Lecture 4 – Spread, Other Loss Functions, Gradient Descent

DSC 40A, Fall 2022 @ UC San Diego

Dr. Truong Son Hy, with help from **many others**

Announcements

- Look at the readings linked on the course website!

- First Discussion: Monday, October 3rd 2022
  First Homework Release: Friday September 30th 2022
  First Groupwork Release: Thursday September 29th 2022
  Groupwork Relsease Day: Thursday afternoon
  Groupwork Submission Day: Monday midnight
  Homework Release Day: Friday after lecture
  Homework Submission Day: Friday before

- See `dsc40a.com/calendar` for the Office Hours schedule.

Agenda

- Recap of empirical risk minimization.
- Center and spread.
- A new loss function.
- Gradient descent.

Recap of empirical risk minimization

Empirical risk minimization

- **Goal**: Given a dataset $y_1, y_2, ..., y_n$, determine the best prediction h^*.

- Strategy:
  1. Choose a **loss function**, $L(h, y)$, that measures how far any particular prediction h is from the "right answer" y.

  2. Minimize **empirical risk** (also known as average loss) over the entire dataset. The value(s) of h that minimize empirical risk are the resulting "best predictions".

$$R(h) = \frac{1}{n} \sum_{i=1}^{n} L(h, y_i)$$

Absolute loss and squared loss

- General form of empirical risk:

$$R(h) = \frac{1}{n} \sum_{i=1}^{n} L(h, y_i)$$

- **Absolute loss**: $L_{\text{abs}}(h, y) = |y - h|$.
  - Empirical risk: $R_{abs}(h) = \frac{1}{n} \sum_{i=1}^{n} |y_i - h|$. Also called "**mean absolute error**".
  - Minimized by $h^* =$ **Median**$(y_1, y_2, ..., y_n)$.

- **Squared loss**: $L_{\text{sq}}(h, y) = (y - h)^2$.
  - Empirical risk: $R_{sq}(h) = \frac{1}{n} \sum_{i=1}^{n} (y_i - h)^2$. Also called "**mean squared error**".
  - Minimized by $h^* =$ **Mean**$(y_1, y_2, ..., y_n)$.

Discussion Question

Consider a dataset $y_1, y_2, ..., y_n$.
Recall,

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

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

Is it true that, for any h, $[R_{abs}(h)]^2 = R_{sq}(h)$?

a) True
b) False

Discussion Question

Consider a dataset $y_1, y_2, ..., y_n$.
Recall,

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

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

Is it true that, for any h, $[R_{abs}(h)]^2 = R_{sq}(h)$?

a) True
b) False

Answer: False. But why?

Absolute and square loss

Cauchy-Schwarz (Bunyakovsky)'s inequality:

$$(a_1 b_1 + a_2 b_2 + \ldots + a_n b_n)^2 \leq (a_1^2 + a_2^2 + \ldots + a_n^2)(b_1^2 + b_2^2 + \ldots + b_n^2)$$

or in summation form:

$$\left(\sum_{i=1}^{n} a_i b_i \right)^2 \leq \left(\sum_{i=1}^{n} a_i^2 \right)\left(\sum_{i=1}^{n} b_i^2 \right)$$

or in vector with inner product & norm form:

$$\langle \underline{a}, \underline{b} \rangle \leq ||\underline{a}|| \cdot ||\underline{b}||$$

where $\underline{a} = (a_1, \ldots, a_n)^T$ and $\underline{b} = (b_1, \ldots, b_n)^T$.

Absolute and square loss

Keep in mind that:

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \leq \left(\sum_{i=1}^{n} a_i^2\right)\left(\sum_{i=1}^{n} b_i^2\right)$$

We have:

$$[R_{abs}(h)]^2 = \left(\sum_{i=1}^{n} \frac{1}{n}|y_i - h|\right)^2 \leq \left(\sum_{i=1}^{n} \frac{1}{n^2}\right)\left(\sum_{i=1}^{n}(y_i - h)^2\right)$$

The right hand side is:

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

Therefore:

$$[R_{abs}(h)]^2 \leq R_{sq}(h)$$

Center and spread

What does it mean?

- General form of empirical risk:

$$R(h) = \frac{1}{n} \sum_{i=1}^{n} L(h, y_i)$$

- The input h^* that minimizes $R(h)$ is some measure of the **center** of the data set.
  - e.g. median, mean, mode.

- The minimum output $R(h^*)$ represents some measure of the **spread**, or variation, in the data set.

Absolute loss

- The empirical risk for the absolute loss is

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

- $R_{abs}(h)$ is minimized at $h^* = \text{Median}(y_1, y_2, \dots, y_n)$.

- Therefore, the minimum value of $R_{abs}(h)$ is

$$\begin{aligned} R_{abs}(h^*) &= R_{abs}(\text{Median}(y_1, y_2, \dots, y_n)) \\ &= \frac{1}{n} \sum_{i=1}^{n} |y_i - \text{Median}(y_1, y_2, \dots, y_n)|. \end{aligned}$$

Mean absolute deviation from the median

- The minimum value of $R_{abs}(h)$ is the **mean absolute deviation from the median**.

$$\frac{1}{n}\sum_{i=1}^{n}|y_i - \text{Median}(y_1, y_2, \dots, y_n)|$$

- It measures how far each data point is from the median, on average.

Discussion Question

For the data set $2, 3, 3, 4$, what is the mean absolute deviation from the median?

a) 0 b) $\frac{1}{2}$ c) 1 d) 2

Mean absolute deviation from the median

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Discussion Question

For the data set $2, 3, 3, 4$, what is the mean absolute deviation from the median?

a) 0 b) $\frac{1}{2}$ c) 1 d) 2

Answer: B.

Squared loss

- The empirical risk for the squared loss is

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

- $R_{\text{sq}}(h)$ is minimized at $h^* = \text{Mean}(y_1, y_2, \dots, y_n)$.

- Therefore, the minimum value of $R_{\text{sq}}(h)$ is

$$\begin{aligned} R_{\text{sq}}(h^*) &= R_{\text{sq}}(\text{Mean}(y_1, y_2, \dots, y_n)) \\ &= \frac{1}{n}\sum_{i=1}^{n}(y_i - \text{Mean}(y_1, y_2, \dots, y_n))^2. \end{aligned}$$

Variance

- The minimium value of $R_{\text{sq}}(h)$ is the mean squared deviation from the mean, more commonly known as the **variance**.

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - \text{Mean}(y_1, y_2, \ldots, y_n))^2$$

- It measures the squared distance of each data point from the mean, on average.

- Its square root is called the **standard deviation.**

0-1 loss

- The empirical risk for the 0-1 loss is

$$R_{0,1}(h) = \frac{1}{n} \sum_{i=1}^{n} \begin{cases} 0, & \text{if } h = y_i \\ 1, & \text{if } h \neq y_i \end{cases}$$

- This is the proportion (between 0 and 1) of data points not equal to h.

- $R_{0,1}(h)$ is minimized at $h^* = \text{Mode}(y_1, y_2, \ldots, y_n)$.

- Therefore, $R_{0,1}(h^*)$ is the proportion of data points not equal to the mode.

A poor way to measure spread

- The minimium value of $R_{0,1}(h)$ is the proportion of data points not equal to the mode.

- A higher value means less of the data is clustered at the mode.

- Just as the mode is a very simplistic way to measure the center of the data, this is a very crude way to measure spread.

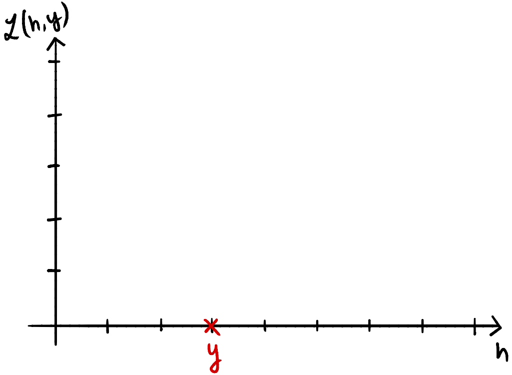
Summary of center and spread

- Different loss functions lead to empirical risk functions that are minimized at various measures of **center**.
- The minimum values of these risk runctions are various measures of **spread**.

A new loss function

Plotting a loss function

- The plot of a loss function tells us how it treats outliers.
- Consider y to be some fixed value. Plot $L_{\text{abs}}(h, y) = |y - h|$:



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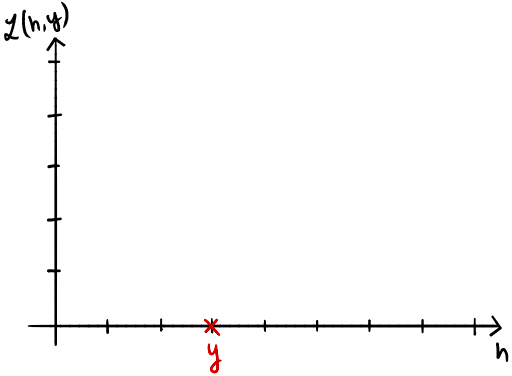


Discussion Question

Suppose L considers all outliers to be equally as bad. What would it look like far away from y?

a) flat

b) rapidly decreasing

c) rapidly increasing

Discussion Question

Suppose L considers all outliers to be equally as bad. What would it look like far away from y?

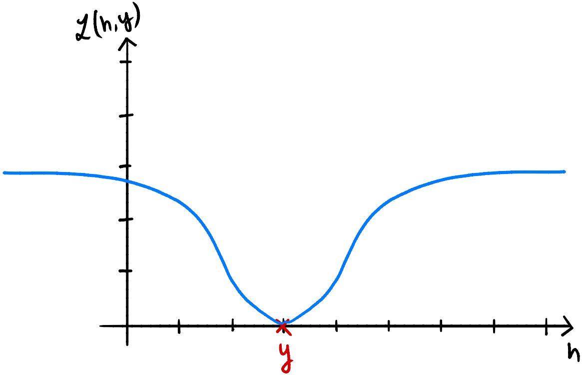
a) flat

b) rapidly decreasing

c) rapidly increasing

Answer: A - Flat.

A very insensitive loss



- We'll call this loss L_{ucsd} because it doesn't have a name.

We want:

$$\lim_{h \to +\infty} L(h, y) = \text{constant} < +\infty$$

$$\lim_{h \to -\infty} L(h, y) = \text{constant} < +\infty$$

Discussion Question

Which of these could be $L_{ucsd}(h, y)$?

a) $e^{-(y-h)^2}$

b) $1 - e^{-(y-h)^2}$

c) $1 - (y - h)^2$

d) $1 - e^{-|y-h|}$

Discussion Question

Which of these could be $L_{ucsd}(h, y)$?

a) $e^{-(y-h)^2}$

b) $1 - e^{-(y-h)^2}$

c) $1 - (y - h)^2$

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Why to reject A?

Discussion Question

Which of these could be $L_{ucsd}(h, y)$?

a) $e^{-(y-h)^2}$

b) $1 - e^{-(y-h)^2}$

c) $1 - (y - h)^2$

d) $1 - e^{-|y-h|}$

Why to reject A?

$$\lim_{h \to +\infty} e^{-(y-h)^2} = 0$$

$h >> y$ is clearly wrong but the loss says it is good.

Discussion Question

Which of these could be $L_{ucsd}(h, y)$?

a) $e^{-(y-h)^2}$

b) $1 - e^{-(y-h)^2}$

c) $1 - (y - h)^2$

d) $1 - e^{-|y-h|}$

Why to reject C?

Discussion Question

Which of these could be $L_{ucsd}(h, y)$?

a) $e^{-(y-h)^2}$

b) $1 - e^{-(y-h)^2}$

c) $1 - (y - h)^2$

d) $1 - e^{-|y-h|}$

Why to reject C?

$$\lim_{h \to +\infty} [1 - (y - h)^2] = -\infty$$

The loss should never be negative.

Discussion Question

Which of these could be $L_{ucsd}(h, y)$?

a) $e^{-(y-h)^2}$

b) $1 - e^{-(y-h)^2}$

c) $1 - (y - h)^2$

d) $1 - e^{-|y-h|}$

D is quite okay:

$$\lim_{h \to +\infty}[1 - e^{-|y-h|}] = 1$$

$$\lim_{h \to -\infty}[1 - e^{-|y-h|}] = 1$$

But $|y - h|$ is not differentiable.

Discussion Question

Which of these could be $L_{ucsd}(h, y)$?

a) $e^{-(y-h)^2}$

b) $1 - e^{-(y-h)^2}$

c) $1 - (y - h)^2$

d) $1 - e^{-|y-h|}$

Answer: B.

$$\lim_{h \to +\infty}[1 - e^{-(y-h)^2}] = 1$$

$$\lim_{h \to -\infty}[1 - e^{-(y-h)^2}] = 1$$

$$L_{ucsd}(y, y) = 0$$

Adding a scale parameter

- Problem: L_{ucsd} has a fixed scale. This won't work for all datasets.
  - If we're predicting temperature, and we're off by 100 degrees, that's bad.
  - If we're predicting salaries, and we're off by 100 dollars, that's pretty good.
  - What we consider to be an outlier depends on the scale of the data.
- Fix: add a **scale parameter**, σ:

$$L_{ucsd}(h, y) = 1 - e^{-(y-h)^2/\sigma^2}$$

Adding a scale parameter

$$L_{ucsd}(h, y) = 1 - e^{-(y-h)^2/\sigma^2}$$

Let's check:

$$\lim_{h\to+\infty} L_{ucsd}(h, y) = 1$$

$$\lim_{h\to-\infty} L_{ucsd}(h, y) = 1$$

$$L_{ucsd}(y, y) = 0$$

Empirical risk minimization

- We have salaries $y_1, y_2, \ldots, y_n$.
- To find prediction, ERM says to minimize the average loss:

$$
\begin{aligned}
R_{ucsd}(h) &= \frac{1}{n} \sum_{i=1}^{n} L_{ucsd}(h, y_i) \\
&= \frac{1}{n} \sum_{i=1}^{n} \left[1 - e^{-(y_i - h)^2 / \sigma^2} \right]
\end{aligned}
$$

Let's plot R_{ucsd}

- Recall:

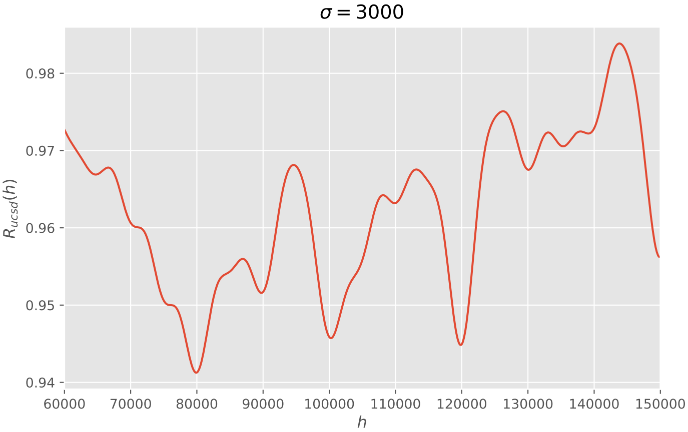
$$R_{ucsd}(h) = \frac{1}{n} \sum_{i=1}^{n} \left[1 - e^{-(y_i - h)^2 / \sigma^2} \right]$$

- Once we have data $y_1, y_2, ..., y_n$ and a scale σ, we can plot $R_{ucsd}(h)$.

- We'll use full the StackOverflow dataset ($n = 1121$).

- Let's try several scales, σ.

Plot of $R_{ucsd}(h)$



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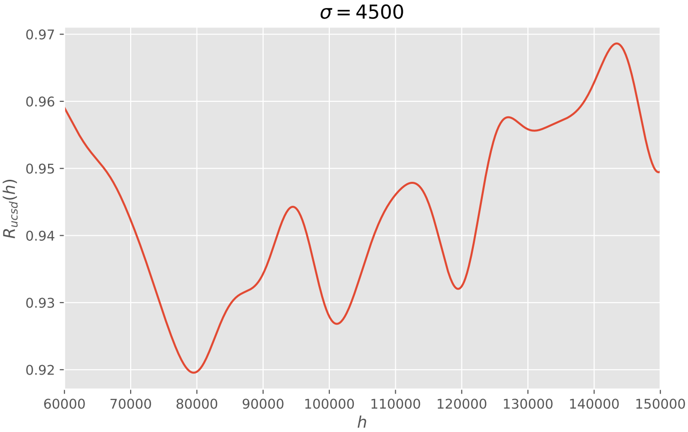

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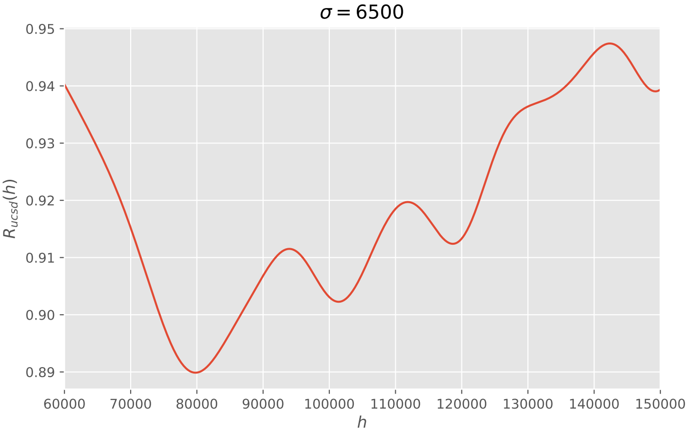

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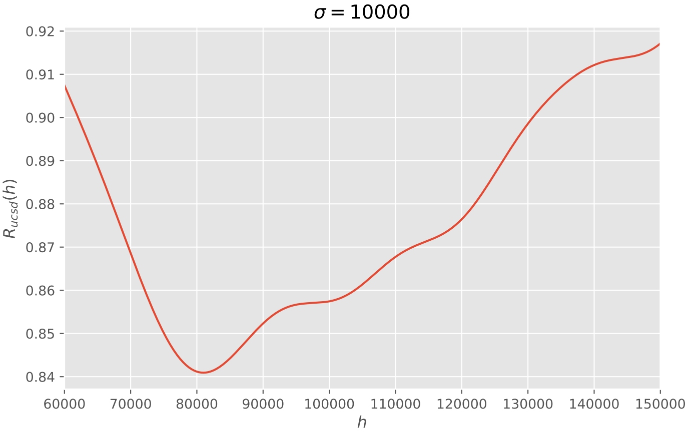

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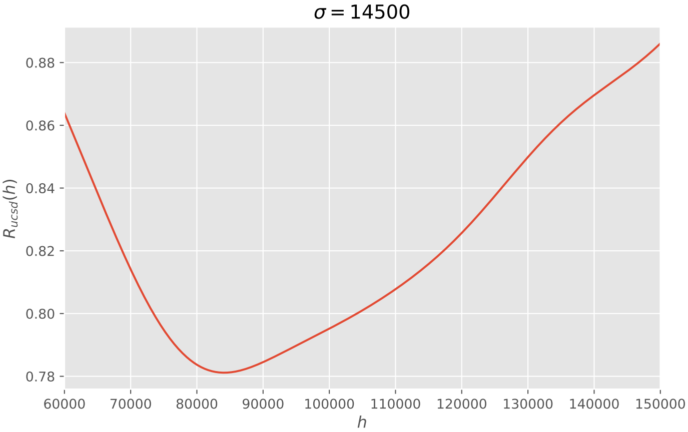

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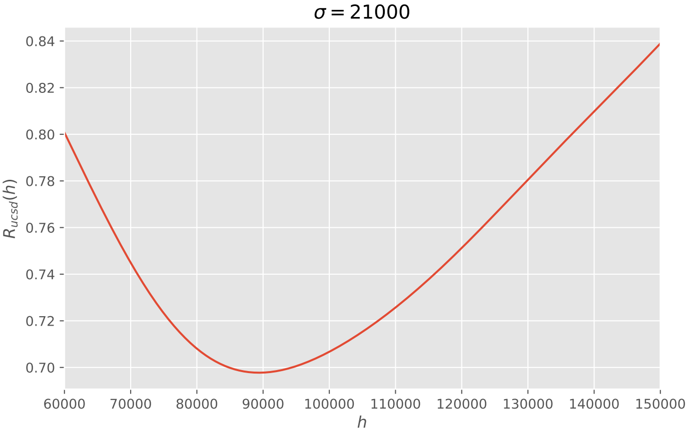

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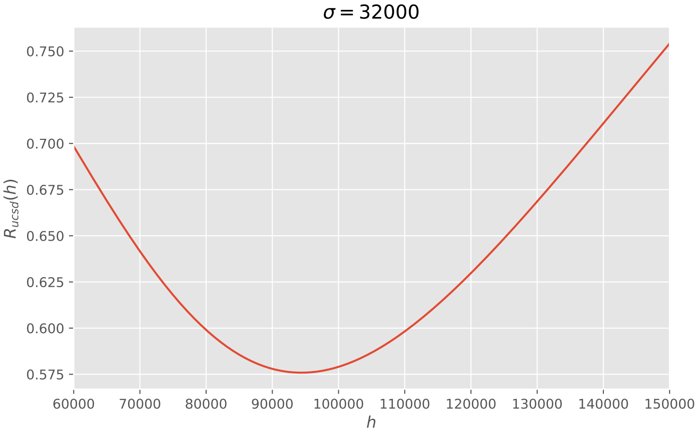

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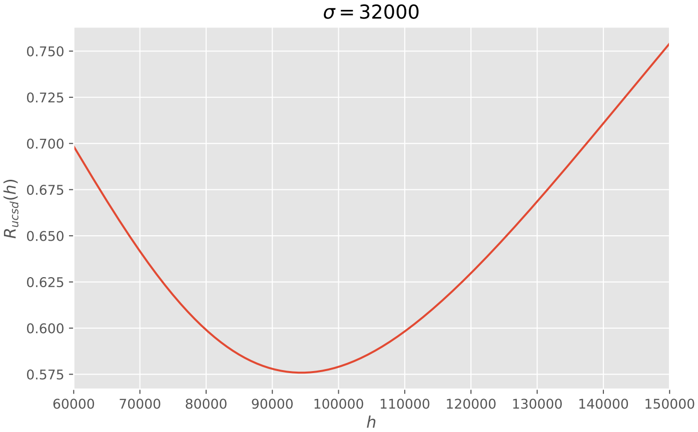

Why when σ large, we see this parabol shape again like for $R_{sq}(h)$?

Minimizing R_{ucsd}

- To find the best prediction, we find h^* minimizing $R_{ucsd}(h)$.
- $R_{ucsd}(h)$ is **differentiable**.
- To minimize: take derivative, set to zero, solve.

Step 1: Taking the derivative

$$\frac{dR_{ucsd}}{dh} = \frac{d}{dh}\left(\frac{1}{n}\sum_{i=1}^{n}\left[1 - e^{-(y_i-h)^2/\sigma^2}\right]\right)$$

Step 1: Taking the derivative

$$\frac{dR_{ucsd}}{dh} = \frac{d}{dh}\left(\frac{1}{n}\sum_{i=1}^{n}\left[1 - e^{-(y_i - h)^2/\sigma^2}\right]\right)$$

$$\Leftrightarrow \frac{dR_{ucsd}}{dh} = \frac{1}{n}\sum_{i=1}^{n}\frac{d}{dh}\left[1 - e^{-(y_i - h)^2/\sigma^2}\right] =$$

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$$\Leftrightarrow \frac{dR_{ucsd}}{dh} = \frac{2}{n\sigma^2}\sum_{i=1}^{n}(h - y_i)\cdot e^{-(y_i-h)^2/\sigma^2}$$

Step 2: Setting to zero and solving

- We found:

$$\frac{d}{dh}(h) = \frac{2}{n\sigma^2}\sum_{i=1}^{n}(h - y_i) \cdot e^{-(h-y_i)^2/\sigma^2}$$

- Now we just set to zero and solve for h:

$$0 = \frac{2}{n\sigma^2}\sum_{i=1}^{n}(h - y_i) \cdot e^{-(h-y_i)^2/\sigma^2}$$

- We **can** calculate derivative, but we **can't** solve for h; we're stuck again.

- Now what???

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- We **can** calculate derivative, but we **can't** solve for h; we're stuck again.

- Now what??? **Iterative algorithm: Gradient Descent**

Gradient descent

The general problem

- **Given:** a differentiable function $R(h)$.
- **Goal:** find the input h^* that minimizes $R(h)$.

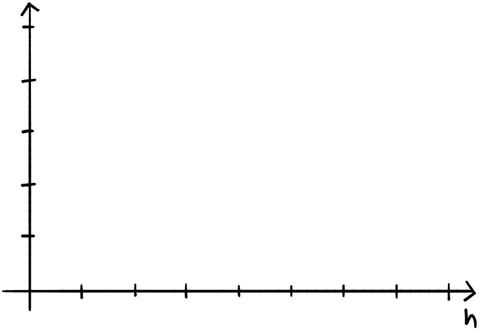
Meaning of the derivative

- We're trying to minimize a **differentiable** function $R(h)$. Is calculating the derivative helpful?

- $\frac{dR}{dh}(h)$ is a function; it gives the **slope** at h.

Key idea behind gradient descent

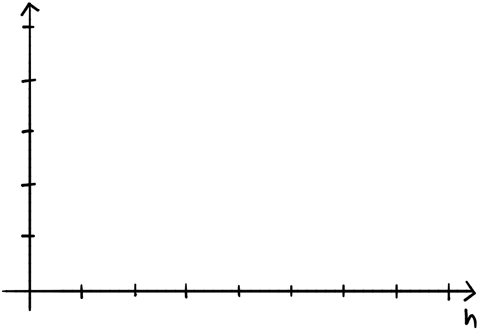
- If the slope of R at h is **positive** then moving to the **left** decreases the value of R.
- i.e., we should **decrease** h.



Key idea behind gradient descent

- If the slope of R at h is **negative** then moving to the **right** decreases the value of R.

- i.e., we should **increase** h.



Key idea behind gradient descent

- Pick a starting place, h_0. Where do we go next?
- Slope at h_0 negative? Then increase h_0.
- Slope at h_0 positive? Then decrease h_0.
- This will work:

$$h_1 = h_0 - \frac{dR}{dh}(h_0)$$

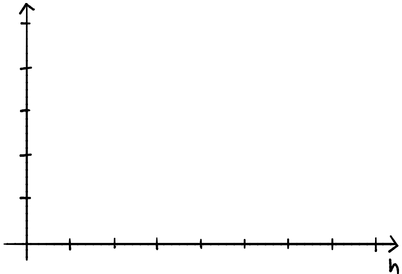
Gradient Descent

- Pick α to be a positive number. It is the **learning rate**, also known as the **step size**.

- Pick a starting prediction, h_0.

- On step i, perform update $h_i = h_{i-1} - \alpha \cdot \frac{dR}{dh}(h_{i-1})$

- Repeat until convergence (when h doesn't change much).



You will not be responsible for implementing gradient descent in this class, but here's an implementation in Python if you're curious:

```
def gradient_descent(derivative, h, alpha, tol=1e-12):
    """Minimize using gradient descent."""
    while True:
        h_next = h - alpha * derivative(h)
        if abs(h_next - h) < tol:
            break
        h = h_next
    return h
```

Example: Minimizing mean squared error

- Recall the mean squared error and its derivative:

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

Discussion Question

Let $y_1 = -4$, $y_2 = -2$, $y_3 = 2$, $y_4 = 4$. Pick $h_0 = 4$ and $\alpha = 1/4$. What is h_1?

a) -1
b) 0
c) 1
d) 2

Solution

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

Data values are $-4, -2, 2, 4$. Pick $h_0 = 4$ and $\alpha = 1/4$. Find h_1.

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Updating step:

$$h_1 = h_0 - \alpha\frac{dR_{sq}}{dh}(h_0) = 4 - \frac{1}{4}\cdot 8 = 2$$

It looks correct, because we move closer to the mean (that is 0).

Summary

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- Different loss functions lead to empirical risk functions that are minimized at various measures of **center**.
- The minimum values of these empirical risk functions are various measures of **spread**.
- We came up with a more complicated loss function, L_{ucsd}, that treats all outliers equally.
  - We weren't able to minimize its empirical risk R_{ucsd} by hand.
- We invented **gradient descent**, which repeatedly updates our prediction by moving in the opposite direction of the derivative.
- **Next Time:** We'll look at gradient descent in action.