CS229: Additional Notes on Backpropagation

1 Forward propagation

Recall that given input x, we define $a^{[0]} = x$. Then for layer $\ell = 1, 2, \ldots, N$, where N is the number of layers of the network, we have

1. $z^{[\ell]} = W^{[\ell]} a^{[\ell-1]} + b^{[\ell]}$
2. $a^{[\ell]} = g^{[\ell]}(z^{[\ell]})$

In these notes we assume the nonlinearities $g^{[\ell]}$ are the same for all layers besides layer N. This is because in the output layer we may be doing regression [hence we might use $g(x) = x$] or binary classification [$g(x) = \text{sigmoid}(x)$] or multiclass classification [$g(x) = \text{softmax}(x)$]. Hence we distinguish $g^{[N]}$ from g, and assume g is used for all layers besides layer N.

Finally, given the output of the network $a^{[N]}$, which we will more simply denote as $\hat{y}$, we measure the loss $J(W, b) = \mathcal{L}(a^{[N]}, y) = \mathcal{L}(\hat{y}, y)$. For example, for real-valued regression we might use the squared loss

$$\mathcal{L}(\hat{y}, y) = \frac{1}{2}(\hat{y} - y)^2$$

and for binary classification using logistic regression we use

$$\mathcal{L}(\hat{y}, y) = -(y \log \hat{y} + (1 - y) \log(1 - \hat{y}))$$

or negative log-likelihood. Finally, for softmax regression over k classes, we use the cross entropy loss

$$\mathcal{L}(\hat{y}, y) = -\sum_{j=1}^{k} \mathbf{1}\{y = j\} \log \hat{y}_j$$

which is simply negative log-likelihood extended to the multiclass setting. Note that $\hat{y}$ is a k-dimensional vector in this case. If we use y to instead denote the k-dimensional vector of zeros with a single 1 at the lth position, where the true label is l, we can also express the cross entropy loss as

$$\mathcal{L}(\hat{y}, y) = -\sum_{j=1}^{k} y_j \log \hat{y}_j$$

2 Backpropagation

Let's define one more piece of notation that'll be useful for backpropagation.[1] We will define

$$\delta^{[\ell]} = \nabla_{z^{[\ell]}} \mathcal{L}(\hat{y}, y)$$

We can then define a three-step "recipe" for computing the gradients with respect to every $W^{[\ell]}, b^{[\ell]}$ as follows:

1. For output layer N, we have

$$\delta^{[N]} = \nabla_{z^{[N]}} \mathcal{L}(\hat{y}, y)$$

   Sometimes we may want to compute $\nabla_{z^{[N]}} \mathcal{L}(\hat{y}, y)$ directly (e.g. if $g^{[N]}$ is the softmax function), whereas other times (e.g. when $g^{[N]}$ is the sigmoid function σ) we can apply the chain rule:

$$\nabla_{z^{[N]}} \mathcal{L}(\hat{y}, y) = \nabla_{\hat{y}} \mathcal{L}(\hat{y}, y) \circ (g^{[N]})'(z^{[N]})$$

   Note $(g^{[N]})'(z^{[N]})$ denotes the elementwise derivative w.r.t. $z^{[N]}$.

2. For $\ell = N-1, N-2, \ldots, 1$, we have

$$\delta^{[\ell]} = ({W^{[\ell+1]}}^\top \delta^{[\ell+1]}) \circ g'(z^{[\ell]})$$

3. Finally, we can compute the gradients for layer ℓ as

$$\begin{aligned} \nabla_{W^{[\ell]}} J(W, b) &= \delta^{[\ell]} {a^{[\ell-1]}}^\top \\ \nabla_{b^{[\ell]}} J(W, b) &= \delta^{[\ell]} \end{aligned}$$

where we use $\circ$ to indicate the elementwise product. Note the above procedure is for a single training example.

You can try applying the above algorithm to logistic regression ($N = 1$, $g^{[1]}$ is the sigmoid function σ) to sanity check steps (1) and (3). Recall that $\sigma'(z) = \sigma(z) \circ (1 - \sigma(z))$ and $\sigma(z^{[1]})$ is simply $a^{[1]}$. Note that for logistic regression, if x is a column vector in $\mathbb{R}^{d \times 1}$, then $W^{[1]} \in \mathbb{R}^{1 \times d}$, and hence $\nabla_{W^{[1]}} J(W, b) \in \mathbb{R}^{1 \times d}$. Example code for two layers is also given at:

`http://cs229.stanford.edu/notes/backprop.py`

[1] These notes are closely adapted from:
`http://ufldl.stanford.edu/tutorial/supervised/MultiLayerNeuralNetworks/`
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