



Slides adapted from Jordan Boyd-Graber

Machine Learning: Chenhao Tan University of Colorado Boulder

Logistics

- HW3 available on Github, due on October 16
- Prelim 1 grades have been released
- Project team match

Outline

Revisiting Logistic Regression

Feed Forward Networks

$$P(Y = 0 \mid \boldsymbol{x}, \beta) = \frac{1}{1 + \exp\left[\beta_0 + \sum_j \beta_j \boldsymbol{x}_j\right]}$$

$$P(Y = 1 \mid \boldsymbol{x}, \beta) = \frac{\exp\left[\beta_0 + \sum_j \beta_j \boldsymbol{x}_j\right]}{1 + \exp\left[\beta_0 + \sum_j \beta_j \boldsymbol{x}_j\right]}$$

$$\mathcal{L} = -\sum_i \log P(y^{(i)} \mid \boldsymbol{x}^{(i)}, \beta)$$

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• Transformation on x (we map class labels from $\{0,1\}$ to $\{1,2\}$):

$$l_k = \beta_k^T x, k = 1, 2$$
 $o_k = \frac{\exp l_k}{\sum_{c \in \{1,2\}} \exp l_c}, k = 1, 2$

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 linear layer $o_k = \frac{\exp l_k}{\sum_{c \in \{1,2\}} \exp l_c}, k = 1, 2$ softmax layer

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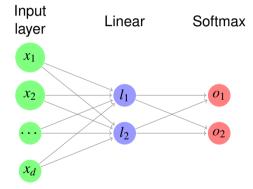
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• Objective function (using cross entropy $-\sum_i p_i \log q_i$):

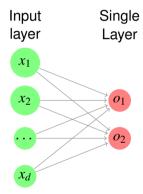
$$\mathscr{L}(Y, \hat{Y}) = -\sum_{i} \left[P(y^{(i)} = 1) \log P(\hat{y}_i = 1 \mid \boldsymbol{x}^{(i)}, \beta) + P(y^{(i)} = 0) \log \hat{P}(y_i = 0 \mid \boldsymbol{x}^{(i)}, \beta) \right]$$

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Logistic Regression as a Single-layer Neural Network



Logistic Regression as a Single-layer Neural Network



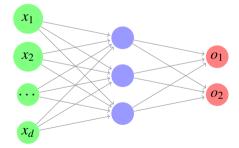
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Revisiting Logistic Regression

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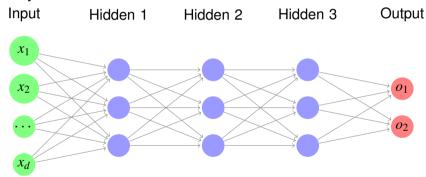
Deep Neural networks

A two-layer example (one hidden layer)
Input Hidden Output



Deep Neural networks

More layers:



Forward propagation algorithm

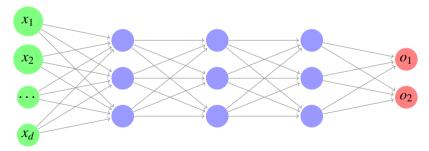
How do we make predictions based on a multi-layer neural network? Store the biases for layer l in b^l , weight matrix in W^l

$$W^1, b^1 W^2, b^2 W^3, b^3$$

$$W^2, b^2$$

$$W^3, b^3$$

$$\pmb{W}^4, \pmb{b}^4$$



Forward propagation algorithm

Suppose your network has L layers Make prediction for an instance x

- 1: Initialize $a^0 = x$
- 2: **for** l = 1 to L **do**
- 3: $\mathbf{z}^l = \mathbf{W}^l \mathbf{a}^{l-1} + \mathbf{b}^l$
- 4: $\boldsymbol{a}^l = g(\boldsymbol{z}^l)$
- 5: end for
- 6: The prediction \hat{y} is simply a^L

Nonlinearity

What happens if there is no nonlinearity?

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Nonlinearity

What happens if there is no nonlinearity? Linear combinations of linear combinations are still linear combinations.

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Neural networks in a nutshell

- Training data $S_{\text{train}} = \{(\boldsymbol{x}, y)\}$
- Network architecture (model)

$$\hat{\mathbf{y}} = f_{\mathbf{w}}(\mathbf{x})$$

Loss function (objective function)

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

Learning (next week)

Nonlinearity Options

Sigmoid

$$f(x) = \frac{1}{1 + \exp(x)}$$

tanh

$$f(x) = \frac{\exp(x) - \exp(-x)}{\exp(x) + \exp(-x)}$$

ReLU (rectified linear unit)

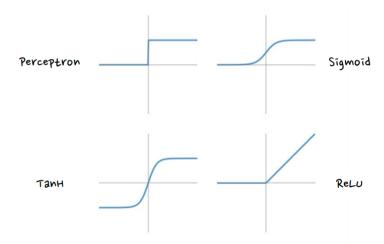
$$f(x) = \max(0, x)$$

softmax

$$x = \frac{\exp(x)}{\sum_{x_i} \exp(x_i)}$$

https://keras.io/activations/

Nonlinearity Options



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Loss Function Options

• ℓ_2 loss

$$\sum_{i} (y_i - \hat{y}_i)^2$$

• ℓ_1 loss

$$\sum_{i} |y_i - \hat{y}_i|$$

Cross entropy (logistic regression)

$$-\sum_{i}y_{i}\log\hat{y}_{i}$$

Hinge loss (more on this during SVM)

$$\max(0, 1 - y\hat{y})$$

https://keras.io/losses/

$$\mathbf{x} = (x_1, x_2), y = f(x_1, x_2)$$







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We consider a simple activation function

$$f(z) = \begin{cases} 1 & z \ge 0 \\ 0 & z < 0 \end{cases}$$

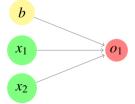
Simple Example: Can we learn OR?

| x_1 | 0 | 1 | 0 | 1 |
|--------------------|---|---|---|---|
| x_2 | 0 | 0 | 1 | 1 |
| $y = x_1 \vee x_2$ | 0 | 1 | 1 | 1 |

Simple Example: Can we learn OR?

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$$\mathbf{w} = (1, 1), b = -0.5$$



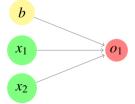
Simple Example: Can we learn AND?

| x_1 | 0 | 1 | 0 | 1 |
|----------------------|---|---|---|---|
| x_2 | 0 | 0 | 1 | 1 |
| $y = x_1 \wedge x_2$ | 0 | 0 | 0 | 1 |

Simple Example: Can we learn AND?

| x_1 | 0 | 1 | 0 | 1 |
|----------------------|---|---|---|---|
| x_2 | 0 | 0 | 1 | 1 |
| $y = x_1 \wedge x_2$ | 0 | 0 | 0 | 1 |

$$\mathbf{w} = (1, 1), b = -1.5$$



Simple Example: Can we learn NAND?

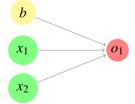
| x_1 | 0 | 1 | 0 | 1 |
|---------------------------|---|---|---|---|
| x_2 | 0 | 0 | 1 | 1 |
| $y = \neg(x_1 \land x_2)$ | 1 | 1 | 1 | 0 |

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Simple Example: Can we learn NAND?

| x_1 | 0 | 1 | 0 | 1 |
|---------------------------|---|---|---|---|
| x_2 | 0 | 0 | 1 | 1 |
| $y = \neg(x_1 \land x_2)$ | 1 | 1 | 1 | 0 |

$$\mathbf{w} = (-1, -1), b = 1.5$$



Simple Example: Can we learn XOR?

| | x_1 | 0 | 1 | 0 | 1 |
|-------|-----------|---|---|---|---|
| | x_2 | 0 | 0 | 1 | 1 |
| x_1 | XOR x_2 | 0 | 1 | 1 | 0 |

Simple Example: Can we learn XOR?

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|-------|-------|-------|---|---|---|---|
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NOPE!

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NOPE! But why?

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NOPE!

But why?

The single-layer perceptron is just a linear classifier, and can only learn things that are linearly separable.

Simple Example: Can we learn XOR?

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NOPE!

But why?

The single-layer perceptron is just a linear classifier, and can only learn things that are linearly separable.

How can we fix this?

Increase the number of layers.

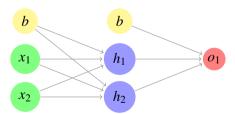
| | x_1 | 0 | 1 | 0 | 1 |
|-------|-----------|---|---|---|---|
| | x_2 | 0 | 0 | 1 | 1 |
| x_1 | XOR x_2 | 0 | 1 | 1 | 0 |

Increase the number of layers.

$$XOR = AND (OR, NAND)$$

Increase the number of layers.

| | x_1 | 0 | 1 | 0 | 1 |
|-------|-----------|---|---|---|---|
| | x_2 | 0 | 0 | 1 | 1 |
| x_1 | XOR x_2 | 0 | 1 | 1 | 0 |



$$\mathbf{W}^{1} = \begin{bmatrix} 1 & 1 \\ -1 & -1 \end{bmatrix}, \mathbf{b}^{1} = \begin{bmatrix} -0.5 \\ 1.5 \end{bmatrix}$$
$$\mathbf{W}^{2} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \mathbf{b}^{2} = -1.5$$

General Expressiveness of Neural Networks

Neural networks with a single hidden layer can approximate any measurable functions [Hornik et al., 1989, Cybenko, 1989].

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Summary

- Logistic regression and perceptron can be seen as special cases of neural networks
- Feed-forward algorithm (forward propagation)

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References

George Cybenko. Approximation by superpositions of a sigmoidal function. *Mathematics of Control, Signals, and Systems (MCSS)*, 2(4):303–314, 1989.

Kurt Hornik, Maxwell Stinchcombe, and Halbert White. Multilayer feedforward networks are universal approximators. *Neural networks*, 2(5):359–366, 1989.

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