TTIC 31230, Fundamentals of Deep Learning

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Multilayer Perceptrons

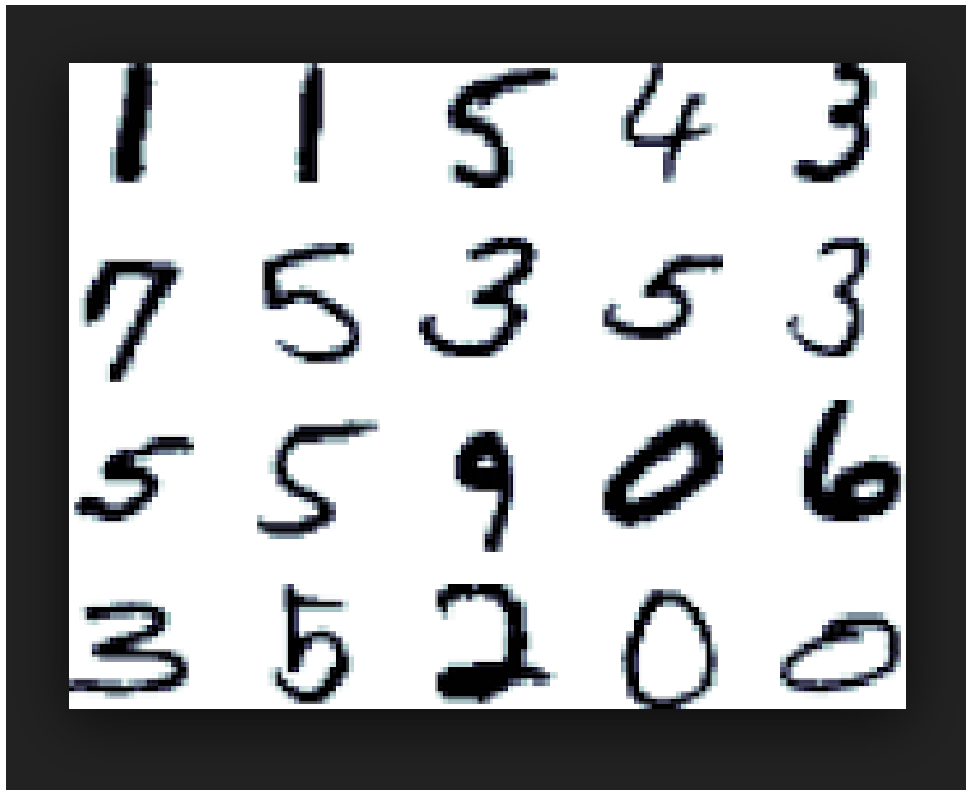
Stochastic Gradient Descent

Multiclass Classification

We will start by considering the problem of multiclass classification.

We consider the problem of taking an input x (such as an image of a hand written digit) and classifying it into some small number of classes (such as the digits 0 through 9).

MNIST



Multiclass Classification

Assume a data distribution D on pairs (x, y) for $x \in \mathbb{R}^d$ and $y \in \mathcal{C}$.

For MNIST x is a 28×28 image which we take to be a 784 dimensional vector giving $x \in \mathbb{R}^{784}$.

For MNIST $\mathcal{C}$ is the set $\{0, \ldots, 9\}$.

Assume a sample (x_0, y_0), $\ldots$, (x_{N-1}, y_{N-1}) drawn from D.

We want to use the sample to construct a rule for predicting y given x.

Class Scores

Assume a sample $(x_0, y_0),\ \ldots,\ (x_{N-1}, y_{N-1})$ drawn from D with $x \in \mathbb{R}^d$ and $y \in \{0, \ldots, K\}$.

For a new x we compute a score $s(\hat{y})$ for each possible label $\hat{y}$.

$$s(\hat{y}) = \sum_{j=1}^{d} W_{\hat{y},j}\; x_j + b_{\hat{y}}$$

or in vector notation

$$s = Wx + b$$

Here $W_{\hat{y},j}$ is the weight on component j of x for predicting class $\hat{y}$ and $b_{\hat{y}}$ is a "bias term" for class $\hat{y}$.

Softmax

We can convert the scores to probabilities using a Gibbs distribution

$$P(\hat{y}) = \frac{1}{Z}\, e^{s(\hat{y})}$$

$$Z = \sum_{\hat{y}} e^{s(\hat{y})}$$

Softmax

In vector notation

$$P = \mathrm{softmax}\ Wx + b$$

$$(\mathrm{softmax}\ s)_i = \frac{1}{Z}\, e^{s_i}$$

$$Z = \sum_i e^{s_i}$$

Log Loss

we have

$$P_{W,b}(\cdot|x) = \text{softmax } Wx + b$$

We can define our "error" or "loss" to be negative log probability of the true label.

$$\textbf{loss}(P(y|x)) = -\log P(y|x) = \log \frac{1}{P(y|x)}$$

We want

$$W^*, b^* = \underset{W,b}{\text{argmin}} \;\; \mathrm{E}_{(x,y)\sim D} \left[\log \frac{1}{P_{W,b}(y|x)} \right]$$

Multiclass Logistic Regression

For now we consider

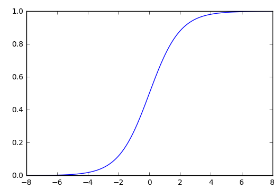
$$W^*, b^* = \operatorname*{argmin}_{W,b} \ \ell_{\mathrm{train}}(W, b)$$

$$\ell_{\mathrm{train}}(W, b) = \frac{1}{N} \sum_n \log \frac{1}{P_{W,b}(y_n | x_n)}$$

This is multiclass logistic regression.

Multi Layer Perceptrons (MLPs)

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



$$\begin{aligned} L^0 &= \sigma(W^0 x + b^0) \\ L^1 &= \mathrm{softmax}(W^1 L^0 + b^1) \end{aligned}$$

In the first equaiton σ is applied to each component of the vector $W^0x + b^0$. In general we will use the notation $f(x)$ where f is a scalar function and x is a vector (or tensor) to denote the vector (or tensor) that results from applying f to each element of x.

MLPs

$$
\begin{aligned}
L^0 &= \sigma(W^0 x + b^0) \\
L^1 &= \text{softmax}(W^1 L^0 + b^1)
\end{aligned}
$$

Here L^0 and L^1 are vectors. We will call the elements of L^0 "channels" (also called units or neurons).

The elements of L^1 are the class probabilities.

We now learn W^0, b^0, W^1 and b^1.

A More General Setting

Consider a system of parameters Θ.

For a two-layer MLP for MNIST we have that Θ is a tuple (W^0, b^0, W^1, b^1).

Consider a scalar loss function $\ell(\Theta, x, y)$.

For MNIST we have

$$\ell(\Theta, x, y) = -\log P_\Theta(y|x) = \log \frac{1}{P_\Theta(y|x)}$$

This is a very common loss function.

Optimizing the Loss Function

We consider minimizing the loss on the training data.

$$\Theta^* = \underset{\Theta}{\operatorname{argmin}} \; \frac{1}{N} \sum_{i=1}^{N} \ell(\Theta, x_i, y_i)$$

We will do this by gradient descent.

Gradients with Respect to Systems of Parameters

$\nabla_\Theta\, \ell(\Theta, x, y)$ denotes the partial derivative of $\ell(\Theta, x, y)$ with respect to the parameter system Θ.

For a scalar loss $\ell(\Theta, x, y)$ we have that $\nabla_\Theta\, \ell(\Theta, x, y)$ has the same shape (scalar, vector, or tensor) as Θ.

For each real number component of Θ there is a corresponding component of $\nabla_\Theta\, \ell(\Theta, x, y)$ giving the partial derivative of $\ell(\Theta, x, y)$ with respect to that component of Θ.

Here can think of Θ as a single vector with

$$(\nabla_\Theta\, \ell(\Theta, x, y))_i = \partial \ell(\Theta, x, y)/\partial \Theta_i$$

Total Gradient Descent

$$\ell_n(\Theta) = \ell(\Theta,\ x_n,\ y_n)$$

$$\ell(\Theta) = \frac{1}{N}\sum_{n=0}^{N-1} \ell_n(\Theta)$$

We want: $\Theta^* = \underset{\Theta}{\operatorname{argmin}}\, \ell(\Theta)$

repeat:

$$\Theta \;\texttt{-=}\; \eta\, \nabla_\Theta\, \ell(\Theta)$$

Stochastic Gradient Descent (SGD)

repeat: Select n at random.

$$\Theta \;\texttt{-=}\; \eta \, \nabla_\Theta \, \ell_n(\Theta)$$

SGD can make progress with only a small subset of the training data.

Note that

$$\mathrm{E}_n \left[\nabla_\Theta \, \ell_n(\Theta)\right] = \sum_n P(n) \, \nabla_\Theta \ell_n(\Theta)$$

$$= \nabla_\Theta \, \ell(\Theta)$$

SGD for MLPs

Consider an MLP

$$\Theta = (W^0, b^0, W^1, b^1)$$

$$L^0 = \sigma(W^0 x_n + b^0)$$

$$L^1 = \mathrm{softmax}(W^1 L^0 + b^1)$$

$$\ell(\Theta, x, y) = -\log(L^1_y)$$

We now need to be able to compute $\frac{\partial \ell(\Theta,x,y)}{\partial \Theta_k}$ for all scalar parameters Θ_k. To be continued ...

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