Lecture 11

Gradient Descent, Continued

DSC 40A, Spring 2024

Announcements

- Midterm Exam scores are available on Gradescope, and regrade requests are due on Tuesday, May 14th at 11:59PM.
- Homework 5 will be released tomorrow, and will be due on Thursday, May 16th at 11:59PM.

Fall 2016

Class	Title	Un.	Gr.
CHEM 1A	General Chemistry	3	B-
CHEM 1AL	General Chemistry Laboratory	1	C+
COMPSCI 61A	The Structure and Interpretation of Computer Programs	4	B+
COMPSCI 70	Discrete Mathematics and Probability Theory	4	A
COMPSCI 195	Social Implications of Computer Technology	1	P
MATH 1A	Calculus	4	A+

Spring 2017

Class	Title	Un.	Gr.
COMPSCI 61B	Data Structures	4	B+
COMPSCI 97	Field Study	1	P
COMPSCI 197	Field Study	1	P
ELENG 16A	Designing Information Devices and Systems I	4	B-
MATH 110	Linear Algebra	4	C
MATH 128A	Numerical Analysis	4	B+

My freshman year transcript.

Fall 2017

Class	Title	Un.	Gr.	Pts.
COMPSCI 170	Efficient Algorithms and Intractable Problems	4.0	B-	10.8
COMPSCI 197	Field Study	2.0	P	0.0
COMPSCI 375	Teaching Techniques for Computer Science	2.0	P	0.0
COMPSCI 399	Professional Preparation: Supervised Teaching of Computer Science	1.0	P	0.0
EECS 126	Probability and Random Processes	4.0	B+	13.2
ENGIN 120	Principles of Engineering Economics	3.0	B+	9.9
SSEASN R5A	Self, Representation, and Nation	4.0	A-	14.8

Spring 2018

Class	Title	Un.	Gr.	Pts.
COMPSCI 174	Combinatorics and Discrete Probability	4.0	B	12.0
COMPSCI 189	Introduction to Machine Learning	4.0	B+	13.2
PHYSICS 7A	Physics for Scientists and Engineers	4.0	B+	13.2
SASIAN R5B	India in the Writer's Eye	4.0	B-	10.8

My sophomore year transcript.

Agenda

- Recap: Gradient descent.
- Convexity.
- More examples.
    - Huber loss.
    - Gradient descent with multiple variables.

Question 🤔

Answer at q.dsc40a.com

Remember, you can always ask questions at q.dsc40a.com!

If the direct link doesn't work, click the "🤔 Lecture Questions" link in the top right corner of dsc40a.com.

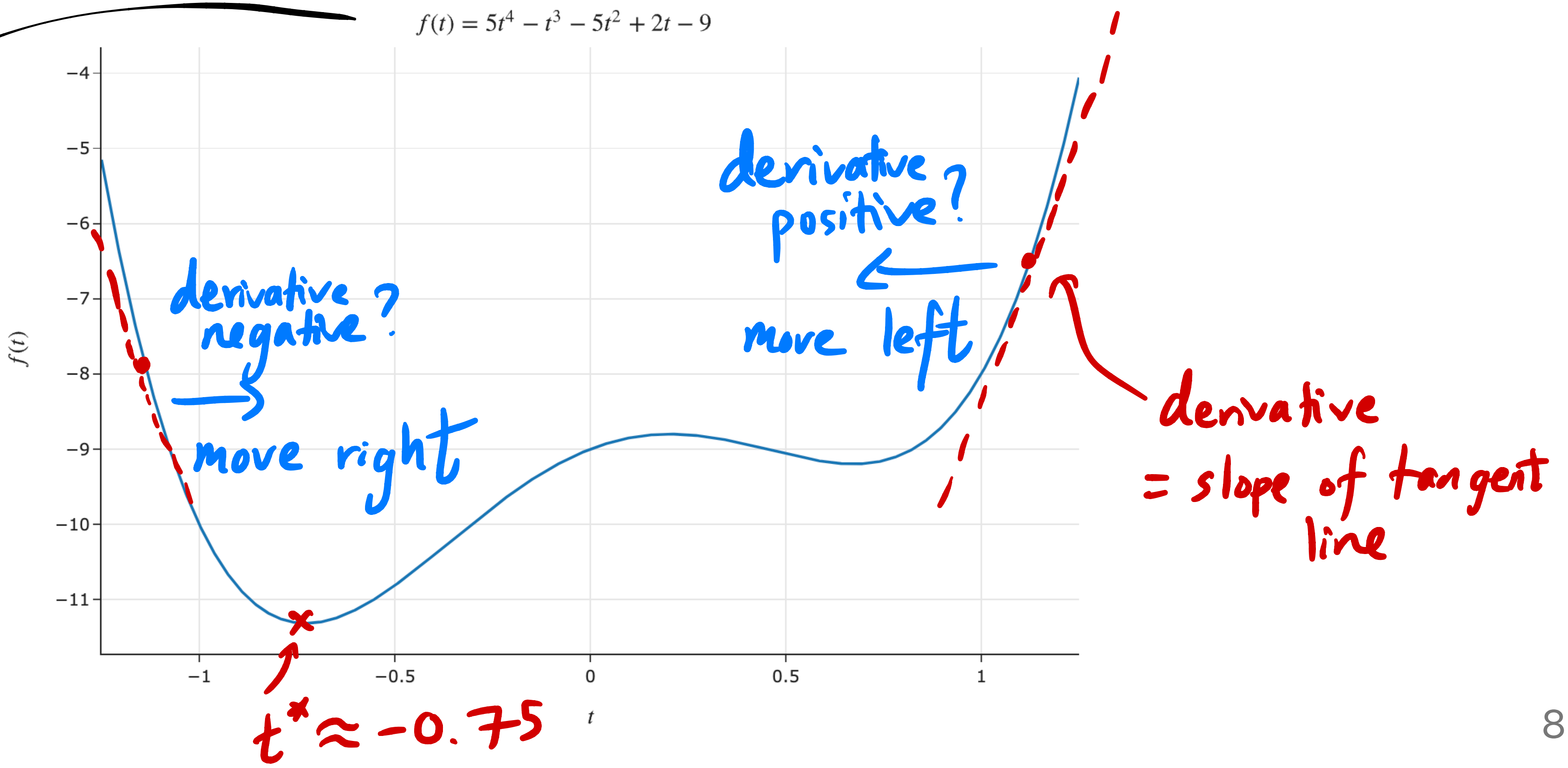
Overview: Gradient descent

derivative exists everywhere!

What's the point?

- **Goal**: Given a **differentiable** function $f(t)$, find the input t^* that minimizes $f(t)$.
- What does $\frac{d}{dt} f(t)$ mean?

Can find $\frac{df}{dt}$, but can't find where $\frac{df}{dt} = 0$.



Gradient descent

To minimize a **differentiable** function f:

- Pick a positive number, α. This number is called the **learning rate**, or **step size**.
- Pick an **initial guess**, t_0.
- Then, repeatedly update your guess using the **update rule**:

learning rate/step size

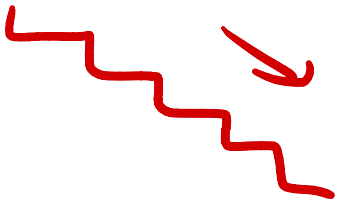
$$t_{i+1} = t_i - \alpha \frac{df}{dt}(t_i)$$

negative, because moving opposite the derivative

- Repeat this process until **convergence** – that is, when t doesn't change much.
- This procedure is called **gradient descent**.

What is gradient descent?

- Gradient descent is a numerical method for finding the input to a function f that minimizes the function.
- Why is it called **gradient** descent?



descending to the bottom!

  - The gradient is the extension of the derivative to functions of multiple variables.
  - We will see how to use gradient descent with multivariate functions next class.
- What is a **numerical** method?
  - A numerical method is a technique for approximating the solution to a mathematical problem, often by using the computer.
- Gradient descent is **widely used** in machine learning, to train models from linear regression to neural networks and transformers (includng ChatGPT)!

See dsc40a.com/resources/lectures/lec10 for animated examples of gradient descent, and see this notebook for the associated code!

Gradient descent and empirical risk minimization

- While gradient descent can minimize other kinds of differentiable functions, its most common use case is in **minimizing empirical risk**.
- For example, consider: squared loss
  - The constant model, $H(x) = h$.
  - The dataset $-4, -2, 2, 4$.
  - The initial guess $h_0 = 4$ and the learning rate $\alpha = \frac{1}{4}$.
- **Exercise**: Find h_1 and h_2.

data: $-4, -2, 2, 4$

$h_0 = 4, \ \alpha = \frac{1}{4}$

$$R_{sq}(h) = \frac{1}{n}\sum_{i=1}^{n}(y_i - h)^2$$

$$\frac{dR_{sq}}{dh} = \frac{1}{n}\sum_{i=1}^{n} 2(y_i - h)(-1)$$

$$= -\frac{2}{n}\sum_{i=1}^{n}(y_i - h)$$

$$= -\frac{2}{n}\Big(\underbrace{\sum_{i=1}^{n} y_i}_{-4-2+2+4 \,=\, 0} - \underbrace{n}_{n=4} h\Big)$$

$$= -\frac{2}{\cancel{4}}(0 - \cancel{4}h) = \boxed{2h}$$

$h_0 = 4$

$$h_1 = h_0 - \alpha \frac{dR_{sq}}{dh}(h_0)$$

$$= 4 - \frac{1}{\cancel{4}} \cdot [2 \cdot \underbrace{\cancel{4}}_{h_0}]$$

$$= 4 - 2 = \boxed{2}$$

$$h_2 = h_1 - \alpha \cdot \frac{dR_{sq}}{dh}(h_1)$$

$$= 2 - \frac{1}{4} \cdot [2 \cdot \underbrace{2}_{h_1}] = 2 - 4 \cdot \frac{1}{4} = \boxed{1}$$

$h_0 = 4$

$h_1 = 2$

$h_2 = 1$

Lingering questions

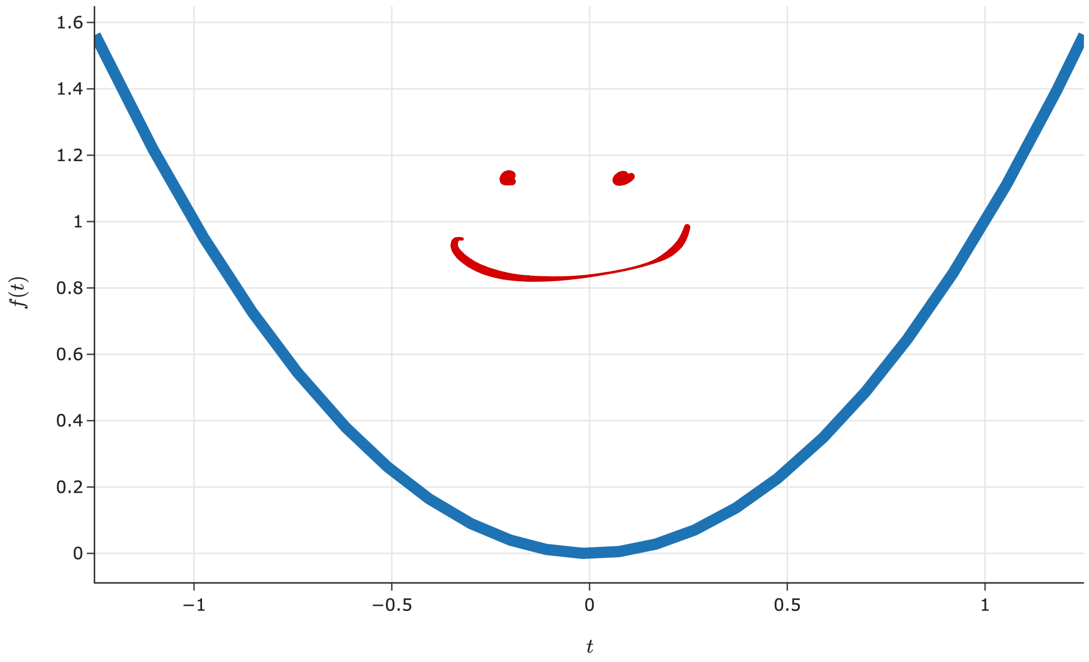
Now, we'll explore the following ideas:

- When is gradient descent *guaranteed* to converge to a global minimum?
  - What kinds of functions work well with gradient descent?
- How do I choose a step size?
- How do I use gradient descent to minimize functions of multiple variables, e.g.:

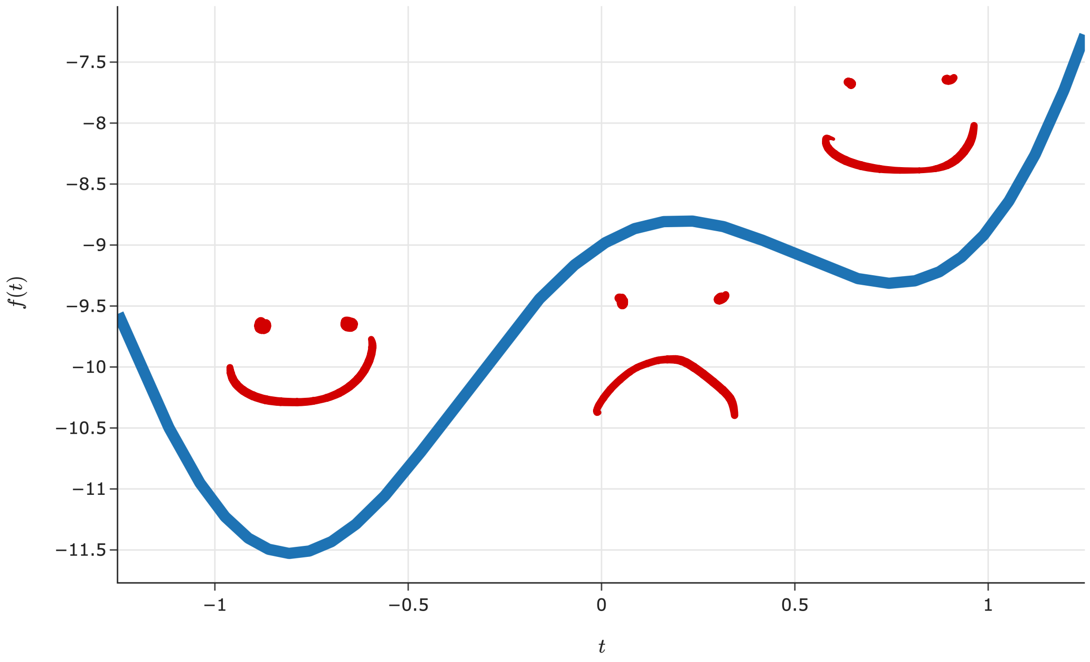
$$R_{\text{sq}}(w_0, w_1) = \frac{1}{n}\sum_{i=1}^{n}(y_i - (w_0 + w_1 x_i))^2$$

When is gradient descent guaranteed to work?

Convex functions



A **convex** function ✅



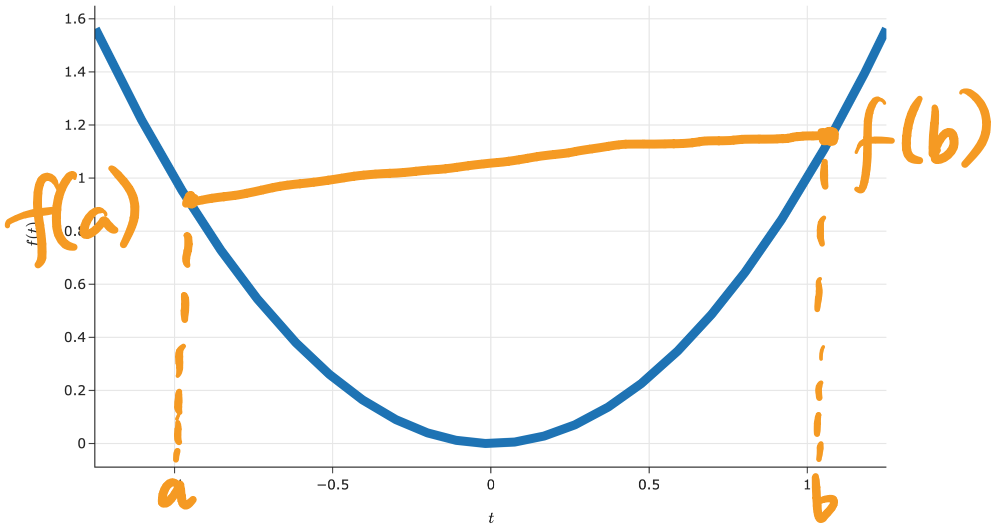
A **non-convex** function ❌

Convexity

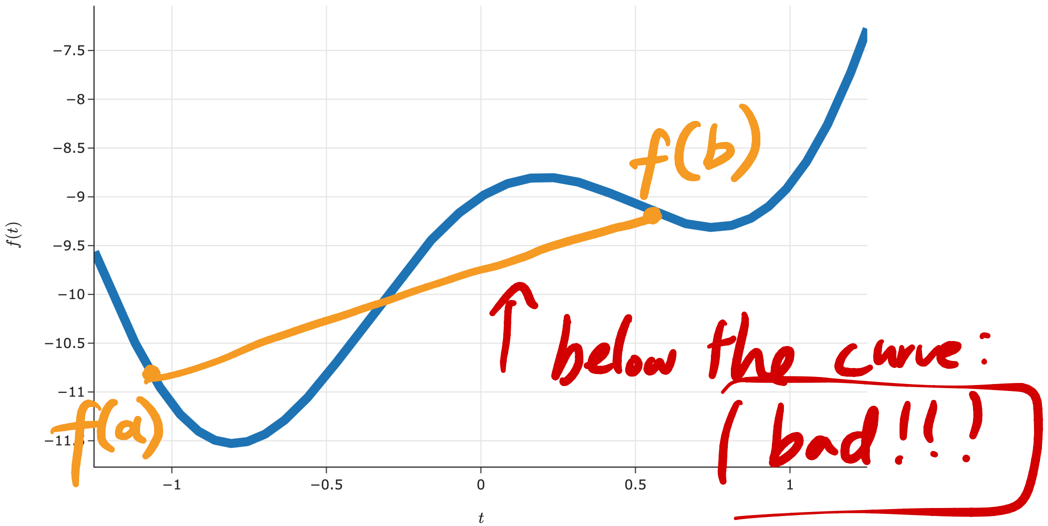
- A function f is **convex** if, for **every** a, b in the domain of f, the line segment between:

$$(a, f(a)) \text{ and } (b, f(b))$$

does not go below the plot of f.



A **convex** function ✅



A **non-convex** function ❌

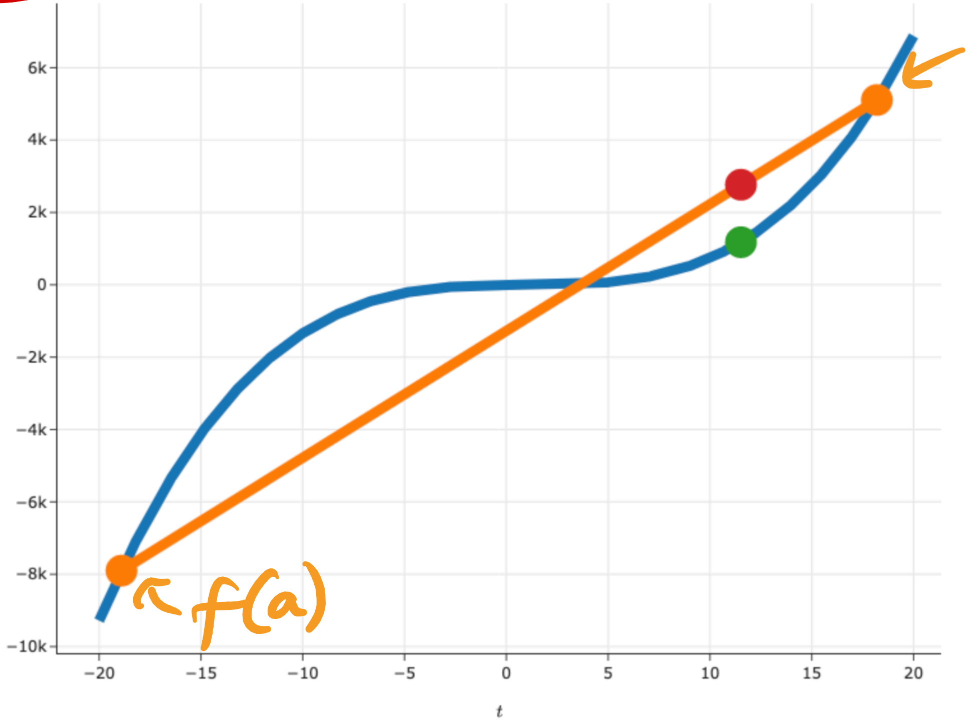
Aside: if $0 \le t \le 1$, what is
$50 + 30t$
$= (1-t)50 + 80t$

(80, 1)
(50, 0)

Formal definition of convexity

- A function $f : \mathbb{R} \to \mathbb{R}$ is **convex** if, for **every** a, b in the domain of f, and for every $t \in [0, 1]$:

$$\underbrace{(1-t)f(a) + tf(b)}_{\text{line between } f(a) \text{ and } f(b)} \geq \underbrace{f((1-t)a + tb)}_{\text{function between } x=a,\ x=b}$$



- This is a formal way of restating the definition from the previous slide.

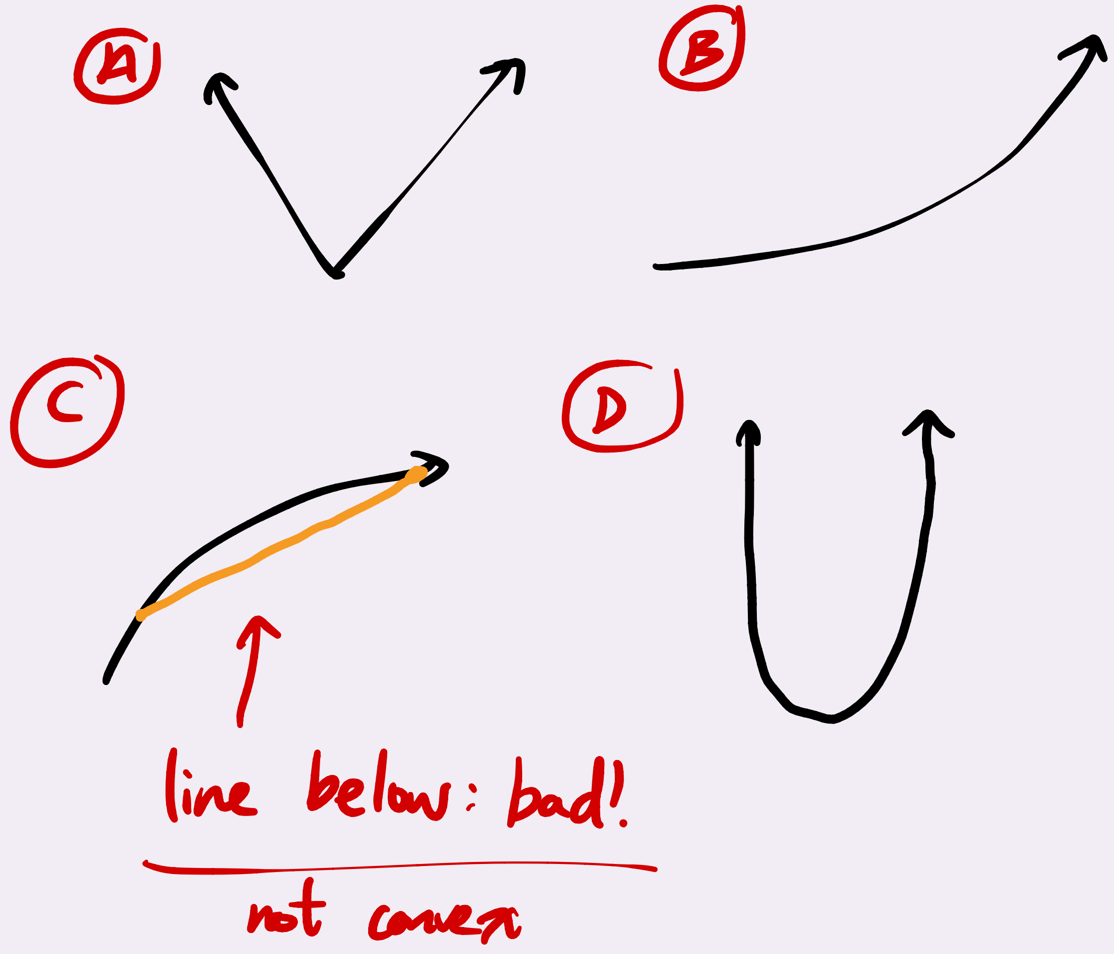
need: line ≥ function
⟺ convex

Question 🤔

Answer at q.dsc40a.com

Which of these functions are **not** convex?

- A. $f(x) = |x|$.
- B. $f(x) = e^x$.
- C. $f(x) = \sqrt{x - 1}$.
- D. $f(x) = (x - 3)^{24}$.
- E. More than one of the above are non-convex.



Second derivative test for convexity

- If $f(t)$ is a function of a single variable and is **twice** differentiable, then $f(t)$ is convex **if and only if**:

$$\frac{d^2 f}{dt^2}(t) \geq 0, \quad \underbrace{\forall}_{\text{"for all"}} t$$

- Example: $f(x) = x^4$ is convex.

$$f'(x) = 4x^3$$

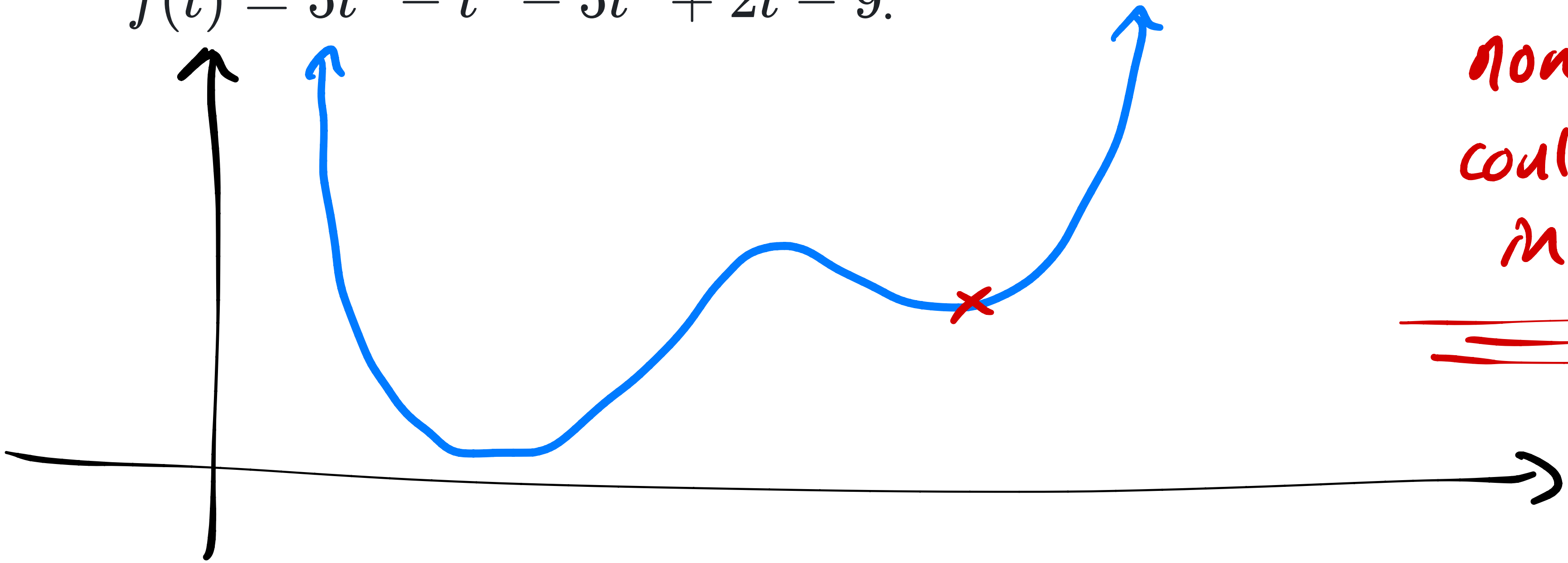
$$f''(x) = 12x^2 \geq 0 \quad \forall x$$

Why does convexity matter?

- Convex functions are (relatively) easy to minimize with gradient descent.
- **Theorem**: If $f(t)$ is convex and differentiable, then gradient descent converges to a **global minimum** of f, as long as the step size is small enough.
- **Why?**
  - Gradient descent converges when the derivative is 0.
  - For convex functions, the derivative is 0 only at one place – the global minimum.
  - In other words, if f is convex, gradient descent won't get "stuck" and terminate in places that aren't global minimums (local minimums, saddle points, etc.).

Nonconvex functions and gradient descent

- We say a function is **nonconvex** if it does not meet the criteria for convexity.
- Nonconvex functions are (relatively) difficult to minimize.
- Gradient descent **might** still work, but it's not guaranteed to find a global minimum.
  - We saw this at the start of the lecture, when trying to minimize $f(t) = 5t^4 - t^3 - 5t^2 + 2t - 9$.



non-convex:
could get stuck
in local minimum

Choosing a step size in practice

- In practice, choosing a step size involves a lot of trial-and-error.
- In this class, we've only touched on "constant" step sizes, i.e. where α is a constant.

$$t_{i+1} = t_i - \underbrace{\alpha \frac{df}{dt}(t_i)}_{}$$

- **Remember**: α is the "step size", but the amount that our guess for t changes is $\alpha \frac{df}{dt}(t_i)$, not just α.
- In future courses, you'll learn about "decaying" step sizes, where the value of α decreases as the number of iterations increases.
  - Intuition: take much bigger steps at the start, and smaller steps as you progress, as you're likely getting closer to the minimum.

More examples

$H(x) = h$

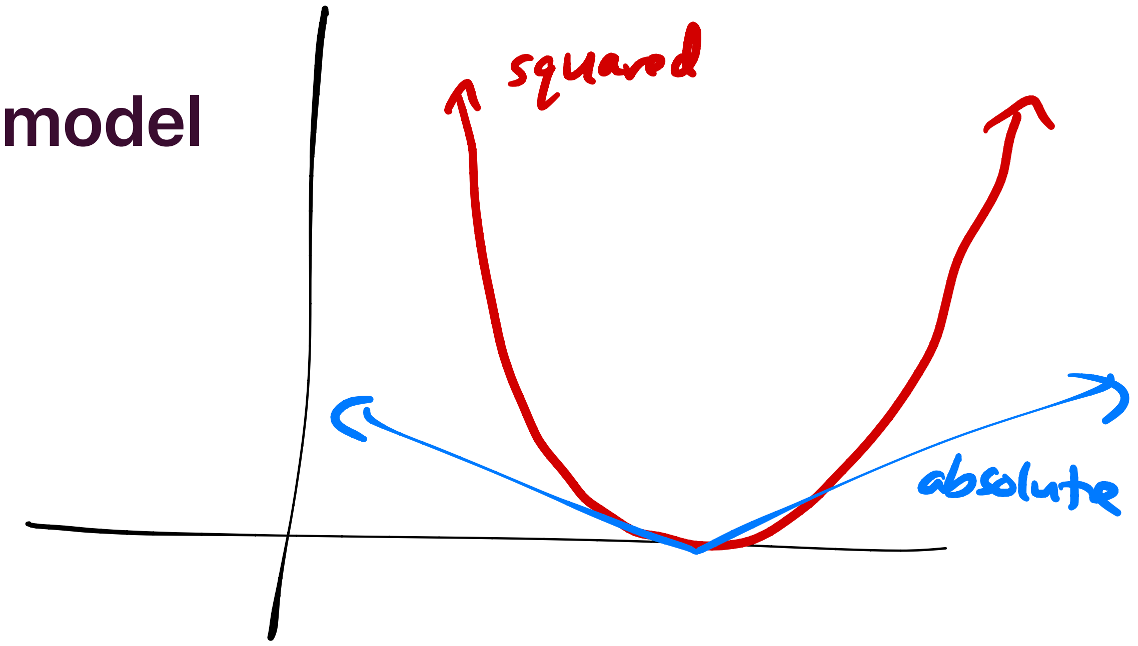
Example: Huber loss and the constant model

- First, we learned about squared loss,

  $L_{\text{sq}}(y_i, H(x_i)) = (y_i - H(x_i))^2.$

pro: differentiable, easy to minimize

con: sensitive to outliers

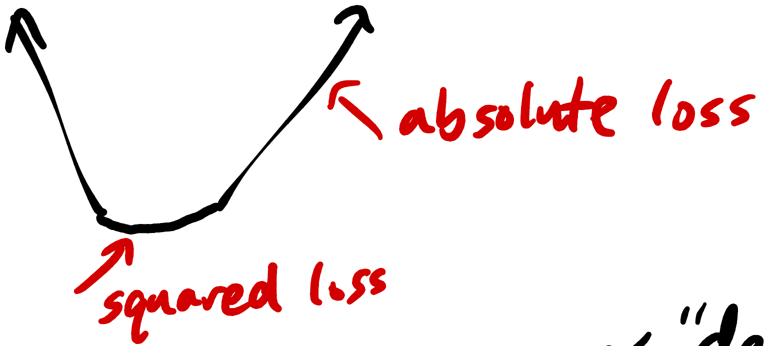


- Then, we learned about absolute loss,

  $L_{\text{abs}}(y_i, H(x_i)) = |y_i - H(x_i)|.$

pro: robust to outliers

con: not differentiable, harder to minimize

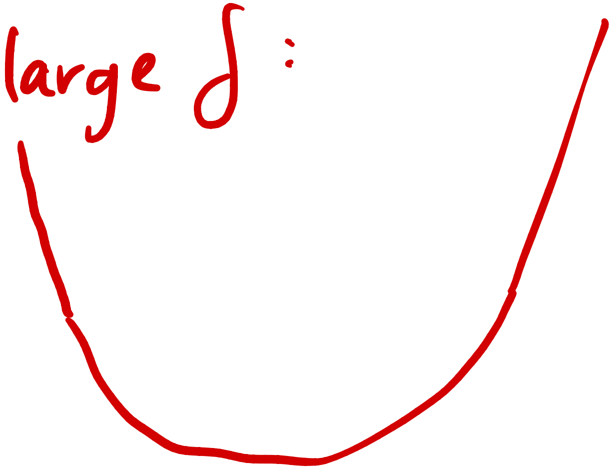


- Let's look at a new loss function, **Huber loss**:

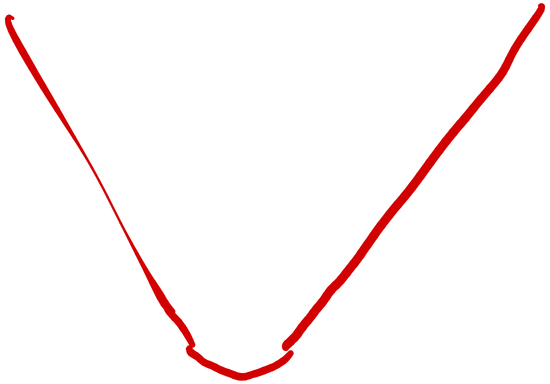
$$L_{\text{huber}}(y_i, H(x_i)) = \begin{cases} \frac{1}{2}(y_i - H(x_i))^2 & \text{if } |y_i - H(x_i)| \leq \delta \\ \delta \cdot \left(|y_i - H(x_i)| - \frac{1}{2}\delta\right) & \text{otherwise} \end{cases}$$

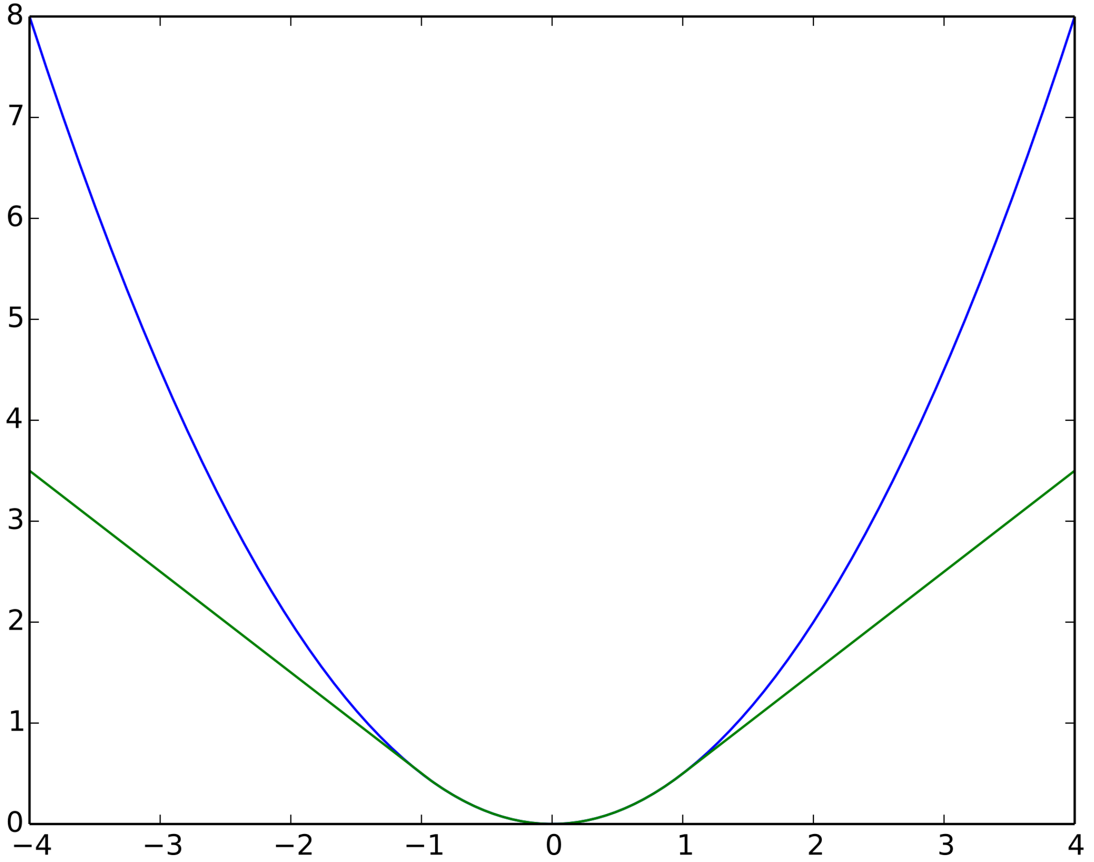
"delta"

large δ:



small δ:





Squared loss in blue, **Huber** loss in green.

Note that both loss functions are convex!

Minimizing average Huber loss for the constant model

- For the constant model, $H(x) = h$:

$$L_{\text{huber}}(y_i, h) = \begin{cases} \frac{1}{2}(y_i - h)^2 & \text{if } |y_i - h| \leq \delta \\ \delta \cdot (|y_i - h| - \frac{1}{2}\delta) & \text{otherwise} \end{cases}$$

$$\implies \quad \frac{\partial L}{\partial h}(h) = \begin{cases} -(y_i - h) & \text{if } |y_i - h| \leq \delta \\ -\delta \cdot \text{sign}(y_i - h) & \text{otherwise} \end{cases}$$

- So, the **derivative** of empirical risk is:

$$\frac{dR_{\text{huber}}}{dh}(h) = \frac{1}{n} \sum_{i=1}^{n} \begin{cases} -(y_i - h) & \text{if } |y_i - h| \leq \delta \\ -\delta \cdot \text{sign}(y_i - h) & \text{otherwise} \end{cases}$$

- It's **impossible** to set $\frac{dR_{\text{huber}}}{dh}(h) = 0$ and solve by hand: we need gradient descent!

Let's try this out in practice! Follow along in this notebook.

Minimizing functions of multiple variables

- Consider the function:

$$f(x_1, x_2) = (x_1 - 2)^2 + 2x_1 - (x_2 - 3)^2$$

- It has two **partial derivatives**: $\frac{\partial f}{\partial x_1}$ and $\frac{\partial f}{\partial x_2}$.

$$\frac{\partial f}{\partial x_1} = 2(x_1 - 2) + 2 = 2x_1 - 4 + 2 = \boxed{2x_1 - 2}$$

$$\frac{\partial f}{\partial x_2} = \boxed{-2(x_2 - 3)}$$

$$\nabla f(\vec{x}) = \begin{bmatrix} 2x_1 - 2 \\ -2(x_2 - 3) \end{bmatrix}$$

"nabla" ∇

The gradient vector

- If $f(\vec{x})$ is a function of multiple variables, then its **gradient**, $\nabla f(\vec{x})$, is a vector containing its partial derivatives.

$$\vec{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$f : \mathbb{R}^2 \to \mathbb{R}$$

- Example:

$$f(\vec{x}) = (x_1 - 2)^2 + 2x_1 - (x_2 - 3)^2$$

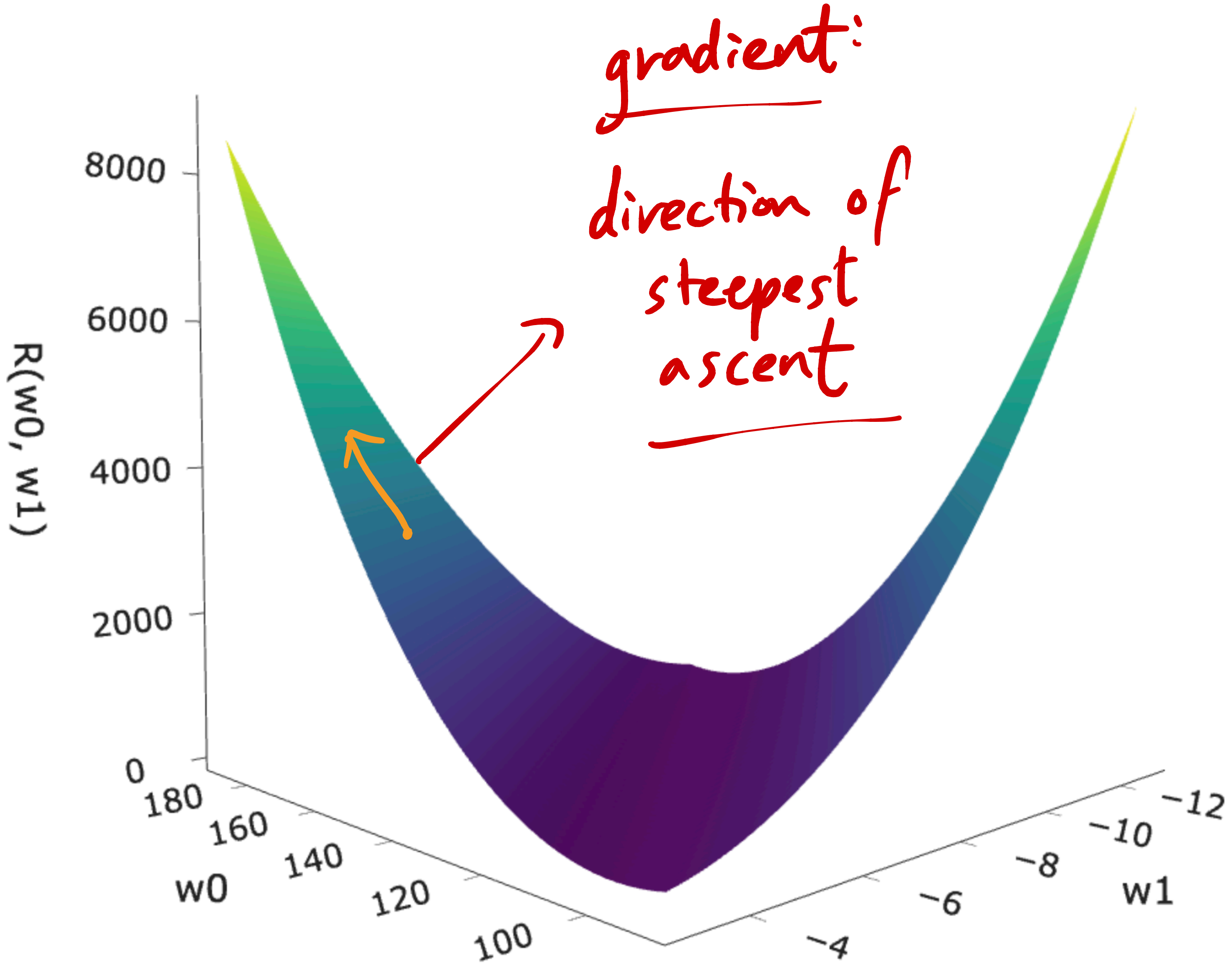
$$\nabla f(\vec{x}) = \begin{bmatrix} 2x_1 - 2 \\ -(2x_2 - 6) \end{bmatrix}$$

- Example:

scalar !

$$f(\vec{x}) = \vec{x}^T \vec{x} = x_1^2 + x_2^2 + \dots + x_n^2 \qquad \frac{\partial f}{\partial x_i} = 2x_i$$

$$\implies \nabla f(\vec{x}) = \begin{bmatrix} 2x_1 \\ 2x_2 \\ \vdots \\ 2x_n \end{bmatrix} = 2\vec{x}$$


gradient:
direction of steepest ascent
R(w0, w1)
8000
6000
4000
2000
0
180
160
140
120
100
w0
−4
−6
−8
−10
−12
w1

Gradient descent for functions of multiple variables

- Example:

$$f(x_1, x_2) = (x_1 - 2)^2 + 2x_1 - (x_2 - 3)^2$$

$$\nabla f(\vec{x}) = \begin{bmatrix} 2x_1 - 2 \\ -(2x_2 - 6) \end{bmatrix}$$

- The minimizer of f is a vector, $\vec{x}^* = \begin{bmatrix} x_1^* \\ x_2^* \end{bmatrix}$.
- We start with an initial guess, $\vec{x}^{(0)}$, and step size α, and update our guesses using:

$$\vec{x}^{(i+1)} = \vec{x}^{(i)} - \alpha \nabla f(\vec{x}^{(i)})$$

Exercise

$$f(x_1, x_2) = (x_1 - 2)^2 + 2x_1 - (x_2 - 3)^2$$

$$\nabla f(\vec{x}) = \begin{bmatrix} 2x_1 - 2 \\ -(2x_2 - 6) \end{bmatrix}$$

$$\vec{x}^{(i+1)} = \vec{x}^{(i)} - \alpha \nabla f(\vec{x}^{(i)})$$

Given an initial guess of $\vec{x}^{(0)} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ and a step size of $\alpha = \frac{1}{3}$, perform **two** iterations of gradient descent. What is $\vec{x}^{(2)}$?

$$\vec{x}^{(1)} = \vec{x}^{(0)} - \alpha \nabla f(\vec{x}^{(0)}) = \begin{bmatrix} 0 \\ 0 \end{bmatrix} - \frac{1}{3}\begin{bmatrix} 2\cdot 0 - 2 \\ -(2\cdot 0 - 6) \end{bmatrix}$$

$$= -\frac{1}{3}\begin{bmatrix} -2 \\ 6 \end{bmatrix} = \begin{bmatrix} 2/3 \\ -2 \end{bmatrix}$$

$$\vec{x}^{(2)} = \begin{bmatrix} 2/3 \\ -2 \end{bmatrix} - \frac{1}{3}\begin{bmatrix} 2\cdot\frac{2}{3} - 2 \\ -(2(-2) - 6) \end{bmatrix}$$

Example: Gradient descent for simple linear regression

- To find optimal model parameters for the model $H(x) = w_0 + w_1 x$ and squared loss, we minimized empirical risk:

$$R_{\text{sq}}(w_0, w_1) = \frac{1}{n} \sum_{i=1}^{n} (y_i - (w_0 + w_1 x_i))^2$$

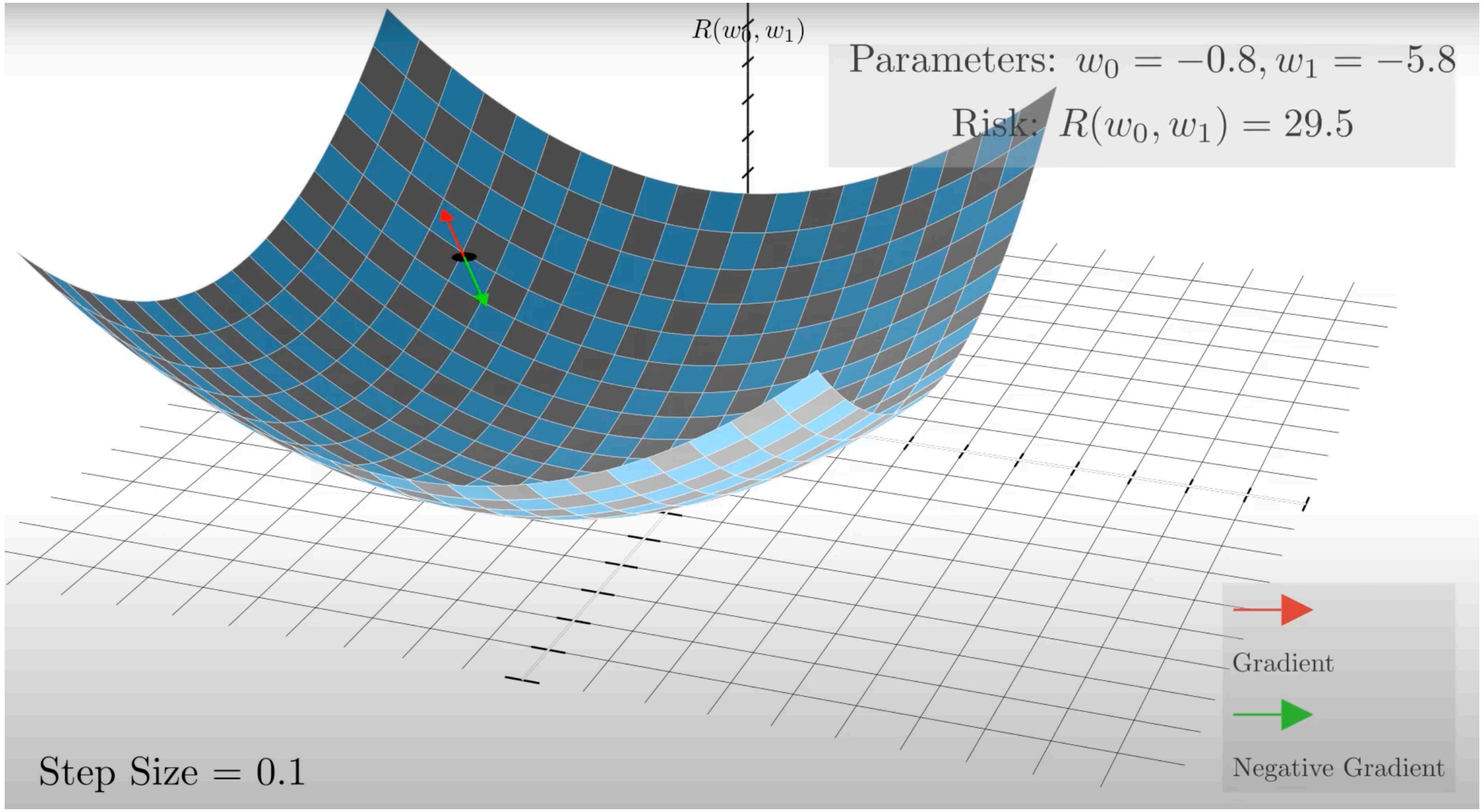
- This is a function of multiple variables, and is differentiable, so it has a gradient!

$$\nabla R(\vec{w}) = \begin{bmatrix} -\frac{2}{n} \sum_{i=1}^{n} (y_i - (w_0 + w_1 x_i)) \\ -\frac{2}{n} \sum_{i=1}^{n} (y_i - (w_0 + w_1 x_i)) x_i \end{bmatrix} \begin{matrix} = 0 \\ = 0 \end{matrix}$$

before:

- **Key idea**: To find w_0^* and w_1^*, we *could* use gradient descent!

Gradient descent for simple linear regression, visualized



Let's watch 🎥 this animation that Jack made.

What's next?

- In Homework 5, you'll see a few questions involving today's material:
  - A question about convexity.
  - A question about implementing gradient descent to find optimal parameters for a model that is **not linear in its parameters**.
- On Tuesday, we'll start talking about probability.
  - Homework 5 will have a probability problem taken from a past DSC 10 exam, to help you refresh.