Data 188: Introduction to Deep Learning

ML Refresher / Softmax Regression

Speaker: Eric Kim
Lecture 02 (Week 01)
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Announcements

- (Week 1) No discussion, no office hours
- (Week 2) Discussion and office hours starts!
- HW0 is released! Start early!
  - See Ed post for more details: "HW0 released!"
  - ~2 weeks to complete it
  - Tip: after today's lecture, you should be able to do HW0
    - Q5: we'll cover two-layer NN's in Lecture 03, but you should be able to still do Q5 without it IMO

Enrollment, Waitlist

- **If you're on the waitlist, and you're a DS senior that is graduating in SP26/SU26 and needs Data 188 to fulfill the MLDM requirement**: please email ds-advising@berkeley.edu to get into the course

- For more info, see Ed post: "Regarding Enrollment, Waitlists"

Reminder: important links

Course Website: Course syllabus, lecture slides, discussion notes, homework assignments, staff bios, office hours times.

Edstem: where announcements are posted, and where you can ask questions.

Gradescope: Where you will submit homework assignments. Exam scores will also be here.

Lecture Zoom link: Zoom link for lectures, TuTh 3:30pm-5pm.

Lecture Recordings: lecture recordings will be uploaded within 1-2 days after lecture.

- Tip: this is the bCourses "Media Gallery".

Outline

Basics of machine learning

Example: softmax regresssion

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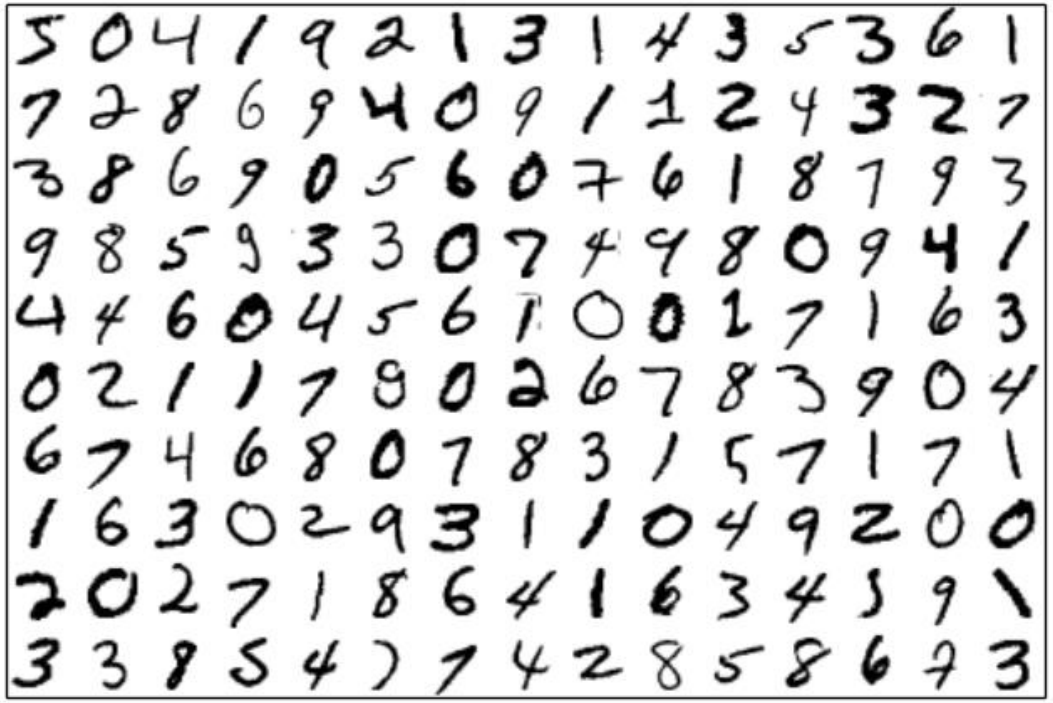
Example: softmax regresssion

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

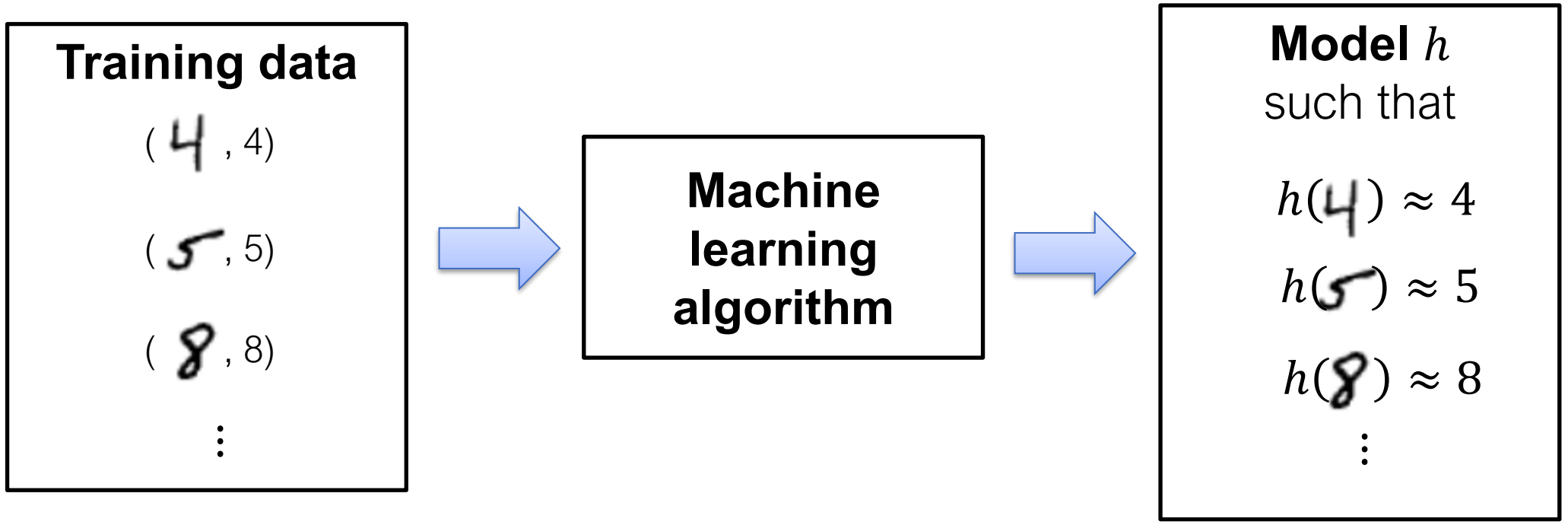
(Despite being a reasonable coder, I don't think I could do this very well)



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

Outline

Basics of machine learning

Example: softmax regresssion

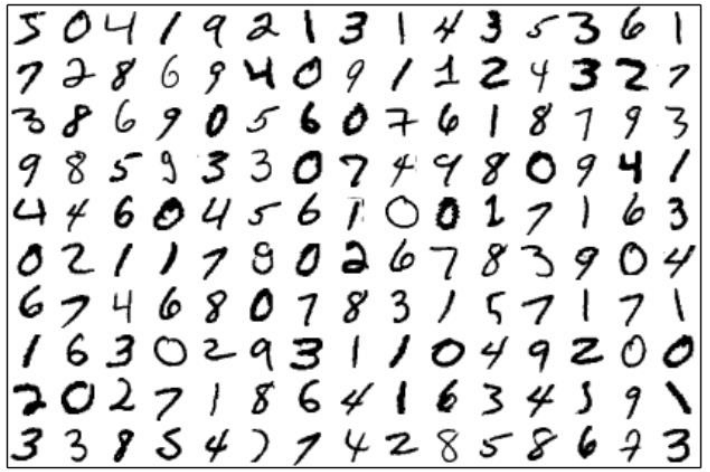
Multi-class classification setting

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

- Training data: $x^{(i)} \in \mathbb{R}^n, y^{(i)} \in \{1, \dots, k\}$ for $i = 1, \dots m$
- $n =$ 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

- $n = 28 \cdot 28 = 784$ (28x28 pixel images)
- $k = 10$ (digits 0-9)
- $m = 60{,}000$



Linear hypothesis function

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

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

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

m: batchsize
n: input dim

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

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

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

[m, n] [n, k]

Loss function #1: classification error

A simple loss function to use in classification is the classification error, i.e., whether the classifier makes a mistake 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

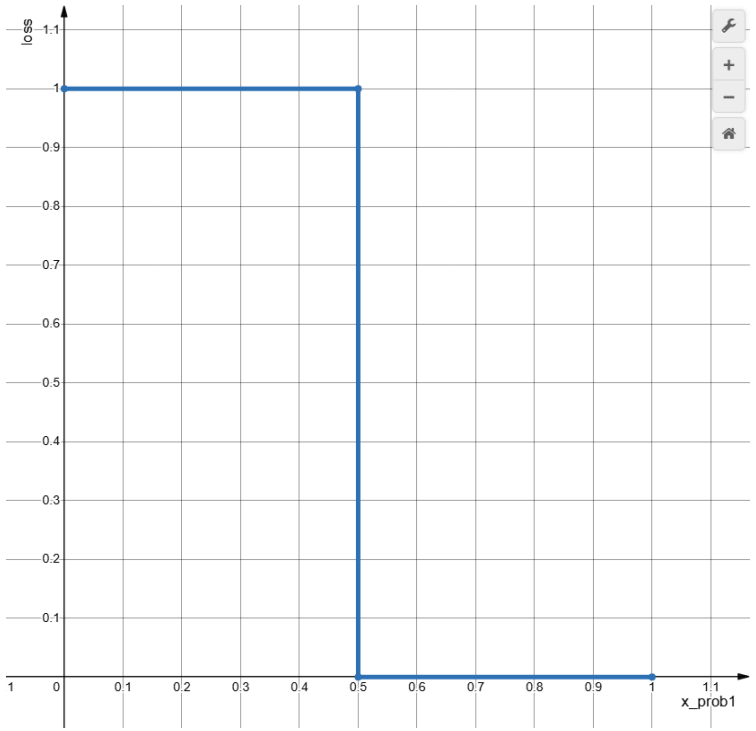
Unfortunately, the error is a bad loss function to use for *optimization*, i.e., selecting the best parameters, because it is not differentiable, and its gradient has little information

Also known as "0/1 loss".

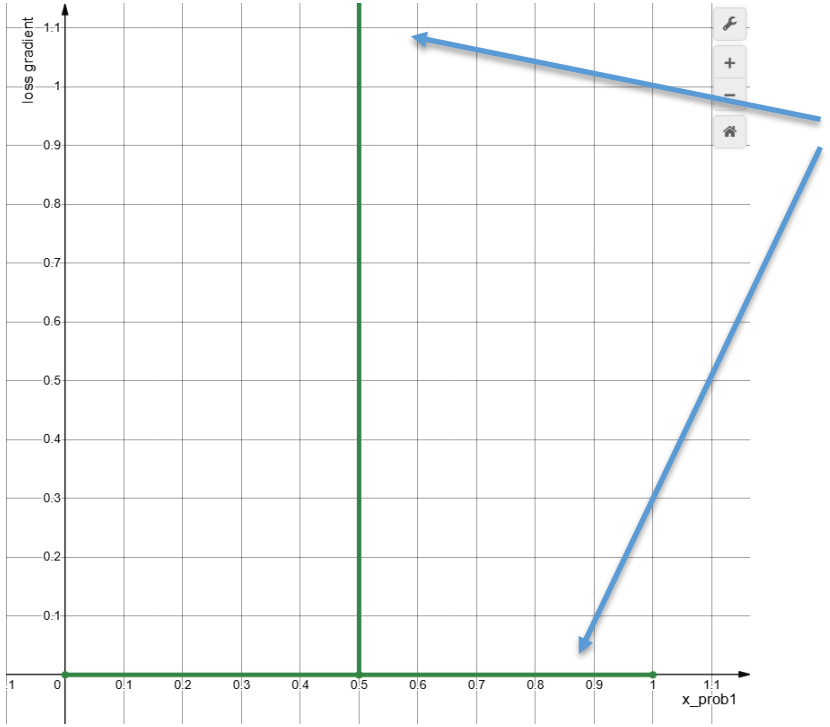
0-1 loss gradient

Suppose we have 2 classes (binary classification). Let p_{class1} denote the probability of class1. Let's view the plots of both the loss and its derivative:

$$\ell_{err}(p_{class1}, y = 1) = \begin{cases} 0 & \text{if } p_{class1} > 0.5 \\ 1 & \text{otherwise} \end{cases}$$



Loss(p_class1, y=1)



Gradient of Loss

Problem: gradient is 0 everywhere, and undefined at p_class1=0.5 (shown as infinity for visualization, though technically is undefined). Gradient descent won't work!

Loss function #2: softmax (aka 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)

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

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

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

Terminology: h(x) is called the "logits". They are values output by your model that get normalized by softmax() to probabilities.

Aside: logits

In this equation, the h(x) are known as **class logits**:

$$p(\text{label} = i) = \frac{\exp\left(h_i(x)\right)}{\sum_{j=1}^{k} \exp\left(h_j(x)\right)} \Leftrightarrow z \equiv \text{softmax}\left(h(x)\right)$$

Unlike probabilities (range [0,1]), logits are unbounded (range [-inf, +inf]).

Typically, we implement classification models by passing **predicted logits** (rather than probabilities) to loss layers (like pytorch's CrossEntropyLoss).

```
Ex: for three classes, suppose our logits are: [1, -2, 3]
>>> logits = np.array([[1, -2, 3]])
>>> probs = softmax_normalize(logits)
>>> probs
array([[0.11849965, 0.00589975, 0.8756006 ]])
>>> probs.sum()  # always sums to 1
np.float64(1.0)
```

Binary Cross Entropy (BCE)

Special case: for binary classification (positive/negative class), can simplify expressions. Let h(x) be the predicted logits for the positive class:

$$p(\text{label} = pos) = \frac{1}{1 + e^{-h(x)}}$$

Aka "sigmoid" or "logistic" function

Then, binary cross-entropy loss is:

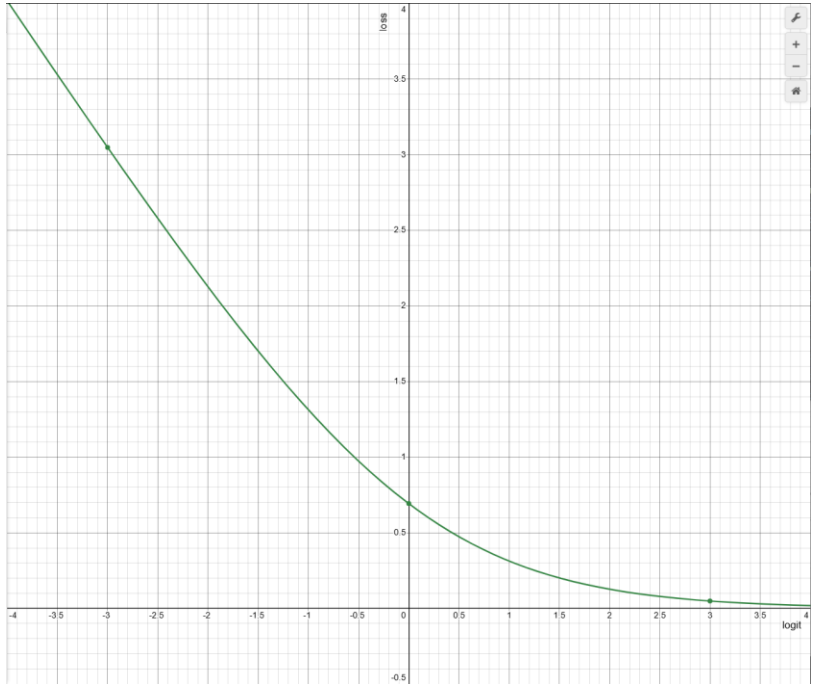
$$\ell_{bce}(h(x), y = pos) = -\log p(\text{label} = pos) = -\log(\frac{1}{1 + e^{-h(x)}})$$

BCE loss gradient

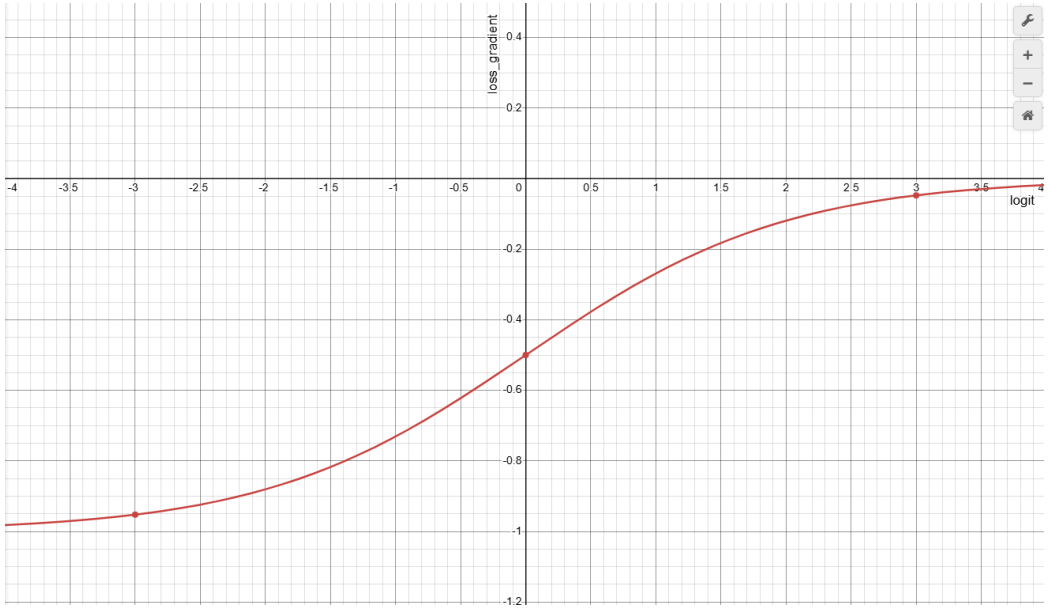
Let's view the BCE loss and its gradient:

$$\ell_{bce}(h(x), y) = -\log(\frac{1}{1 + e^{-h(x)}})$$

$$\frac{\partial}{\partial h(x)} \ell_{bce}(h(x), y = pos) = -\frac{1}{e^{h(x)} + 1}$$



Loss(p_class1, y=1)



Gradient of Loss

Gradient is smooth, continuous, and provides a "healthy" training signal! Gradient descent will work well here.

Observation: gradient is large for **confidently wrong preds**, and small for **correct preds**. Good property!

Note: dots indicate logit vals where prob=5%, 50%, and 95% confidence.

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

$$\underset{\theta}{\text{minimize}} \frac{1}{m} \sum_{i=1}^{m} \ell\left(\underbrace{h_\theta\left(x^{(i)}\right)}_{\text{model prediction}}, \underbrace{y^{(i)}}_{\text{ground truth label}}\right)$$

Means: find the model parameters θ that minimizes the training loss

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

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

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

Definition: Jacobians

For a multi-input function, multi-output function $f: \mathbb{R}^n \to \mathbb{R}^k$, the **Jacobian** of f is defined as the collection of all partial derivatives:

$$\nabla f(x) \in \mathbb{R}^{n \times k} = \begin{bmatrix} \frac{\partial f(x)_1}{\partial x_1} & \cdots & \frac{\partial f(x)_k}{\partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial f(x)_1}{\partial x_n} & \cdots & \frac{\partial f(x)_k}{\partial x_n} \end{bmatrix}$$

Note: this uses the "denominator" convention for the Jacobian, eg [n, k]. The "numerator" convention instead uses [k, n].
Different places can use different conventions, so take care!
In this course, we'll use the "denominator" convention.

Ex: if $f(x_1, x_2) = [x_1 + 3x_2,\ 2x_1x_2,\ 42], f: \mathbb{R}^2 \to \mathbb{R}^3$, then its Jacobian would be:

$$\nabla f(x) \in \mathbb{R}^{2 \times 3} = \begin{bmatrix} \frac{\partial(x_1 + 3x_2)}{\partial x_1} & \frac{\partial(2x_1x_2)}{\partial x_1} & \frac{\partial(42)}{\partial x_1} \\ \frac{\partial(x_1 + 3x_2)}{\partial x_2} & \frac{\partial(2x_1x_2)}{\partial x_2} & \frac{\partial(42)}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 1 & 2x_2 & 0 \\ 3 & 2x_1 & 0 \end{bmatrix}$$

Intuition: how much does f(x) change with respect to each of its inputs?

In ML: how much does my loss f(x) change with respect to each of its model parameters?

Tip: Jacobian "proper" shapes

Warning: in this class, we will often work with functions that accept matrices as input/output. When we define the Jacobian of these matrix-valued functions, the "true" shape of the Jacobian is still 2D, not 3D/4D.

Example: suppose f takes an [n x k] matrix, and outputs a scalar. Its Jacobian $\nabla f(x)$ has shape [n*k, 1], where the first dimension is "flattened" (eg row-wise).

Notably, the shape of $\nabla f(x)$ is NOT [n, k].

However, for convenience, people sometimes represent $\nabla f(x)$ as a matrix (shape=[n, k]) rather than as a tall vector (shape=[n*k, 1]). This is fine, as long as you recognize when this happens!

This will be important later, where it's important to keep track of matrix/Jacobian shapes.

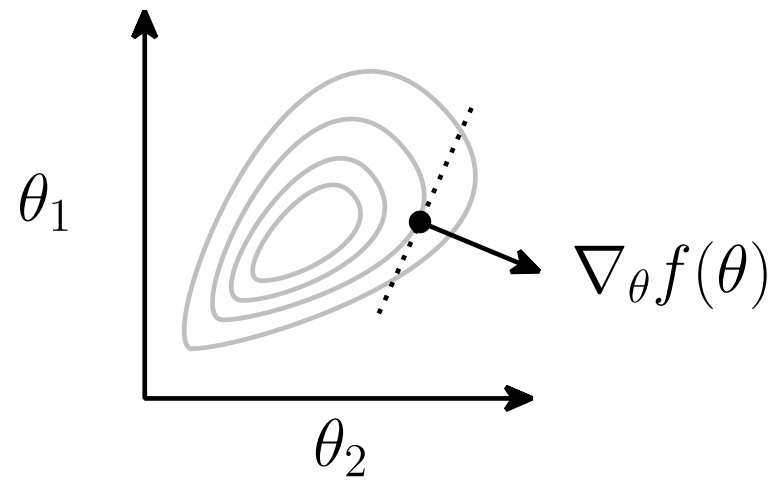
(Apologies if this doesn't make much sense right now, but it will in a few days...)

Optimization: gradient descent (1/2)

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

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

Note: the shape is actually [n*k, 1], but visualized here as [n, k] for visual clarity



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

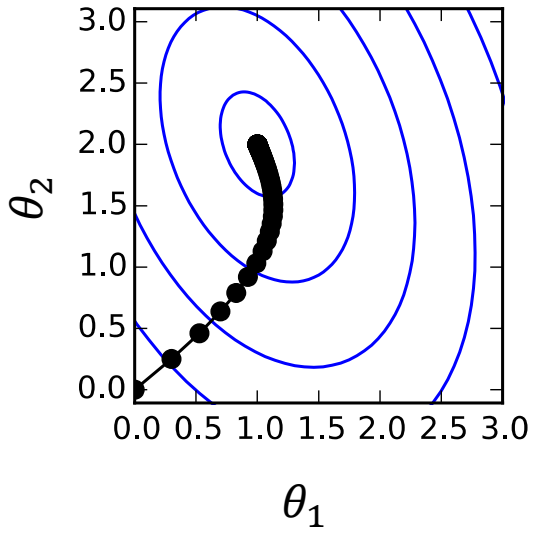
In ML, θ is our model parameters, and f is our loss function. Thus, $\nabla_\theta f(\theta)$ tells us: if I want to minimize the loss f, in which direction should I adjust my model parameters θ?

Optimization: gradient descent (2/2)

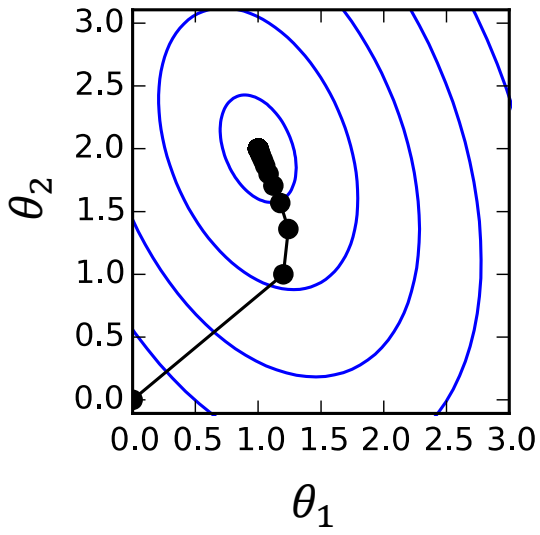
To *minimize* a function, the gradient descent algorithm proceeds by iteratively taking steps in the direction of the negative gradient

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

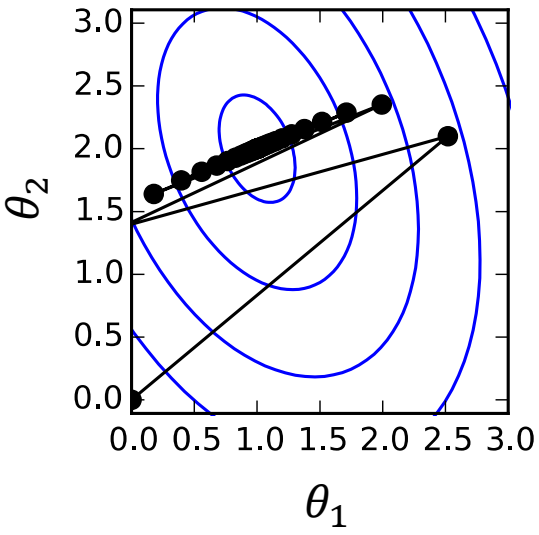
where $\alpha > 0$ is a *step size* or *learning rate*



$\alpha = 0.05$



$\alpha = 0.2$



$\alpha = 0.42$

The art of picking a good learning rate:
Too small: overly long training jobs.
Too large: unstable training, overshooting.

In practice: set empirically (a hyperparameter), eg "try a bunch of step sizes, choose the one that performs best".

"Stochastic" gradient descent (aka mini-batches)

If our objective (as is the case in machine learning) is the *sum* of individual losses, we typically 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

Repeat:

Sample a minibatch of data $X \in \mathbb{R}^{B \times n}, y \in \{1, \dots, k\}^B$

Update parameters $\theta := \theta - \frac{\alpha}{B} \sum_{i=1}^{B} \nabla_\theta \ell\left(h_\theta\left(x^{(i)}\right), y^{(i)}\right)$

Jargon: a pass over the entire dataset is called an "epoch"

The gradient of the softmax objective

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

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

One way: "brute force". Write out $\ell_{ce}(\theta^T x, y)$, and directly (by hand!) differentiate it with respect to model parameters θ. Aka "plug and chug". Labor intensive!

A more convenient way: utilize the **(multivariate) chain rule** to simplify calculations.

Multivariate chain rule

Suppose we have $z = f(y), y = g(x)$. Then:

$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y} * \frac{\partial y}{\partial x}$$

Shapes: [z.shape, x.shape] [z.shape, y.shape] [y.shape, x.shape]

Note: unlike scalar chain rule, these quantities are **matrices**, and this is **matrix multiplication**. See how the shapes are compatible with each other! Important to keep track of shapes.

Intuition: x changes z indirectly via intermediate function g(x). To find out how changes in x modify z ($\frac{\partial z}{\partial x}$): first find out how changes in y affect z ($\frac{\partial z}{\partial y}$), then scale it by how changes in x affect y ($\frac{\partial y}{\partial x}$).

Decomposes $\frac{\partial z}{\partial x}$ in terms of two (hopefully easier) derivatives $\frac{\partial z}{\partial y}, \frac{\partial y}{\partial x}$.

Spoiler alert: this will be very useful for deep learning ("backprop!")

Softmax gradient: chain rule (first term)

Let $h = \theta^T x$ (aka pred logits). Using the chain rule, the softmax loss gradient is:

$$\frac{\partial \ell_{ce}(h,y)}{\partial \theta} = \frac{\partial \ell_{ce}(h,y)}{\partial h} * \frac{\partial h}{\partial \theta}$$

[1, dim(theta)] [1, k] [k, dim(theta)]

Let's start by computing the first term:

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

[1, 1]

$$= -1\{i = y\} + \frac{\exp h_i}{\sum_{j=1}^{k} \exp h_j}$$

Means: 1 if i=y, 0 otherwise. Also written as: ∂_{iy}

e_y is the **one-hot encoding** of y, eg vector of all 0's except a 1 at index for ground-truth class y.

In vector form: $\frac{\partial \ell_{ce}(h,y)}{\partial h} = \left(z - e_y\right)^T$, where $z = \text{softmax}(h)$

[1, k]

Softmax gradient: chain rule (second term)

Recall: θ shape is [d, k], x shape is [d, 1], k is num classes.

To compute the second term $\frac{\partial h}{\partial \theta}$ (where $h = \theta^T * x$):

$$\theta^T x = \begin{bmatrix} \theta^T[0,:] * x \\ \theta^T[1,:] * x \\ \vdots \\ \theta^T[k,:] * x \end{bmatrix}$$

Tip: X[i,:] means "the i-th row", eg numpy-like notation

Observation: h[i] only depends on the i-th row of θ^T.

$$\frac{\partial h[0]}{\partial \theta} = \begin{bmatrix} \vdots & \vdots & \vdots & \vdots \\ x & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix} \quad \frac{\partial h[1]}{\partial \theta} = \begin{bmatrix} \vdots & \vdots & \vdots & \vdots \\ 0 & x & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix} \quad \cdots$$

Note: shape is [1, d*k], but for clarity I've reshaped to [d, k]

Technically, at this point we are "done"! We can calculate each of the terms of this chain rule expression to get what we want. What could go wrong...?

$$\frac{\partial \ell_{ce}(h,y)}{\partial \theta} = \frac{\partial \ell_{ce}(h,y)}{\partial h} * \frac{\partial h}{\partial \theta}$$

Shape: [1, dim(θ)] [1, k] [k, dim(θ)]

Issue: $\frac{\partial h}{\partial \theta}$ is large! Ex: ImageNet-1k has 1000 classes. Classification with >10K classes is quite common now. Can we do better?

Recall: θ shape is [d, k], x shape is [d, 1], k is num classes.

Trick: exploit structure

Let's see if we can calculate $\frac{\partial \ell_{ce}(h,y)}{\partial \theta}$ without having to explicitly create $\frac{\partial h}{\partial \theta}$:

$$\frac{\partial \ell_{ce}(h,y)}{\partial h} * \frac{\partial h}{\partial \theta} = \sum_{i=1}^{k} \frac{\partial \ell_{ce}}{\partial h[i]} * \frac{\partial h[i]}{\partial \theta} = \left(\begin{bmatrix} \vdots & \vdots & \vdots & \vdots \\ c_0 x & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix} + \begin{bmatrix} \vdots & \vdots & \vdots & \vdots \\ 0 & c_1 x & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix} + \ldots \right)$$

Where $c_i = \frac{\partial \ell_{ce}}{\partial h[i]} = z - e_y$

$$= \begin{bmatrix} \vdots & \vdots & \vdots & \vdots \\ c_0 x & c_1 x & \cdots & c_k x \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

Tip: matrix-vector mult A*x can be expressed as scaling the i-th column of A by the i-th entry in x, and summing each scaled column:

$$A * x = \sum_{i=1}^{k} A[:, i] * x[i]$$

$$= x * \left(\frac{\partial \ell_{ce}}{\partial h} \right) = x * (z - e_y)^T$$

Much easier to calculate this!

Observe that:

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} * \begin{bmatrix} y_1 & y_2 \end{bmatrix} = \begin{bmatrix} x_1 y_1 & x_1 y_2 \\ x_2 y_1 & x_2 y_2 \\ x_3 y_1 & x_3 y_2 \end{bmatrix} = \begin{bmatrix} \vdots & \vdots \\ y_1 x & y_2 x \\ \vdots & \vdots \end{bmatrix}$$

Shape check: [d, 1] * [1, k] -> [d, k] (which, when flattened row-wise) leads to [1, d*k]!

What we've done: we've taken advantage of the structure of $\frac{\partial \ell_{ce}(h,y)}{\partial h}$ and $\frac{\partial h}{\partial \theta}$ to calculate $\frac{\partial \ell_{ce}(h,y)}{\partial \theta}$ in an efficient manner.

Time, memory complexity

k classes, n input dimensionality, shape(θ)=[n, k]

$$\frac{\partial \ell_{ce}(h,y)}{\partial \theta} = \frac{\partial \ell_{ce}(h,y)}{\partial h} * \frac{\partial h}{\partial \theta}$$

Shape: [1, n∗ k] [1, k] [k, $n * k$]

Approach 1: "naive". Directly instantiate each term, and do matrix multiply.
Approach 2: Exploit structure to calculate efficiently.

	Memory	Time
Approach 1	$O(k^2n + k)$	$O(k^2n)$
Approach 2	$O(nk)$	$O(kn)$
Reduction factor	$k + \frac{1}{n} \cong k$	k

Recall: matrix multiplication of [m,n] and [n,p] matrix is O(m*n*p)

Approach 2 is k times better than Approach 1 (in both time and space!)

Data point: ResNet-50, ImageNet-1k

ResNet-50: standard convnet (2015)
ImageNet-1k: standard image classification dataset.

k=1000 classes
n=1000 (fc6)
shape(θ)=[n, k]=[1000, 1000]

$$\frac{\partial \ell_{ce}(h,y)}{\partial \theta} = \frac{\partial \ell_{ce}(h,y)}{\partial h} * \frac{\partial h}{\partial \theta}$$

Shape: [1, n∗ k] [1, k] [k, $n * k$]

Approach 1: "naive". Directly instantiate each term, and do matrix multiply.
Approach 2: Exploit structure to calculate efficiently.

	Memory (fp32), batchsize=1	Time
Approach 1	$O(k^2n + k) = 4$ GB	$O(k^2n)$
Approach 2	$O(nk) = 4\ MB$	$O(kn)$
Reduction factor	$k + \frac{1}{n} \cong k = 1000x$	$k = 1000x$

Approach 2 is **1000x** times better than Approach 1 (in both time and space!)

To train a resnet50 model on imagenet1k in pytorch: ~306 MB GPU memory (batchsize=1), (~14 GB batchsize=96)

4 GB to store $\frac{\partial h}{\partial \theta}$ is way too expensive! batchsize=96 would require 4*96=384 GB (!)

Top-of-the-line GPU cards (server) max out at **80 GB memory** (Nvidia H100, ~$25k each as of Jan 2026)

Softmax gradient: recap

Let $h = \theta^T x$ (aka pred logits). The softmax loss gradient is:

$$\frac{\partial \ell_{ce}(h, y)}{\partial \theta} = \frac{\partial \ell_{ce}(h, y)}{\partial h} * \frac{\partial h}{\partial \theta} = x * \left(z - e_y\right)^T$$

Note: shape should be [1,dim(θ)], but here it is [d, k] for clarity.

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

$$\nabla_\theta \ell_{ce}(X\theta, y) \in \mathbb{R}^{B \times k} = X^T\left(Z - I_y\right), \qquad Z = \text{softmax}(X\theta)$$

Where B is the number of samples in our batch.

I_y is the [B,k] matrix of one-hot encodings stacked on top of each other.
X has shape [B, d].
θ shape is [d, k]

Putting it all together

Despite a (somewhat long) derivation, it's neat how *simple* the final algorithm is

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

Step size

This is: $\frac{\partial \ell_{ce}(h,y)}{\partial \theta}$, aka $\nabla_\theta loss(h, y)$

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)