Deep Learning Systems: Algorithms and Implementation

ML Refresher / Softmax Regression

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Outline

Basics of machine learning

Example: softmax regresssion

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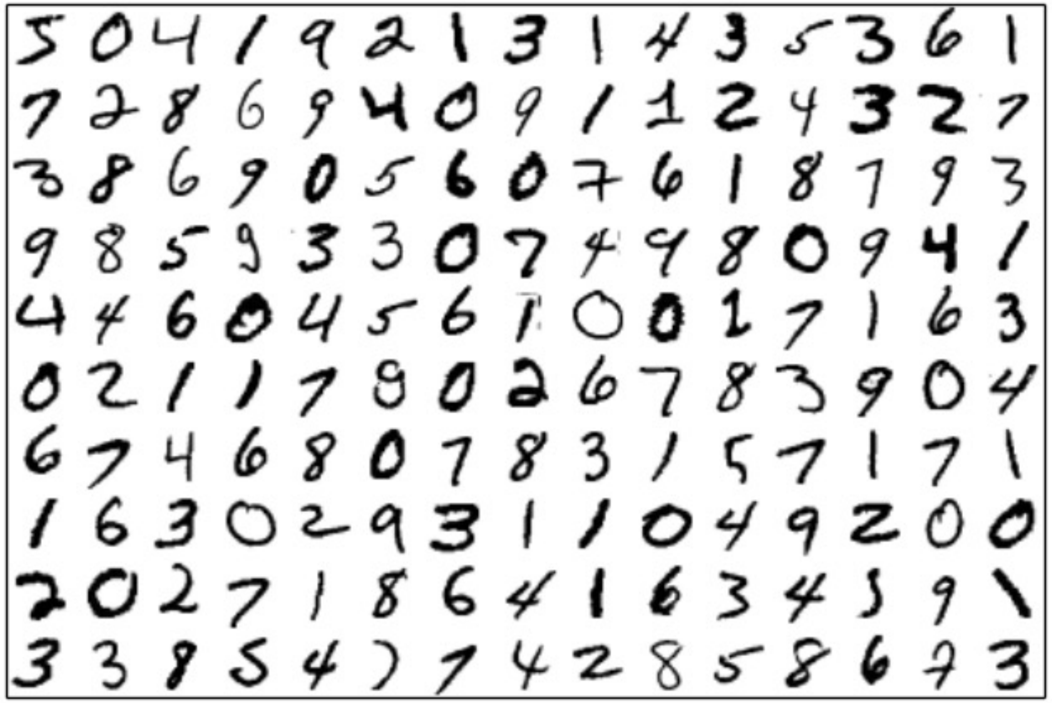
Example: softmax regresssion

Machine learning as data-driven programming

Suppose you want to write a program that will classify handwritten drawing of digits into their appropriate category: 0,1,…,9

You *could*, think hard about the nature of digits, try to determine the logic of what indicates what kind of digit, and write a program to codify this logic

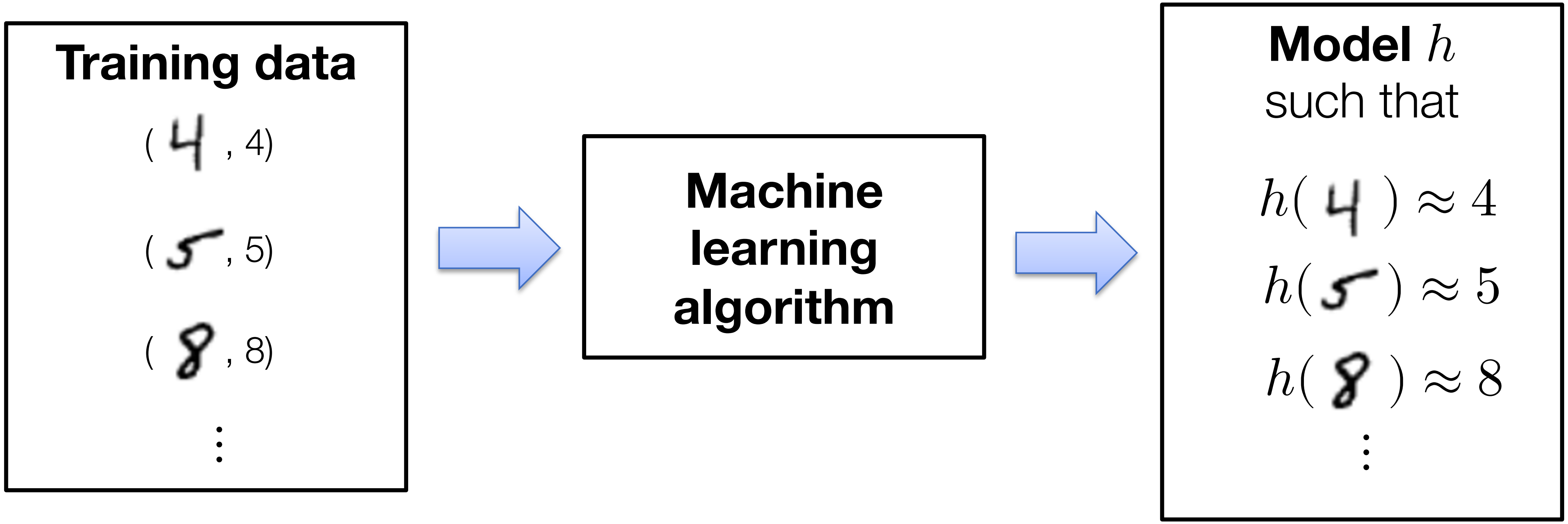
(Despite being a reasonable coder, I don't think I could do this very well)



MNIST Dataset

Machine learning as data-driven programming

The (supervised) ML approach: collect a *training set* of images with known labels and feed these into a *machine learning algorithm*, which will (if done well), automatically produce a “program” that solves this task



Three ingredients of a machine learning algorithm

Every machine learning algorithm consists of three different elements:

1. **The hypothesis class:** the “program structure”, parameterized via a set of *parameters*, that describes how we map inputs (e.g., images of digits) to outputs (e.g., class labels, or probabilities of different class labels)

2. **The loss function:** a function that specifies how “well” a given hypothesis (i.e., a choice of parameters) performs on the task of interest

3. **An optimization method:** a procedure for determining a set of parameters that (approximately) minimize the sum of losses over the training set

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Multi-class classification setting

Let's consider a *k-class classification setting,* where we have

- Training data: $x^{(i)} \in \mathbb{R}^n, y^{(i)} \in \{1, \ldots, k\}$ for $i = 1, \ldots m$
- $n =$ dimensionality of the input data
- $k =$ number of different classes / labels
- $m =$ number of points in the training set

Example: classification of 28x28 MNIST digits

- $n = 28 \cdot 28 = 784$
- $k = 10$
- $m = 60{,}000$

Linear hypothesis function

Our hypothesis function maps inputs $x \in \mathbb{R}^n$ to k-dimensional vectors

$$h: \mathbb{R}^n \rightarrow \mathbb{R}^k$$

where $h_i(x)$ indicates some measure of "belief" in how much likely the label is to be class i (i.e., "most likely" prediction is coordinate i with largest $h_i(x)$).

A **linear hypothesis function** uses a *linear* operator (i.e. matrix multiplication) for this transformation

$$h_\theta(x) = \theta^T x$$

for *parameters* $\theta \in \mathbb{R}^{n \times k}$

Matrix batch notation

Often more convenient (and this is how you want to code things for efficiency) to write the data and operations in *matrix batch* form

$$X \in \mathbb{R}^{m \times n} = \begin{bmatrix} - & {x^{(1)}}^T & - \\ & \vdots & \\ - & {x^{(m)}}^T & - \end{bmatrix}, \qquad y \in \{1, \ldots, k\}^m = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$

Then the linear hypothesis applied to this batch can be written as

$$h_\theta(X) = \begin{bmatrix} - & h_\theta(x^{(1)})^T & - \\ & \vdots & \\ - & h_\theta(x^m)^T & - \end{bmatrix} = \begin{bmatrix} - & {x^{(1)}}^T \theta & - \\ & \vdots & \\ - & {x^{(m)}}^T \theta & - \end{bmatrix} = X\theta$$

Loss function #1: classification error

The simplest loss function to use in classification is just the classification error, i.e., whether the classifier makes a mistake a or not

$$\ell_{err}(h(x), y) = \begin{cases} 0 & \text{if } \operatorname{argmax}_i h_i(x) = y \\ 1 & \text{otherwise} \end{cases}$$

We typically use this loss function to assess the *quality* of classifiers

Unfortunately, the error is a bad loss function to use for *optimization*, i.e., selecting the best parameters, because it is not differentiable

Loss function #2: softmax / cross-entropy loss

Let's convert the hypothesis function to a "probability" by exponentiating and normalizing its entries (to make them all positive and sum to one)

$$z_i = p(\text{label} = i) = \frac{\exp\big(h_i(x)\big)}{\sum_{j=1}^{k} \exp\big(h_j(x)\big)} \Longleftrightarrow z \equiv \text{normalize}(\exp(h(x)))$$

Then let's define a loss to be the (negative) log probability of the true class: this is called *softmax* or *cross-entropy* loss

$$\ell_{ce}(h(x), y) = -\log p(\text{label} = y) = -h_y(x) + \log \sum_{j=1}^{k} \exp\big(h_j(x)\big)$$

The softmax regression optimization problem

The third ingredient of a machine learning algorithm is a method for solving the associated optimization problem, i.e., the problem of minimizing the average loss on the training set

$$\underset{\theta}{\text{minimize}} \ \frac{1}{m}\sum_{i=1}^{m} \ell(h_\theta(x^{(i)}), y^{(i)})$$

For softmax regression (i.e., linear hypothesis class and softmax loss):

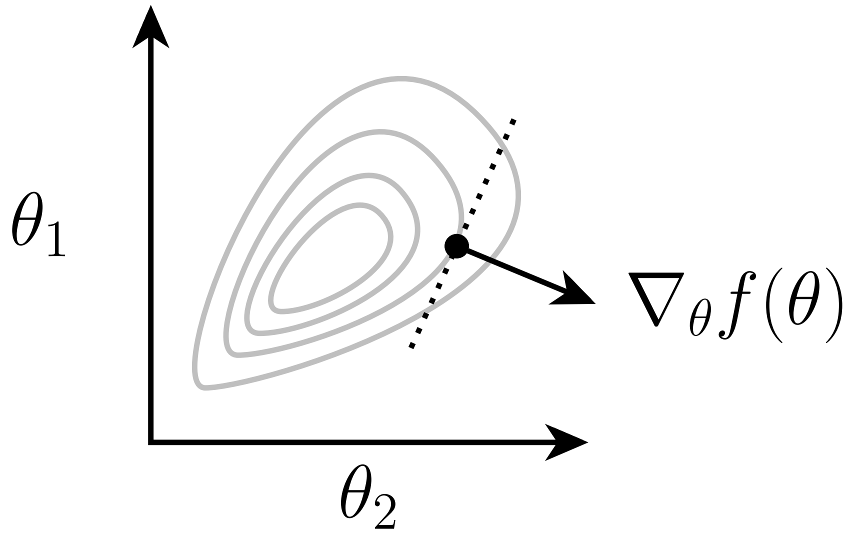
$$\underset{\theta}{\text{minimize}} \ \frac{1}{m}\sum_{i=1}^{m} \ell_{ce}(\theta^T x^{(i)}, y^{(i)})$$

So how do we find θ that solves this optimization problem?

Optimization: gradient descent

For a matrix-input, scalar output function $f\colon \mathbb{R}^{n\times k} \to \mathbb{R}$, the *gradient* is defined as the matrix of partial derivatives

$$\nabla_\theta f(\theta) \in \mathbb{R}^{n\times k} = \begin{bmatrix} \frac{\partial f(\theta)}{\partial \theta_{11}} & \cdots & \frac{\partial f(\theta)}{\partial \theta_{1k}} \\ \vdots & \ddots & \vdots \\ \frac{\partial f(\theta)}{\partial \theta_{n1}} & \cdots & \frac{\partial f(\theta)}{\partial \theta_{nk}} \end{bmatrix}$$



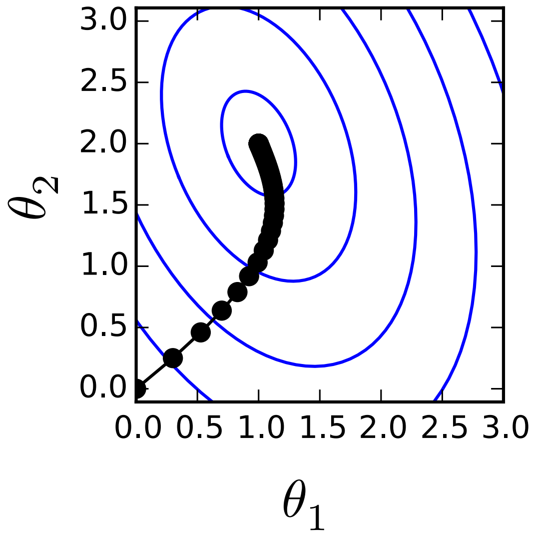
Gradient points in the direction that most *increases* f (locally)

Optimization: gradient descent

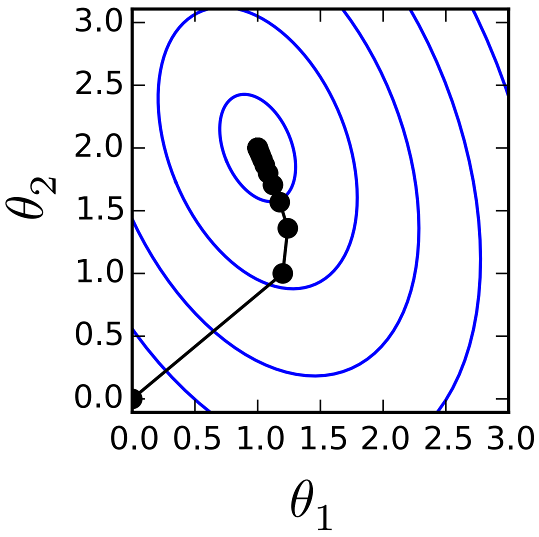
To *minimize* a function, the gradient descent algorithm proceeds by iteratively taking steps in the direction of the negative gradient

$$\theta := \theta - \alpha \nabla_\theta f(\theta)$$

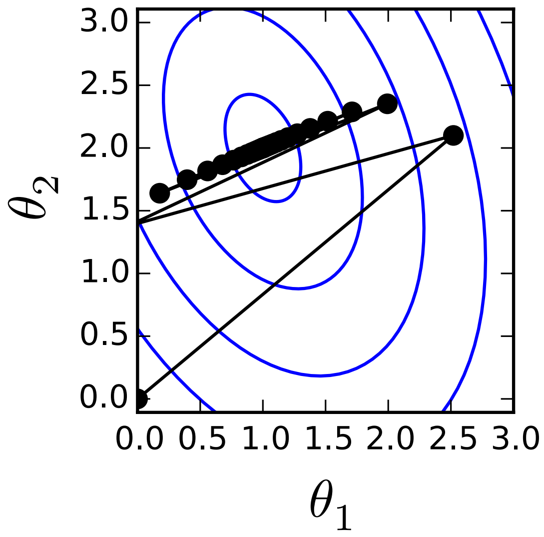
where $\alpha > 0$ is a *step size* or *learning rate*



$\alpha = 0.05$



$\alpha = 0.2$



$\alpha = 0.42$

Stochastic gradient descent

If our objective (as is the case in machine learning) is the *sum* of individual losses, we don't want to compute the gradient using all examples to make a single update to the parameters

Instead, take many gradient steps each based upon a *minibatch* (small partition of the data), to make many parameter updates using a single "pass" over data

$$
\begin{aligned}
&\text{Repeat:}\\
&\qquad \text{Sample a minibatch of data } X \in \mathbb{R}^{B \times n}, y \in \{1, \ldots, k\}^B\\
&\qquad \text{Update parameters } \theta := \theta - \frac{\alpha}{B} \sum_{i=1}^{B} \nabla_\theta \ell(h_\theta(x^{(i)}), y^{(i)})
\end{aligned}
$$

The gradient of the softmax objective

So, how do we compute the gradient for the softmax objective?

$$\nabla_\theta \ell_{ce}(\theta^T x, y) = ?$$

Let's start by deriving the gradient of the softmax loss itself: for vector $h \in \mathbb{R}^k$

$$\begin{aligned}\frac{\partial \ell_{ce}(h,y)}{\partial h_i} &= \frac{\partial}{\partial h_i}\left(-h_y + \log \sum_{j=1}^{k} \exp h_j\right) \\ &= -1\{i = y\} + \frac{\exp h_i}{\sum_{j=1}^{k} \exp h_j}\end{aligned}$$

So, in vector form: $\nabla_h \ell_{ce}(h,y) = z - e_y$, where $z = \mathrm{normalize}(\exp(\mathrm{h}))$

The gradient of the softmax objective

So how do we compute the gradient $\nabla_\theta \ell_{ce}(\theta^T x, y)$?

- The chain rule of multivariate calculus … but the dimensions of all the matrices and vectors get pretty cumbersome

Approach #1 (a.k.a. the right way): Use matrix differential calculus, Jacobians, Kronecker products, and vectorization

Approach #2 (a.k.a. the hacky quick way that everyone actually does): Pretend everything is a scalar, use the typical chain rule, and then rearrange / transpose matrices/vectors to make the sizes work 😱 (and check your answer numerically)

The slide I'm embarrassed to include…

Let's compute the "derivative" of the loss:

$$\frac{\partial}{\partial \theta} \ell_{ce}(\theta^T x, y) = \frac{\partial \ell_{ce}(\theta^T x, y)}{\partial \theta^T x} \frac{\partial \theta^T x}{\partial \theta}$$

$$= (z - e_y)(x), \qquad \left(\text{where } z = \text{normalize}(\exp(\theta^T x))\right)$$

(k-dimensional) (n-dimensional)

So to make the dimensions work…

$$\nabla_\theta \ell_{ce}(\theta^T x, y) \in \mathbb{R}^{n \times k} = x(z - e_y)^T$$

Same process works if we use "matrix batch" form of the loss

$$\nabla_\theta \ell_{ce}(X\theta, y) \in \mathbb{R}^{n \times k} = X^T(Z - I_y), \qquad Z = \text{normalize}(\exp(X\theta))$$

Putting it all together

Despite a fairly complex derivation, we should highly just how *simple* the final algorithm is

- Repeat until parameters / loss converges
    1. Iterate over minibatches $X \in \mathbb{R}^{B \times n}$, $y \in \{1, \ldots, k\}^B$ of training set
    2. Update the parameters $\theta := \theta - \frac{\alpha}{B} X^T (Z - I_y)$

That is the entirety of the softmax regression algorithm

As you will see on the homework, this gets less than 8% error in classifying MNIST digits, runs in a couple seconds

Up next time: neural networks (a.k.a. fancier hypothesis classes)