CS559 Machine Learning
Neural Networks

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Week 12

Outline

- Basics of neural network
- Implementation of Simple NN

Basics of Neural Networks

Some Reviews

- Last few lectures, we focused on **unsupervised learning** problems (e.g., density estimation, clustering etc), and we discussed the general algorithm and model for that (e.g., EM algorithm for latent variable model). We also show that the model can be represented and do inference using *Bayesian Network* which encodes conditional relations between different random variables.

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- Back to the **supervised learning** scenarios, but consider *non-linear* models on that.

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- Back to the **supervised learning** scenarios, but consider *non-linear* models on that.
- One way is to use *Neural Network* which presents *non-linear* transformation/mapping of the input.

Summary of supervised learning

$$\underbrace{\mathbf{w}^T\mathbf{x} + b}_{\text{score}}$$

	Classification	Regression
Predictor	sign	score
Relate to y	margin (score, y)	residual (score, y)
Loss	zero-one, logistic	squared, absolute deviation
Algorithm	GD	GD

Review: Optimization problem

Minimize Training Loss

$$\min_{\mathbf{w}\in\mathbb{R}^d} \mathsf{TrainLoss}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N} L(\mathbf{x}_n, y_n, \mathbf{w})$$

Review: Optimization problem

Gradient Descent (GD)

$$\mathbf{w} \leftarrow \mathbf{w} - \underbrace{\eta}_{\text{step size}} \underbrace{\nabla_{\mathbf{w}} \text{TrainLoss}(\mathbf{w})}_{\text{gradient}}$$

$\nabla_{\mathbf{w}}$TrainLoss denotes the gradient of the (average) total training loss with respect to $\mathbf{w}$

Review: Optimization problem

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Stochastic Gradient Descent (SGD)

For each $(x, y) \in D_{train}$

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla_{\mathbf{w}} \mathsf{L}(x, y, \mathbf{w})$$

$\nabla_{\mathbf{w}} L$ denotes the gradient of one example loss with respect to w

Notation clarification

- $\mathbf{w}, \mathbf{x}$: bold letters are usually vectors in dimension d
- w_i: the i-th element in vector $\mathbf{w}$
- $\mathbf{x}_n$: the n-th example in the training data set, its corresponding target value: y_n
- x_i: feature i in current example $\mathbf{x}$
- x_{ni}: feature i in the n-th example
- V, W: capital letters usually denote matrices.

What is Neural Network?

- Often associated with biological devices (brains), electronic devices, or network diagrams;
- But the best conceptualization for this presentation is none of these: think of a neural network as a mathematical function.

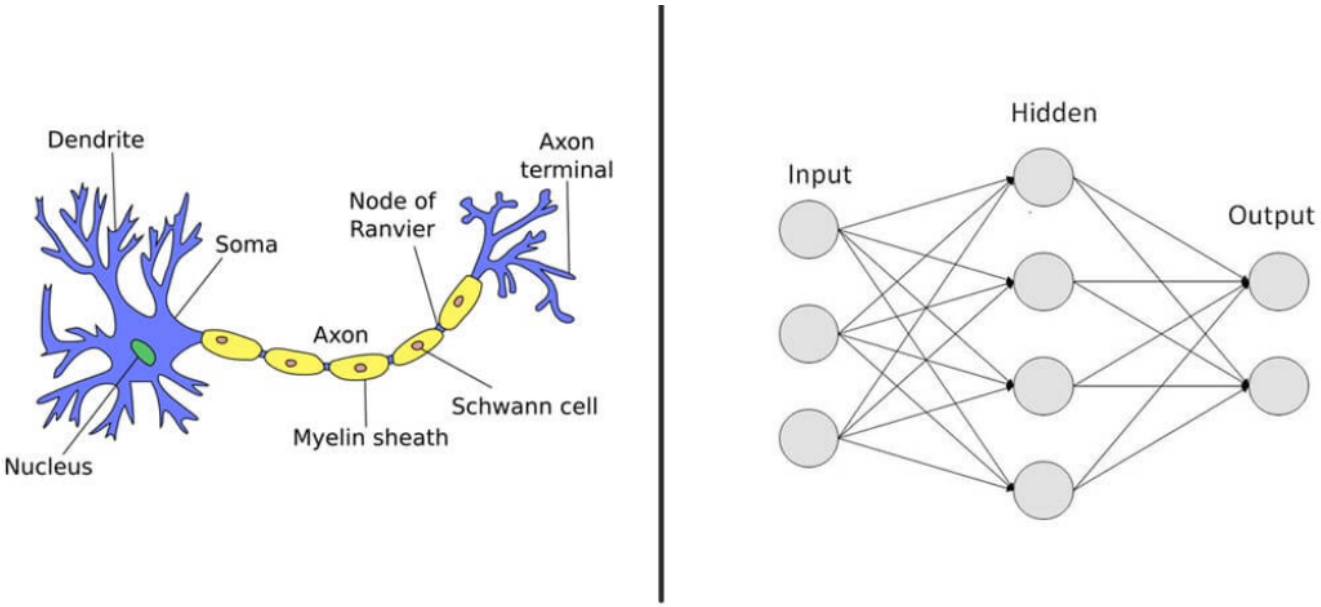


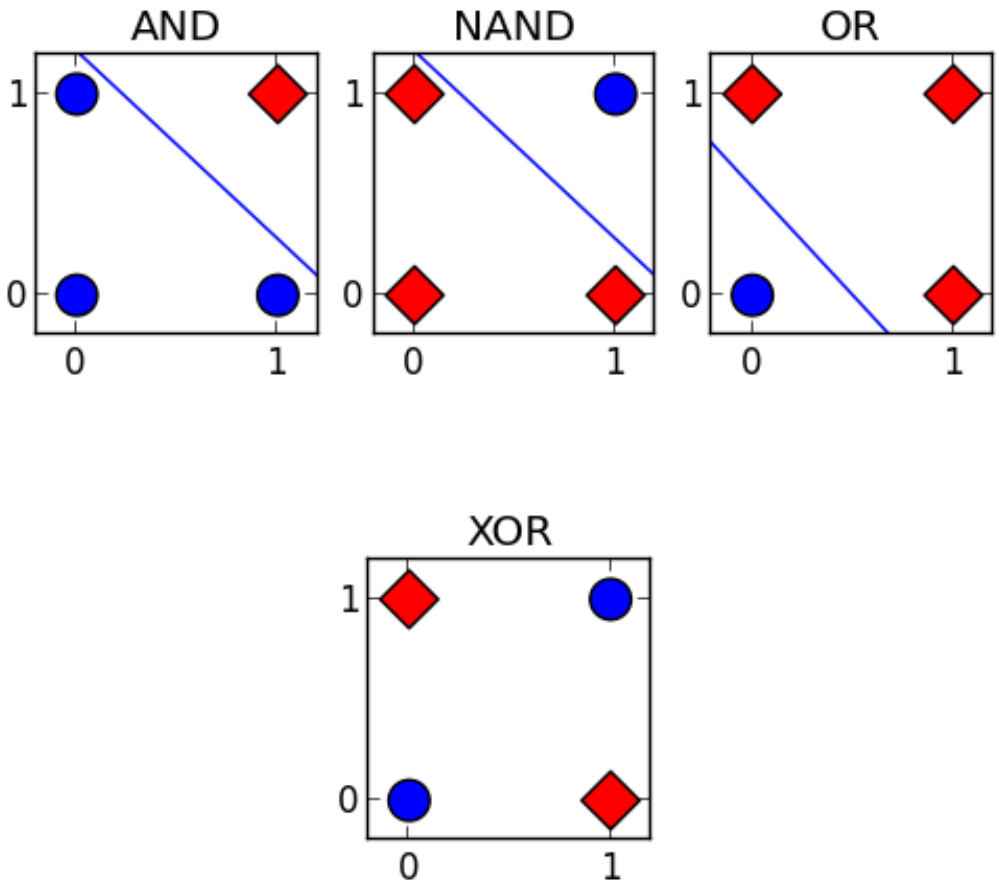
Figure: [Jacob Joseph]

The pros of Neural Network

- Successfully used on a variety of domains: computer vision, speech recognition, gaming etc.
- Can provide solutions to very complex and nonlinear problems;
- If provided with sufficient amount of data, can solve classification and detection problems accurately and easily
- Once trained, prediction is fast;

Motivation

- Perceptron: limitations;
- Feedforward networks and Backpropagation;

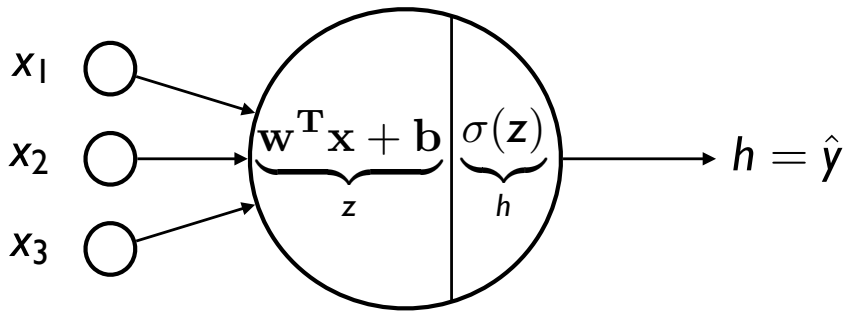


Motivation

- Allow to learn non linearly separable transformations from input to output;
- A single hidden layer allows to compute any input/output transformation;

No Hidden Units: Logistic Regression

- Sigmoid activation function:



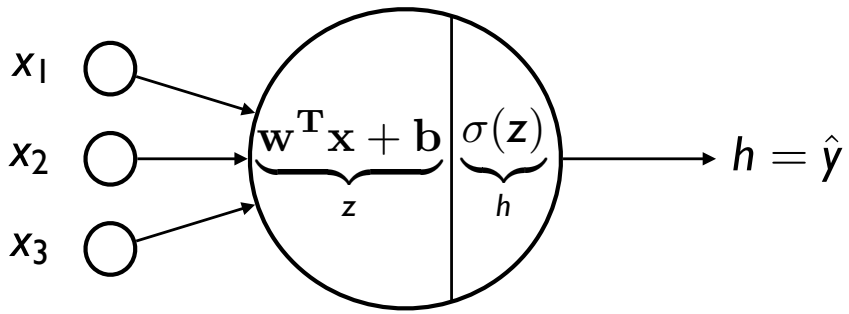
- Output score: sigmoid function $\hat{y} = \sigma(\mathbf{w}^T\mathbf{x} + b)$
- Recall sigmoid function:

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

Derivative:

No Hidden Units: Logistic Regression

- Sigmoid activation function:



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- Recall sigmoid function:

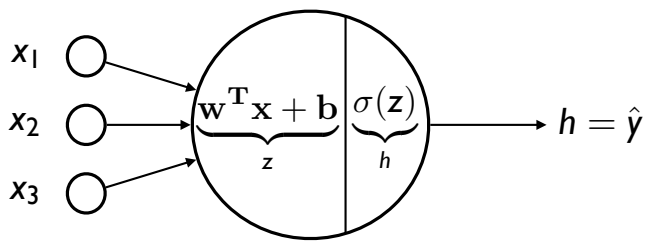
$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

Derivative:

$$\sigma'(z) = \sigma(z)(1 - \sigma(z))$$

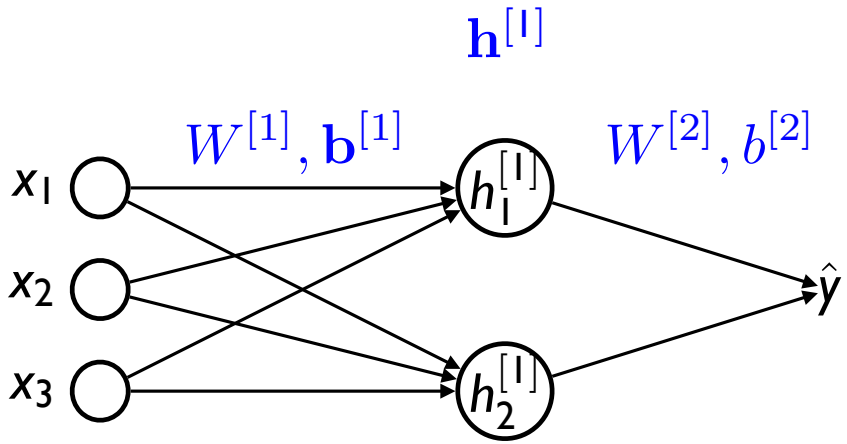
Learning Algorithm: No hidden units

- Logistic loss: $J(\mathbf{x}, y, \mathbf{w}) = -y \log(\hat{y}) - (1-y)\log(1-\hat{y})$
- $\hat{y} = \frac{1}{1+e^{-\mathbf{w}^T\mathbf{x}}} = \sigma(\mathbf{w}^T\mathbf{x})$
- $\frac{\partial \hat{y}}{\partial w_i} = \hat{y}(1-\hat{y})x_i$
- $\frac{\partial J}{\partial w_i} = \frac{\partial J}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial w_i} = (\hat{y}-y)x_i$
- Applying gradient descent (η is the learning rate):
  - Element (feature) operation: $w_i^{t+1} = w_i^t - \eta \frac{\partial J}{\partial w_i}$
  - Vector operation: $\mathbf{w}^{t+1} = \mathbf{w}^t - \eta \frac{\partial J}{\partial \mathbf{w}}$



Neural Networks: one hidden layer

- One hidden layer:



- Hidden layer representation

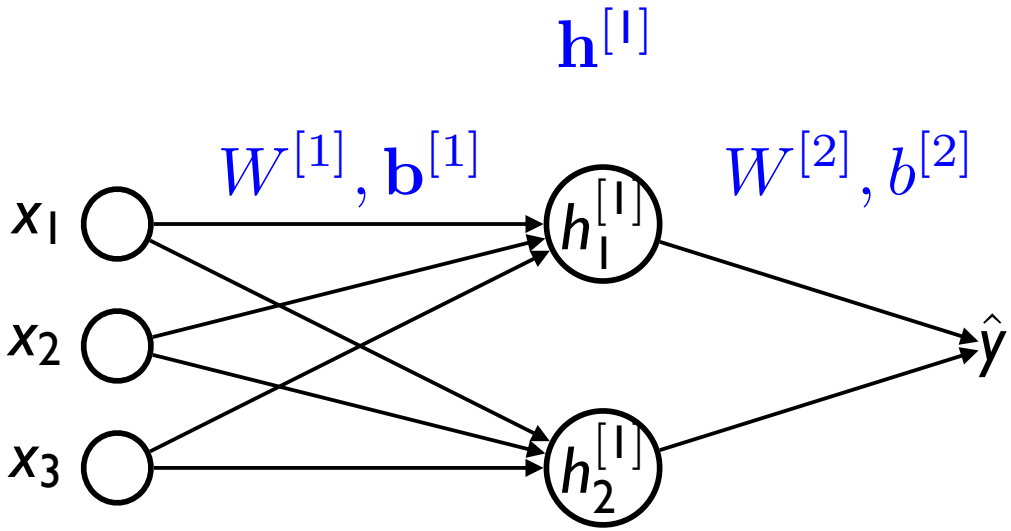
$$z_1^{[1]} = \mathbf{w}_1^{[1]T}\mathbf{x} + b_1^{[1]}, h_1^{[1]} = \sigma(z_1^{[1]})$$
$$z_2^{[1]} = \mathbf{w}_2^{[1]T}\mathbf{x} + b_2^{[1]}, h_2^{[1]} = \sigma(z_2^{[1]})$$

$\Rightarrow$

$$\mathbf{z}^{[1]} = \underbrace{W^{[1]}}_{2\times 3}\underbrace{\mathbf{x}}_{3\times 1} + \underbrace{\mathbf{b}^{[1]}}_{2\times 1}$$
$$\mathbf{h}^{[1]} = \sigma(\mathbf{z}^{[1]})$$

Neural Networks: one hidden layer

- One hidden layer:



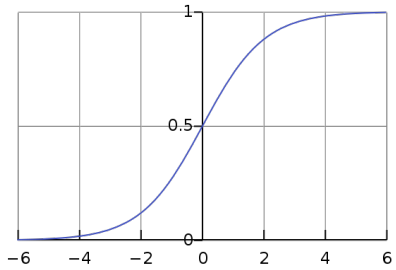
- Output layer

$$z^{[2]} = \underbrace{W^{[2]}}_{1\times 2}\underbrace{\mathbf{h}^{[1]}}_{2\times 1} + b^{[2]}$$

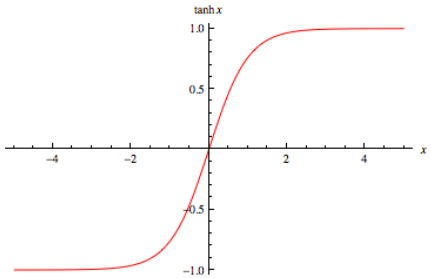
$$\hat{y} = \sigma(z^{[2]})$$

Activation Functions

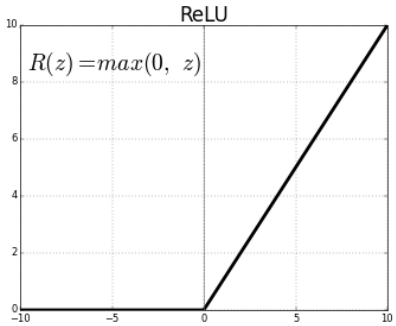
Sigmoid: $f(x) = \sigma(x) = \frac{1}{1+e^{-x}}$



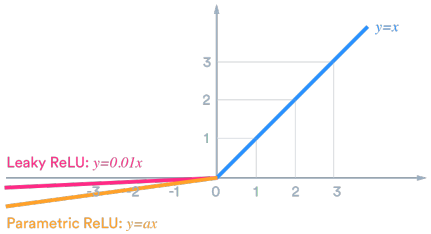
tanh: $f(x) = 2\sigma(2x) - 1$



ReLU: $f(x) = \max(0, x)$



Leaky ReLU: $f(x) = \max(\alpha x, x)$

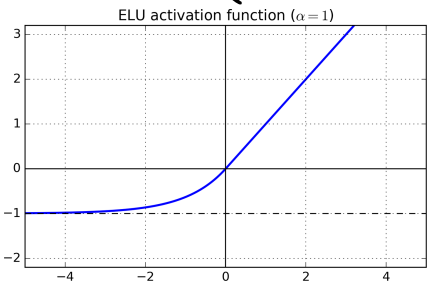


Maxout

$$\max(\mathbf{w}_1^T \mathbf{x} + b_1, \mathbf{w}_2^T \mathbf{x} + b_2)$$

ELU:

$$f(x) = \begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Neural Networks: one hidden layer

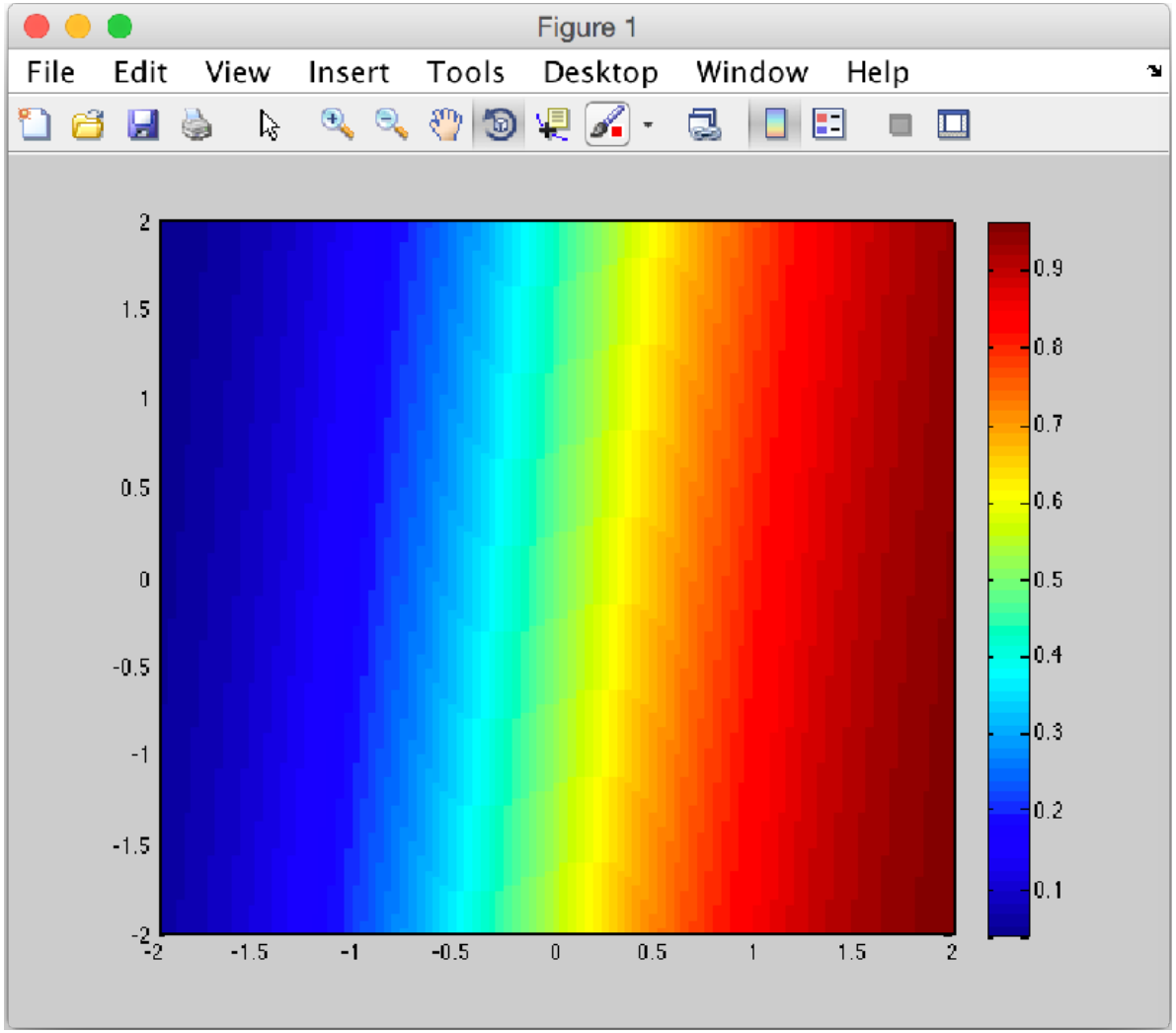
- Think of intermediate hidden units as learned features of a linear predictor.
- Feature learning: manually specified features:

$$\mathbf{x}$$

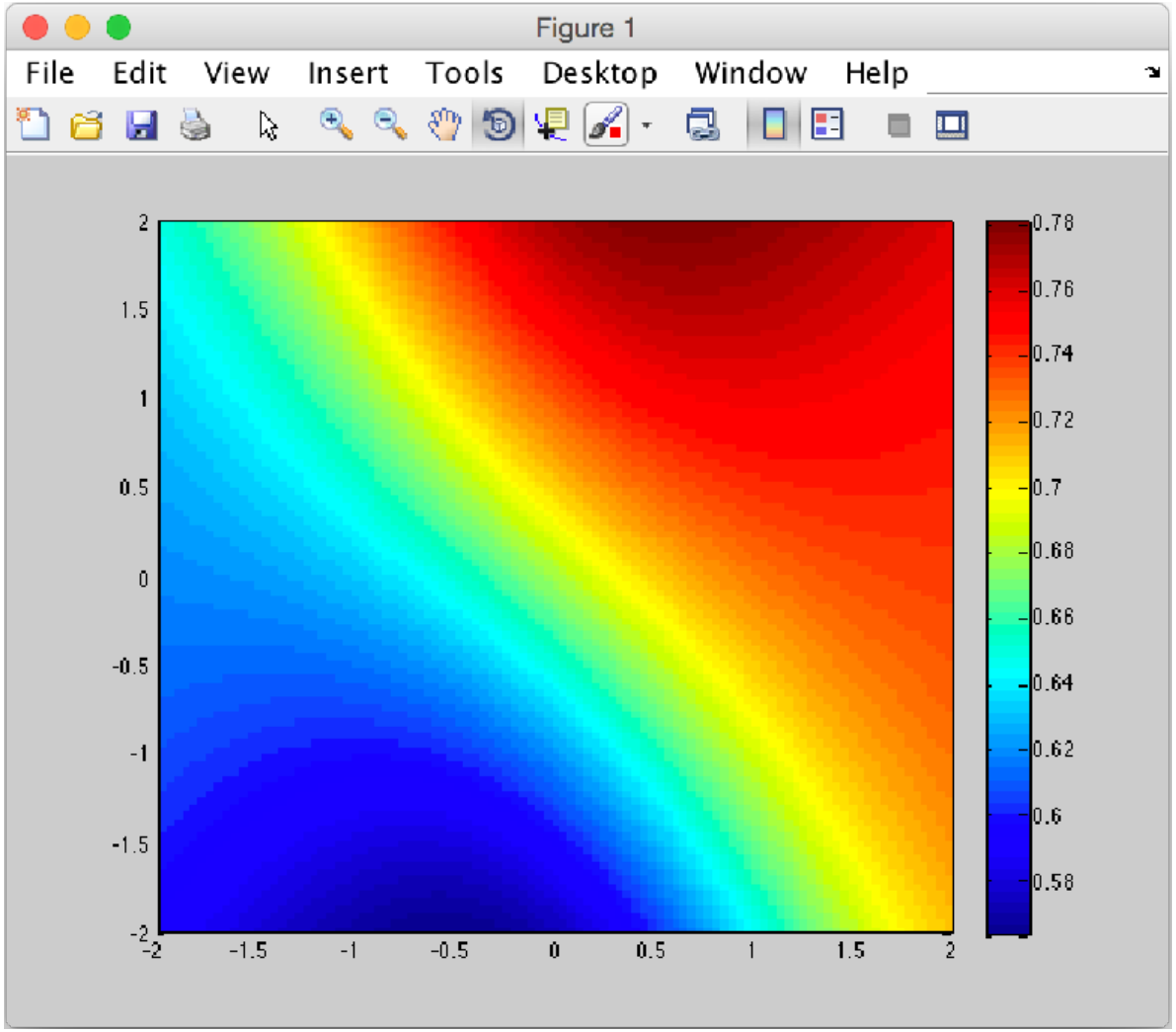
automatically learned features:

$$h(\mathbf{x}) = [h_1(\mathbf{x}), ..., h_k(\mathbf{x})]$$

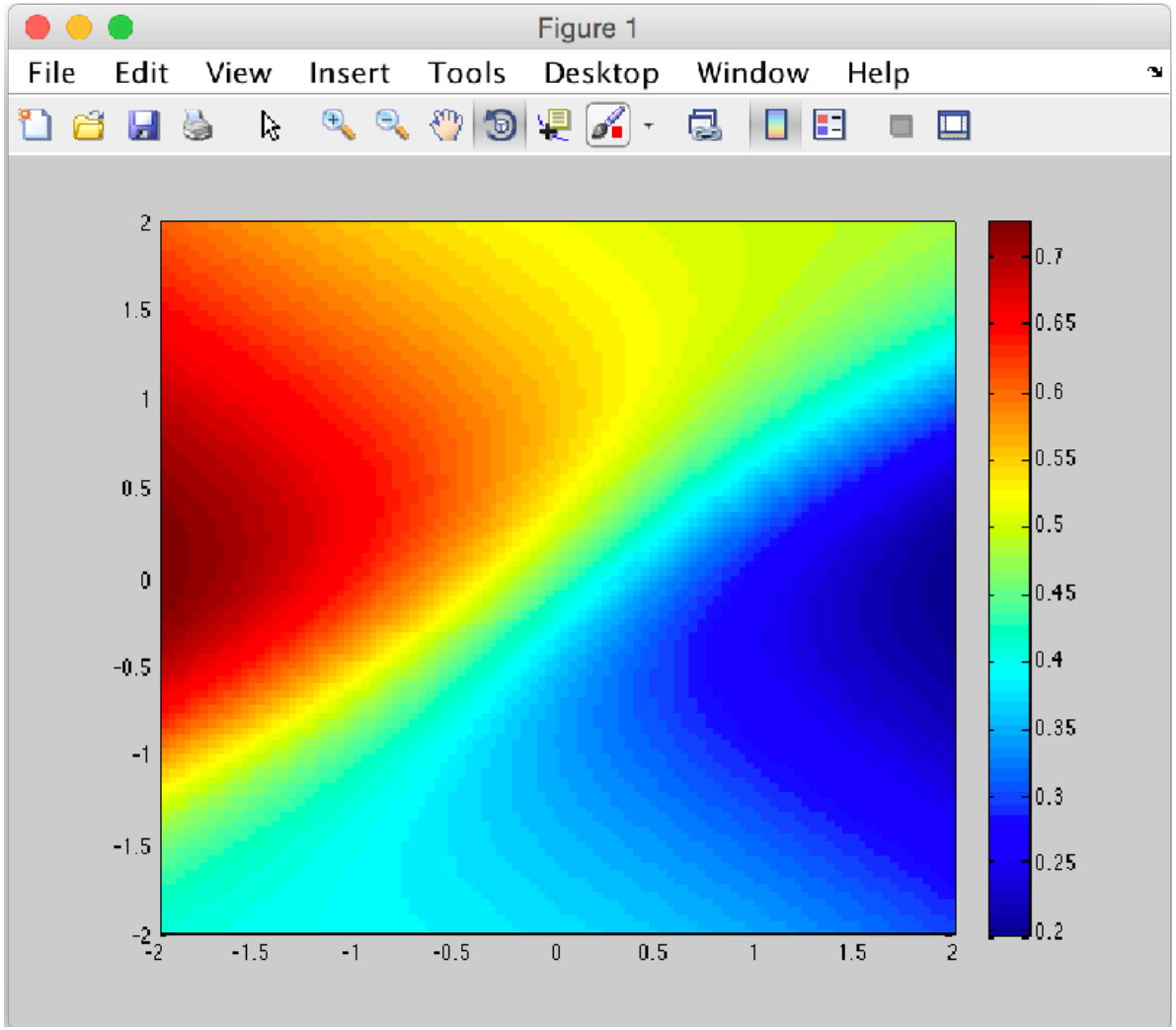
Decision Boundary: Logistic Regression



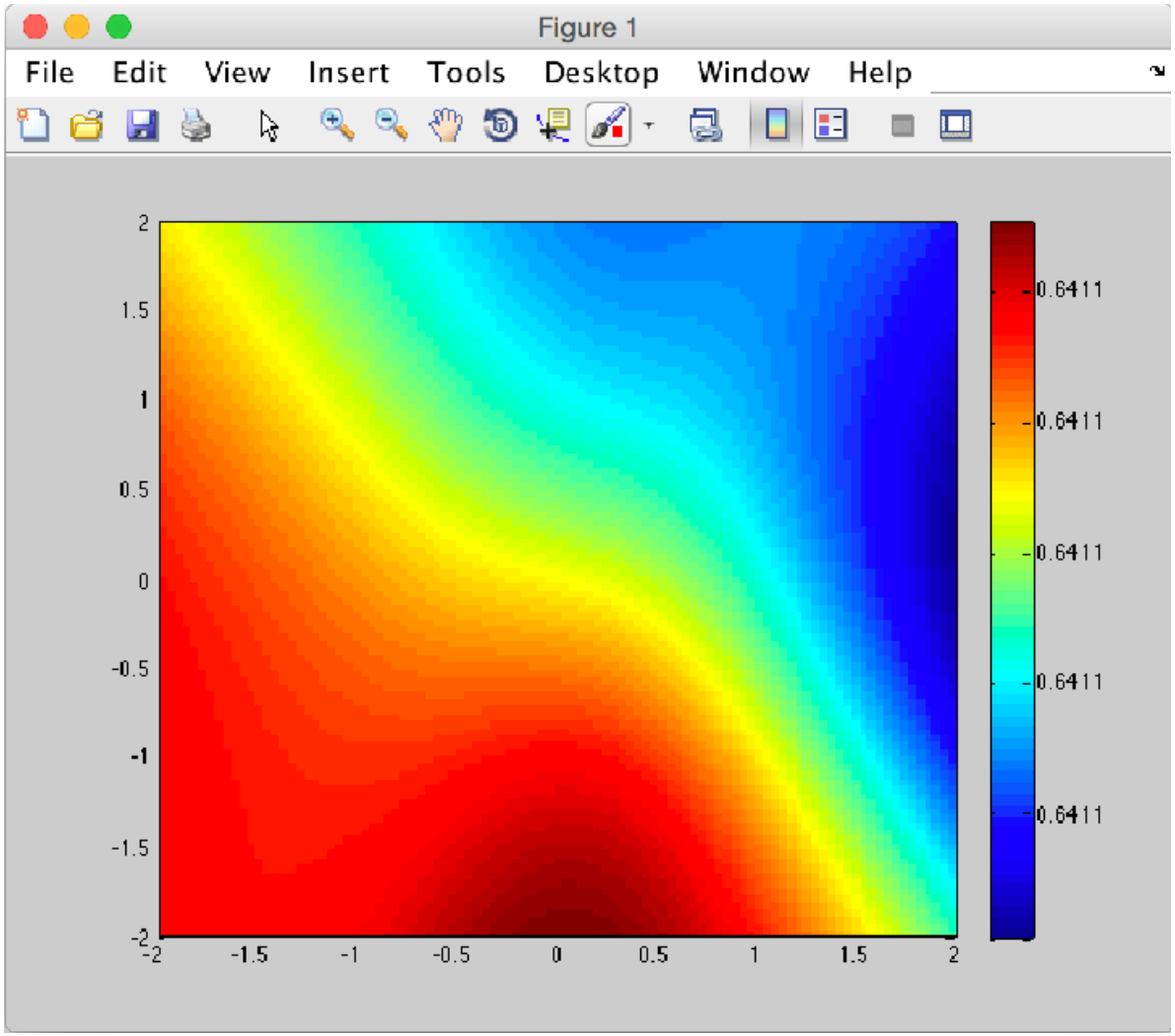
Decision Boundary: 2 hidden layers, 2 hidden units



Decision Boundary: 2 hidden layers, 3 hidden units



Decision Boundary: 10 hidden layers, 5 hidden units



Loss Minimization

- Optimization problem

$$\text{TrainLoss}(\mathbf{W}, \mathbf{b}) = \frac{1}{|\mathcal{D}_{train}|} \sum_{(\mathbf{x},y)\in\mathcal{D}_{train}} \text{Loss}(\mathbf{x}, y, \mathbf{W}, \mathbf{b})$$

$$J = \text{Loss}(\mathbf{x}, y, \mathbf{W}, \mathbf{b}) = -y \log(\hat{y}) - (1-y) \log(1-\hat{y})$$

$$\hat{y} = h^{[2]}$$

- Goal: compute gradient

$$\nabla_{\mathbf{W},\mathbf{b}} J(\mathbf{W}, \mathbf{b})$$

Stochastic Gradient Descent

- Goal: compute gradient

$$\nabla_{\mathbf{W},\mathbf{b}} J(\mathbf{W}, \mathbf{b})$$

- Repeat, given a sample $(\mathbf{x}^{(i)}, y^{(i)})$:

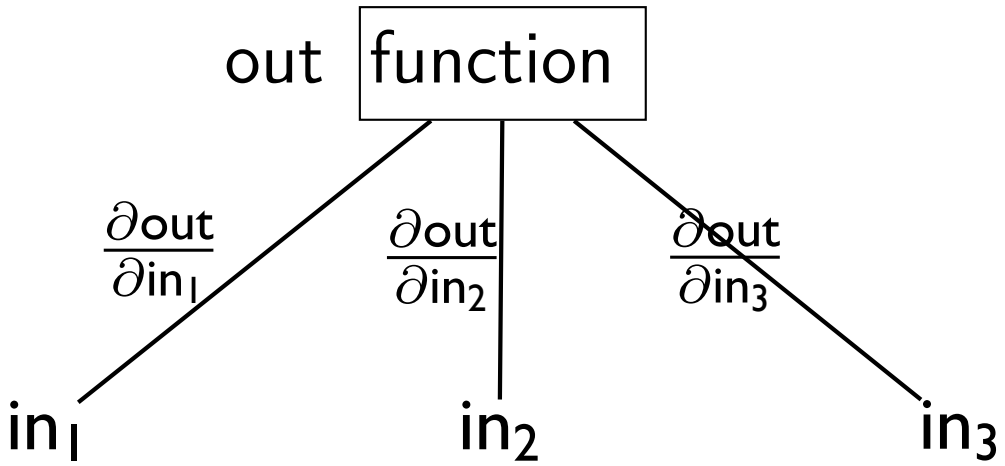
$$dW^{[1]} = \frac{\partial J}{\partial W^{[1]}}, \quad W^{[1]} = W^{[1]} - \eta dW^{[1]}$$
$$d\mathbf{b}^{[1]} = \frac{\partial J}{\partial \mathbf{b}^{[1]}}, \quad \mathbf{b}^{[1]} = \mathbf{b}^{[1]} - \eta d\mathbf{b}^{[1]}$$
$$dW^{[2]} = \frac{\partial J}{\partial W^{[2]}}, \quad W^{[2]} = W^{[2]} - \eta dW^{[2]}$$
$$db^{[2]} = \frac{\partial J}{\partial b^{[2]}}, \quad b^{[2]} = b^{[2]} - \eta db^{[2]}$$

Approach

- Mathematical: just grind through the chain rule
- Next: visualize the computation using a computation graph
- Advantages:
  - Avoid long equations
  - Reveal structure of computations (modularity, efficiency, dependencies)

Functions as boxes

- Partial derivatives (gradients): how much does the output change if an input changes?



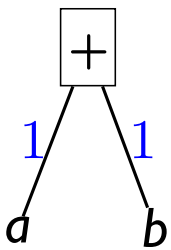
- Example:

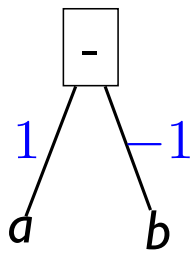
$$\text{out} = 2\text{in}_1 + \text{in}_2\text{in}_3$$

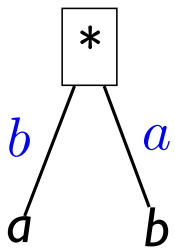
$$2\text{in}_1 + (\text{in}_2 + \epsilon)\text{in}_3 = \text{out} + \epsilon\text{in}_3$$

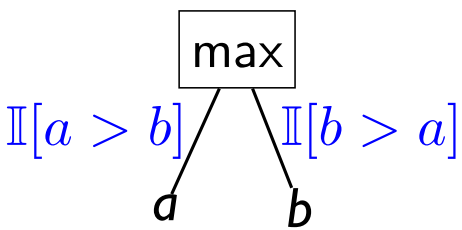
- Partial derivatives (gradients): a measure of sensitivity

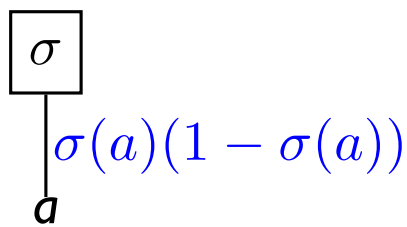
Basic building blocks



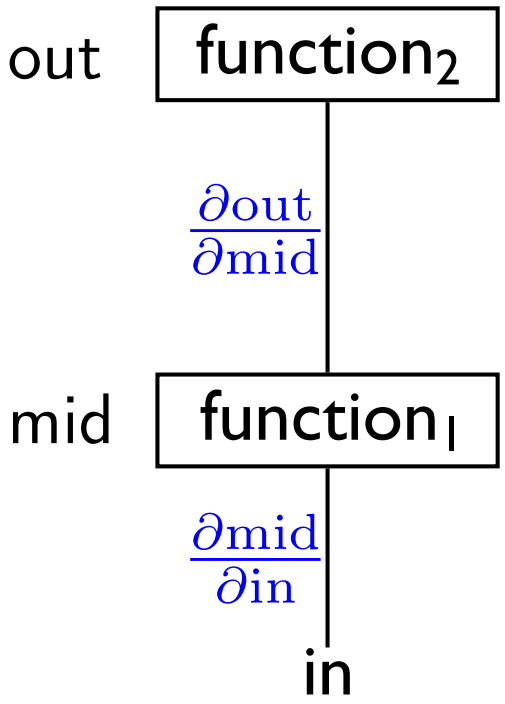








Composing Functions



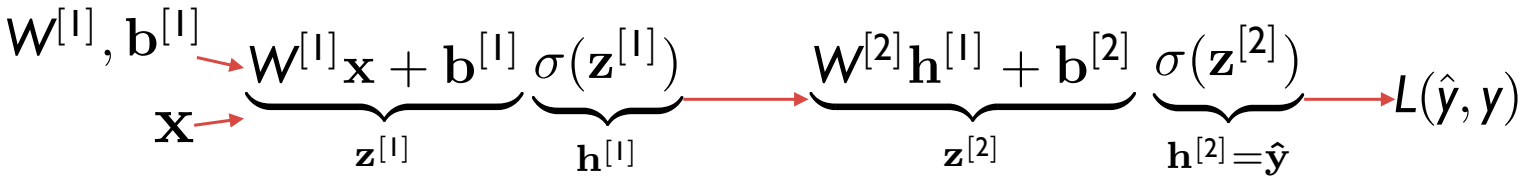
Chain rule

$$\frac{\partial \text{out}}{\partial \text{in}} = \frac{\partial \text{out}}{\partial \text{mid}} \frac{\partial \text{mid}}{\partial \text{in}}$$

Back propagation

- Goal: learn the weights so that the loss (error) is minimized.
- It provides an efficient procedure to compute derivatives.
- For a fixed sample $(\mathbf{x}, y)$, we want to learn $\hat{y} = f(\mathbf{x})$
- Negative Log-likelihood over input $\mathbf{x}_n$ is (assume $y_n \in \{0, 1\}$):
  $L_n = -y_n \log(\hat{y}_n) - (1 - y_n) \log(1 - \hat{y}_n)$
- Total error of training examples is $E = \sum_n L_n$

Back propagation



Loss function : $L = -y \log(\hat{y}) - (1 - y) \log(1 - \hat{y})$

$$d\mathbf{z}^{[1]} = \frac{\partial L}{\partial \mathbf{h}^{[1]}} \frac{\partial \mathbf{h}^{[1]}}{\partial \mathbf{z}^{[1]}} = {W^{[2]}}^T dz^{[2]} \circ \mathbf{h}^{[1]} \circ (1 - \mathbf{h}^{[1]})$$

$$dW^{[1]} = d\mathbf{z}^{[1]} \mathbf{x}^T$$

$$d\mathbf{b}^{[1]} = d\mathbf{z}^{[1]}$$

$$dz^{[2]} = \frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z^{[2]}} = \hat{y} - y$$

$$dW^{[2]} = dz^{[2]} {\mathbf{h}^{[1]}}^T$$

$$db^{[2]} = dz^{[2]}$$

Summary: computing derivatives

Forward propagation:

$$\mathbf{z}^{[1]} = W^{[1]}\mathbf{x} + b^{[1]}$$
$$\mathbf{h}^{[1]} = \sigma(\mathbf{z}^{[1]})$$
$$z^{[2]} = W^{[2]}\mathbf{h}^{[1]} + b^{[2]}$$
$$\hat{y} = h^{[2]} = \sigma(z^{[2]})$$

Backpropagation

$$dz^{[2]} = h^{[2]} - y$$
$$dW^{[2]} = dz^{[2]}{\mathbf{h}^{[1]}}^T$$
$$db^{[2]} = dz^{[2]}$$
$$d\mathbf{z}^{[1]} = {W^{[2]}}^T dz^{[2]} \circ \mathbf{h}^{[1]} \circ (1 - \mathbf{h}^{[1]})$$
$$dW^{[1]} = d\mathbf{z}^{[1]}\mathbf{x}^T$$
$$d\mathbf{b}^{[1]} = d\mathbf{z}^{[1]}$$

Vectorizing across multiple examples - forward

for $n = 1$ to N:

$$\mathbf{z}_n^{[1]} = W^{[1]}\mathbf{x}_n + b^{[1]}$$
$$\mathbf{h}_n^{[1]} = \sigma(\mathbf{z}_n^{[1]})$$
$$z_n^{[2]} = W^{[2]}\mathbf{h}_n^{[1]} + b^{[2]}$$
$$h_n^{[2]} = \sigma(z_n^{[2]})$$

Vectorizing
(Row: hidden units,
column: examples):

$$Z^{[1]} = W^{[1]}X + \mathbf{b}^{[1]}$$
$$H^{[1]} = \sigma(Z^{[1]})$$
$$Z^{[2]} = W^{[2]}H^{[1]} + b^{[2]}$$
$$H^{[2]} = \sigma(Z^{[2]})$$

Vectorizing across multiple examples - backpropagation

Given one data point:

$$dz^{[2]} = h^{[2]} - y$$
$$dW^{[2]} = dz^{[2]}\mathbf{h}^{[1]^T}$$
$$db^{[2]} = dz^{[2]}$$
$$d\mathbf{z}^{[1]} = dz^{[2]}W^{[2]^T} \circ \mathbf{h}^{[1]} \circ (1 - \mathbf{h}^{[1]})$$
$$dW^{[1]} = d\mathbf{z}^{[1]}\mathbf{x}^T$$
$$d\mathbf{b}^{[1]} = d\mathbf{z}^{[1]}$$

Vectorizing:

$$dZ^{[2]} = H^{[2]} - \mathbf{y}$$
$$dW^{[2]} = \frac{1}{N} dZ^{[2]} H^{[1]^T}$$
$$db^{[2]} = \frac{1}{N} \sum dZ^{[2]}$$
$$dZ^{[1]} = W^{[2]^T} dZ^{[2]} \circ H^{[1]} \circ (1 - H^{[1]})$$
$$dW^{[1]} = \frac{1}{N} dZ^{[1]} X^T$$
$$d\mathbf{b}^{[1]} = \frac{1}{N} \sum d\mathbf{z}^{[1]}$$

Adaptive learning rates

- Popular and simple idea: reduce the learning rate by some factor every few epochs.
  - At the beginning, we are far from the destination, so we use larger learning rate
  - After several epochs, we are close to the destination, so we reduce the learning rate
  - E.g. $1/t$ decay: $\eta^t = \frac{\eta}{\sqrt{t+1}}$
- Learning rate cannot be one-size-fits-all
  - Giving different parameters different learning rates.

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  - E.g. $1/t$ decay: $\eta^t = \frac{\eta}{\sqrt{t+1}}$
- Learning rate cannot be one-size-fits-all
  - Giving different parameters different learning rates.
  - Adagrad, RMSprop, Adam etc

Implementation of simple NN

Implementation

Python (Numpy) for 1 hidden layer neural network. (Link)

Implementation

Implementation

Deep Learning packages (e.g., Tensorflow, Pytorch MXNet) for multiple layer (convolutional) neural network.

Usefully resources: Tensorflow web, Pytorch web

Acknowledgement and Further Reading

Slides are adapted from Dr. Y. Ning's Spring 19 offering of CS-559.