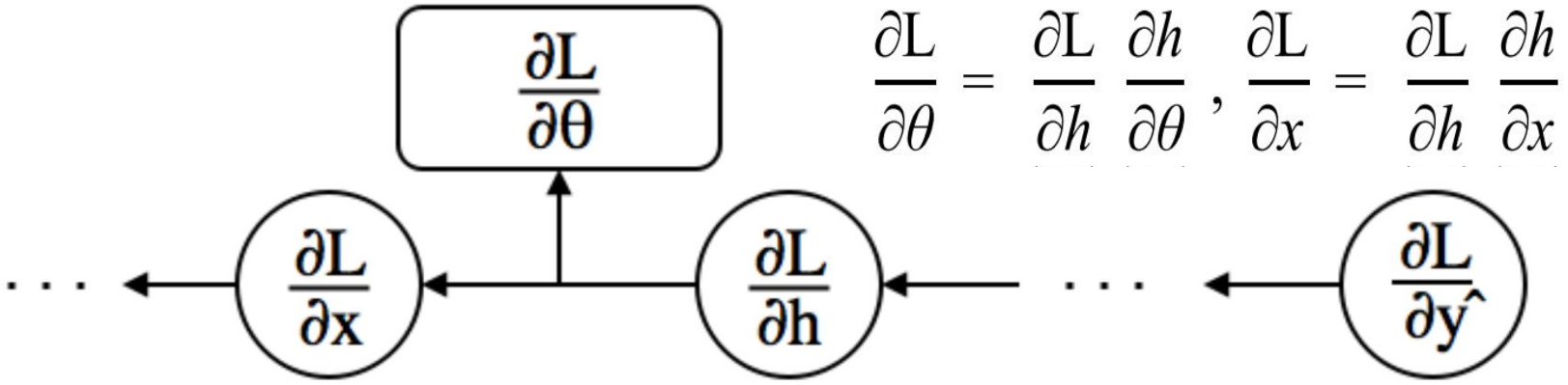
- Assuming that $\frac{\partial L}{\partial h}$ is given, use the **chain rule** to compute the gradients



$$\frac{\partial L}{\partial \theta} = \underbrace{\frac{\partial L}{\partial h}}_{\text{given}}\underbrace{\frac{\partial h}{\partial \theta}}_{\text{easy}}, \quad \frac{\partial L}{\partial x} = \underbrace{\frac{\partial L}{\partial h}}_{\text{given}}\underbrace{\frac{\partial h}{\partial x}}_{\text{easy}}$$

Idea behind backpropagation

- We need only $\frac{\partial \mathrm{L}}{\partial \theta}$ for gradient descent. Why compute $\frac{\partial \mathrm{L}}{\partial x}$?
  - The previous layer needs it because x is the output of the previous layer.



Slide credit: Junhyuk Oh, Jacob Abernethy

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

Forward Propagation

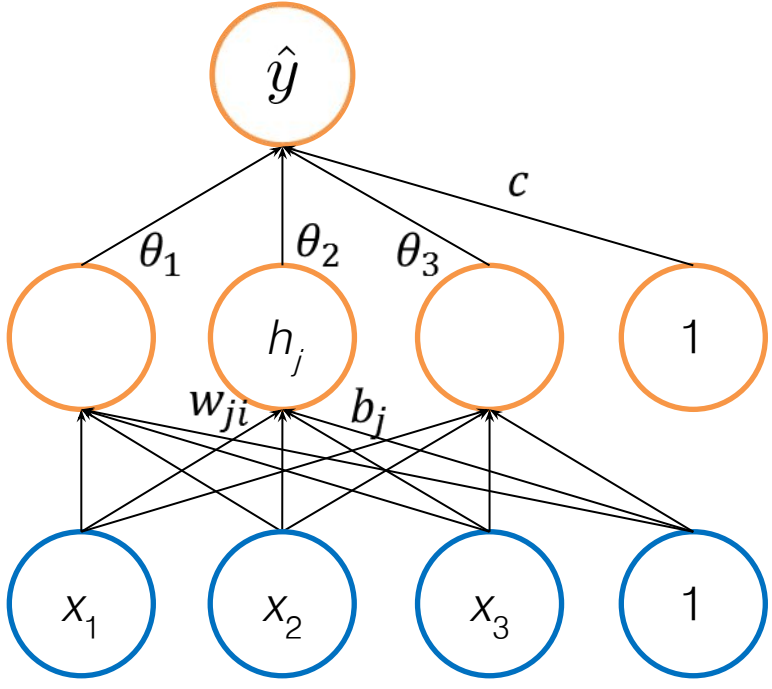
- **Example: a network with 1 hidden layer**
  - Input: $\mathbf{x}$
  - Output: $\hat{y}$
  - Target: y
  - Loss function: square error $(\hat{y} - y)^2$

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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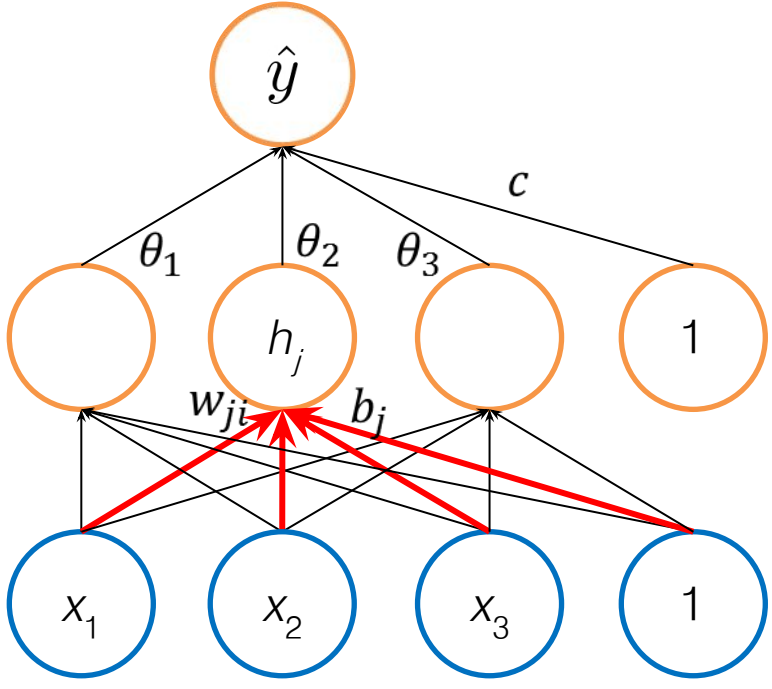

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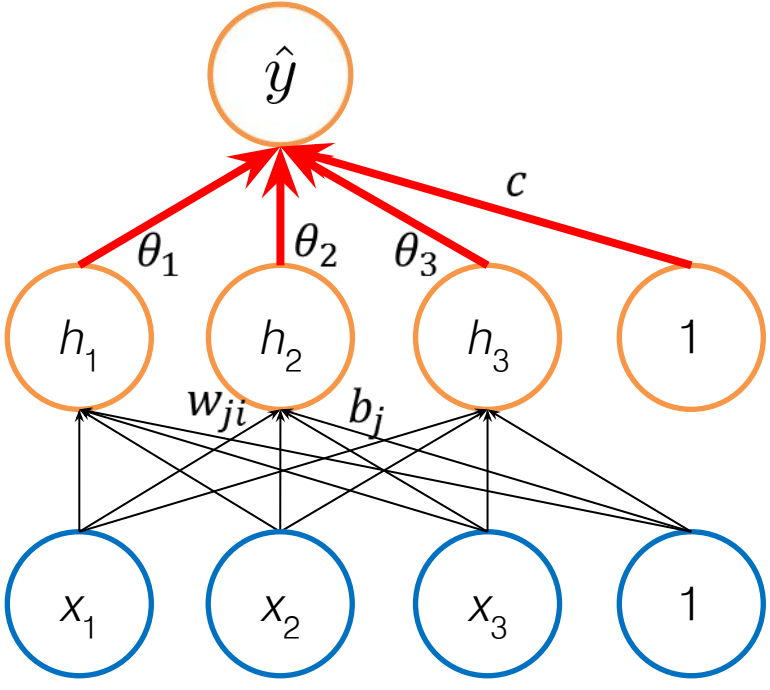

Backpropagation

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

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

$$L = (\hat{y} - y)^2$$

- Goal: Compute gradient w.r.t. parameters $\{W, b, \theta, c\}$
- Main idea: Apply a chain rule recursively!

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

$$\frac{\partial L}{\partial \theta_j} = \frac{\partial \hat{y}}{\partial \theta_j}\frac{\partial L}{\partial \hat{y}} = h_j \frac{\partial L}{\partial \hat{y}}$$

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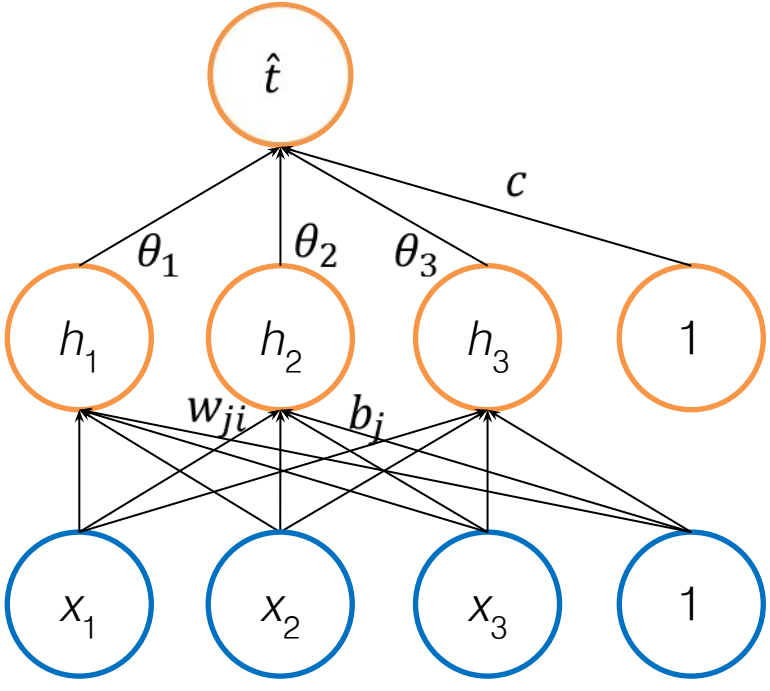
$$\frac{\partial L}{\partial w_{ji}} = \frac{\partial h_j}{\partial w_{ji}}\frac{\partial L}{\partial h_j} = f' x_i \frac{\partial L}{\partial h_j}$$

$$\text{where } f' = f'(\sum_i w_{ji} x_i + b_j)$$



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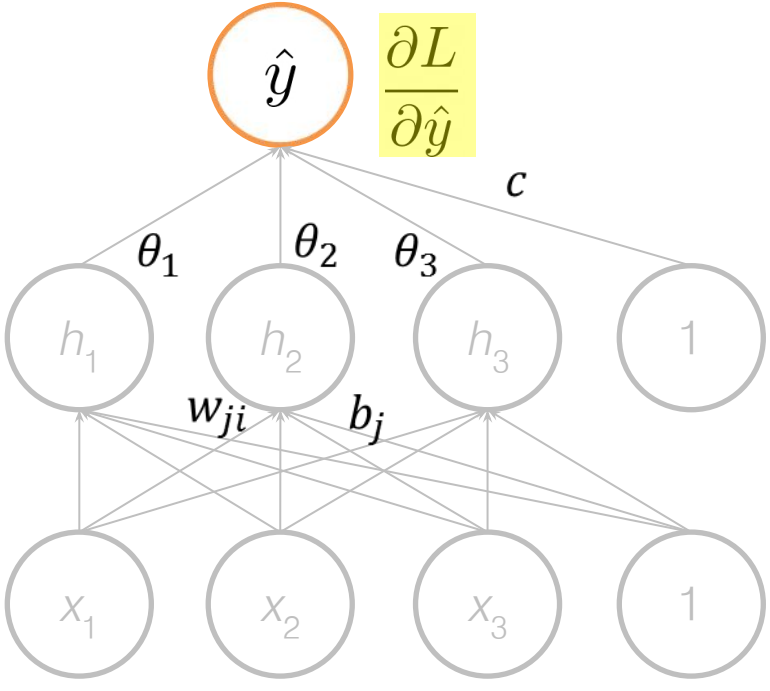

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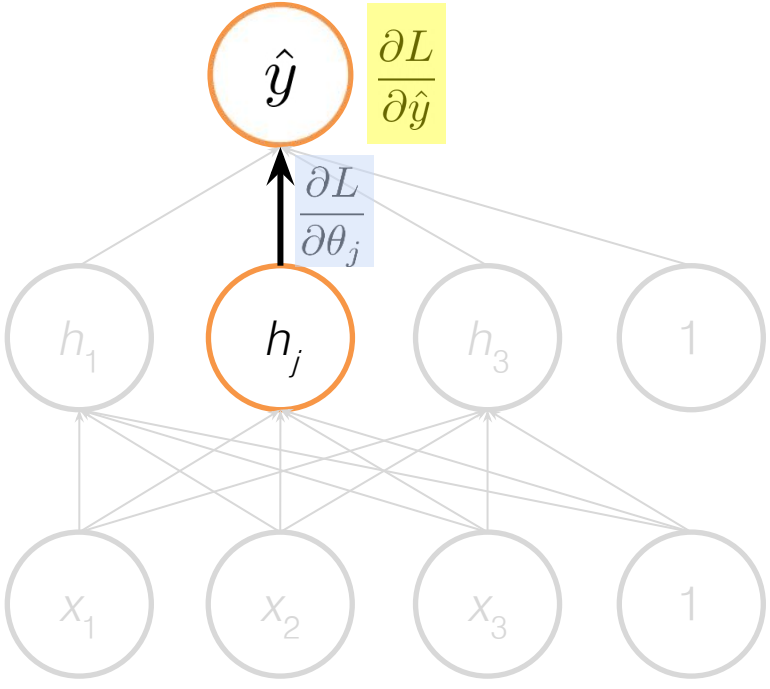

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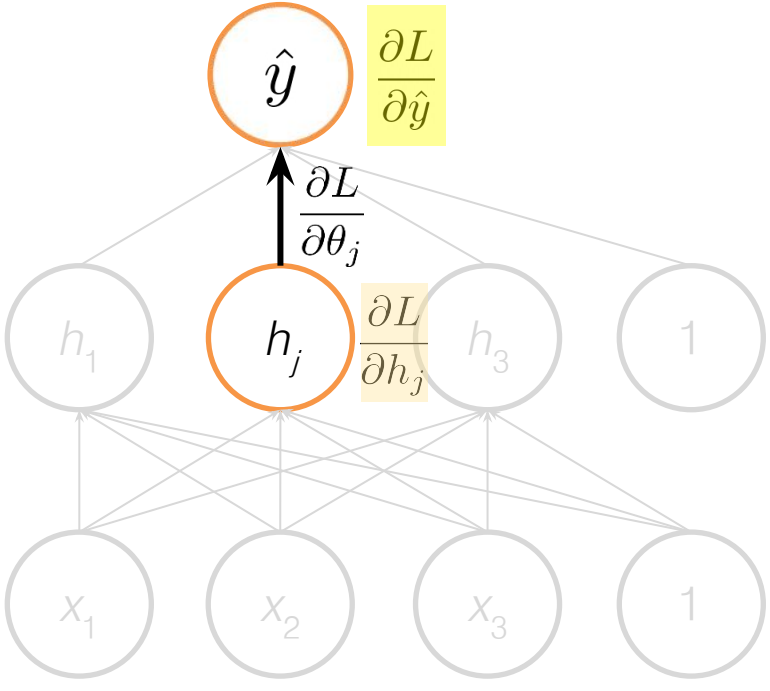

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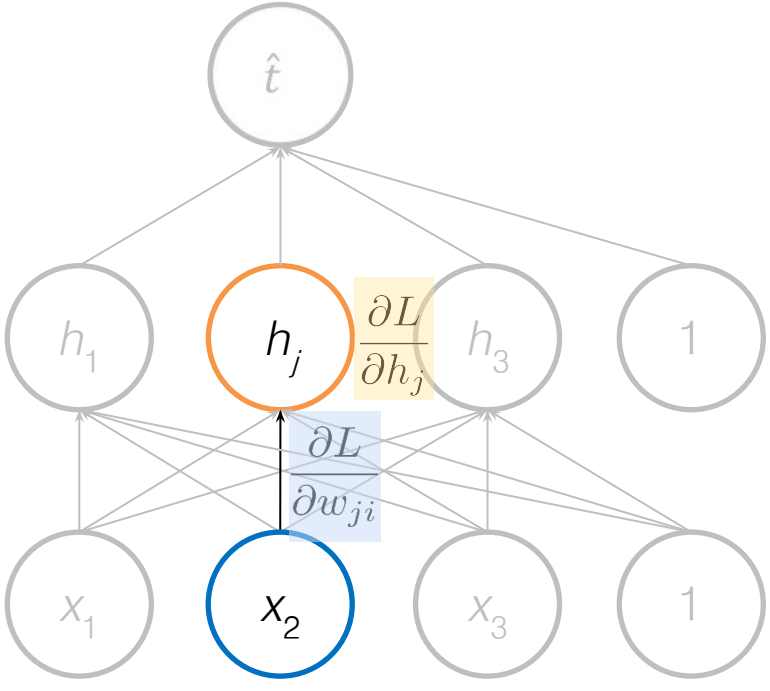


Backpropagation: examples
(NN with 2-hidden layer for regression)

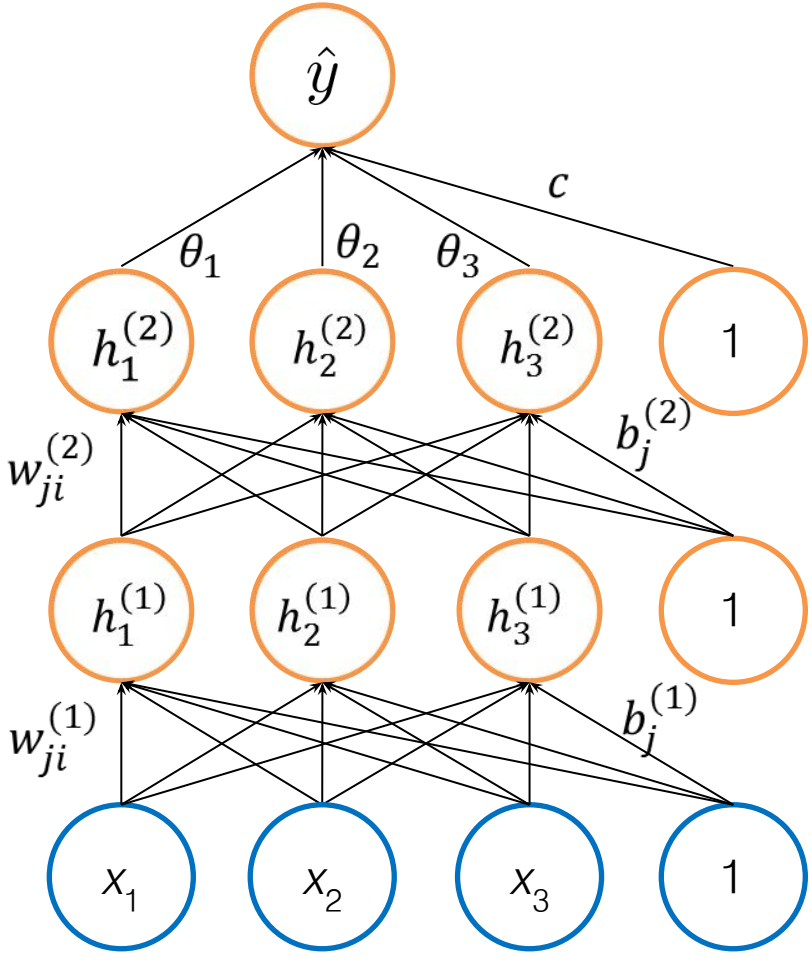
Multilayer neural network

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

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

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

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



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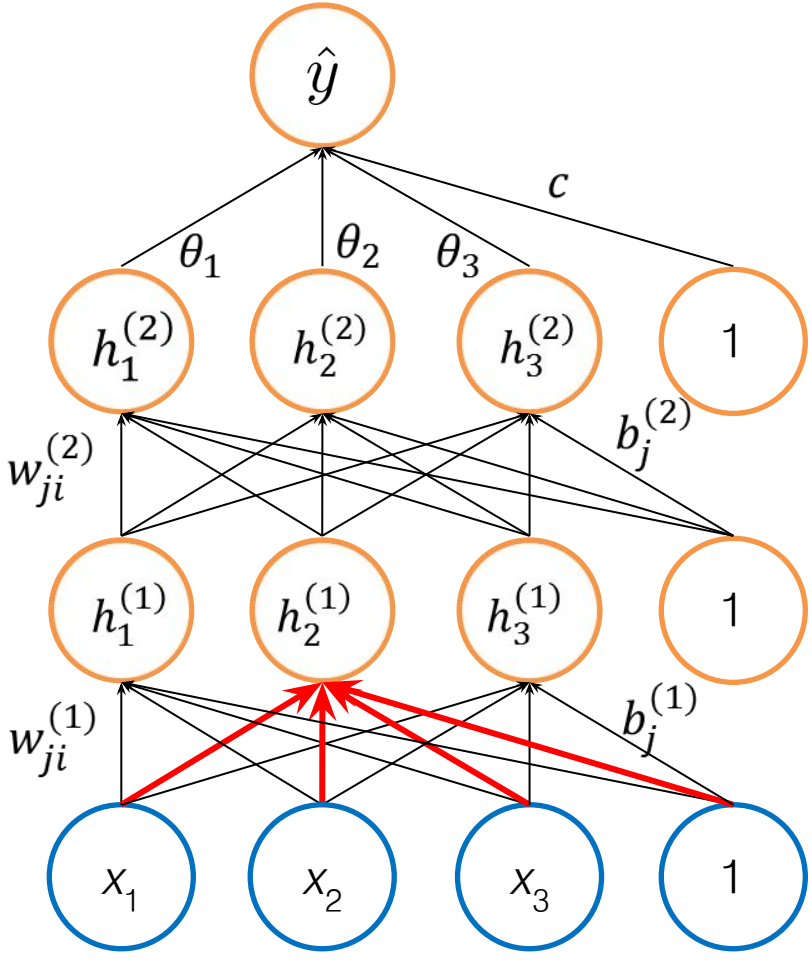

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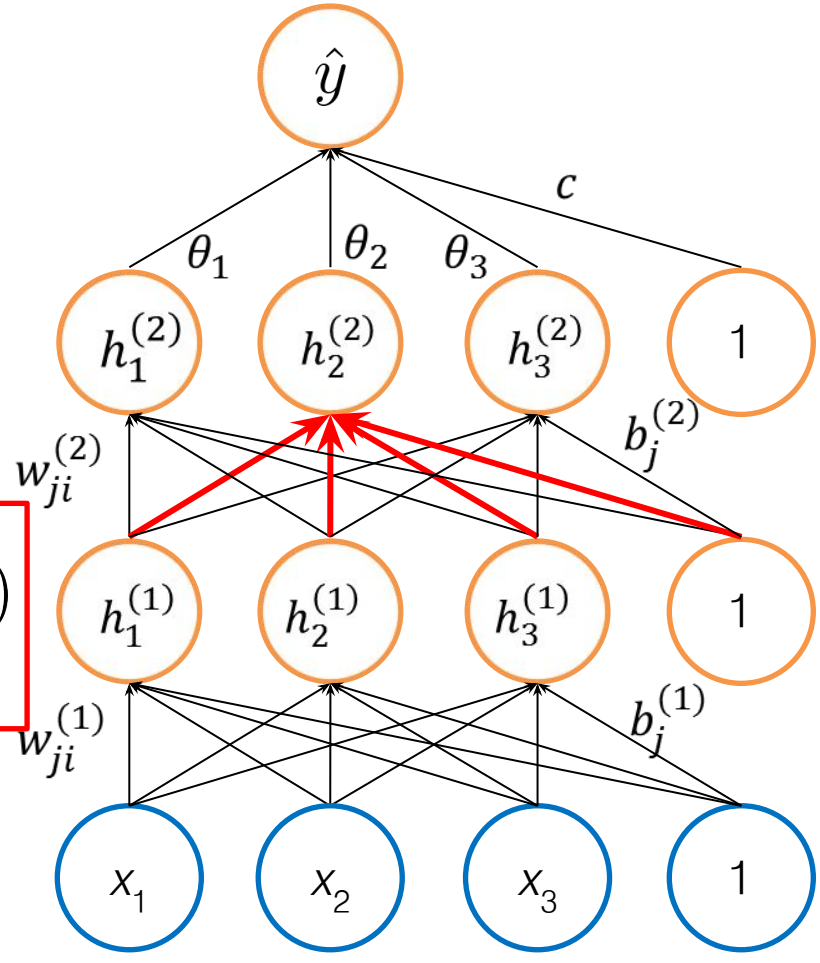


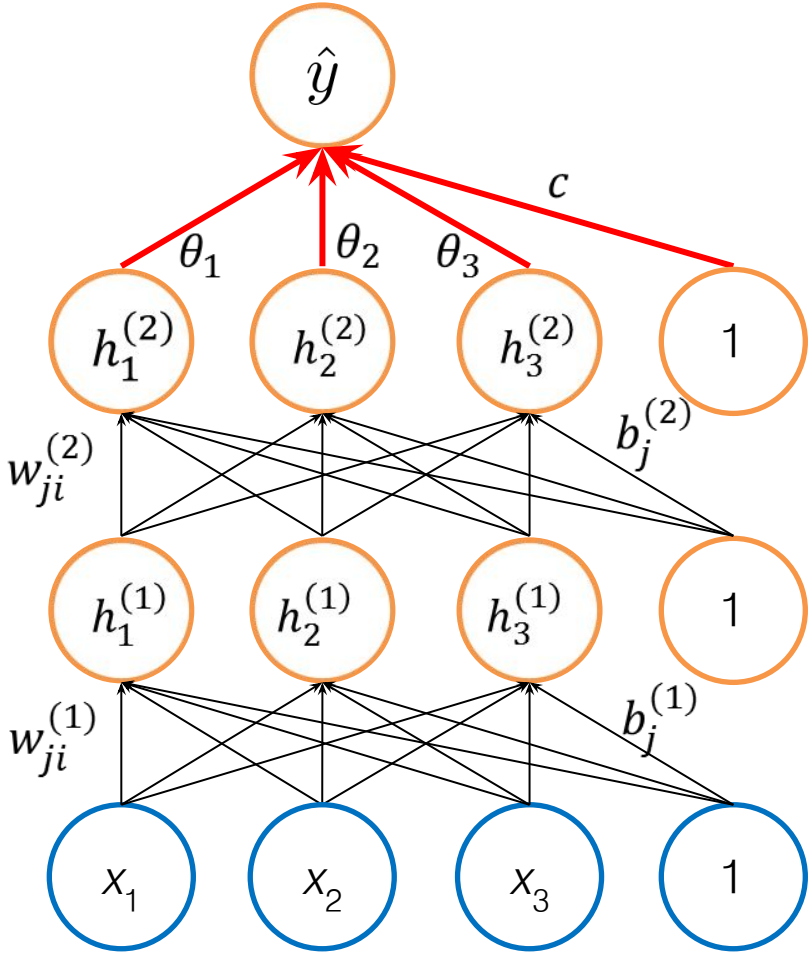
Multilayer neural network

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

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

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

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



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

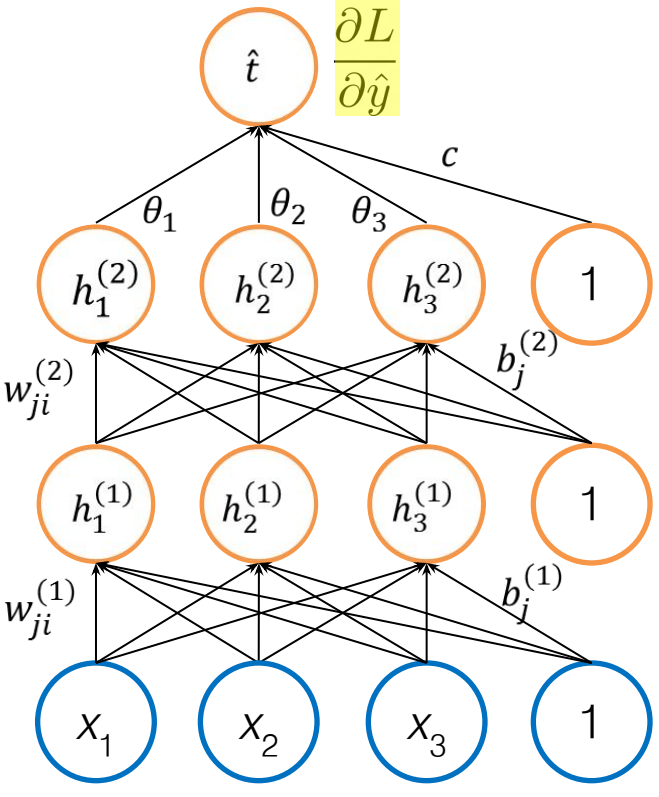
$$\frac{\partial L}{\partial \hat{y}} = 2(\hat{y} - y)$$

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

$$h_j^{(2)} = f(\sum_i w_{ji}^{(2)} h_i^{(i)} + b_j^{(2)}), \forall j$$

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

$$L = (\hat{y} - y)^2$$



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

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

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

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

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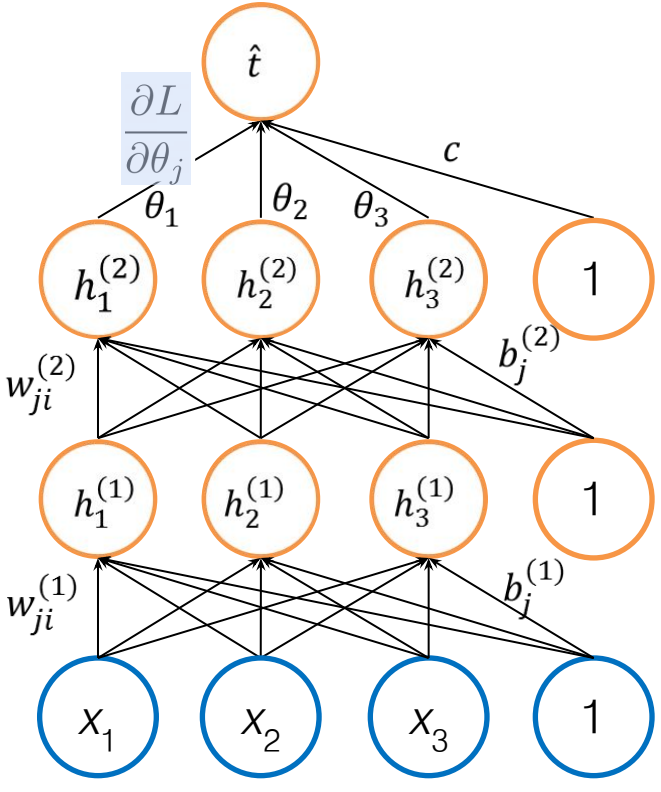

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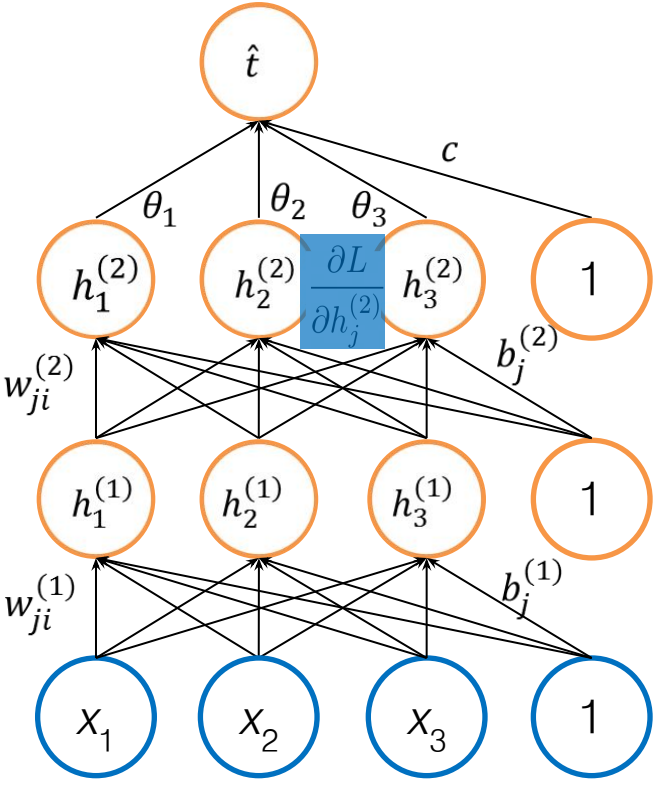

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$$\frac{\partial L}{\partial w_{ji}^{(2)}} = \frac{\partial h_j^{(2)}}{\partial w_{ji}^{(2)}}\frac{\partial L}{\partial h_j^{(2)}} = f'(z_j^{(2)})h_i^{(1)}\frac{\partial L}{\partial h_j^{(2)}}$$

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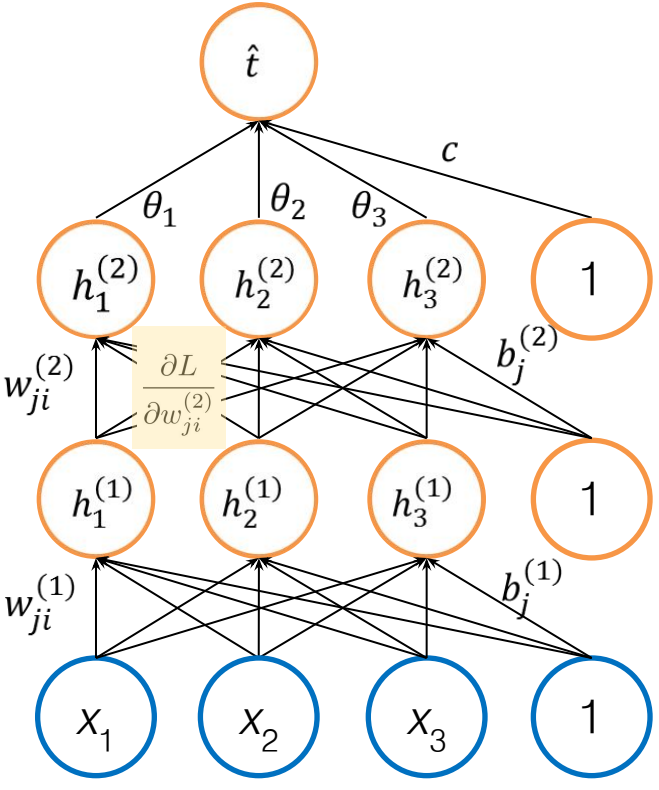

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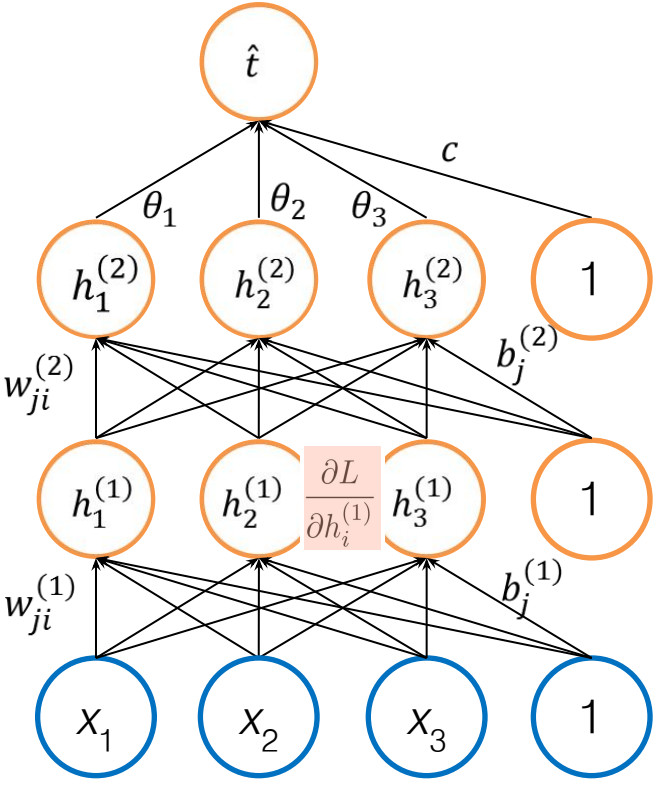

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$$\frac{\partial L}{\partial w_{ik}^{(1)}} = \frac{\partial h_i^{(1)}}{\partial w_{ik}^{(1)}}\frac{\partial L}{\partial h_i^{(1)}} = f'(z_i^{(1)})x_k\frac{\partial L}{\partial h_i^{(1)}}$$

where

$$z_j^{(2)} = \sum_i h_i^{(1)}w_{ji}^{(2)} + b_j^{(2)}$$

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

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

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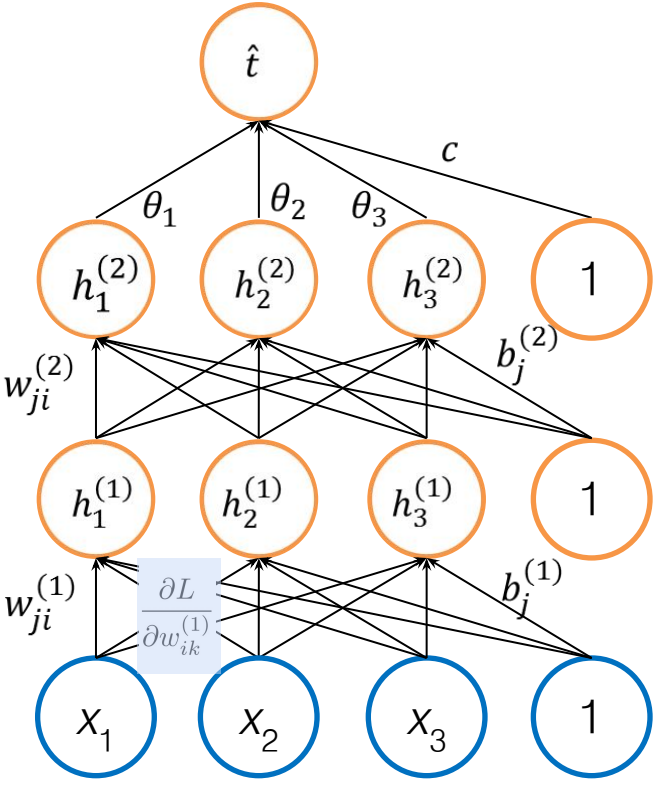


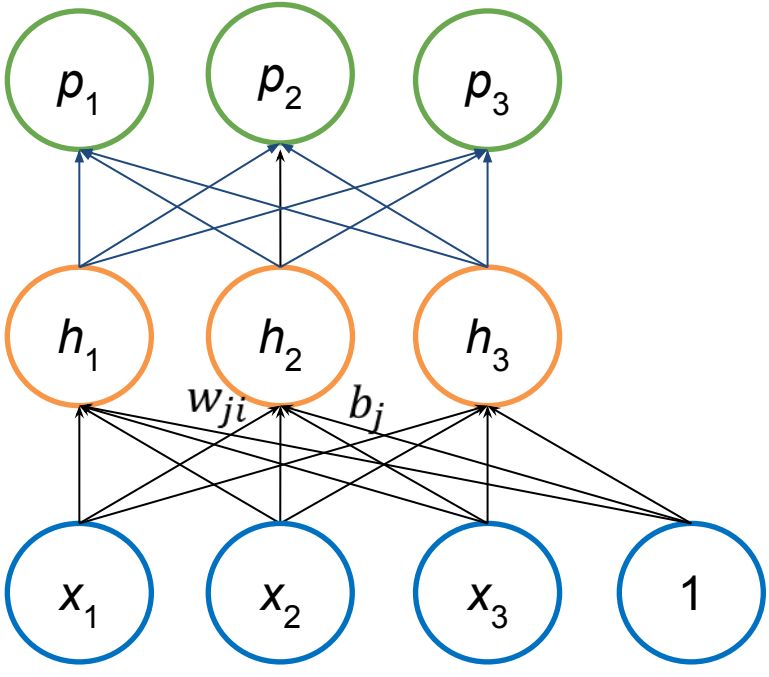
Backpropagation: examples
(NN with 1-hidden layer for classification)

Forward Propagation

- **Example: a network with 1 hidden layer**
  - Input: $\mathbf{x}$
  - Output: $\mathbf{p}$
  - Target: $\mathbf{y}$
  - Loss function: cross entropy $-\sum_i y_i \log p_i$

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

Output $p_i = \frac{e^{h_i}}{\sum_j e^{h_j}}$



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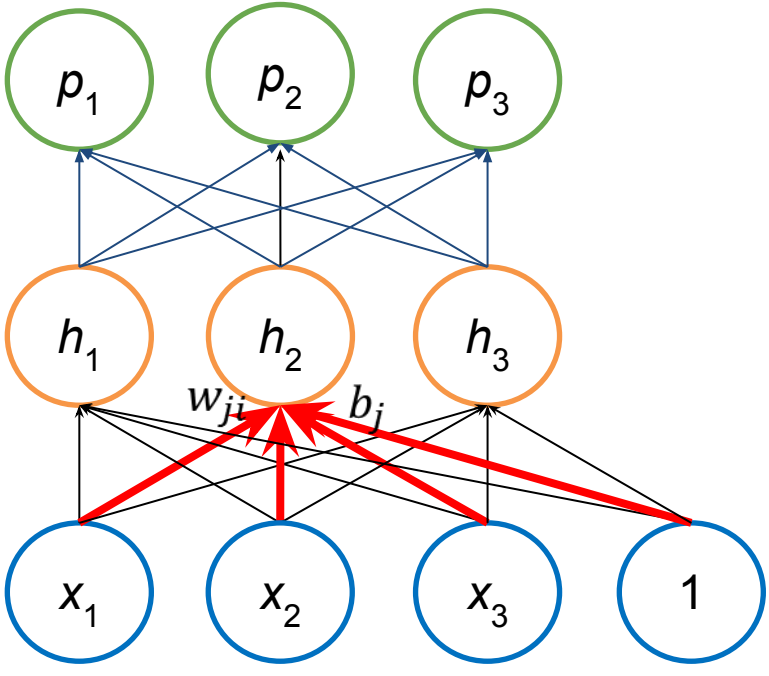

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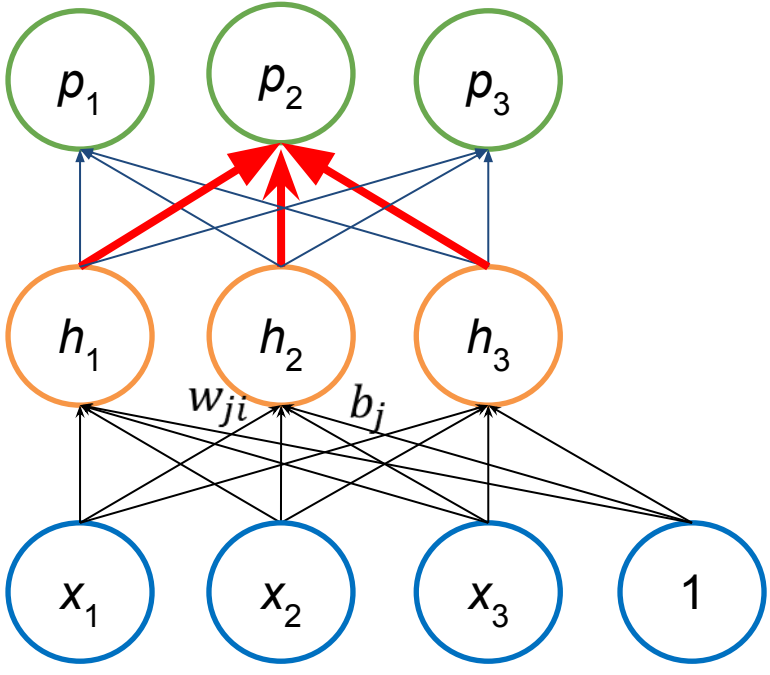


Backpropagation

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

$$L = -\sum_i y_i \log p_i = -\sum_i y_i \log \frac{e^{h_i}}{\sum_k e^{h_k}}$$

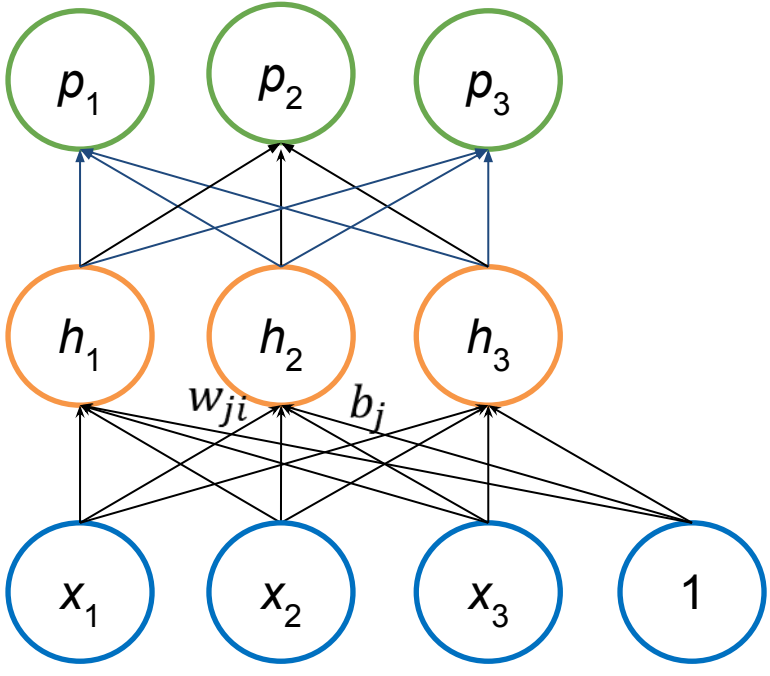
$$= -\sum_i y_i h_i + (\sum_i y_i) \log(\sum_k e^{h_k})$$

$$= \log(\sum_k e^{h_k}) - \sum_k y_k h_k$$

$$\frac{\partial L}{\partial h_j} = \frac{e^{h_j}}{\sum_k e^{h_k}} - y_j = p_j - y_j$$

$$\frac{\partial L}{\partial w_{ji}} = \frac{\partial h_j}{\partial w_{ji}} \frac{\partial L}{\partial h_j} = f' x_i \frac{\partial L}{\partial h_j}$$

where $f' = f'(\sum_i w_{ji} x_i + b_j)$



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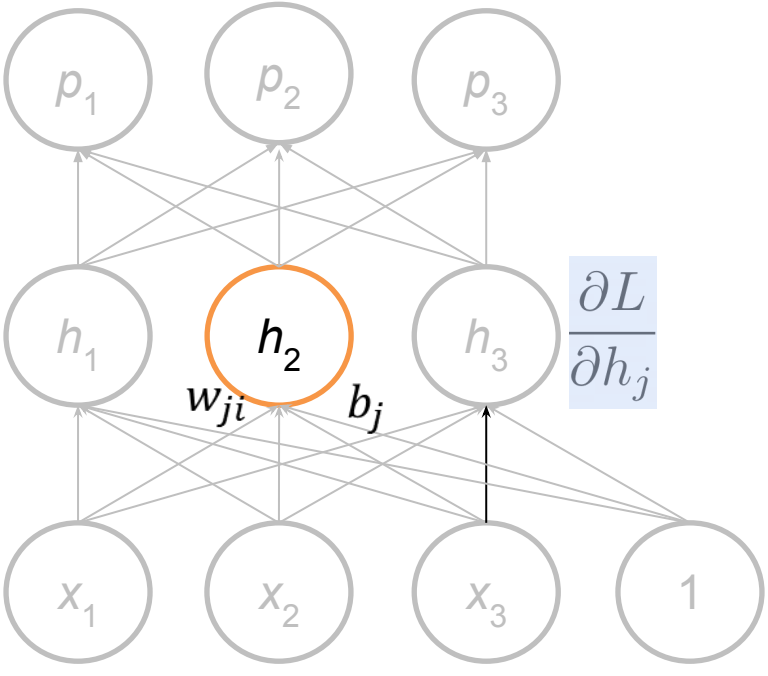
$$\frac{\partial L}{\partial h_j} = \frac{e^{h_j}}{\sum_k e^{h_k}} - y_j = p_j - y_j$$



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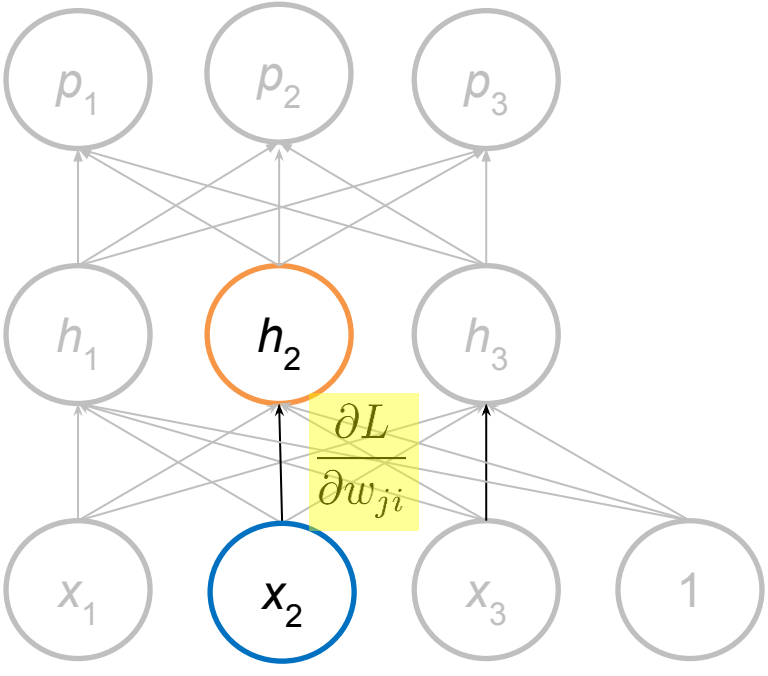


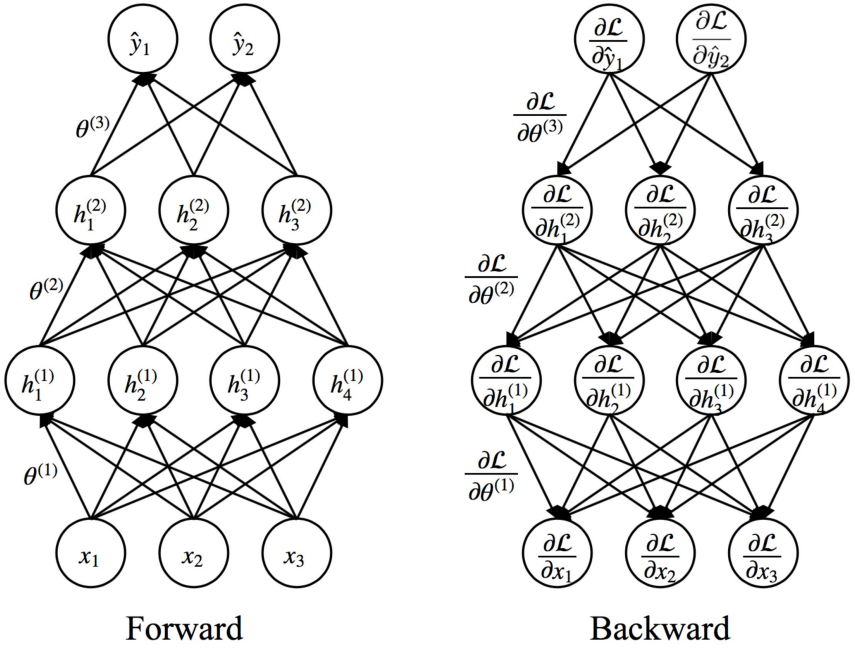
Deep Neural Networks

- Construction is straightforward: recursively stacking the blocks of layers

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

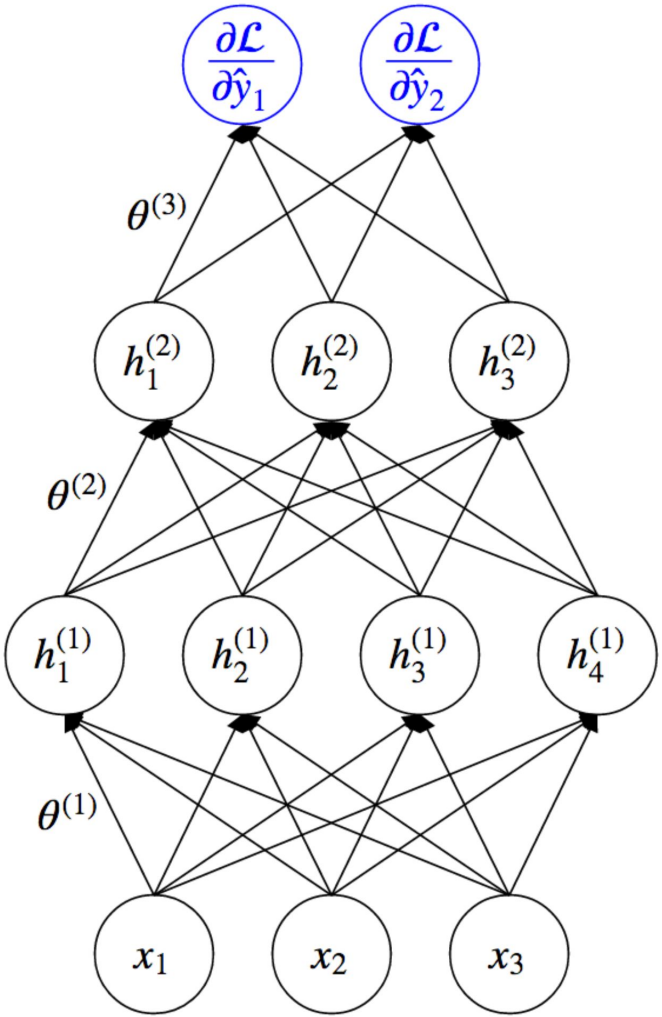
Backpropagation for deep neural nets

- 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**



Slide credit: Junhyuk Oh, Jacob Abernethy

Backpropagation (for deep neural nets)



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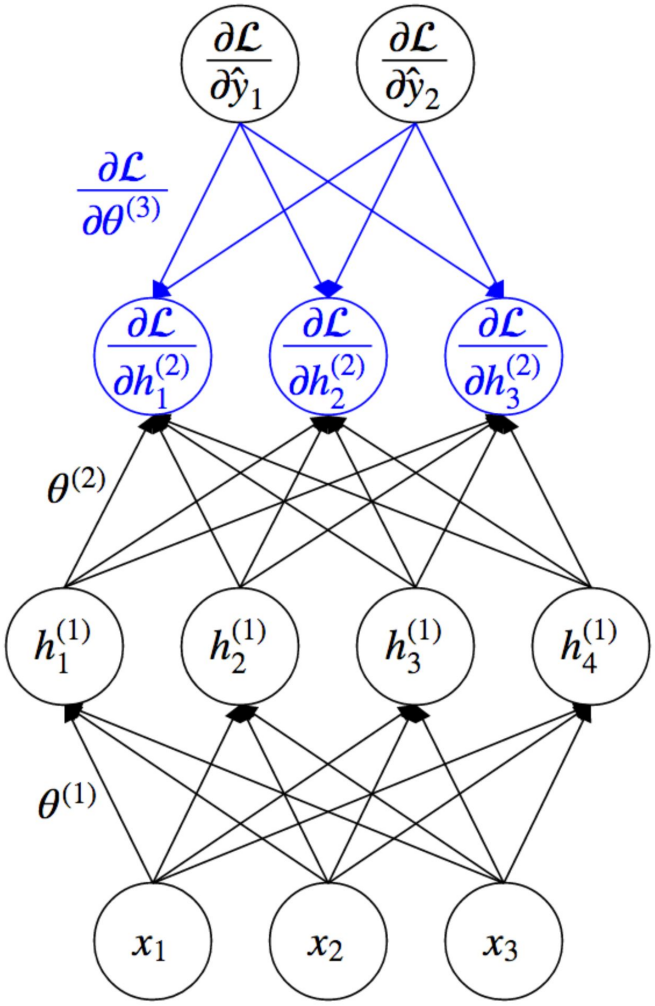
Backpropagation (for deep neural nets)



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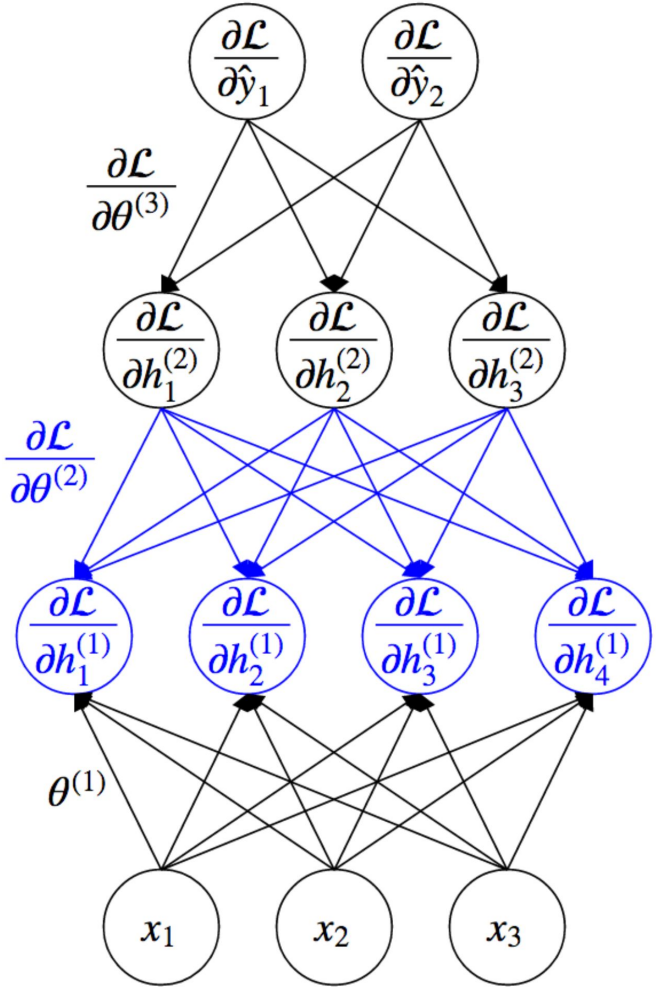
Backpropagation (for deep neural nets)



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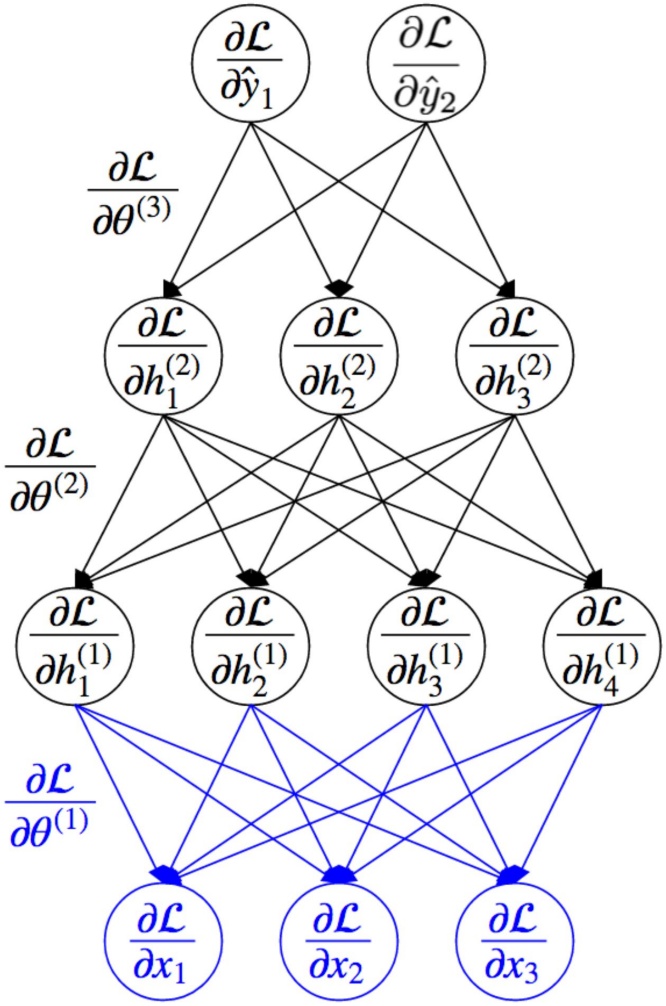


Slide credit: Junhyuk Oh, Jacob Abernethy

Back-Propagation Algorithm

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

$$\nabla_{\mathbf{W}} \mathcal{L} = \nabla_{\mathbf{h}} \mathcal{L} \nabla_{\mathbf{W}} \mathbf{h}$$
$$\nabla_{\mathbf{x}} \mathcal{L} = \nabla_{\mathbf{h}} \mathcal{L} \nabla_{\mathbf{x}} \mathbf{h}$$

Slide credit: Junhyuk Oh, Jacob Abernethy

Practice: Linear

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

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

$$\nabla_{\mathbf{b}} \mathcal{L} = \nabla_{\mathbf{h}} \mathcal{L}$$

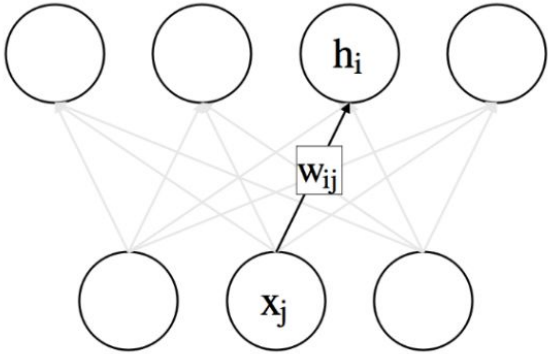
- Gradient w.r.t. inputs

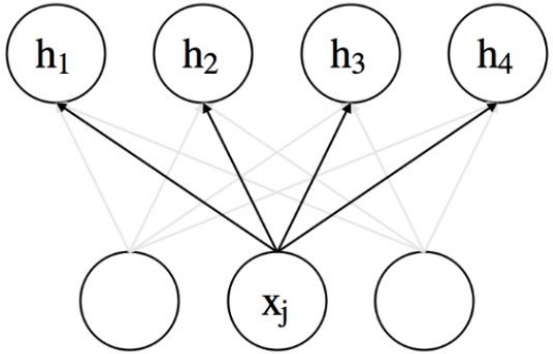
$$\frac{\partial \mathcal{L}}{\partial x_j} = \sum_i \frac{\partial \mathcal{L}}{\partial h_i}\frac{\partial h_i}{\partial x_j} = \sum_i \frac{\partial \mathcal{L}}{\partial h_i} w_{ij} \iff \nabla_{\mathbf{x}} \mathcal{L} = \mathbf{W}^\top \nabla_{\mathbf{h}} \mathcal{L}$$

$$Y = W \cdot X$$

$$\frac{\partial \mathcal{L}}{\partial W} = \frac{\partial \mathcal{L}}{\partial Y} X^\top$$

$$\frac{\partial \mathcal{L}}{\partial X} = W^\top \frac{\partial \mathcal{L}}{\partial Y}$$





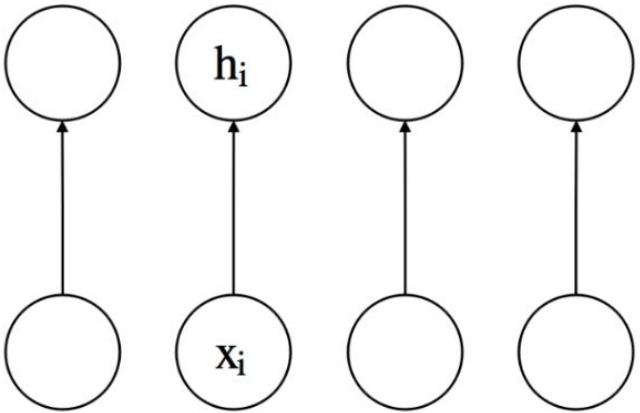
Note: In the lecture, we use column vector notation. However, PyTorch / NumPy typically uses row vector notation (please also see the note in the HW4).

Practice: Non-Linear Activation (Sigmoid)

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

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

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



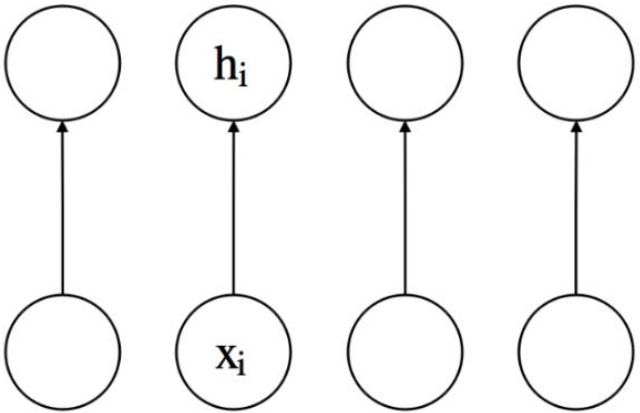
Slide credit: Junhyuk Oh, Jacob Abernethy

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

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

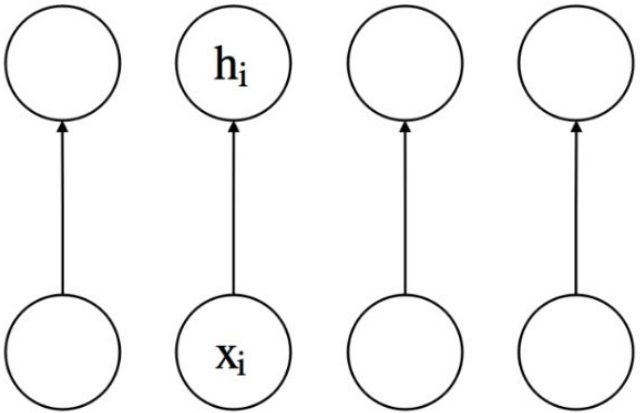
$$\nabla_{\mathbf{x}}\mathcal{L} = \nabla_{\mathbf{h}}\mathcal{L} \odot (\mathbf{1} - \mathbf{h} \odot \mathbf{h})$$



Practice: Non-Linear Activation (relu)

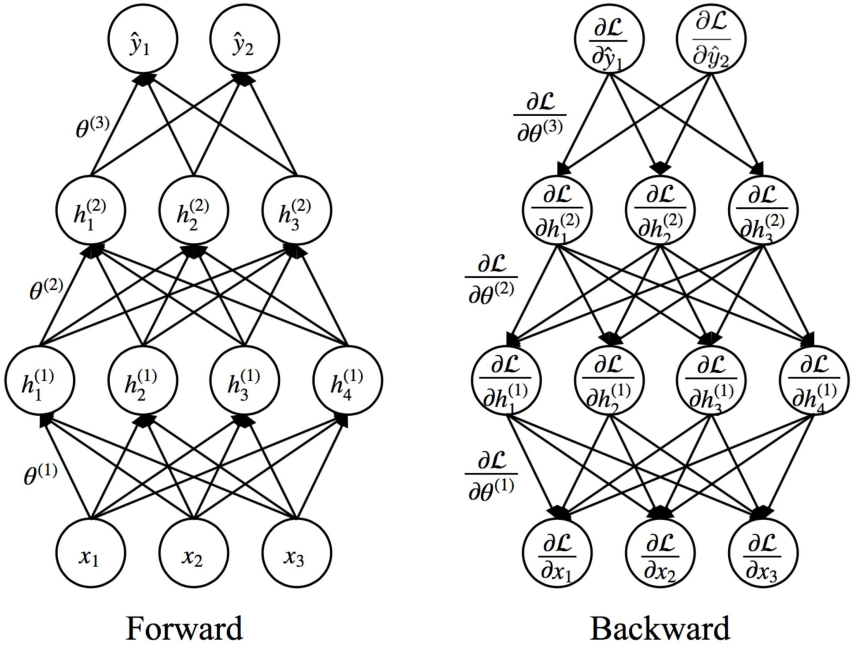
- Forward: $h_i = \text{relu}(x_i) = \max(x_i, 0) \iff \mathbf{h} = \text{relu}(\mathbf{x})$
- Gradient w.r.t inputs

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



Backpropagation for deep neural nets

- 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**



Slide credit: Junhyuk Oh, Jacob Abernethy

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)

End of lecture Quiz

https://forms.gle/Y7vxojrpPwzBrCB5A