CS540 Introduction to Artificial Intelligence
Lecture 4

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Based on lecture slides by Jerry Zhu and Yingyu Liang

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Neural Network Diagram

Review

Multi-Layer Neural Network Diagram

Review

Stochastic Gradient Descent

Motivation

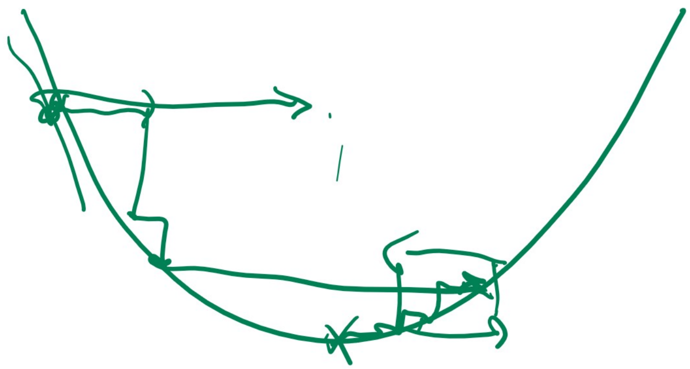
$$\frac{\partial C}{\partial w} = \sum_{i=1}^{n} a_i (1-a_i) x \cdots \qquad n \leftarrow \text{\# of training data}$$

$$\frac{\partial C_i}{\partial w} = a_i (1-a_i) \cdots$$

- Each gradient descent step requires the computation of gradients for all training instances $i = 1, 2, ..., n$. It is very costly.
- Stochastic gradient descent picks one instance x_i randomly, compute the gradient, and update the weights and biases.
- When a batch of instances is selected randomly each time, it is called mini batch gradient descent.

Stochastic Gradient Descent Diagram

Motivation



for each instance

grad direction on average is same as grad

Stochastic Gradient Descent, Part 1

Algorithm

- Inputs, Outputs: same as backpropagation.
- Initialize the weights.
- Randomly permute (shuffle) the training set. Evaluate the activation functions at one instance at a time.
- Compute the gradient using the chain rule.

random selection, without replace

no sum,

$$\frac{\partial C}{\partial w_{j'j}^{(l)}} = \delta_{ij}^{(l)} a_{ij'}^{(l-1)}$$

$$\frac{\partial C}{\partial b_j^{(l)}} = \delta_{ij}^{(l)}$$

Stochastic Gradient Descent, Part 2

Algorithm

- Update the weights and biases using gradient descent.

For $l = 1, 2, ..., L$

$$w_{j'j}^{(l)} \leftarrow w_{j'j}^{(l)} - \alpha \frac{\partial C}{\partial w_{j'j}^{(l)}}, j' = 1, 2, ..., m^{(l-1)}, j = 1, 2, ..., m^{(l)}$$

$$b_{j}^{(l)} \leftarrow b_{j}^{(l)} - \alpha \frac{\partial C}{\partial b_{j}^{(l)}}, j = 1, 2, ..., m^{(l)}$$

- Repeat the process until convergent.

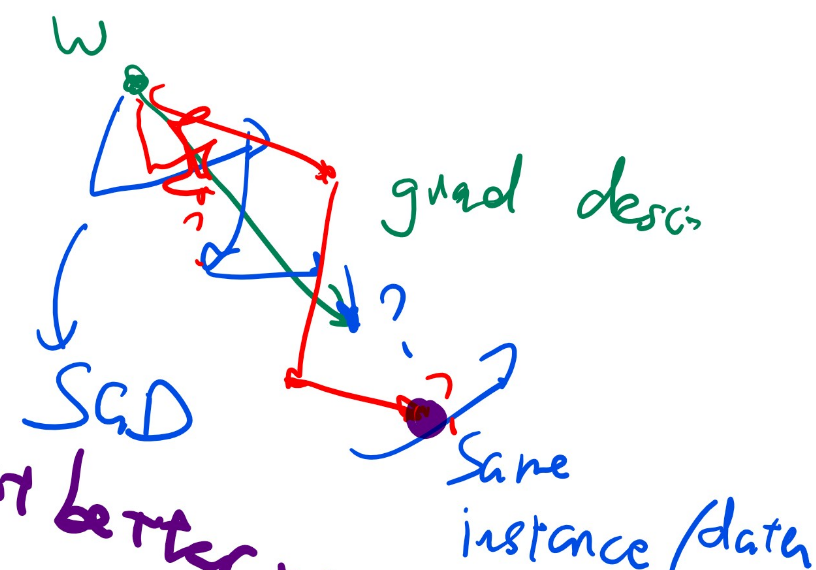
$$|C - C^{\text{prev}}| < \varepsilon$$

Q 10

Stochastic vs Full Gradient Descent

Quiz (Participation)

- Given the same initial weights and biases, stochastic gradient descent with instances picked randomly without replacement and full gradient descent lead to the same updated weights.
- A: Do not choose this.
- B: True.
- C: Do not choose this.
- D: False.
- E: Do not choose this.



Start at better w

$w = w - \alpha \frac{\partial C_1}{\partial w}$ $\quad w = w - \alpha \frac{\partial C_2}{\partial w}$

$w = w - \alpha \sum \frac{\partial C_i}{\partial w}$ $\quad E\left[\frac{\partial C_i}{\partial w}\right] = \sum \frac{\partial C_i}{\partial w}$

Generalization Error

Motivation

- With a large number of hidden units and small enough learning rate α, a multi-layer neural network can fit every finite training set perfectly.
- It does not imply the performance on the test set will be good.
- This problem is called overfitting.

Generalization Error Diagram

Motivation

Method 1, Validation Set

Discussion

- Set aside a subset of the training set as the validation set.
- During training, the cost (or accuracy) on the training set will always be decreasing until it hits 0.
- Train the network until the cost (or accuracy) on the validation set begins to increase.

Validation Set Diagram

Discussion

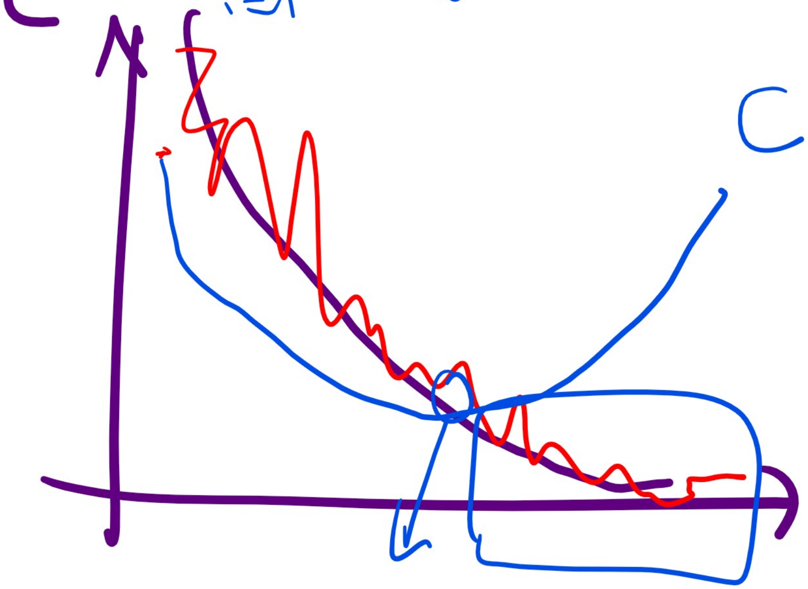
train

$$C = \sum_{i=1}^{n} (a_i - y_i)^2$$

C on validation

$$\approx \sum_{i=1}^{N} (a_i - y_i)^2$$

validation



$\boxed{\text{Stop}}$

trying to fit training too closely

not general.

Method 2, Drop Out

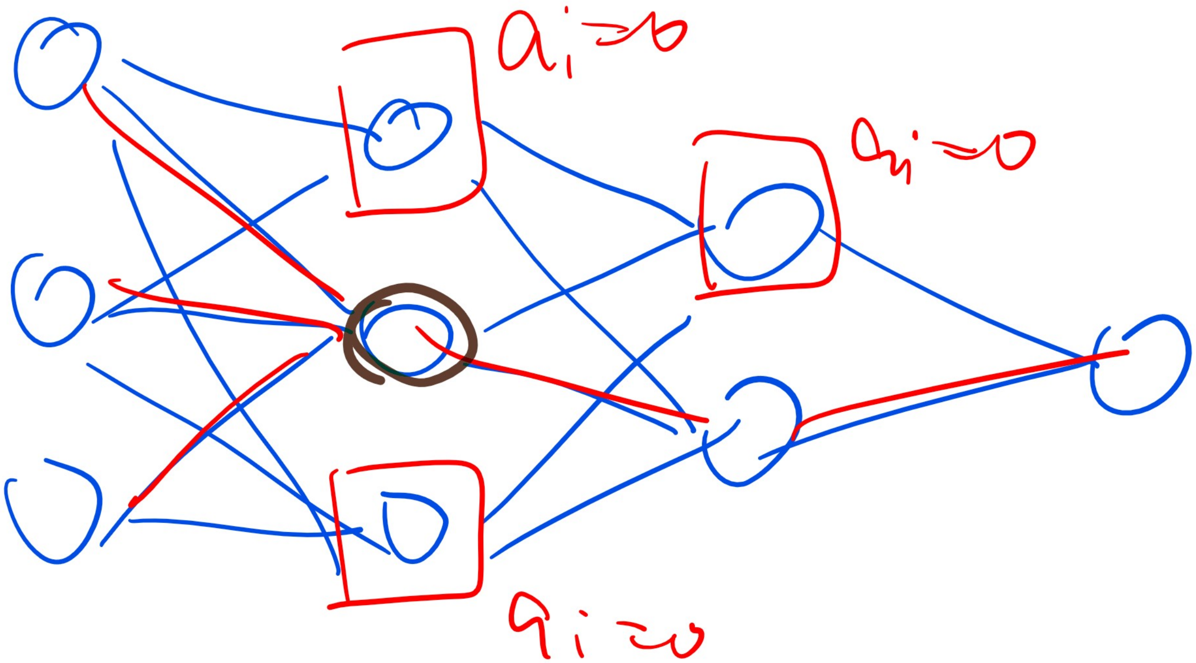
Discussion

- At each hidden layer, a random set of units from that layer is set to 0.
- For example, each unit is retained with probability $p = 0.5$. During the test, the activations are reduced by $p = 0.5$ (or 50 percent).
- The intuition is that if a hidden unit works well with different combinations of other units, it does not rely on other units and it is likely to be individually useful.

Drop Out Diagram

Discussion

goal not make it faster



Method 3, L1 and L2 Regularization

Discussion

- The idea is to include an additional cost for non-zero weights.
- The models are simpler if many weights are zero.
- For example, if logistic regression has only a few non-zero weights, it means only a few features are relevant, so only these features are used for prediction.

Method 3, L1 Regularization

Discussion

- For L1 regularization, add the 1-norm of the weights to the cost.

$$C = \sum_{i=1}^{n} (a_i - y_i)^2 + \lambda \left\| \begin{bmatrix} w \\ b \end{bmatrix} \right\|_1$$

$$= \underbrace{\sum_{i=1}^{n} (a_i - y_i)^2}_{\text{mistake}} + \underbrace{\lambda \left(\sum_{i=1}^{m} |w_i| + |b| \right)}_{\text{weights} \neq 0}$$

cost of non-zero weight.

min

- Linear regression with L1 regularization is called LASSO (least absolute shrinkage and selection operator).

Method 3, L2 Regularization

Discussion

- For L2 regularization, add the 2-norm of the weights to the cost.

$$
\begin{aligned}
C &= \sum_{i=1}^{n} (a_i - y_i)^2 + \lambda \left\| \begin{bmatrix} w \\ b \end{bmatrix} \right\|_2^2 \\
&= \underbrace{\sum_{i=1}^{n} (a_i - y_i)^2}_{} + \lambda \left(\sum_{i=1}^{m} w_i^2 + b^2 \right)
\end{aligned}
$$

L2

$$\frac{\partial C}{\partial w} = \frac{\partial (a_i - y_i)^2}{\partial w} + 2w$$

$$w = w - \alpha \frac{\partial}{\partial w} - 2\alpha w$$

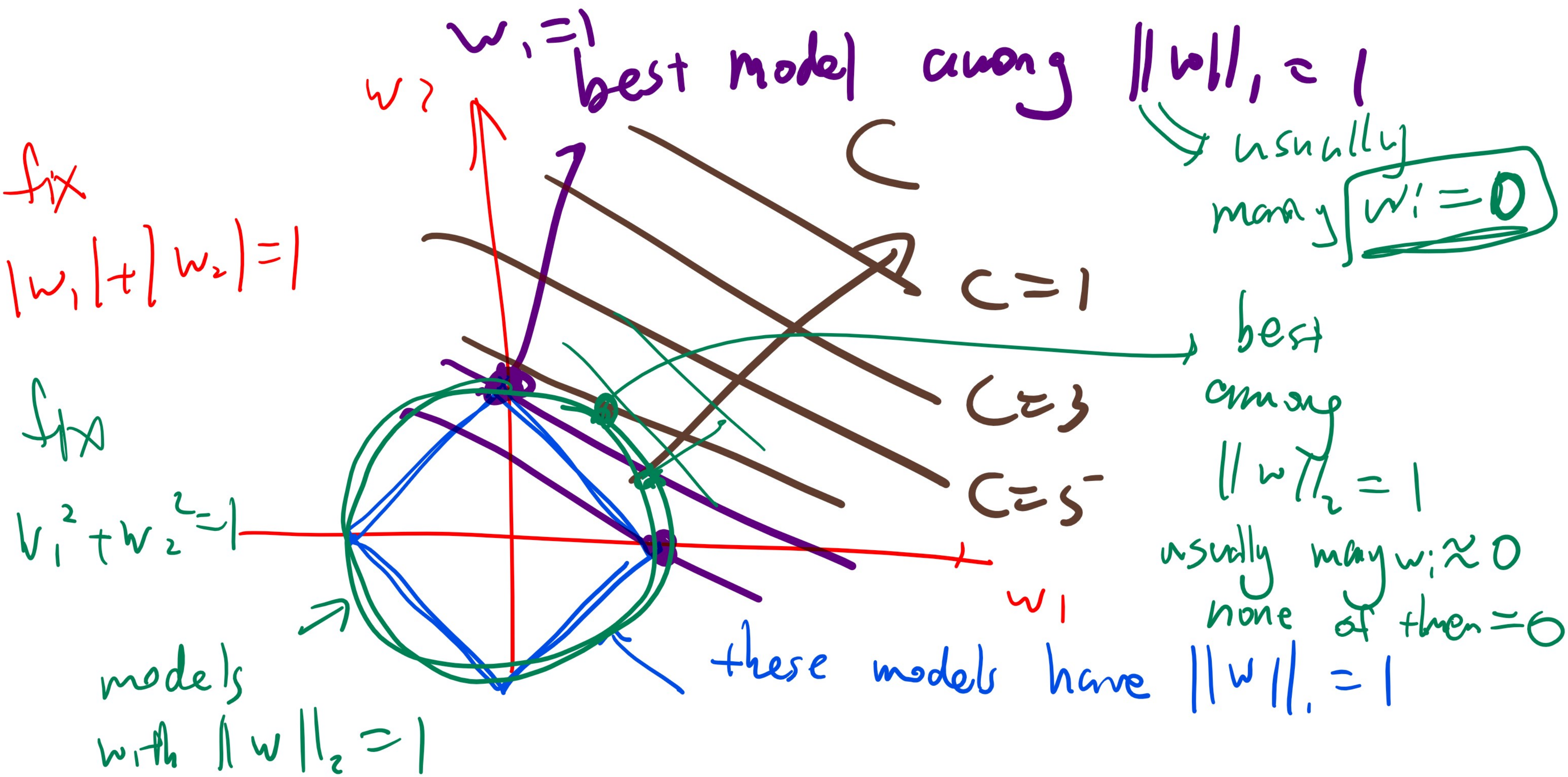
L1 and L2 Regularization Comparison

Discussion

- L1 regularization leads to more weights that are exactly 0. It is useful for feature selection.
- L2 regularization leads to more weights that are close to 0. It is easier to do gradient descent because 1-norm is not differentiable.

L1 and L2 Regularization Diagram

Discussion



Method 4, Data Augmentation

Discussion

- More training data can be created from the existing ones, for example, by translating or rotating the handwritten digits.

Hyperparameters

Discussion

- It is not clear how to choose the learning rate α, the stopping criterion ε, and the regularization parameters.
- For neural networks, it is also not clear how to choose the number of hidden layers and the number of hidden units in each layer.
- The parameters that are not parameters of the functions in the hypothesis space are called hyperparameters.

K Fold Cross Validation

Discussion

- Partition the training set into K groups.
- Pick one group as the validation set.
- Train the model on the remaining training set.
- Repeat the process for each of the K groups.
- Compare accuracy (or cost) for models with different hyperparameters and select the best one.

5 Fold Cross Validation Example

Discussion

- Partition the training set S into 5 subsets S_1, S_2, S_3, S_4, S_5

$$S_i \cap S_j = \emptyset \text{ and } \bigcup_{i=1}^{5} S_i = S$$

Same hyperparam

Same structure

different parameter

Iteration	Training	Validation
1	$S_2 \cup S_3 \cup S_4 \cup S_5$	S_1
2	$S_1 \cup S_3 \cup S_4 \cup S_5$	S_2
3	$S_1 \cup S_2 \cup S_4 \cup S_5$	S_3
4	$S_1 \cup S_2 \cup S_3 \cup S_5$	S_4
5	$S_1 \cup S_2 \cup S_3 \cup S_4$	S_5

Leave One Out Cross Validation

Discussion

- If $K = n$, each time exactly one training instance is left out as the validation set. This special case is called Leave One Out Cross Validation (LOOCV).

Cross Validation, Part II

Quiz (Graded)

x

y = 0 1 1 0 1

$\hat{y} = 1$

- March 2018 Midterm Q9
- Consider the majority classifier that predict $\hat{y}$ = mode of the training data labels. What is the 2-fold cross validation accuracy (percentage of correct classification) on the following training set.

S_1 S_2

x	1	2	3	4	5	6	7	8	9	10
y	1	1	0	1	1	0	0	1	0	0

20%

- A: 0 percent, B: 10 percent, C: 20 percent
- D: 50 percent, E: 100 percent

correct correct.

Cross Validation, Part I

Quiz (Graded)

K = 10

- March 2018 Midterm Q9
- Consider the majority classifier that predict $\hat{y}$ = mode of the training data labels. What is the LOOCV accuracy (percentage of correct classification) on the following training set.

S_{10}

x	1	2	3	4	5	6	7	8	9	10
y	1	1	0	1	1	0	0	1	0	0

- A: 0 percent, B: 10 percent, C: 20 percent
- D: 50 percent, E: 100 percent

Multi-Class Classification

Discussion

- When there are K categories to classify, the labels can take K different values, $y_i \in \{1, 2, ..., K\}$.
- Logistic regression and neural network cannot be directly applied to these problems.

Method 1, One VS All

Discussion

0 not 0

1 not 1

2 not 2

- Train a binary classification model with labels $y_i' = \mathbb{1}_{\{y_i = j\}}$ for each $j = 1, 2, ..., K$.
- Given a new test instance x_i, evaluate the activation function $a_i^{(j)}$ from model j.

$$\hat{y}_i = \arg\max_j a_i^{(j)}$$

- One problem is that the scale of $a_i^{(j)}$ may be different for different j.

Method 2, ~~One VS One~~

Discussion

0 vs 1 1 vs 2
0 vs 2 1 vs 3
0 vs 3
⋮ ⋮

- Train a binary classification model with for each of the $\dfrac{K(K-1)}{2}$ pairs of labels.
- Given a new test instance x_i, apply all $\dfrac{K(K-1)}{2}$ models and output the class that receives the largest number of votes.

$$\hat{y}_i = \arg\max_j \sum_{j' \neq j} \hat{y}_i^{(j \text{ vs } j')}$$

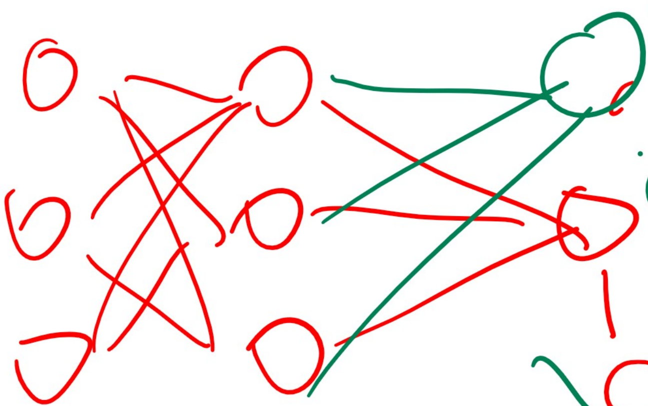
- One problem is that it is not clear what to do if multiple classes receive the same number of votes.

One Hot Encoding

$y = 1, 2, 3,$

- If y is not binary, use one-hot encoding for y.
- For example, if y has three categories, then

$$y_i \in \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\}$$



$a_{i1}^{(2)}$

$a_{i2}^{(2)}$

here?

classes

$$C = \sum_{i=1}^{n} \sum_{j=1}^{K} \left(a_{ij}^{(2)} - y_{ij}\right)^2$$

$$\cancel{C = \sum \left(a_i^{(2)} - y_i\right)^2}$$

$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$

Method 3, Softmax Function

Discussion

- For both logistic regression and neural network, the last layer will have K units, a_{ij}, for $j = 1, 2, ..., K$ and the softmax function is used instead of the sigmoid function.

$$a_{ij} = g\left(w_j^T x_i + b_j\right) = \frac{\exp\left(w_j^T x_i + b_j\right)}{\sum_{j'=1}^{K} \exp\left(w_{j'}^T x_i + b_{j'}\right)}, j = 1, 2, ..., K$$

$$\frac{1}{1 + e^{-w^T x + b}}$$

Back Propagation

Quiz (Graded)

8

- 2018 May Final Exam Q4
- Which one best describes backpropagation?
- A: Activation values are propagated from input nodes to output nodes. feed forward
- B: Activation values are propagated from output nodes to input nodes.
- C: Do not choose this.
- D: Weights are modified based on values propagated from input nodes to output nodes.
- E: Weights are modified based on values propagated from output nodes to input nodes. back prop.

Backpropogation, Part 1

Algorithm

- Inputs: instances: $\{x_i\}_{i=1}^n$ and $\{y_i\}_{i=1}^n$, number of hidden layers L with units $m^{(1)}, m^{(2)}, ..., m^{(L-1)}$, with $m^{(0)} = m, m^{(L)} = 1$, and activation function g is the sigmoid function.
- Outputs: weights and biases:

$$w_{j'j}^{(l)}, b_j^{(l)}, j' = 1, 2, ..., m^{(l-1)}, j = 1, 2, ..., m^{(l)}, l = 1, 2, ..., L$$

- Initialize the weights.

$$w_{j'j}^{(l)}, b_j^{(l)} \sim \text{ Unif } [0, 1]$$

Backpropogation, Part 2

Algorithm

- Evaluate the activation functions.

$$a_i = g\left(\sum_{j=1}^{m^{(L-1)}} a_{ij}^{(L-1)} w_j^{(L)} + b^{(L)}\right)$$

$$a_{ij}^{(l)} = g\left(\sum_{j'=1}^{m^{(l-1)}} a_{ij'}^{(l-1)} w_{j'j}^{(l)} + b_j^{(l)}\right), l = 1, 2, ..., L-1$$

$$a_{ij}^{(0)} = x_{ij}$$

Backpropogation, Part 3

Algorithm

- Compute the δ to simplify the expression of the gradient.

$$\delta_i^{(L)} = (y_i - a_i)\, a_i\, (1 - a_i)$$

$$\delta_{ij}^{(l)} = \sum_{j'=1}^{m^{(l+1)}} \delta_{j'}^{(l+1)} w_{jj'}^{(l+1)} a_{ij}^{(l)} \left(1 - a_{ij}^{(l)}\right), l = 1, 2, ..., L-1$$

- Compute the gradient using the chain rule.

$$\frac{\partial C}{\partial w_{j'j}^{(l)}} = \sum_{i=1}^{n} \delta_{ij}^{(l)} a_{ij'}^{(l-1)}, l = 1, 2, ..., L$$

$$\frac{\partial C}{\partial b_j^{(l)}} = \sum_{i=1}^{n} \delta_{ij}^{(l)}, l = 1, 2, ..., L$$

Backpropogation, Part 4

Algorithm

- Update the weights and biases using gradient descent.

For $l = 1, 2, ..., L$

$$w_{j'j}^{(l)} \leftarrow w_{j'j}^{(l)} - \alpha \frac{\partial C}{\partial w_{j'j}^{(l)}}, j' = 1, 2, ..., m^{(l-1)}, j = 1, 2, ..., m^{(l)}$$

$$b_{j}^{(l)} \leftarrow b_{j}^{(l)} - \alpha \frac{\partial C}{\partial b_{j}^{(l)}}, j = 1, 2, ..., m^{(l)}$$

- Repeat the process until convergent.

$$|C - C^{\text{prev}}| < \varepsilon$$

$$\min \quad C + \lambda \|w_1\|$$

Lagrange

$$\min \quad C \quad \text{st} \quad \|w_1\| = d$$