EECS 545: Machine Learning

Lecture 11. Neural Networks and Deep Learning

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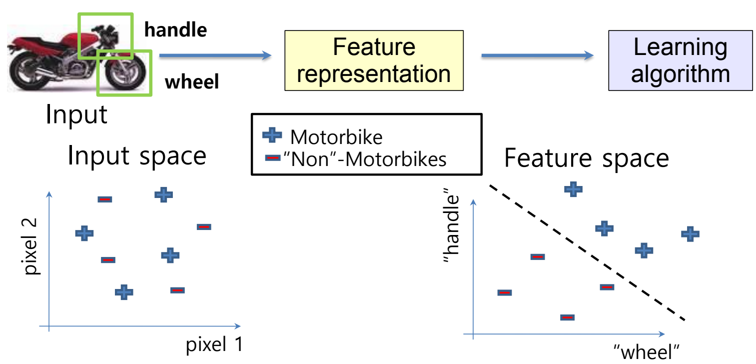
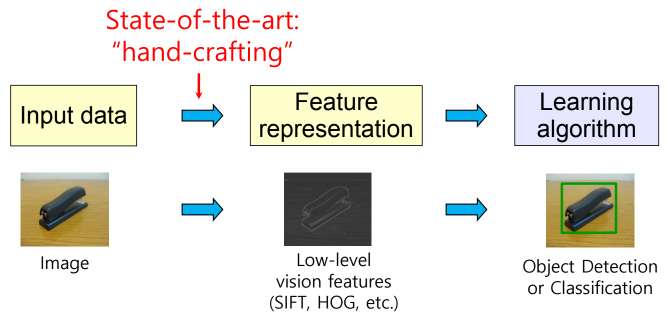
Representing Data

- 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 **<u>automatically</u>**?

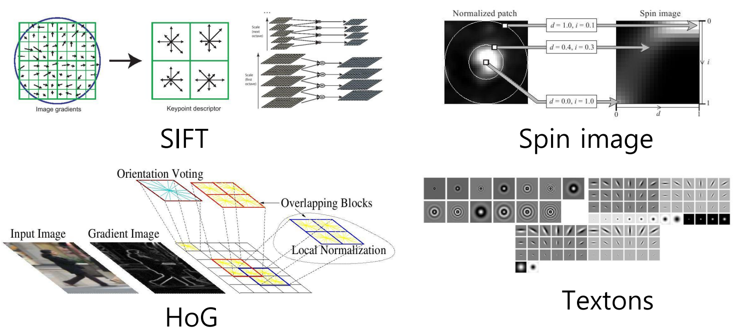
Feature representations



How is computer perception done?



Computer Vision Features



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

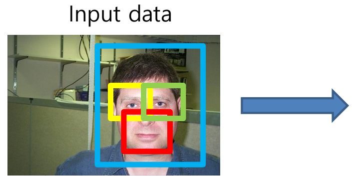
Learning Feature Representations

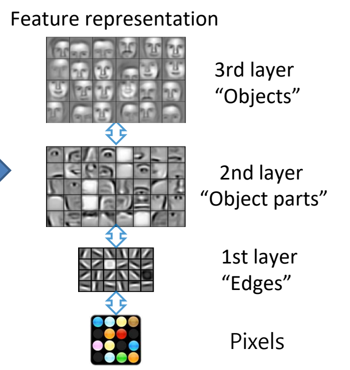
- Key idea of **Deep Learning**:
  - Learn <u>multiple levels</u> of representation of increasing complexity/abstraction.
  - The representations can be learned in both **supervised** and/or **unsupervised** settings.
  - These features can be used for downstream tasks.

Example: Learning Feature Hierarchy

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

Input data





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

Taxonomy of machine learning methods

Supervised

Shallow

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

Deep

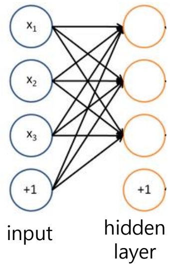
- Deep Neural Network
- Convolutional Neural Network*
- Recurrent Neural Network*
- Variational Autoencoder*
- Generative Adversarial Network
- Transformers*
- Diffusion Models*

Unsupervised

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

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

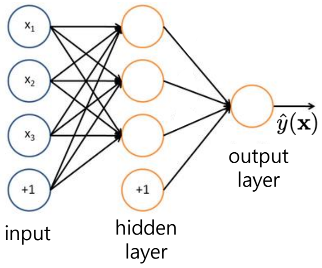


But we don't have to decide ahead of time what variables these logistic regressions are trying to predict!

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

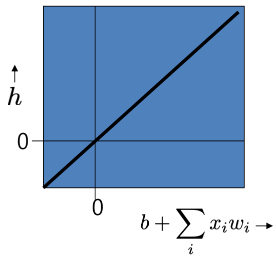
Types of Neurons: Linear Neurons

- 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



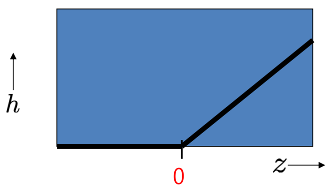
Slide Credit: Geoff Hinton

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.

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

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



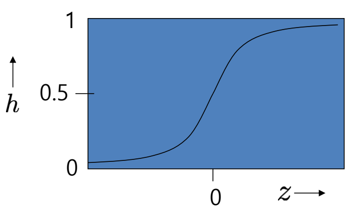
Slide Credit: Geoff Hinton

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

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

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



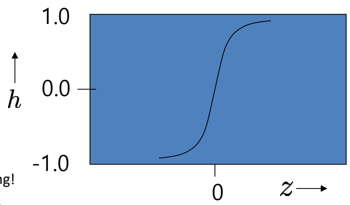
Slide Credit: Geoff Hinton

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

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

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



Note: tanh and sigmoid is equivalent after shifting and scaling!

$\sigma(z) = \frac{1}{2} + \frac{1}{2}\tanh\left(\frac{z}{2}\right)$ or $\tanh(z) = 2\sigma(2z) - 1$

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

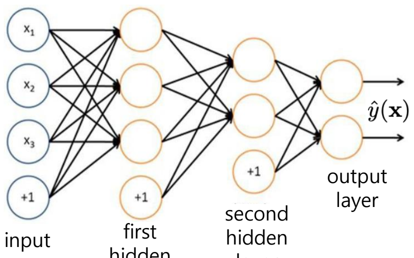
$$h_j = \frac{e^{z_j}}{\sum_k e^{z_k}}$$

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

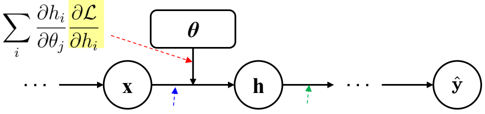
- Recall: Deep Neural Network represents a complex function with nested, composite functions (represented by layer-wise operation and nonlinearity, etc.)
- Q. How can we compute the gradient of the complex function?
- A. Backpropagation:
  - Computing gradient via **chain rule** for compositional function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

Backpropagation

- 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)

$$\frac{\partial \mathcal{L}}{\partial \theta_j} = \sum_i \frac{\partial h_i}{\partial \theta_j} \frac{\partial \mathcal{L}}{\partial h_i}$$



$$\frac{\partial \mathcal{L}}{\partial x_k} = \sum_i \frac{\partial h_i}{\partial x_k} \frac{\partial \mathcal{L}}{\partial h_i} \qquad \nabla_{\mathbf{h}} \mathcal{L} = \left[\frac{\partial \mathcal{L}}{\partial h_1}, \cdots, \frac{\partial \mathcal{L}}{\partial h_N}\right]^T$$

"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
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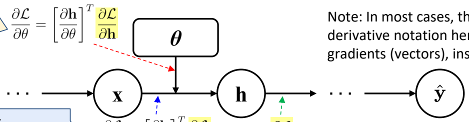
same as $\frac{\partial \mathcal{L}}{\partial \theta_j} = \sum_i \frac{\partial h_i}{\partial \theta_j} \frac{\partial \mathcal{L}}{\partial h_i}$

$$\frac{\partial \mathcal{L}}{\partial \theta} = \left[\frac{\partial \mathbf{h}}{\partial \theta}\right]^T \frac{\partial \mathcal{L}}{\partial \mathbf{h}}$$

Note: In most cases, the short-hand partial derivative notation here is Jacobian (matrices) or gradients (vectors), instead of scalars.



same as $\frac{\partial \mathcal{L}}{\partial x_k} = \sum_i \frac{\partial h_i}{\partial x_k} \frac{\partial \mathcal{L}}{\partial h_i}$

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

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

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

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

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

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

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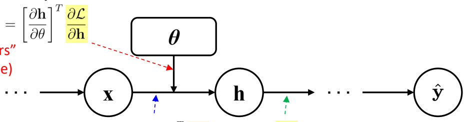
Backpropagation

- 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, but we can derive a recursion rule for the gradient.

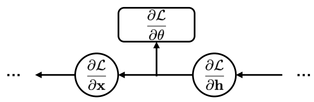
$$\frac{\partial \mathcal{L}}{\partial \theta} = \left[\frac{\partial \mathbf{h}}{\partial \theta}\right]^T \frac{\partial \mathcal{L}}{\partial \mathbf{h}}$$

"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) $\frac{\partial \mathcal{L}}{\partial \mathbf{x}} = \left[\frac{\partial \mathbf{h}}{\partial \mathbf{x}}\right]^T \frac{\partial \mathcal{L}}{\partial \mathbf{h}}$ $\quad \frac{\partial \mathcal{L}}{\partial \mathbf{h}}$ "gradient w.r.t. hidden layer above" (given)

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



$$\frac{\partial \mathcal{L}}{\partial \theta} = \underbrace{\left[\frac{\partial \mathbf{h}}{\partial \theta}\right]^T}_{\text{easy}} \underbrace{\frac{\partial \mathcal{L}}{\partial \mathbf{h}}}_{\text{given}} \qquad \frac{\partial \mathcal{L}}{\partial \mathbf{x}} = \underbrace{\left[\frac{\partial \mathbf{h}}{\partial \mathbf{x}}\right]^T}_{\text{easy}} \underbrace{\frac{\partial \mathcal{L}}{\partial \mathbf{h}}}_{\text{given}}$$

- Repeat recursion backwards (until reaching the bottom layers).

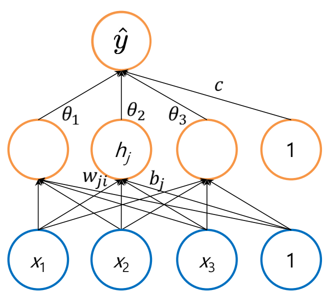
Backpropagation: Examples (NN with 1-hidden layer for regression)

Forward Propagation

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

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

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



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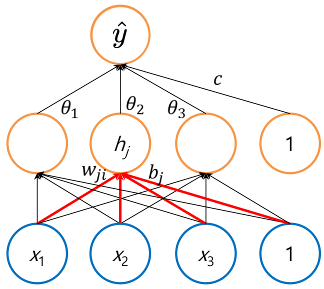

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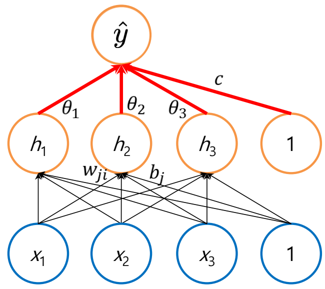

Backpropagation

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

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

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

- Goal: Compute gradient w.r.t. parameters $\{W, b, \theta, c\}$
- 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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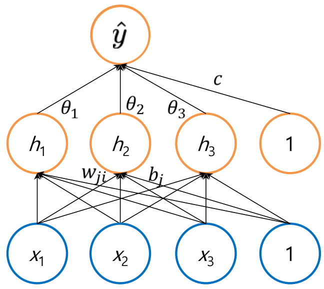
$$\frac{\partial \mathcal{L}}{\partial w_{ji}} = \frac{\partial h_j}{\partial w_{ji}}\frac{\partial \mathcal{L}}{\partial h_j} = f' x_i \frac{\partial \mathcal{L}}{\partial h_j}$$

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



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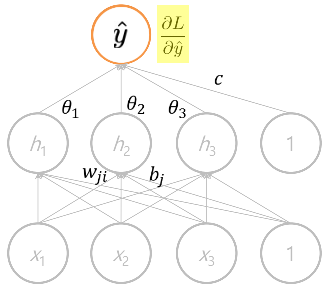

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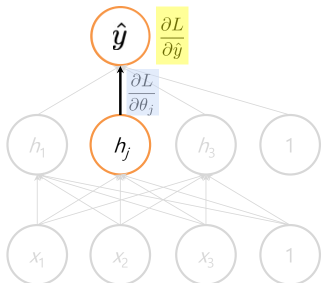

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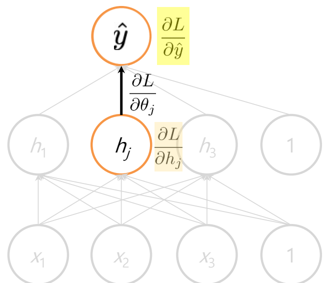

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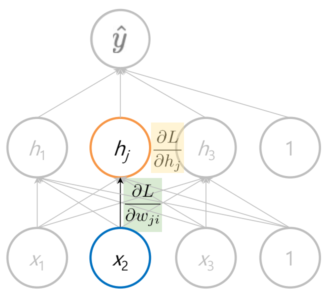


Backpropagation: examples
(NN with 2-hidden layer for regression)

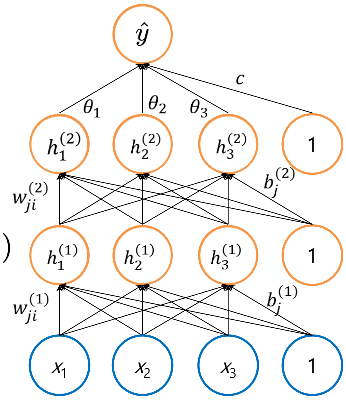
Multilayer neural network

- **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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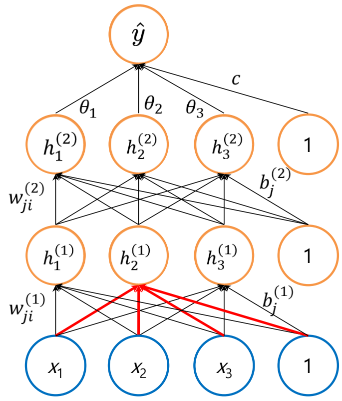

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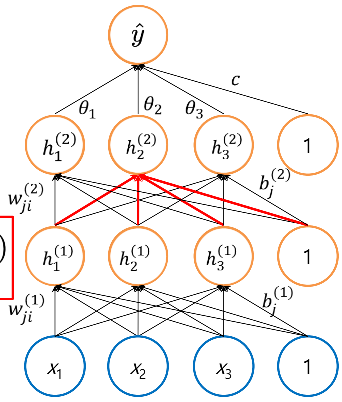

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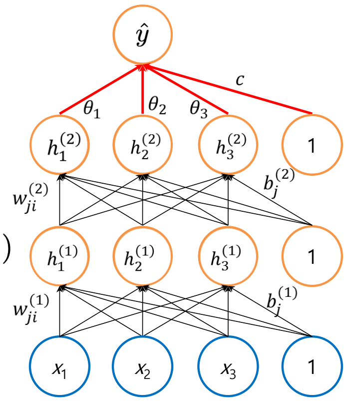
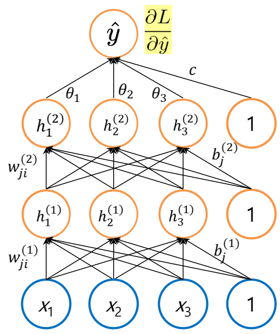
$\boxed{\text{Output } \hat{y} = \sum_j \theta_j h_j^{(2)} + c}$



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

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

$$h_j^{(1)} = f(\sum_i w_{ji}^{(1)} x_i + b_j^{(1)}), \forall j$$
$$h_j^{(2)} = f(\sum_i w_{ji}^{(2)} h_i^{(1)} + b_j^{(2)}), \forall j$$
$$\hat{y} = \sum_j \theta_j h_j^{(2)} + c$$
$$\mathcal{L} = (\hat{y}-y)^2$$



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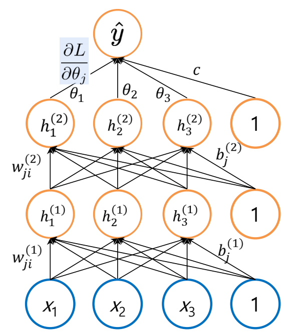

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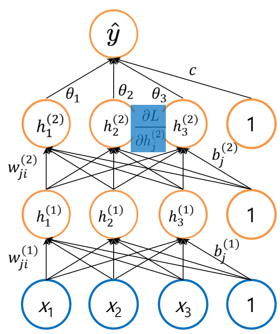

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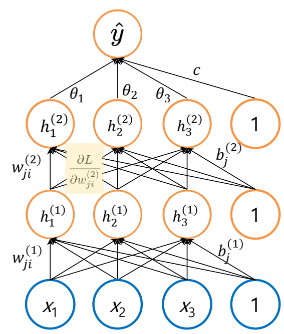

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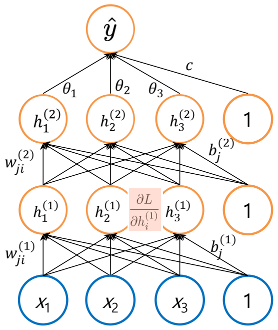

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$$\frac{\partial \mathcal{L}}{\partial w_{ik}^{(1)}} = \frac{\partial h_i^{(1)}}{\partial w_{ik}^{(1)}}\frac{\partial \mathcal{L}}{\partial h_i^{(1)}} = f'(z_i^{(1)})x_k\frac{\partial \mathcal{L}}{\partial h_i^{(1)}}$$

$$\text{where } z_j^{(2)} = \sum_i h_i^{(1)}w_{ji}^{(2)} + b_j^{(2)}$$
$$z_i^{(1)} = \sum_k x_k w_{ik}^{(1)} + b_i^{(1)}$$

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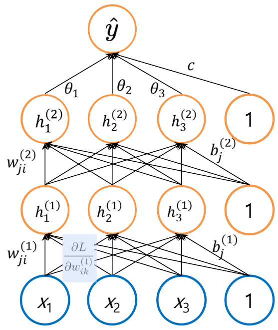


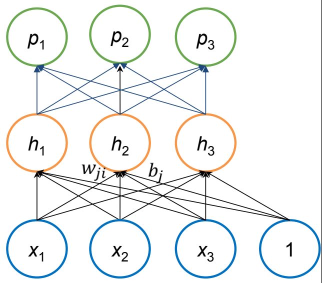
Backpropagation: examples (NN with 1-hidden layer for classification)

Forward Propagation

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

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

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



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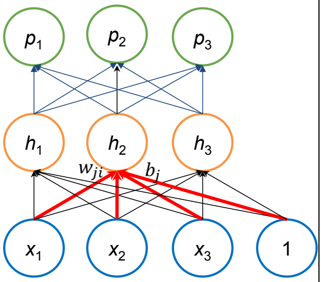

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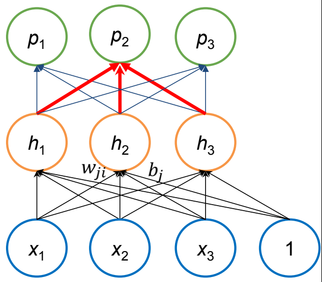


Backpropagation

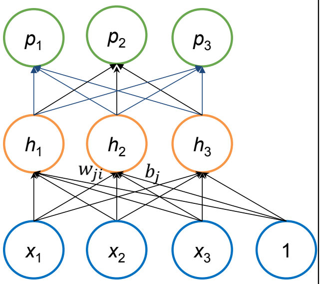
- **Example: a network with 1 hidden layer**
  - Goal: Compute Gradients w.r.t parameters $\{\boldsymbol{W}, \boldsymbol{b}\}$
  - Main Idea: Apply Chain Rule recursively

$$\mathcal{L} = -\sum_i y_i \log p_i = -\sum_i y_i \log \frac{e^{h_i}}{\sum_k e^{h_k}}$$
$$= -\sum_i y_i h_i + (\sum_i y_i)\log(\sum_k e^{h_k})$$
$$= \log(\sum_k e^{h_k}) - \sum_k y_k h_k$$

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

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

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



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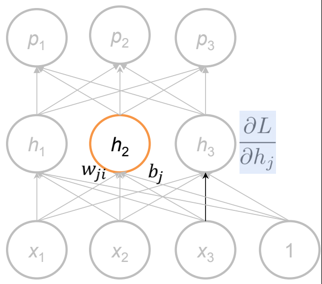

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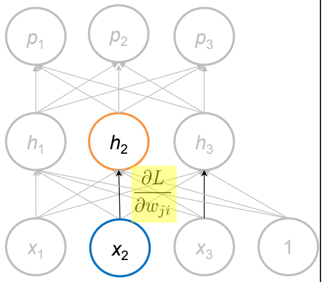
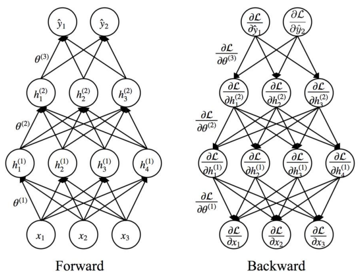


Deep Neural Networks

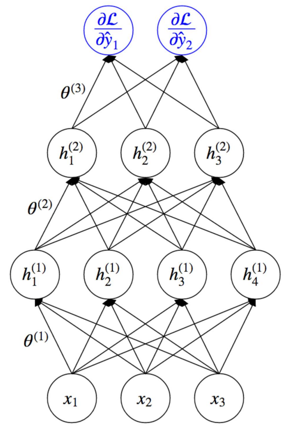
- Construction is straightforward: recursively stacking the blocks of layers
- Computing gradient is straightforward (via back propagation)
  - For general formula, see Bishop's book.

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**



Backpropagation (for deep neural nets)



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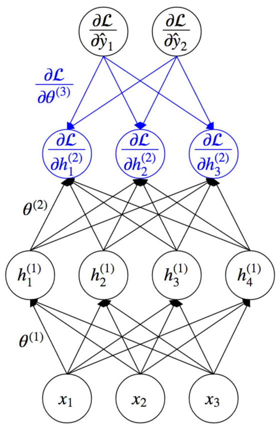

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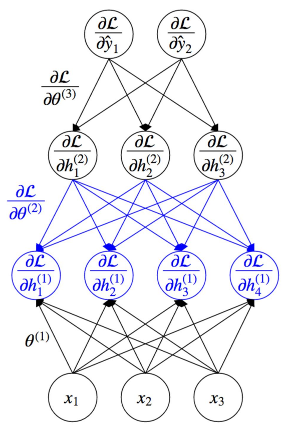
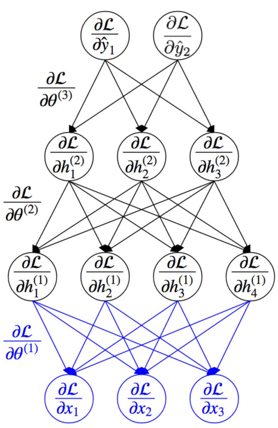


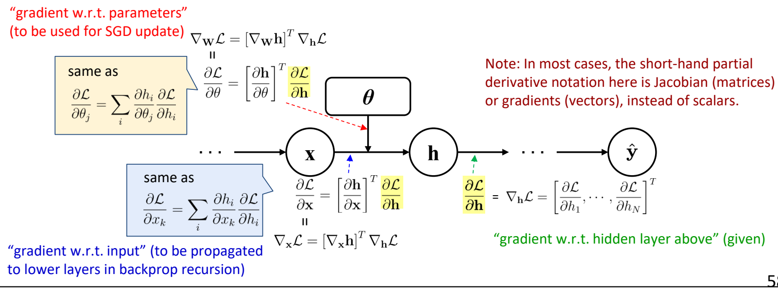
Backpropagation (for deep neural nets)



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 $\mathbf{W}$,
  - Assuming that $\nabla_{\mathbf{h}} \mathcal{L}$ is given, compute gradients using the **chain rule** as:

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



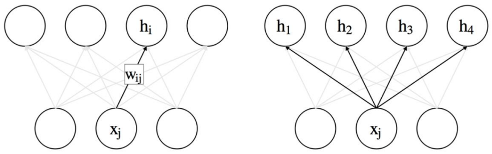
Practice: Linear

- 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

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



Note 1: In the lecture, we use **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**.

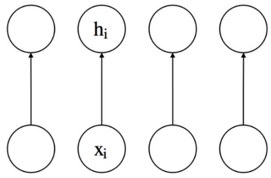
Note 2: In HW3 and HW4, we will ask you to do additional vectorization for backpropagation using multiple input examples (i.e., input/output of a layer can be represented as matrix, not a vector)

Practice: Non-Linear Activation (Sigmoid)

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

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

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

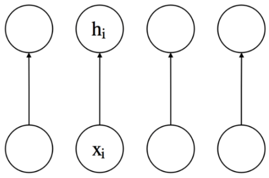


Practice: Non-Linear Activation (tanh)

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

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

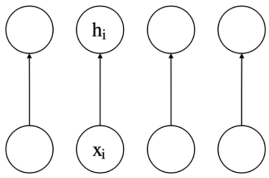
$$\nabla_{\mathbf{x}}\mathcal{L} = \nabla_{\mathbf{h}}\mathcal{L} \odot (1 - \mathbf{h} \odot \mathbf{h})$$



Practice: Non-Linear Activation (ReLU)

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

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



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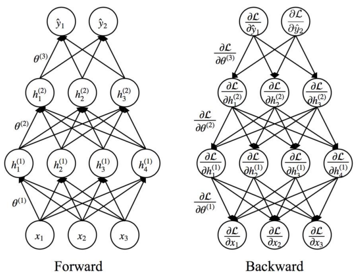

Problems with Back Propagation

- 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)