# DSC 140A

## Probabilistic Modeling & Machine Learning

Lecture 4 | Part 1

## Introduction

# Empirical Risk Minimization (ERM)

- Step 1: choose a **hypothesis class**
  - We've chosen linear predictors.
- Step 2: choose a **loss function**
- Step 3: find $H$ minimizing **empirical risk**

# Minimizing Empirical Risk

- We want to minimize the **empirical risk**:

$$R(\vec{w}) = \frac{1}{n}\sum_{i=1}^{n} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

$$= \frac{1}{n}\sum_{i=1}^{n} \ell(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w}, y_i)$$

- For some choices of loss function, we can find a formula for the minimizer.

# Example: Least Squares

- With the square loss, risk becomes:

$$R(\vec{w}) = \frac{1}{n}\sum_{i=1}^{n}(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i)^2$$

- Setting gradient to zero, solving for $\vec{w}$ gives:

$$\vec{w}^* = (X^T X)^{-1} X^T \vec{y}$$

# Gradient Descent

- But sometimes we **can't** solve for $\vec{w}$ **directly**.
  - It's too costly.
  - There's no closed-form solution.

- **Idea:** use **gradient descent** to iteratively minimize risk.

# Gradient Descent

- Starting from an initial guess $\vec{w}^{(0)}$, iteratively update:

$$\vec{w}^{(t+1)} = \vec{w}^{(t)} - \eta \frac{dR}{d\vec{w}}(\vec{w}^{(t)})$$

# Today

We'll address two issues with gradient descent.

1. Can be **expensive** to compute the exact gradient.
   - Especially when we have a large data set.
   - **Solution:** **stochastic gradient descent**.
2. Doesn't work as-is if risk is **not differentiable**.
   - Such as with the absolute loss.
   - **Solution:** **subgradient descent**.

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Probabilistic Modeling & Machine Learning

Lecture 4 | Part 2

## Motivation: Large Scale Learning

# Example

- Suppose you're doing **least squares regression** on a medium-to-large data set.
- Say, $n = 200{,}000$ examples, $d = 5{,}000$ features.
- Encoded as 64 bit floats, $X$ is 8 GB.
    - Fits in your laptop's memory, but barely.
- **Example:** predict sentiment from text.

# Attempt 0: Normal Equations

- You start by solving the normal equations:

```
np.linalg.solve(X.T @ X, X.T @ y)
```

- **Time:** 30.7 seconds.
- **Mean Squared Error:** $7.2 \times 10^{-7}$.
- Can we speed this up?

# Attempt 1: Gradient Descent

- Recall[1] that the gradient of the MSE is:

$$\frac{dR}{d\vec{w}}(\vec{w}) = \frac{2}{n}\sum_{i=1}^{n}\left(\text{Aug}(\vec{x}^{(i)})\cdot\vec{w} - y_i\right)\text{Aug}(\vec{x}^{(i)})$$
$$= \frac{1}{n}\left(2X^T X\vec{w} - 2X^T\vec{y}\right)$$

- You code up a function:[2]

```
def gradient(w):
    n = len(y)
    return (2/n) * X.T @ (X @ w - y)
```

[1] From Lecture 02, where we derived this.
[2] There's a good and a bad way to do this.

# Attempt 1: Gradient Descent

- You plug this into `gradient_descent` from last lecture, run it, and...

- **Time:** **8.6 seconds** total
  - 14 iterations
  - ≈ 0.6 seconds per iteration

- **Mean Squared Error:** $9.4 \times 10^{-7}$.

# Trivia: why is it faster?

- **Solving normal equations** takes $\Theta(nd^2 + d^3)$ time.
  - $\Theta(nd^2)$ time to compute $X^T X$.
  - $\Theta(d^3)$ time to solve the system.

- **Gradient descent** takes $\Theta(nd)$ time per iteration.
  - $\Theta(nd)$ time to compute $X\vec{w}$.
  - $\Theta(nd)$ time to compute $X^T(X\vec{w} - \vec{y})$.

# Looking Ahead

- What if you had a **larger** data set?
- Say, $n = 10{,}000{,}000$ examples, $d = 5{,}000$ features.
- Encoded as 64 bit floats, $X$ is **400 GB**.
  - Doesn't fit in your laptop's memory!
  - Barely fits on your hard drive.

# Approach 0: Normal Equations

- You can try solving the normal equations:

```
np.linalg.solve(X.T @ X, X.T @ y)
```

- One of three things will happen:
  1. You will receive an **out of memory** error.
  2. The process will be killed (or your OS will freeze).
  3. It will run, but take a **very long time** (paging).

# Approach 1: Gradient Descent

- We can't store the data in memory all at once.
- But we can **still** compute the **gradient**, $\frac{dR}{d\vec{w}}$.
  - Read a little bit of data at once.
  - Or, distribute the computation to several machines.
- Computing gradient involves a loop over data:

$$\frac{dR}{d\vec{w}}(\vec{w}) = \frac{2}{n}\sum_{i=1}^{n}\left(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i\right)\text{Aug}(\vec{x}^{(i)})$$

# Problem

$$\frac{dR}{d\vec{w}}(\vec{w}) = \frac{2}{n}\sum_{i=1}^{n}\left(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i\right)\text{Aug}(\vec{x}^{(i)})$$

- In machine learning, the number of training points $n$ can be **very large**.
- Computing the gradient can be **expensive** when $n$ is large.
    - So each step of gradient descent is **expensive**.

# Idea

- Don’t worry about computing the **exact** gradient.
- An **approximation** will do.

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Probabilistic Modeling & Machine Learning

Lecture 4 | Part 3

## Stochastic Gradient Descent

# Gradient Descent for Minimizing Risk

- In ML, we often want to minimize a **risk function**:

$$R(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

# Observation

- The gradient of the risk is the average of the gradient of the losses:

$$\frac{d}{d\vec{w}} R(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} \frac{d}{d\vec{w}} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

- The averaging is over **all training points**.

- This can take a long time when $n$ is large.[3]

[3] Trivia: this usually takes $\Theta(nd)$ time.

# Idea

- The (full) gradient of the risk uses all of the training data:

$$\frac{d}{d\vec{w}} R(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} \frac{d}{d\vec{w}} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

- **Idea:** instead of using all $n$ training points, randomly choose a smaller set, $B$:

$$\frac{d}{d\vec{w}} R(\vec{w}) \approx \frac{1}{|B|} \sum_{i \in B} \frac{d}{d\vec{w}} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

# Stochastic Gradient

- The smaller set $B$ is called a **mini-batch**.
- We now compute a **stochastic gradient**:

$$\frac{d}{d\vec{w}} R(\vec{w}) \approx \frac{1}{|B|} \sum_{i \in B} \frac{d}{d\vec{w}} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

- "Stochastic," because it is a random.

# Stochastic Gradient

$$\frac{d}{d\vec{w}} R(\vec{w}) \approx \frac{1}{|B|} \sum_{i \in B} \frac{d}{d\vec{w}} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

- The stochastic gradient is an **approximation** of the full gradient.
- When $|B| \ll n$, it is **much faster** to compute.
- But the approximation is **noisy**.

# Stochastic Gradient Descent for ERM

To minimize empirical risk $R(\vec{w})$:

- Pick starting weights $\vec{w}^{(0)}$, learning rate $\eta > 0$, batch size $m$.
- Until convergence, repeat:
  - **Randomly sample** a batch $B$ of $m$ training data points.
  - **Compute stochastic gradient:**

$$\vec{g} = \frac{1}{|B|} \sum_{i \in B} \frac{d}{d\vec{w}} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

  - **Update:** $\vec{w}^{(t+1)} = \vec{w}^{(t)} - \eta \vec{g}$
- When converged, return $\vec{w}^{(t)}$.

# Note

- A **new batch** should be randomly sampled on each iteration!

- This way, the entire training set is used over time.

- Size of batch should be **small** compared to $n$.
  - Think: $m = 64$, $m = 32$, or even $m = 1$.

# Example: Least Squares

- We can use SGD to perform least squares regression.

- Need to compute the gradient of the square loss:

$$\ell_{\text{sq}}(H(\vec{x}^{(i)}; \vec{w}), y_i) = \left(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i\right)^2$$

## Exercise

What is the gradient of the square loss of a linear predictor? That is, what is $\frac{d}{d\vec{w}}\left(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i\right)^2$?

# Example: Least Squares

- The gradient of the square loss of a linear predictor is:

$$
\begin{aligned}
&\frac{d}{d\vec{w}} \ell_{\text{sq}}(H(\vec{x}^{(i)}; \vec{w}), y_i) \\
&\qquad = \frac{d}{d\vec{w}} \left(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i\right)^2 \\
&\qquad = 2\left(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i\right) \frac{d}{d\vec{w}} \left(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i\right) \\
&\qquad = 2\left(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i\right) \text{Aug}(\vec{x}^{(i)})
\end{aligned}
$$

# Example: Least Squares

- Therefore, on each step we compute the stochastic gradient:

$$\vec{g} = \frac{2}{m} \sum_{i \in B} \left( \text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i \right) \text{Aug}(\vec{x}^{(i)})$$

- The update rule is:

$$\vec{w}^{(t+1)} = \vec{w}^{(t)} - \eta \vec{g}$$

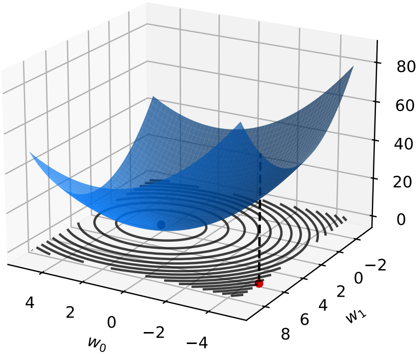
# Example: Least Squares

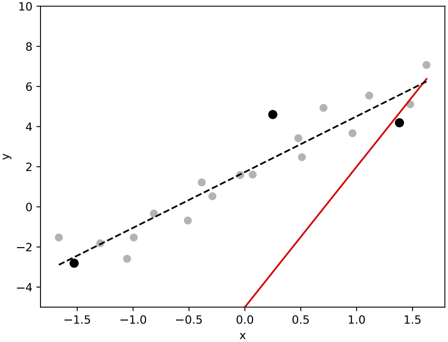
- We can write in matrix-vector form, too:
  - Let $X_B$ be the design matrix using only the examples in batch $B$.
  - Let $y_B$ be the corresponding vector of labels.

- Then:

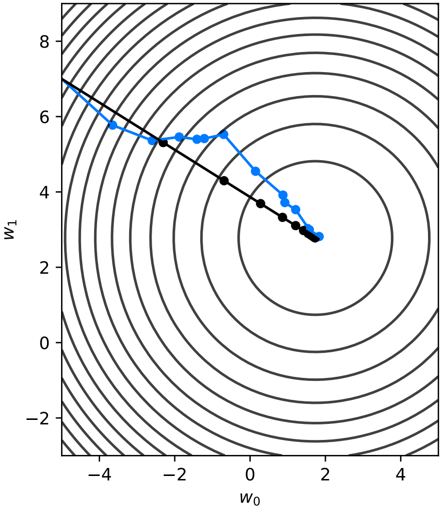
$$\vec{g} = \frac{2}{m} X_B^T (X_B \vec{w} - y_B)$$

# Example: SGD



# SGD vs. GD



# Tradeoffs

- In each step of GD, move in the “best” direction.
  - But **slowly!**
- In each step of SGD, move in a “good” direction.
  - But **quickly!**
- SGD may take more steps to converge, but can be faster overall.

# Example

- Suppose you're doing **least squares regression** on a medium-to-large data set.
- Say, $n = 200{,}000$ examples, $d = 5{,}000$ features.
- Encoded as 64 bit floats, $X$ is 8 GB.
  - Fits in your laptop's memory, but barely.
- **Example:** predict sentiment from text.

# We saw...

- Solving the normal equations took **30.7 seconds**.
- Gradient descent took **8.6 seconds**.
  - 14 iterations, ≈ 0.6 seconds per iteration.
- Stochastic gradient descent takes **3 seconds**.
  - Batch size $m = 16$.
  - 13,900 iterations, ≈ 0.0002 seconds per iteration.

# Aside: Terminology

- Some people say “stochastic gradient descent” only when batch size is 1.
- They say “mini-batch gradient descent” for larger batch sizes.
- **In this class**: we’ll use “SGD” for any batch size, as long as it’s chosen randomly.

# Aside: A Popular Variant

- One variant of SGD uses **epochs**.
- During each epoch, we:
  - Randomly shuffle the training data.
  - Divide the training data into $n/m$ mini-batches.
  - Perform one step for each mini-batch.

# Usefulness of SGD

- SGD **enables** learning on **massive** data sets.
  - Billions of training examples, or more.
- Useful even when exact solutions available.
  - E.g., least squares regression / classification.

# History: ADALINE

# DSC 140A

## Probabilistic Modeling & Machine Learning

Lecture 4 | Part 4

## Motivation: Minimizing Absolute Loss

# Empirical Risk Minimization (ERM)

- Step 1: choose a **hypothesis class**
  - We've chosen linear predictors.
- Step 2: choose a **loss function**
- Step 3: find $H$ minimizing **empirical risk**

# Loss Functions

- The **absolute loss** is a natural first choice for regression.

- The empirical risk becomes:

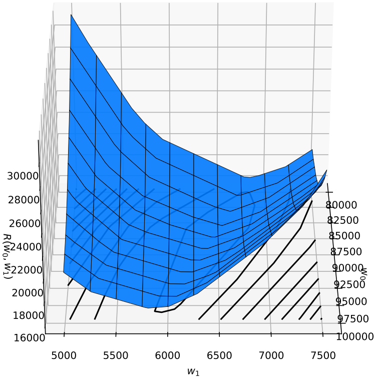
$$
\begin{aligned}
R_{\text{abs}}(\vec{w}) &= \frac{1}{n} \sum_{i=1}^{n} |H(\vec{x}^{(i)}) - y_i| \\
&= \frac{1}{n} \sum_{i=1}^{n} |\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) - y_i|
\end{aligned}
$$

# Minimizing the Risk

$$R(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} |\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) - y_i|$$

- We might try computing the gradient, setting to zero, and solving.
- But the risk is **not differentiable**.

# Risk for the Absolute Loss



# Gradient Descent?

- **Question**: can we use gradient descent if the risk is not differentiable?
- **Answer**: **yes**, with a slight modification.

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Probabilistic Modeling & Machine Learning

Lecture 4 | Part 5

## Subgradient Descent

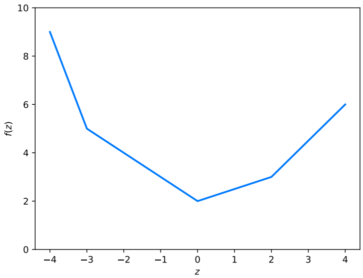
# Differentiability

- A function $f(z)$ is **differentiable** if the derivative exists at every point.
- That is, it has a well-defined slope at every point.

# Exercise

Where is the derivative **not** defined?

$$f(z) = \begin{cases} -4z - 7 & \text{if } z < -3 \\ -z + 2 & \text{if } -3 \leq z < 0 \\ 0.5z + 2 & \text{if } 0 \leq z < 2 \\ 3z/2 & \text{if } z \geq 2 \end{cases}$$

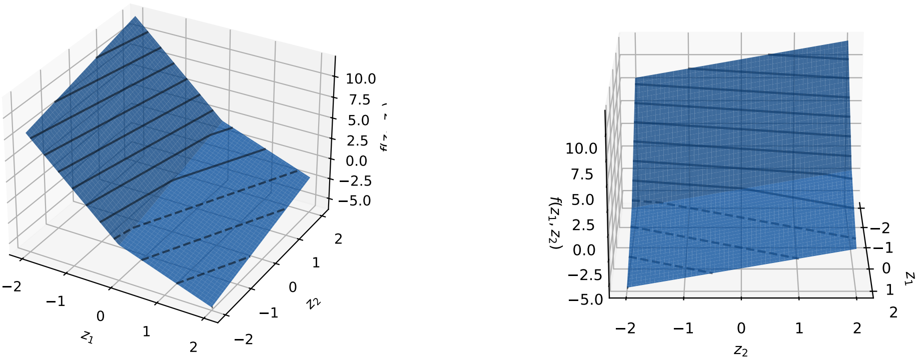


# Differentiability

- A function $f(\vec{z})$ is **differentiable** if the **gradient** exists at every point.
- In other words, all of the slopes are well-defined:
  - $\partial f / \partial z_1, \partial f / \partial z_2, \ldots$

# Example

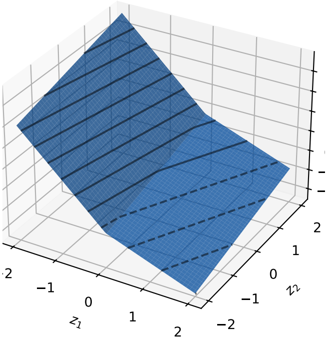
- $f(z_1, z_2) = \begin{cases} -5z_1 + z_2 & \text{if } z_1 \leq 0 \\ -2z_1 + z_2 & \text{if } z_1 > 0 \end{cases}$



## Exercise

What is the gradient at (-1, -1)? (1, -1)? (0, 1)?

$$f(z_1, z_2) = \begin{cases} -5z_1 + z_2 & \text{if } z_1 \leq 0 \\ -2z_1 + z_2 & \text{if } z_1 > 0 \end{cases}$$

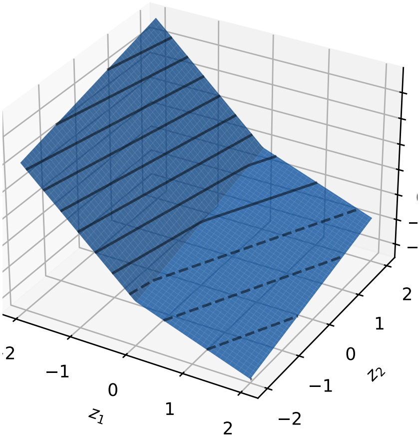


# Answer

- $\frac{d}{d\vec{w}} f(\vec{z})$ is defined everywhere except along $z_1 = 0$.

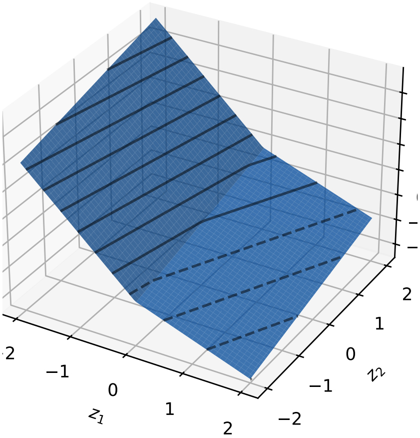
- If $z_1 < 0$, $f(\vec{z}) = -5z_1 + z_2$.
  - gradient is $(-5, 1)^T$ here

- If $z_1 > 0$, $f(\vec{z}) = -2z_1 + z_2$.
  - gradient is $(-2, 1)^T$ here



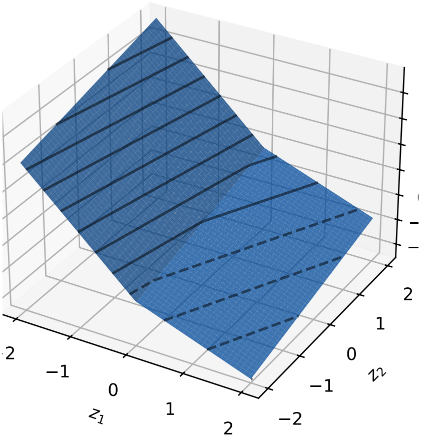
# Answer

$$\frac{df}{d\vec{z}}(\vec{z}) = \begin{cases} (-5, 1)^T, & \text{if } z_1 < 0, \\ (-2, 1)^T, & \text{if } z_1 > 0, \\ \text{undefined}, & \text{if } z_1 = 0. \end{cases}$$



# Problem

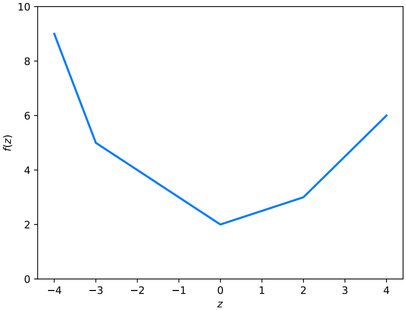
- We can try running gradient descent.
- But what do we do if we reach a point where the gradient is **not defined**?
- We need a **replacement** for the gradient that tells us where to go.



# Idea

- Slope is undefined at $z_1 = -3$.
  - To the left, slope is -4
  - To the right, slope is -1

$$f(z) = \begin{cases} -4z - 7 & \text{if } z < -3 \\ -z + 2 & \text{if } -3 \leq z < 0 \\ 0.5z + 2 & \text{if } 0 \leq z < 2 \\ 3z/2 & \text{if } z \geq 2 \end{cases}$$



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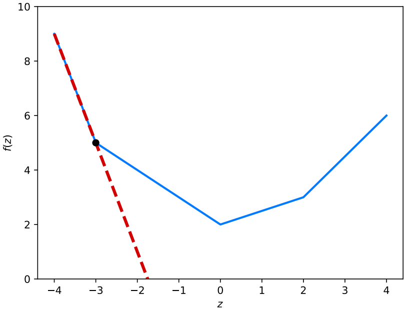

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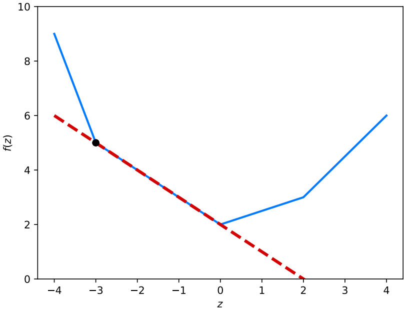

# Idea

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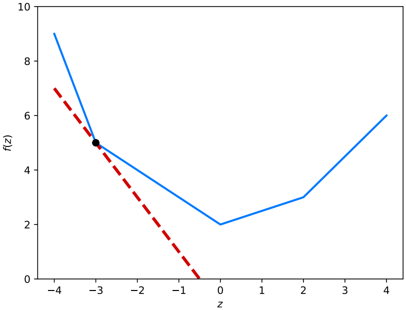
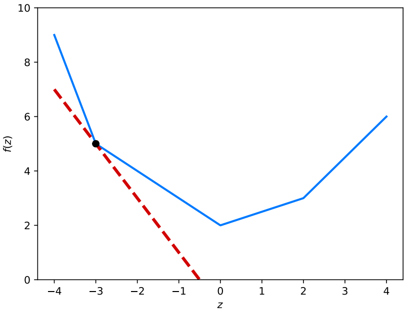


# Idea

- Any number between -4 and -1 adequately describes the behavior of $f$ at $z = -3$.

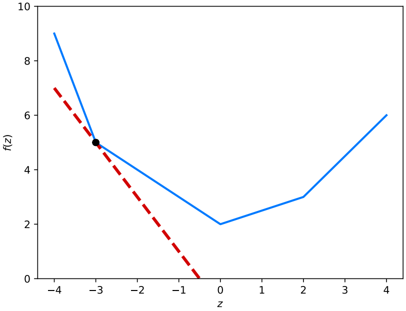
$$f(z) = \begin{cases} -4z - 7 & \text{if } z < -3 \\ -z + 2 & \text{if } -3 \le z < 0 \\ 0.5z + 2 & \text{if } 0 \le z < 2 \\ 3z/2 & \text{if } z \ge 2 \end{cases}$$



# Idea

- Any number between -4 and -1 is a **subderivative** of $f$ at $z = -3$.

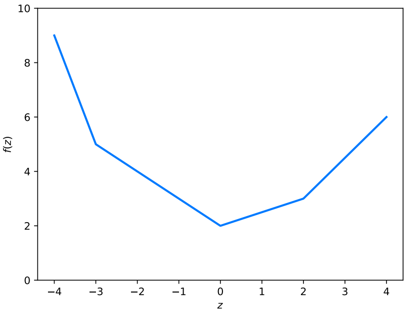
$$f(z) = \begin{cases} -4z - 7 & \text{if } z < -3 \\ -z + 2 & \text{if } -3 \le z < 0 \\ 0.5z + 2 & \text{if } 0 \le z < 2 \\ 3z/2 & \text{if } z \ge 2 \end{cases}$$



## Exercise

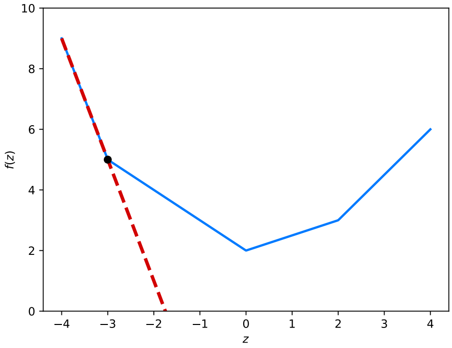
What are the valid subderivatives of $f$ at $z = 2$?

$$f(z) = \begin{cases} -4z - 7 & \text{if } z < -3 \\ -z + 2 & \text{if } -3 \le z < 0 \\ 0.5z + 2 & \text{if } 0 \le z < 2 \\ 3z/2 & \text{if } z \ge 2 \end{cases}$$



# Subderivatives

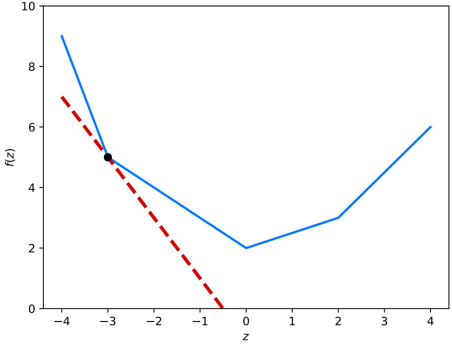
- Any valid subderivative defines a line that lies below the function.



# Subderivatives

- The equation of this line is:

$$f_s(z) = f(z_0) + s(z - z_0)$$



# Subderivatives

- A number $s$ is a subderivative of $f$ at $z_0$ if:

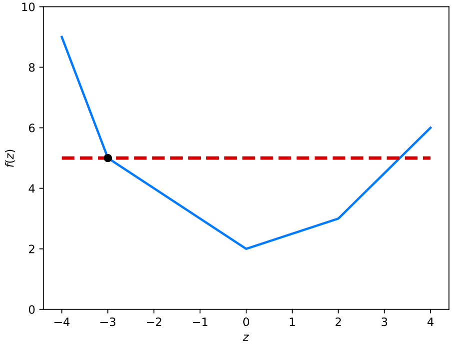
$$f(z) \geq f_s(z) \quad \text{for all } z$$

- That is, if:

$$f(z) \geq f(z_0) + s(z - z_0)$$

## Exercise

Is 0 a valid subderivative of $f$ at $z = 2$?



# Intuition

- The **subderivative** tells us how the function changes when the slope doesn't exist.
- We can sometimes use it in place of a derivative.

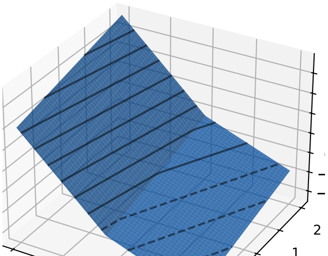
# Subgradient

- In higher dimensions, we have multiple slopes to worry about.
- We can use a **subgradient** to generalize the concept of a subderivative.

# Example

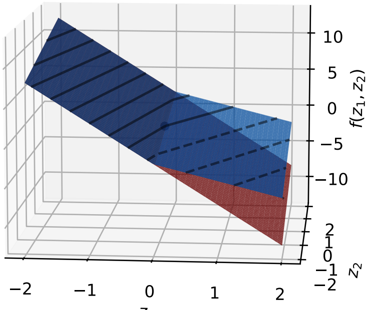
- There's no well-defined gradient at $z_1 = (0, 0)$.
  - The slope in the $z_1$ direction is undefined
  - Between -5 and -2?
  - The slope in the $z_2$ direction is 1
- We will call any vector $(s_1, 1)$ with $-5 \leq s_1 \leq -2$ a **subgradient** at $(0, 0)$.

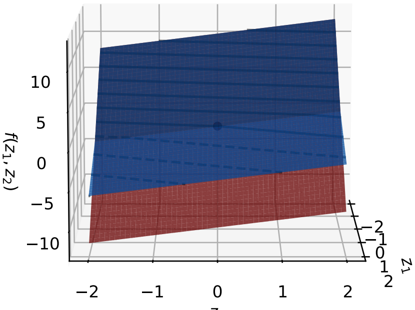
$$f(z_1, z_2) = \begin{cases} -5z_1 + z_2 & \text{if } z_1 \leq 0 \\ -2z_1 + z_2 & \text{if } z_1 > 0 \end{cases}$$



# Subgradient

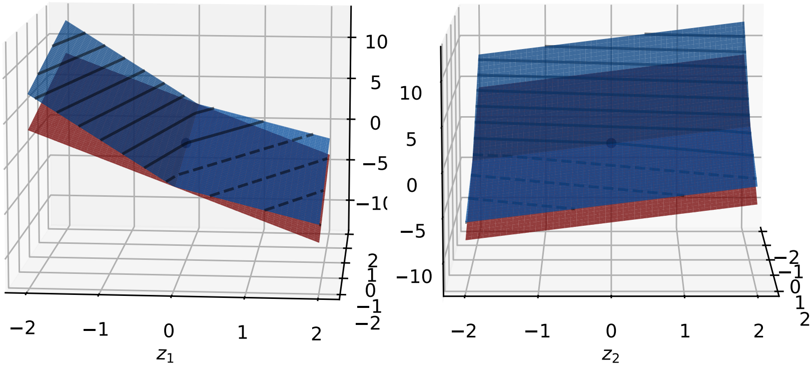
- A vector $\vec{s}$ defines a plane:
  - Example: $(-5, 1)^T$
  - Example: $(-2, 1)^T$
  - Example: $(-3, 1)^T$



# Subgradient

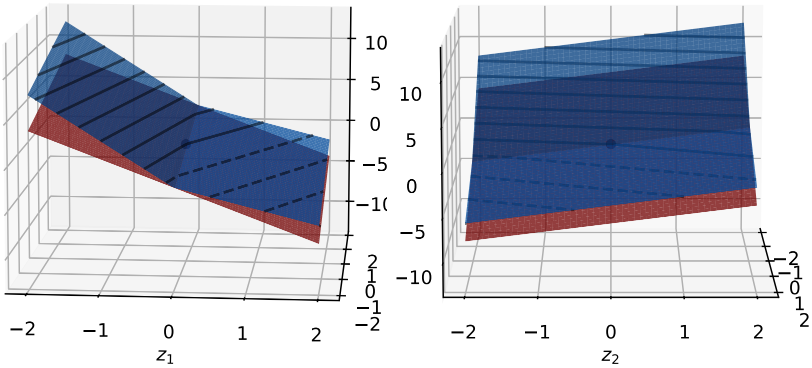
- A vector $\vec{s}$ is a valid **subgradient** at $\vec{z}^{(0)}$ if the plane it defines lies at or below the function $f$.
  - Example: $(-3, 1)^T$



# Subgradient

- The equation of the plane defined by $\vec{s}$ at $\vec{z}^{(0)}$ is:

$$f_s(\vec{z}) = f(\vec{z}^{(0)}) + \vec{s} \cdot (\vec{z} - \vec{z}^{(0)})$$



# Subgradients

- $\vec{s}$ is a **subgradient** of $f(\vec{z})$ at $\vec{z}^{(0)}$ if:

$$f(\vec{z}) \geq f_s(\vec{z}) \quad \text{for all } \vec{z}$$

- That is, if:

$$f(\vec{z}) \geq f(\vec{z}^{(0)}) + \vec{s} \cdot (\vec{z} - \vec{z}^{(0)})$$

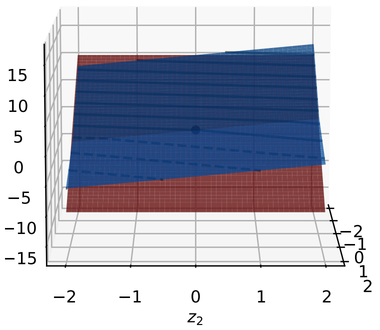
# Finding Subgradients

- Here are two suggested ways to check that $\vec{s}$ is a valid subgradient.
- 1) Visualize it.
- 2) Check if the inequality holds.

# Example

$$f(z_1, z_2) = \begin{cases} -5z_1 + z_2 & \text{if } z_1 \leq 0 \\ -2z_1 + z_2 & \text{if } z_1 > 0 \end{cases}$$

- Is $(-5, 0)^T$ a valid subgradient?



# Example

$$f(z_1, z_2) = \begin{cases} -5z_1 + z_2 & \text{if } z_1 \le 0 \\ -2z_1 + z_2 & \text{if } z_1 > 0 \end{cases}$$

- Is $(-5, 0)^T$ a valid subgradient at the point (0,0)?
- Is $f(0,0) + (-5,0)^T \cdot ((z_1, z_2) - (0,0)^T) \le f(z_1, z_2) \quad$ for all $z_1, z_2$?

# Tip

- If the slope is defined in a direction, the corresponding entry of the subgradient must be that slope.

# Intuition

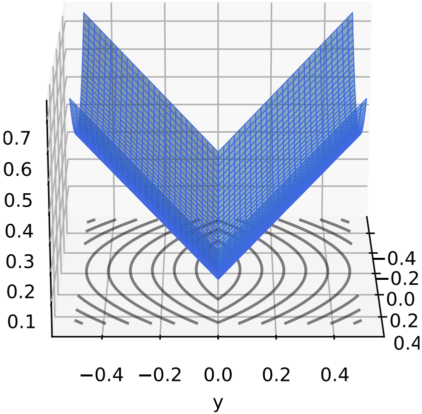
- A **subgradient** tells us where to go when the gradient is undefined.
- We can use it instead of the gradient in gradient descent.

# Example

- $f(z_1, z_2) = z_1^2 + |z_2|$

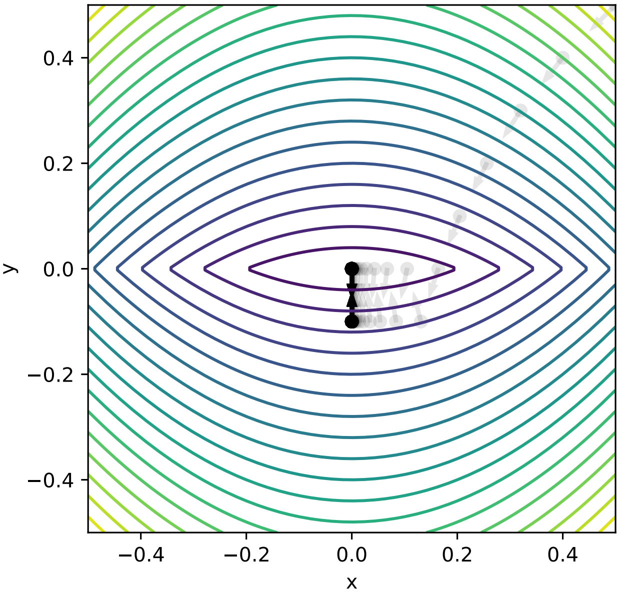
- A subgradient:

$$\vec{s}(z_1, z_2) = \begin{cases} (2z_1, 1)^T & , \text{if } z_2 > 0, \\ (2z_1, -1)^T & , \text{if } z_2 < 0, \\ (2z_1, 0)^T & , \text{if } z_2 = 0. \end{cases}$$



# Example

- Subgradient descent on $f(z_1, z_2) = z_1^2 + |z_2|$
- Starting point: $(1/2, 1/2)^T$
- Learning rate: $\eta = 0.1$.



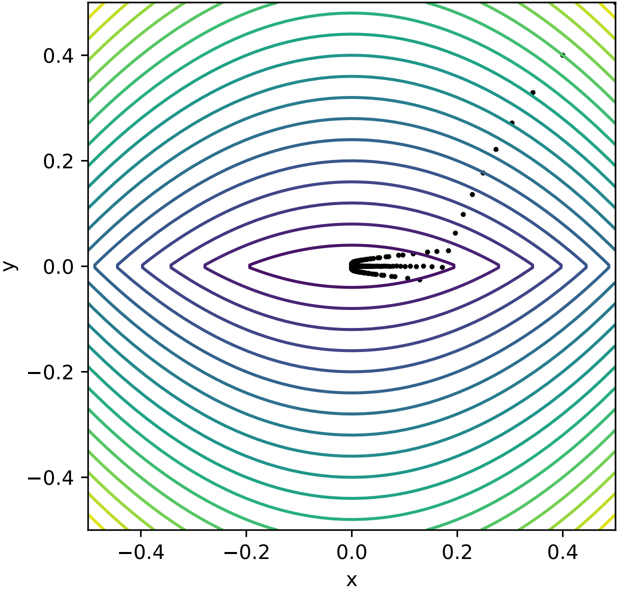
0.4
0.2
0.0
−0.2
−0.4
y
−0.4
−0.2
0.0
0.2
0.4
x

# Problem

- Does not converge! Why?
- If $f$ is differentiable, gradient gets smaller as we approach the minimum.
  - Naturally take smaller steps.
- Not true if the function is not differentiable!
  - Steps may stay the same size (too large).

# Fix

- Decrease learning rate with each iteration.
- That is, choose a decreasing **learning rate schedule** $\eta(t) > 0$.
- **Theory:** choose $\eta(t) = c/\sqrt{t}$, where $t$ is iteration #, $c$ is a positive constant.



0.4
0.2
0.0
−0.2
−0.4
y
−0.4
−0.2
0.0
0.2
0.4
x

# Subgradient Descent

To minimize $f(\vec{z})$:

- Pick arbitrary starting point $\vec{z}^{(0)}$, a decreasing **learning rate schedule** $\eta(t) > 0$.
- Until convergence, repeat:
  - **Compute a subgradient** $\vec{s}$ of $f$ at $\vec{z}^{(i)}$.
  - Update $\vec{z}^{(t+1)} = \vec{z}^{(t)} - \eta(t)\vec{s}$
- When converged, return $\vec{z}^{(t)}$.

# Next Time

- When is (S)GD guaranteed to converge?