Convex Optimization

Lecture 16 - Softmax Regression and Neural Networks

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Today's Lecture

1. Softmax Regression

2. Neural Networks

Outline

1. Softmax Regression
2. Neural Networks

Softmax Regression

extend logistic regression to multi-class classification

training data $(a^{(i)}, b^{(i)}),\ \ i = 1, \ldots, m$

labels with K values: $b^{(i)} \in \{1, \ldots, K\}$

hypothesis:

$$h_x(a) = \begin{bmatrix} P(b = 1 \mid a; x) \\ \vdots \\ P(b = K \mid a; x) \end{bmatrix} = \frac{1}{\sum_{k=1}^{K} \exp(x^{(k)T} a)} \begin{bmatrix} \exp(x^{(1)T} a) \\ \vdots \\ \exp(x^{(K)T} a) \end{bmatrix}$$

parameters to learn:

$$x = [x^{(1)}, \ldots, x^{(K)}] \in \mathbb{R}^{n \times K}$$

Maximum Log-Likelihood Estimator

given training data $(a^{(i)}, b^{(i)})_{i=1}^{m}$, the probability of this sequence is

$$\prod_{i=1}^{m}\prod_{k=1}^{K}\left[\frac{\exp(x^{(k)T}a^{(i)})}{\sum_{j=1}^{K}\exp(x^{(j)T}a^{(i)})}\right]^{\mathbf{1}_{\{b^{(i)}=k\}}}$$

log-likelihood is

$$\ell(x)=\sum_{i=1}^{m}\sum_{k=1}^{K}\mathbf{1}_{\{b^{(i)}=k\}}\cdot\log\frac{\exp(x^{(k)T}a^{(i)})}{\sum_{j=1}^{K}\exp(x^{(j)T}a^{(i)})}$$

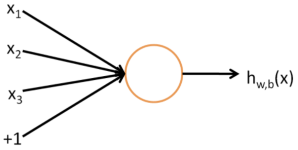
gradient is

$$\frac{\partial\ell(x)}{\partial x^{(k)}}=\sum_{i=1}^{m}a^{(i)}\cdot\left(\mathbf{1}_{\{b^{(i)}=k\}}-\frac{\exp(x^{(k)T}a^{(i)})}{\sum_{j=1}^{K}\exp(x^{(j)T}a^{(i)})}\right)$$

Outline

Neural Networks – A Single Neuron

fit a training example (x, y) with a neuron:



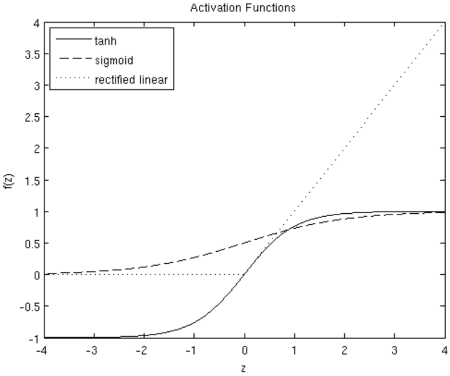
- input: x and a normalization term $+1$
- output: $h_{w,b}(x) = f(w^T x + b)$
- f is the activation function

some choices of activation function:

- sigmoid: $f(z) = \frac{1}{1+e^{-z}}$ (as in logistic regression)
- tanh: $f(z) = \tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$
- rectified linear: $f(z) = \max\{0, x\}$ (deep neural networks)

Neural Networks – Activation Functions

illustration of activation functions

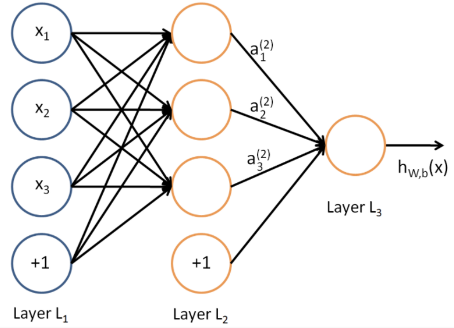


- tanh: rescaled sigmoid
- rectified linear: unbounded

Neural Networks – Basic Architecture

neural network: network of neurons

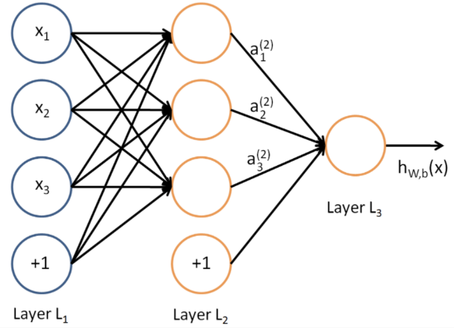
a three-layer neural network:



- input layer: the leftmost layer
- output layer: the rightmost layer
- hidden layer: the layers in the middle

Neural Networks – Parameters to Learn

a three-layer neural network:

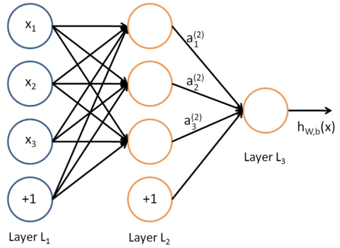


number of layers $n_\ell = 3$

weight of link from unit j in layer ℓ and unit i in layer $\ell + 1$: W_{ij}^{ℓ}

parameters to learn: $(W^{(1)}, b^{(1)}, \ldots, W^{(n_\ell)}, b^{(n_\ell)})$

Neural Networks – Example



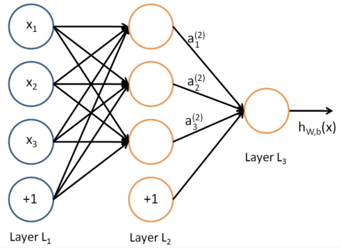
the activation (i.e., output) of unit i at layer ℓ: $a_i^{(\ell)}$

computation:

$$
\begin{aligned}
a_1^{(2)} &= f(W_{11}^{(1)}x_1 + W_{12}^{(1)}x_2 + W_{13}^{(1)}x_3 + b_1^{(1)}) \\
a_2^{(2)} &= f(W_{21}^{(1)}x_1 + W_{22}^{(1)}x_2 + W_{23}^{(1)}x_3 + b_2^{(1)}) \\
a_3^{(2)} &= f(W_{31}^{(1)}x_1 + W_{32}^{(1)}x_2 + W_{33}^{(1)}x_3 + b_3^{(1)}) \\
h_{W,b}(x) &= a_1^{(3)} = f(W_{11}^{(2)}a_1^{(2)} + W_{12}^{(2)}a_2^{(2)} + W_{13}^{(2)}a_3^{(2)} + b_3^{(2)})
\end{aligned}
$$

Neural Networks – Compact Representation

a three-layer neural network:



define weighted sum of inputs to unit i in layer ℓ as

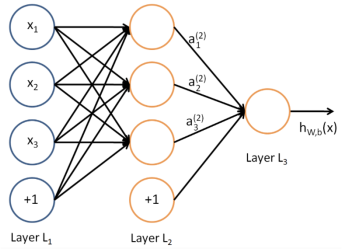
$$z_i^{(\ell)} = \sum_{j=1}^{n} W_{ij}^{(\ell-1)} a_j^{(\ell-1)} + b_i^{(\ell-1)},$$

where

$$a_j^{(\ell-1)} = f(z_j^{(\ell-1)})$$

Neural Networks – Compact Representation

a three-layer neural network:



compact representation: (forward propagation)

$$
\begin{aligned}
z^{(\ell+1)} &= W^{(\ell)} a^{(\ell)} + b^{(\ell)} \\
a^{(\ell+1)} &= f(z^{(\ell+1)})
\end{aligned}
$$

Neural Networks – Extensions

may have different architectures (i.e., network topology)

- different numbers s_ℓ of units in each layer ℓ
- different connectivity

may have loops

may have multiple output units

Neural Networks – Optimization

minimize the prediction error while promoting sparsity:

$$J(W,b) = \left[\frac{1}{m} \sum_{i=1}^{m} J(W,b;x^{(i)},y^{(i)}) \right] + \frac{\lambda}{2} \sum_{\ell=1}^{n_\ell - 1} \sum_{j=1}^{s_\ell} \sum_{i=1}^{s_{\ell+1}} \left(W_{ij}^{(\ell)} \right)^2$$

where $J(W,b;x^{(i)},y^{(i)})$ is the prediction error of sample i

$$J(W,b;x^{(i)},y^{(i)}) = \frac{1}{2} \left\| h_{W,b}(x^{(i)}) - y^{(i)} \right\|^2$$

characteristics:

- nonconvex – gradient descent used in practice
- initialization: small random values near 0 (but not all zeros)

Neural Networks – Calculating Gradients

need to compute gradients:

$$\frac{\partial J(W,b)}{\partial W_{ij}^{(\ell)}} = \left[\frac{1}{m}\sum_{i=1}^{m}\frac{\partial J(W,b;x^{(i)},y^{(i)})}{\partial W_{ij}^{(\ell)}}\right] + \lambda W_{ij}^{(\ell)}$$

$$\frac{\partial J(W,b)}{\partial b_{i}^{(\ell)}} = \frac{1}{m}\sum_{i=1}^{m}\frac{\partial J(W,b;x^{(i)},y^{(i)})}{\partial b_{i}^{(\ell)}}$$

backpropagation to compute $\frac{\partial J(W,b;x^{(i)},y^{(i)})}{\partial W_{ij}^{(\ell)}}$ and $\frac{\partial J(W,b;x^{(i)},y^{(i)})}{\partial b_{i}^{(\ell)}}$

Neural Networks – Backpropagation

for the output layer: (the superscript of sample index removed)

$$\begin{aligned}
&\frac{\partial J(W,b;x,y)}{\partial W_{ij}^{(n_\ell-1)}} \\
=\;& \frac{\partial}{\partial W_{ij}^{(n_\ell-1)}} \left\{ \frac{1}{2} \left[y_i - \underbrace{h_{W,b}\left(\sum_{j=1}^{n} W_{ij}^{(n_\ell-1)} a_j^{(n_\ell-1)} + b_i^{(n_\ell-1)} \right)}_{=f(z_i^{(n_\ell)})=a_i^{(n_\ell)}} \right]^2 \right\} \\
=\;& \left(y_i - a_i^{(n_\ell)} \right) \cdot \left[-f'\left(z_i^{(n_\ell)} \right) \right] \cdot \frac{\partial z_i^{(n_\ell)}}{\partial W_{ij}^{(n_\ell-1)}} \\
=\;& -\underbrace{\left(y_i - a_i^{(n_\ell)} \right) \cdot f'\left(z_i^{(n_\ell)} \right)}_{\triangleq \delta_i^{(n_\ell)}} \cdot a_j^{(n_\ell-1)}
\end{aligned}$$

Neural Networks – Backpropagation

for the middle layer $n_\ell - 1$: (the superscript of sample index removed)

$$
\begin{aligned}
&\frac{\partial J(W,b;x,y)}{\partial W_{ij}^{(n_\ell-2)}} \\
= \ & \frac{\partial}{\partial W_{ij}^{(n_\ell-2)}} \left\{ \frac{1}{2} \sum_{k=1}^{s_{n_\ell}} \left[y_k - f(z_k^{(n_\ell)}) \right]^2 \right\} \\
= \ & \sum_{k=1}^{s_{n_\ell}} \left(y_k - a_k^{(n_\ell)} \right) \cdot \left[-f'\left(z_k^{(n_\ell)} \right) \right] \cdot \frac{\partial z_k^{(n_\ell)}}{\partial a_i^{(n_\ell-1)}} \cdot \frac{\partial a_i^{(n_\ell-1)}}{\partial z_i^{(n_\ell-1)}} \cdot \frac{\partial z_i^{(n_\ell-1)}}{\partial W_{ij}^{(n_\ell-2)}} \\
= \ & \underbrace{\sum_{k=1}^{s_{n_\ell}} \delta_k^{(n_\ell)} \cdot W_{ki}^{(n_\ell-1)} \cdot f'\left(z_i^{(n_\ell-1)} \right)}_{\triangleq \delta_i^{(n_\ell-1)}} \cdot a_j^{(n_\ell-2)}
\end{aligned}
$$

Neural Networks – Backpropagation

backpropagation:

- a forward propagation to determine all the $a_i^{(\ell)}, z_i^{(\ell)}$
- for the output layer, set

$$\delta_i^{(n_\ell)} = -(y_i - a_i^{(n_\ell)}) \cdot f'(z_i^{(n_\ell)})$$

- for middle layers $\ell = n_\ell - 1, \ldots, 2$ and each node i in layer ℓ, set

$$\delta_i^{(\ell)} = \left(\sum_{j=1}^{s_{\ell+1}} W_{ji}^{(\ell)} \delta_j^{(\ell+1)} \right) f'(z_i^{(\ell)})$$

- compute gradients

$$\frac{\partial J(W, b; x, y)}{\partial W_{ij}^{(\ell)}} = a_j^{(\ell)} \delta_i^{(\ell+1)}$$

$$\frac{\partial J(W, b; x, y)}{\partial b_i^{(\ell)}} = \delta_i^{(\ell+1)}$$