CS-GY 6923: Lecture 5 Linear Classification, Logistic Regression, Gradient Descent

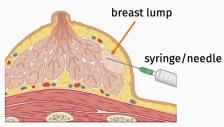
NYU Tandon School of Engineering, Prof. Christopher Musco

- We will release solutions to HW1 shortly and I will go over solutions next week in office hours.
- Lab 3 due next Tuesday.
- Written Homework 2 due the day after that. <u>No slip days</u> for this one.
- Midterm exam on Friday 10/18. We will do an optional lecture on a miscellaneous topic after the midterm.

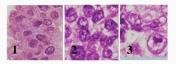
MOTIVATING PROBLEM

Breast Cancer Biopsy: Determine if a breast lump in a patient is <u>malignant</u> (cancerous) or <u>benign</u> (safe).

- Collect cells from lump using fine needle biopsy.
- Stain and examine cells under microscope.
- Based on certain characteristics (shape, size, cohesion) determine if likely malignant or not).



cross section



MOTIVATING PROBLEM

Demo: demo_breast_cancer.ipynb

Data: UCI machine learning repository

Breast Cancer Wisconsin (Original) Data Set

Download: Data Folder, Data Set Description

Abstract: Original Wisconsin Breast Cancer Database



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Data Set Characteristics:	Multivariate	Number of Instances:	699	Area:	Life
Attribute Characteristics:	Integer	Number of Attributes:	10	Date Donated	1992-07-15
Associated Tasks:	Classification	Missing Values?	Yes	Number of Web Hits:	564320

Features: 10 numerical scores about cell characteristics (Clump Thickness, Uniformity, Marginal Adhesion, etc.)

Data: $(x_1, y_1), \ldots, (x_n, y_n).$

 $\mathbf{x}_i = [1, 5, 4 \dots, 2]$ contains score values.

Label $y_i \in \{0, 1\}$ is 0 if benign cells, 1 if malignant cells.

Goal: Based on scores (which would be collected manually, or even learned on their own using an ML algorithm) predict if a sample of cells is malignant or benign.

Approach:

 Naive Bayes Classifier can be extended to x with numerical values (instead of binary values as seen before). Will see on Homework 2.

What are other classification algorithms people have heard of?

k-**NN algorithm:** a simple but powerful baseline for classification.

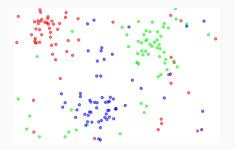
Training data: $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)$ where $y_1, \dots, y_n \in \{1, \dots, q\}$. Classification algorithm:

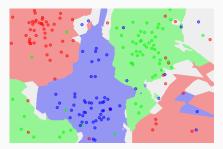
Given new input **x**_{new},

- Compute $sim(\mathbf{x}_{new}, \mathbf{x}_1), \dots, sim(\mathbf{x}_{new}, \mathbf{x}_n)$.¹
- Let $\mathbf{x}_{j_1}, \ldots, \mathbf{x}_{j_k}$ be the training data vectors with highest similarity to \mathbf{x}_{new} .
- Predict y_{new} as majority(y_{j1},..., y_{jk}). Break ties any way you want.

 $sim(\mathbf{x}_{new}, \mathbf{x}_i)$ is any chosen similarity function, like $\langle \mathbf{x}_{new}, \mathbf{x}_i \rangle$ or $-\|\mathbf{x}_{new} - \mathbf{x}_i\|_2$.

k-nearest neighbor method



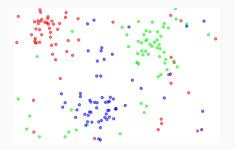


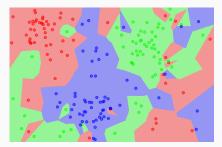
Data

5-NN classifier

- Smaller *k*, more complex classification function.
- Larger *k*, more robust to noisy labels/class overlap.

k-nearest neighbor method



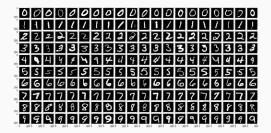


Data

1-NN classifier

- Smaller *k*, more complex classification function.
- Larger *k*, more robust to noisy labels/class overlap.

Especially good for large datasets with lots of repetition. Works well on MNIST for example:



pprox 95% Accuracy out-of-the-box.

Can be improved to 99.5% with a fancy similarity function!²

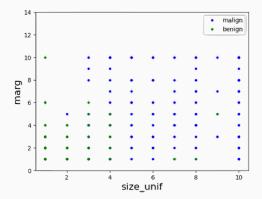
One issue is that prediction can be computationally intensive...

²We will revisit this when we talk about kernel methods.

LINEAR CLASSIFICATION

BEGIN BY PLOTTING DATA

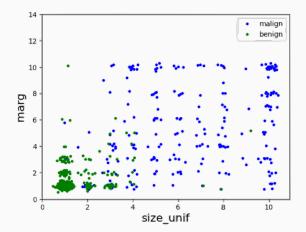
We pick two variables, <u>Marginal Adhesion</u> and <u>Size Uniformity</u> and plot a scatter plot. Points with label 1 (malignant) are plotted in blue, those with label 2 (benign) are plotted in green.



Lots of overlapping points! Hard to get a sense of the data.

PLOTTING WITH JITTER

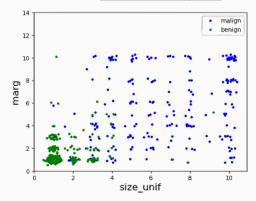
Simple + Useful Trick: data <u>jittering</u>. Add tiny random noise (using e.g. **np.random.randn**) to data to prevent overlap.



Noise is only for plotting. It is not added to the data for

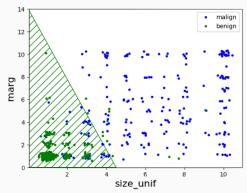
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Any ideas for possible classification rules for this data?



Given vector of predictors $\mathbf{x}_i \in \mathbb{R}^d$ (here d = 2) find a parameter vector $\boldsymbol{\beta} \in \mathbb{R}^d$ and threshold λ .

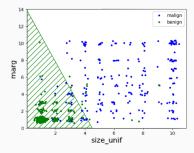
- Predict $y_i = 0$ if $\langle \mathbf{x}_i, \boldsymbol{\beta} \rangle \leq \lambda$.
- Predict $y_i = 1$ if $\langle \mathbf{x}_i, \boldsymbol{\beta} \rangle > \lambda$



Line has equation $\langle \mathbf{x}, \boldsymbol{\beta} \rangle = \lambda$.

As long as we append a 1 onto each data vector **x**_i (i.e. a column of ones onto the data matrix **X**) like we did for linear regression, an equivalent function is:

- Predict $y_i = 0$ if $\langle \mathbf{x}_i, \boldsymbol{\beta} \rangle \leq 0$.
- Predict $y_i = 1$ if $\langle \mathbf{x}_i, \boldsymbol{\beta} \rangle > 0$



Line has equation $\langle \mathbf{x}, \boldsymbol{\beta} \rangle = 0$.

$0-1 \ \mathrm{Loss}$

Question: How do we find a good linear classifier automatically?

Loss minimization approach (first attempt):

• Model³:

$$f_{\boldsymbol{\beta}}(\mathbf{x}) = \mathbb{1}\left[\langle \mathbf{x}, \boldsymbol{\beta} \rangle > 0\right]$$

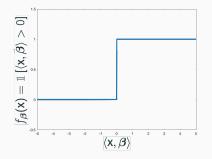
Loss function: "0 − 1 Loss"

$$L(\boldsymbol{\beta}) = \sum_{i=1}^{n} |f_{\boldsymbol{\beta}}(\mathbf{x}_i) - y_i|$$

³1[event] is the indicator function: it evaluates to 1 if the argument inside is true, 0 if false.

$0-1 \, \mathrm{Loss}$

Problem with 0 - 1 loss:



- The loss function $L(\beta)$ is not differentiable because $f_{\beta}(\mathbf{x})$ is discontinuous.
- Impossible to take the gradient, very hard to minimize loss to find optimal *β*.
- Non-convex function (will make more sense next lecture).

Loss minimization approach (second attempt):

• Model:

$$f_{\boldsymbol{\beta}}(\mathbf{x}) = \mathbb{1}\left[\langle \mathbf{x}, \boldsymbol{\beta} \rangle > 1/2\right]$$

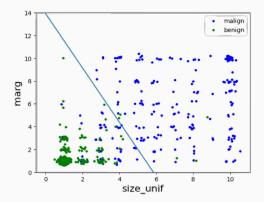
• Loss function: "Square Loss"

$$L(\boldsymbol{\beta}) = \sum_{i=1}^{n} (\langle \mathbf{x}, \boldsymbol{\beta} \rangle - y_i)^2$$

Intuitively tries to make $\langle \mathbf{x}, \boldsymbol{\beta} \rangle$ close to 0 for examples in class 0, close to 1 for examples in class 1.

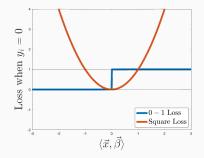
LINEAR CLASSIFIER VIA SQUARE LOSS

We can solve for β by just solving a least squares multiple linear regression problem.



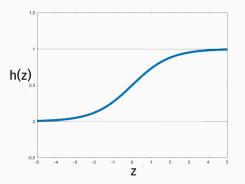
Do you see any issues here?

Problem with square loss:



- Loss increases if $\langle \mathbf{x}, \boldsymbol{\beta} \rangle > 1$ even if correct label is 1. Or if $\langle \mathbf{x}, \boldsymbol{\beta} \rangle < 0$ even if correct label is 0.
- Intuitively we don't want to "punish" these cases.





As discussed in previous lecture, can think of this function as mapping $\mathbf{x}^T \boldsymbol{\beta}$ to a probability that the true label is 1. If $\mathbf{x}^T \boldsymbol{\beta} \gg 0$ then the probability is close to 1, if $\mathbf{x}^T \boldsymbol{\beta} \ll 0$ then the probability is close to 0. Loss minimization approach (this works!):

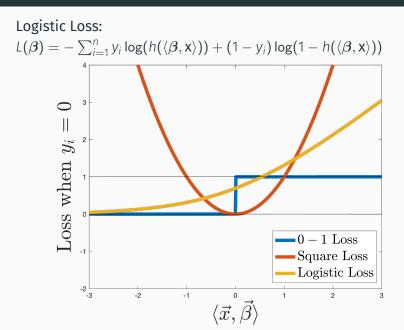
• Model:
$$h(\langle \beta, \mathbf{x} \rangle) = \frac{1}{1+e^{-\langle \beta, \mathbf{x} \rangle}}$$
.
 $f_{\beta}(\mathbf{x}) = \mathbb{1} [h(\langle \beta, \mathbf{x} \rangle) > 1/2]$

• Loss function: "Logistic loss" aka "binary cross-entropy loss"

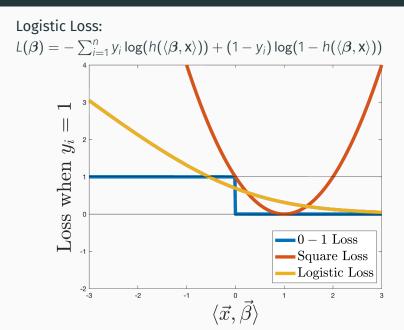
$$L(\boldsymbol{\beta}) = -\sum_{i=1}^{n} y_i \log(h(\langle \boldsymbol{\beta}, \mathbf{x} \rangle)) + (1 - y_i) \log(1 - h(\langle \boldsymbol{\beta}, \mathbf{x} \rangle))$$

 $= \mathbb{1}[\langle \mathbf{X}, \boldsymbol{\beta} \rangle > 0]$

LOGISTIC LOSS



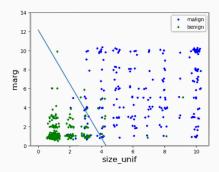
LOGISTIC LOSS



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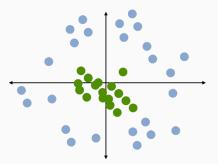
LOGISTIC LOSS

- Convex function in *β*, can be minimized using gradient descent.
- Works well in practice.
- Good Bayesian motivation (discussed last class).



Fit using logistic regression/log loss.

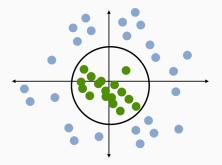
How would we learn a classifier for this data using logisitic regression?



This data is not <u>linearly separable</u> or even approximately linearly separable.

NON-LINEAR TRANSFORMATIONS

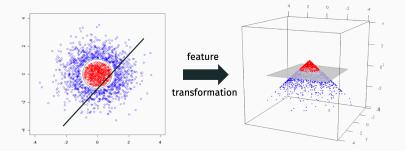
Transform each $\mathbf{x} = [x_1, x_2]$ to $\mathbf{x} = [1, x_1, x_2, x_1^2, x_2^2, x_1x_2]$



- Predict class 1 if $x_1^2 + x_2^2 \ge \lambda$.
- Predict class 0 if $x_1^2 + x_2^2 < \lambda$.

This is a <u>linear classifier</u> on our transformed data set. Logisitic regression might learn $\beta = [-\lambda, 0, 0, 1, 1, 0]$.

View as mapping data to a higher dimensional space, where it is linearly separable.

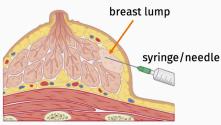


Lots more on this in future lecture!

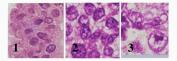
Once we have a classification algorithm, how do we judge its performance?

- **Simplest answer:** Error rate = fraction of data examples misclassified in test set.
- What are some issues with this approach?

Think back to motivating problem of breast cancer detection.



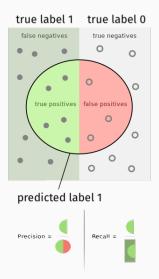
cross section



ERROR IN CLASSIFICATION

- **Precision:** Fraction of positively labeled examples (label 1) which are correct.
- **Recall:** Fraction of true positives that we labeled correctly with label 1.

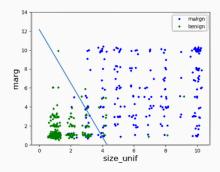
Question: Which should we optimize for medical diagnosis? (Here "positive" label means the patient has the disease.)



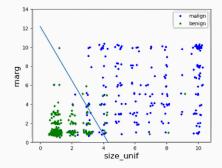
ERROR IN CLASSIFICATION

Possible logistic regression workflow:

- \cdot Learn eta using logistic loss.
- Predict $y_i = 0$ if $\langle \beta, \mathbf{x} \rangle < \lambda$, $y_i = 1$ if $\langle \beta, \mathbf{x} \rangle \ge \lambda$ where $\lambda = 0$ to start.
- Increase λ to improve precision. Decrease λ to improve recall.



CLASS IMBALANCE



One very common cause of poor precision or recall is <u>class</u> <u>imbalance</u>. A common way of dealing with this is to subsample down the larger class.

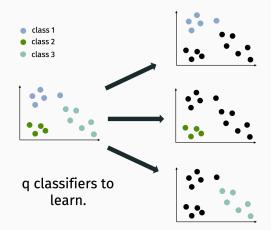
This is actually what was done with the breast cancer dataset.

What about when $y \in \{1, ..., q\}$ instead of $y \in \{0, 1\}$.

Two common options for reducing multi-class problems to binary problems:

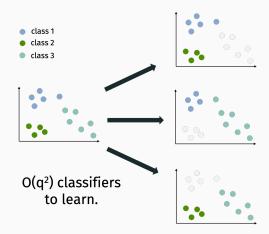
- One-vs.-all (most common, also called one-vs.-rest)
- One-vs.-one (slower, but can be more effective)

ONE VS. REST



- For q classes train q classifiers. Obtain parameters $\beta^{(1)}, \ldots, \beta^{(q)}$.
- Assign y to class i if $\langle \beta^{(i)}, \mathbf{x} \rangle \ge 0$. Could be ambiguous!
- Better: Assign y to class i with maximum value of $\langle \beta^{(i)}, \mathbf{x} \rangle$.

ONE VS. REST



- For q classes train $\frac{q(q-1)}{2}$ classifiers.
- Assign y to class which *i* which wins in the most number of head-to-head comparisons.

Hard case for one-vs.-all.



• One-vs.-one would be a better choice here.

But one-vs.-one can be super expensive! E.g when q = 100 or q = 1000.

More common modern alternative: If we have q classes, train a single model with q parameter vectors $\beta^{(1)}, \ldots, \beta^{(q)}$, and predict class $i = \arg \max_i \langle \beta^{(i)}, \mathbf{x} \rangle$.

Same idea as one-vs.-rest, but we treat $[\beta^{(1)}, \ldots, \beta^{(q)}]$ as a single length qd parameter vector which we optimize to minimize a <u>single joint loss function</u>. We do not train the parameter vectors separately.

What's a good loss function?

Softmax function:

$$\begin{bmatrix} \langle \boldsymbol{\beta}^{(1)}, \mathbf{x} \rangle \\ \vdots \\ \langle \boldsymbol{\beta}^{(q)}, \mathbf{x} \rangle \end{bmatrix} \xrightarrow{\text{softmax}} \begin{bmatrix} e^{\langle \boldsymbol{\beta}^{(1)}, \mathbf{x} \rangle} / \sum_{i=1}^{q} e^{\langle \boldsymbol{\beta}^{(i)}, \mathbf{x} \rangle} \\ \vdots \\ e^{\langle \boldsymbol{\beta}^{(q)}, \mathbf{x} \rangle} / \sum_{i=1}^{q} e^{\langle \boldsymbol{\beta}^{(i)}, \mathbf{x} \rangle} \end{bmatrix}$$

<u>Softmax</u> takes in a vector of numbers and converts it to a vector of probabilities:

$$\begin{bmatrix} -10 & 4 & 1 & 0 & -5 \end{bmatrix} \rightarrow \begin{bmatrix} .00 & .93 & .04 & .02 & .01 \end{bmatrix}$$

Multi-class cross-entropy:

$$L(\boldsymbol{\beta}^{(1)},\ldots,\boldsymbol{\beta}^{(q)}) = -\sum_{i:y_{i}=1}\log\frac{e^{\langle \boldsymbol{\beta}^{(1)},\mathbf{x}_{i}\rangle}}{\sum_{j=1}^{q}e^{\langle \boldsymbol{\beta}^{(j)},\mathbf{x}_{i}\rangle}} - \ldots - \sum_{i:y_{i}=q}\log\frac{e^{\langle \boldsymbol{\beta}^{(q)},\mathbf{x}_{i}\rangle}}{\sum_{j=1}^{q}e^{\langle \boldsymbol{\beta}^{(j)},\mathbf{x}_{i}\rangle}}$$
$$= -\sum_{i=1}^{n}\sum_{\ell=1}^{q}\mathbb{1}[y_{i}=\ell] \cdot \log\frac{e^{\langle \boldsymbol{\beta}^{(\ell)},\mathbf{x}_{i}\rangle}}{\sum_{j=1}^{q}e^{\langle \boldsymbol{\beta}^{(j)},\mathbf{x}_{i}\rangle}}$$

Binary cross-entropy:

$$L(\boldsymbol{\beta}) = -\sum_{i=1}^{n} y_i \log(h(\langle \boldsymbol{\beta}, \mathbf{x}_i \rangle)) + (1 - y_i) \log(1 - h(\langle \boldsymbol{\beta}, \mathbf{x}_i \rangle))$$
$$= -\sum_{i: y_i=1} \log(h(\langle \boldsymbol{\beta}, \mathbf{x}_i \rangle)) - \sum_{i: y_i=0} \log(1 - h(\langle \boldsymbol{\beta}, \mathbf{x}_i \rangle))$$

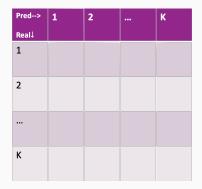
Not exactly the same... but can show equivalent if you set $\beta^{(0)} = \beta$ and $\beta^{(1)} = -\beta$.

Multi-class cross-entropy:

$$egin{aligned} &L(oldsymbol{eta}) = -\sum_{i=1}^n y_i \log(h(\langleeta, \mathbf{x}_i
angle)) + (1-y_i) \log(1-h(\langleeta, \mathbf{x}_i
angle))) \ &= -\sum_{i:y_i=1} \log(h(\langleeta, \mathbf{x}_i
angle)) - \sum_{i:y_i=0} \log(1-h(\langleeta, \mathbf{x}_i
angle))) \end{aligned}$$

ERROR IN (MULTICLASS) CLASSIFICATION

Confusion matrix for k classes:



- Entry *i*, *j* is the fraction of class *i* items classified as class *j*.
- Useful to see whole matrix to visualize where errors occur.

OPTIMIZATION

Goal: Minimize the logistic loss:

$$L(\boldsymbol{\beta}) = -\sum_{i=1}^{n} y_i \log(h(\boldsymbol{\beta}^T \mathbf{x}_i)) + (1 - y_i) \log(1 - h(\boldsymbol{\beta}^T \mathbf{x}_i))$$

I.e. find $\beta^* = \arg \min L(\beta)$. How should we do this?

$$L(\boldsymbol{\beta}) = -\sum_{i=1}^{n} y_i \log(h(\boldsymbol{\beta}^T \mathbf{x}_i)) + (1 - y_i) \log(1 - h(\boldsymbol{\beta}^T \mathbf{x}_i))$$

Let $\mathbf{X} \in \mathbb{R}^{d \times n}$ be our data matrix with $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$ as rows. Let $\mathbf{y} = [y_1, \dots, y_n]$. A calculation gives (see notes on webpage):

 $\nabla L(\boldsymbol{\beta}) = \mathbf{X}^{\mathsf{T}}(h(\mathbf{X}\boldsymbol{\beta}) - \mathbf{y})$

where $h(X\beta) = \frac{1}{1+e^{-X\beta}}$. Here all operations are entrywise. I.e in Python you would compute:

1 h = 1/(1 + np.exp(-X@beta))
2 grad = np.transpose(X)@(h - y)

LOGISTIC REGRESSION GRADIENT

To find β minimizing $L(\beta)$ we typically start by finding a β where:

$$\nabla L(\boldsymbol{\beta}) = \mathbf{X}^{\mathsf{T}} (h(\mathbf{X}\boldsymbol{\beta}) - \mathbf{y}) = \mathbf{0}$$

- In contrast to what we saw when minimizing the squared loss for linear regression, there's no simple closed form expression for such a β!
- This is <u>the typical situation</u> when minimizing loss in machine learning: linear regression was a lucky exception.
- Main question: How do we minimize a loss function L(β) when we can't explicitly compute where it's gradient is 0?

Always an option: Brute-force search. Test our many possible values for β and just see which gives the smallest value of $L(\beta)$.

- As we saw on Lab 1, this actually works okay for low-dimensional problems (e.g. when β has 1 or 2 entries).
- **Problem:** Super computationally expensive in high-dimension. For $\beta \in \mathbb{R}^d$, run time grows as:

Much Better idea. Some sort of guided search for a good of β .

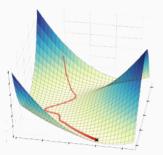
- Start with some $\beta^{(0)}$, and at each step try to change β slightly to reduce $L(\beta)$.
- Hopefully find an approximate minimizer for L(β) much more quickly than brute-force search.
- Concrete goal: Find $\boldsymbol{\beta}$ with

$$L(\boldsymbol{\beta}) < \min_{\boldsymbol{\beta}} L(\boldsymbol{\beta}) + \epsilon$$

for some small error term ϵ .

GRADIENT DESCENT

Gradient descent: A greedy search algorithm for minimizing functions of multiple variables (including loss functions) that often works amazingly well.



The single most important computational tool in machine learning. And it's remarkable simple + easy to implement.

OPTIMIZATION ALGORITHMS



Just one method in a huge class of algorithms for <u>numerical</u> <u>optimization</u>. All of these methods are important in ML.

First order oracle model: Given a function *L* to minimize, assume we can:

- Function oracle: Evaluate $L(\beta)$ for any β .
- Gradient oracle: Evaluate $\nabla L(\beta)$ for any β .

These are very general assumptions. Gradient descent will not use <u>any other information</u> about the loss function *L* when trying to find a β which minimizes *L*.

GRADIENT DESCENT

Basic Gradient descent algorithm:

- Choose starting point $\beta^{(0)}$.
- For i = 0, ..., T:

•
$$\boldsymbol{\beta}^{(i+1)} = \boldsymbol{\beta}^{(i)} - \eta \nabla L(\boldsymbol{\beta}^{(i)})$$

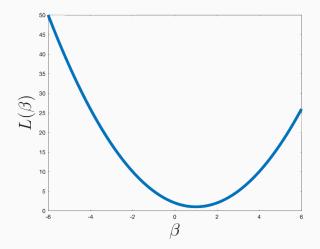
• Return $\beta^{(T)}$.

 $\eta > 0$ is a step-size parameter. Also called the learning rate.

Why does this method work?

First observation: if we actually reach the minimizer β^* then we stop.

Consider a 1-dimensional loss function. I.e. where β is just a single value. Our update step is $\beta^{(i+1)} = \beta^{(i)} - \eta L'(\beta^{(i)})$



GRADIENT DESCENT IN 1D

Mathematical way of thinking about it:

By definition, $L'(\beta) = \lim_{\Delta \to 0} \frac{L(\beta + \Delta) - L(\beta)}{\Delta}$. So for small values of Δ , we expect that:

$$L(\beta + \Delta) - L(\beta) \approx \Delta \cdot L'(\beta).$$

We want $L(\beta + \Delta)$ to be <u>smaller</u> than $L(\beta)$, so we want $\Delta \cdot L'(\beta)$ to be negative.

This can be achieved by choosing $\Delta = -L'(\beta)$, or really $\Delta = -\eta \cdot L'(\beta)$ for positive step size η .

$$\boldsymbol{\beta}^{(i+1)} = \boldsymbol{\beta}^{(i)} - \eta L'(\boldsymbol{\beta}^{(i)})$$

For high dimensional functions ($\beta \in \mathbb{R}^d$), our update involves a vector $\mathbf{v} \in \mathbb{R}^d$. At each step:

$$\boldsymbol{eta} \leftarrow \boldsymbol{eta} + \boldsymbol{\mathsf{v}}.$$

Question: When **v** is small, what's an approximation for $L(\beta + \mathbf{v}) - L(\beta)$?

$$L(eta + v) - L(eta) pprox$$

DIRECTIONAL DERIVATIVES

We have

$$L(\boldsymbol{\beta} + \mathbf{v}) - L(\boldsymbol{\beta}) \approx \frac{\partial L}{\partial \beta_1} v_1 + \frac{\partial L}{\partial \beta_2} v_2 + \ldots + \frac{\partial L}{\partial \beta_d} v_d$$
$$= \langle \nabla L(\boldsymbol{\beta}), \mathbf{v} \rangle.$$

How should we choose v so that $L(\beta + v) < L(\beta)$?

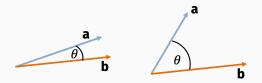
³Formally, you might remember that we can define the **directional derivative** of a multivariate function: $D_{v}L(\beta) = \lim_{\Delta \to 0} \frac{l(\beta + \Delta v) - l(\beta)}{\Delta}$.

STEEPEST DESCENT

Claim (Gradient descent = Steepest descent⁴) $\frac{-\nabla L(\beta)}{\|\nabla L(\beta)\|_2} = \arg \min_{\mathbf{v}, \|\mathbf{v}\|_2 = 1} \langle \nabla L(\beta), \mathbf{v} \rangle$

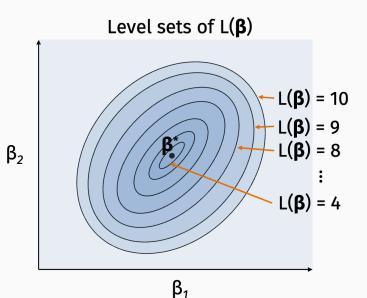
Recall: For two vectors a, b,

 $\langle \mathbf{a}, \mathbf{b} \rangle = \|\mathbf{a}\|_2 \|\mathbf{b}\|_2 \cdot \cos(\theta)$



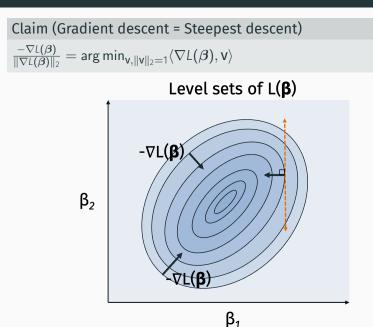
⁴We could have restricted **v** using a different norm. E.g. $\|\mathbf{v}\|_1 \leq 1$ or $\|\mathbf{v}\|_{\infty} = 1$. These choices lead to variants of generalized steepest descent...

VISUALIZING IN 2D



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STEEPEST DESCENT



Basic Gradient descent (GD) algorithm:

- Choose starting point $\beta^{(0)}$.
- For i = 0, ..., T:
 - $\boldsymbol{\beta}^{(i+1)} = \boldsymbol{\beta}^{(i)} \eta \nabla L(\boldsymbol{\beta}^{(i)})$
- Return $\beta^{(T)}$.
- **Theoretical questions:** Does gradient descent always converge to the minimum of the loss function *L*? Can you prove how quickly?
- **Practical questions:** How to choose η? Any other modifications needed for good practical performance?