

DSC 140A

Probabilistic Modeling & Machine Learning

Lecture 5 | Part 1

Introduction

Minimizing Empirical Risk

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

$$\begin{aligned} R(\vec{w}) &= \frac{1}{n} \sum_{i=1}^n \ell(H(\vec{x}^{(i)}; \vec{w}), y_i) \\ &= \frac{1}{n} \sum_{i=1}^n \ell(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w}, y_i) \end{aligned}$$

Minimizing Empirical Risk

- ▶ For some losses there's a formula for the best \vec{w} .
 - ▶ **Example:** square loss.
 - ▶ But it might be **too costly** to use!
- ▶ For others, there isn't.
 - ▶ **Example:** absolute loss, Huber loss.
- ▶ In either case, we might use **gradient descent**.

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.**

Today

- ▶ Answer two remaining questions:
 1. How do we minimize the risk with respect to non-differentiable losses, like the **absolute loss**?
 2. When is gradient descent **guaranteed** to work?

DSC 140A

Probabilistic Modeling & Machine Learning

Lecture 5 | Part 2

Subgradient Descent

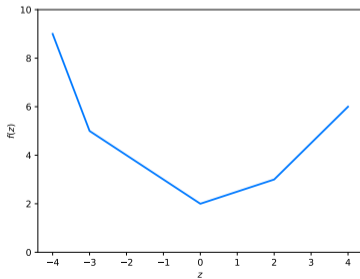
Differentiability

- ▶ 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?

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

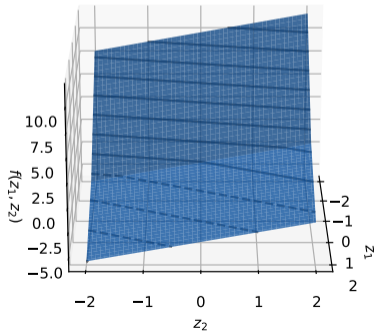
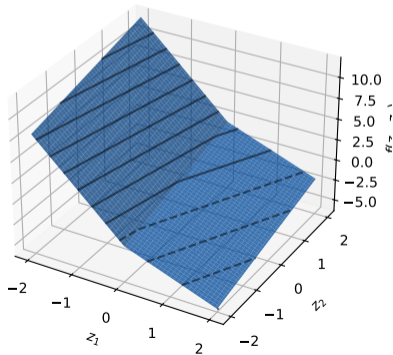


Differentiability

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

Example

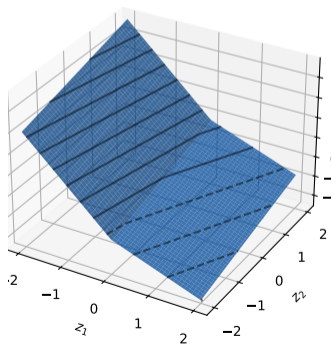
$$\blacktriangleright f(z_1, z_2) = \begin{cases} -5z_1 + z_2 & \text{if } z_1 \leq 0 \\ -2z_1 + z_2 & \text{if } z_1 > 0 \end{cases}$$



Exercise

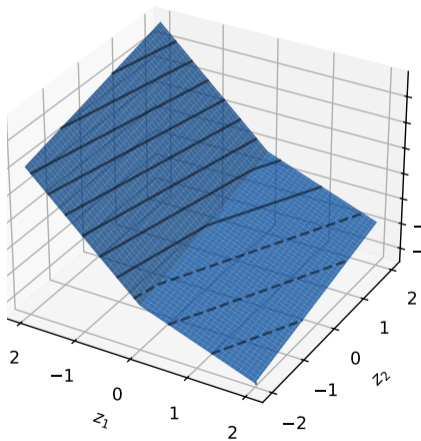
What is the gradient at $(-1, -1)$? $(1, -1)$? $(0, 1)$?

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



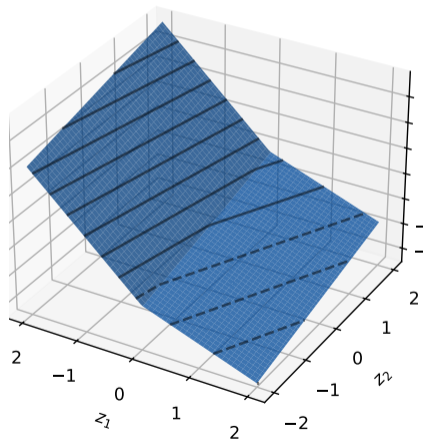
Answer

- ▶ $\vec{\nabla} f(\vec{z})$ 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



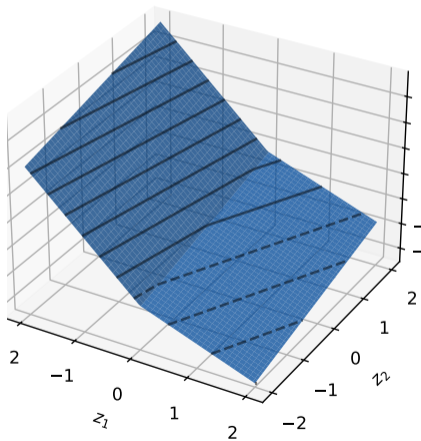
Answer

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



Problem

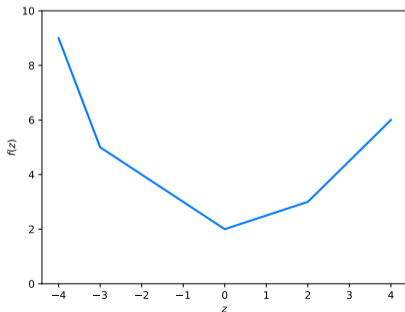
- ▶ We can try running gradient descent.
- ▶ But what do we do if we reach a point where the gradient is **not defined**?
- ▶ We need a **replacement** for the gradient that tells us where to go.



Idea

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

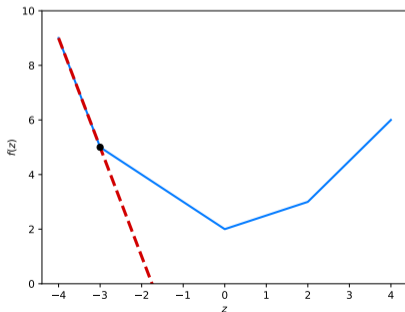
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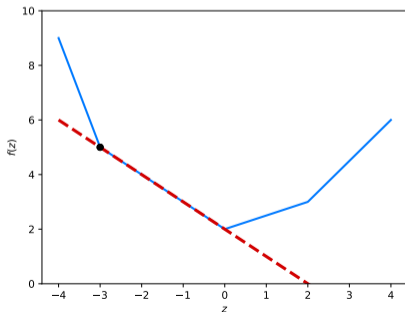
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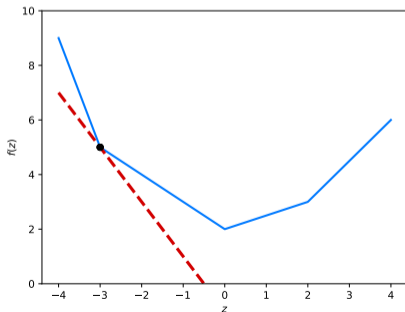
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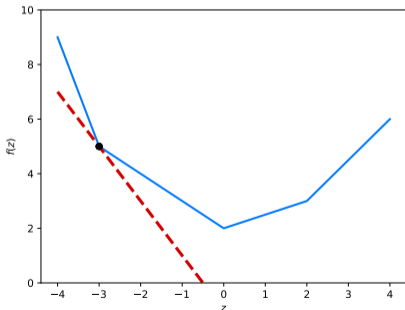
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Idea

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

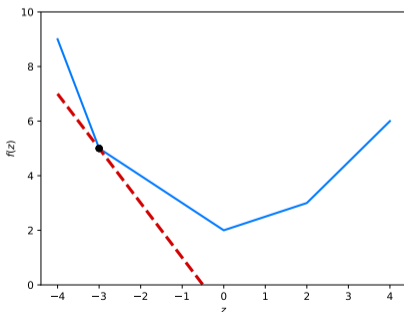
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Idea

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

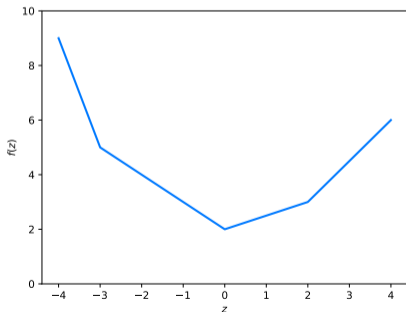
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Exercise

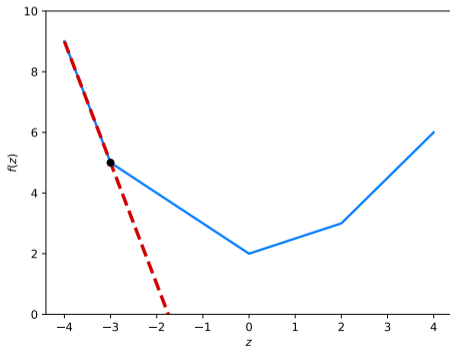
What are the valid subderivatives of f at $z = 2$?

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



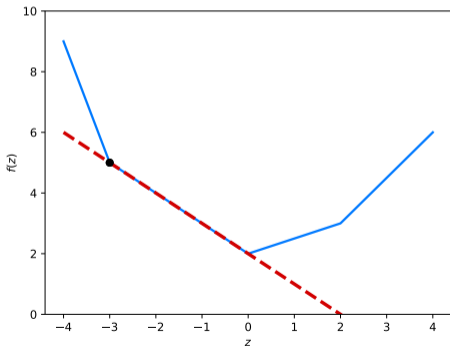
Subderivatives

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



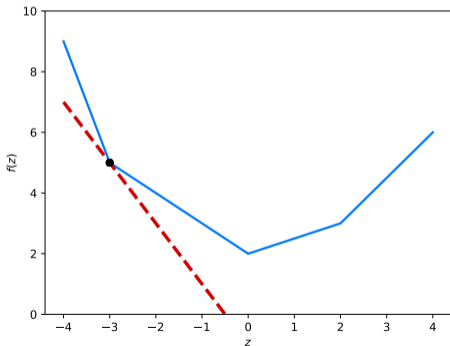
Subderivatives

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



Subderivatives

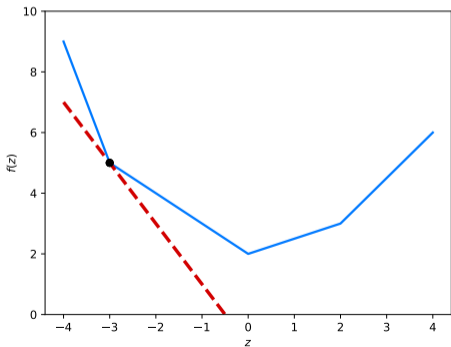
- ▶ Any valid subderivative defines a line that lies below the function.



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:

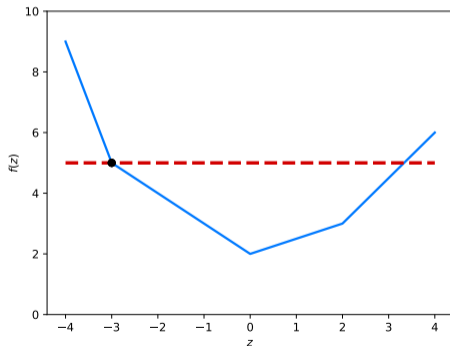
$$f(z) \geq f_s(z) \quad \text{for all } z$$

- ▶ 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.

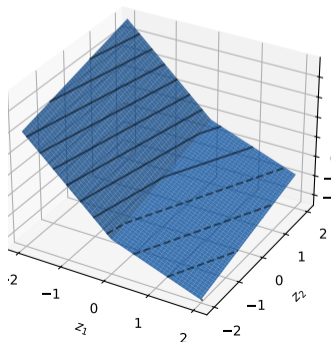
Subgradient

- ▶ 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

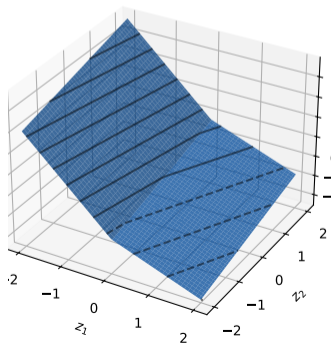
$$f(z_1, z_2) = \begin{cases} -5z_1 + z_2 & \text{if } z_1 \leq 0 \\ -2z_1 + z_2 & \text{if } z_1 > 0 \end{cases}$$



Example

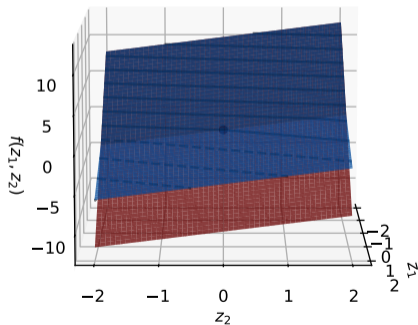
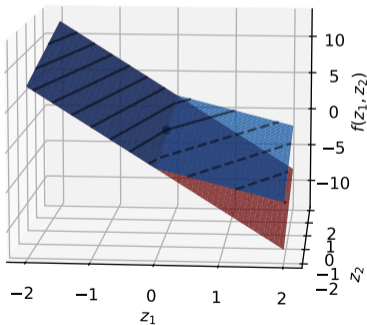
- ▶ We will call any vector $(s_1, 1)$ with $-5 \leq s_1 \leq -2$ a **subgradient** at $(0, 0)$.

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



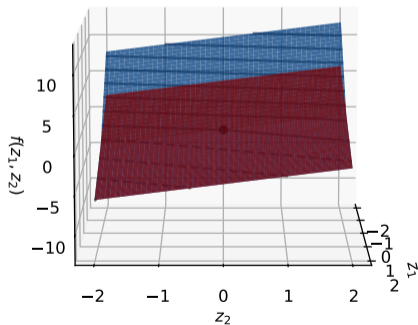
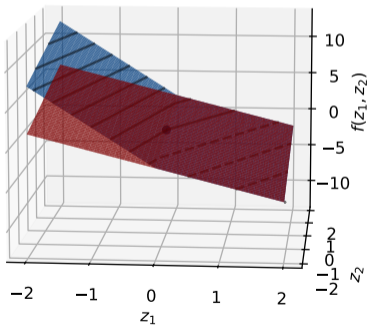
Subgradient

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



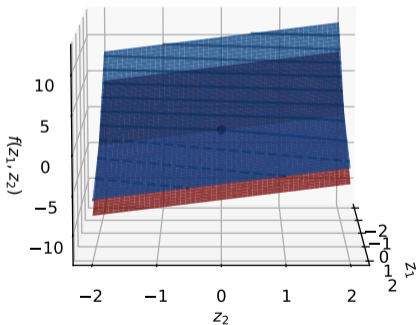
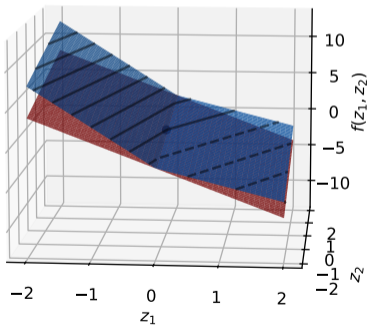
Subgradient

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



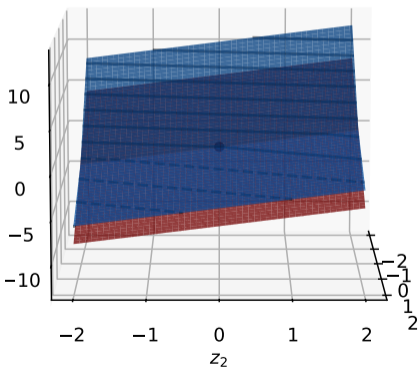
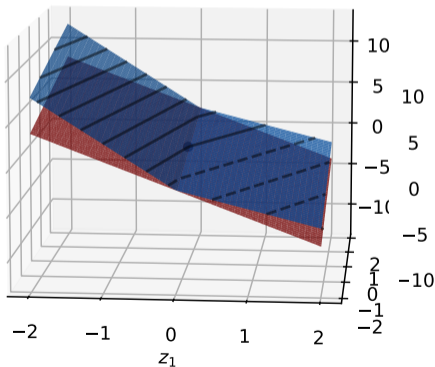
Subgradient

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



Subgradient

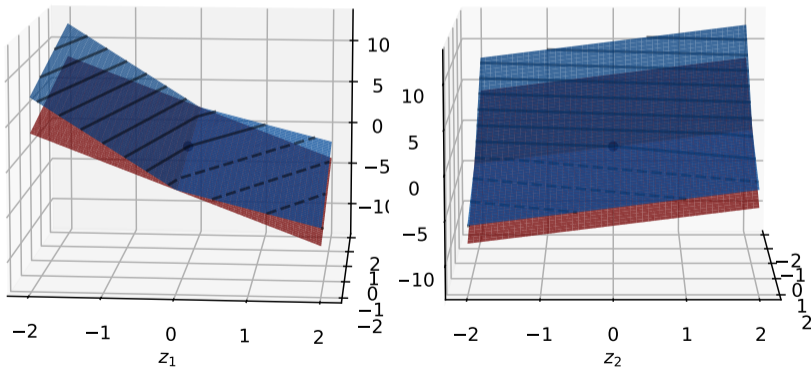
- ▶ A vector \vec{s} is a valid **subgradient** at $\vec{z}^{(0)}$ if the plane it defines lies at or below the function f .
 - ▶ Example: $(-3, 1)^T$



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:

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

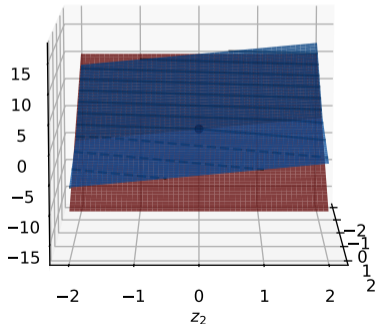
Finding Subgradients

- ▶ 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 at $(0, 0)$?



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 at the point $(0, 0)$?
- ▶ Is $f(0, 0) + (-5, 0)^T \cdot ((z_1, z_2) - (0, 0)^T) \leq f(z_1, z_2)$ 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

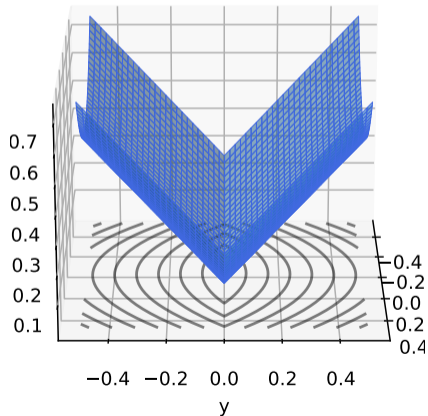
- ▶ A **subgradient** tells us where to go when the gradient is undefined.
- ▶ We can use it instead of the gradient in gradient descent.

Example

► $f(z_1, z_2) = z_1^2 + |z_2|$

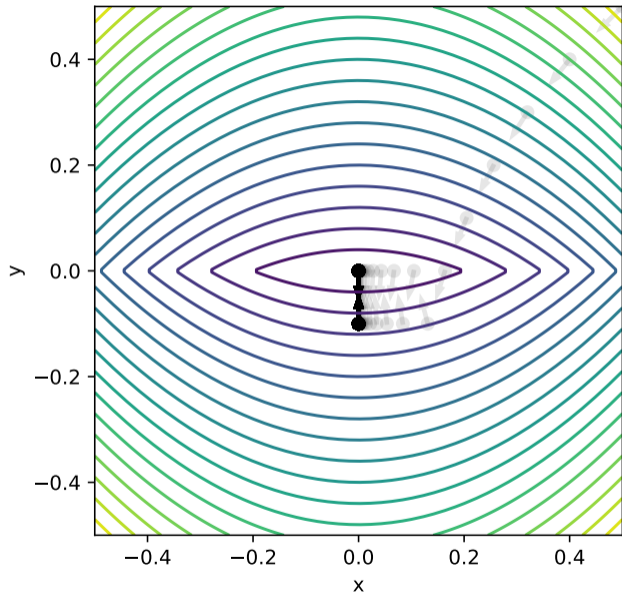
► A subgradient:

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



Example

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

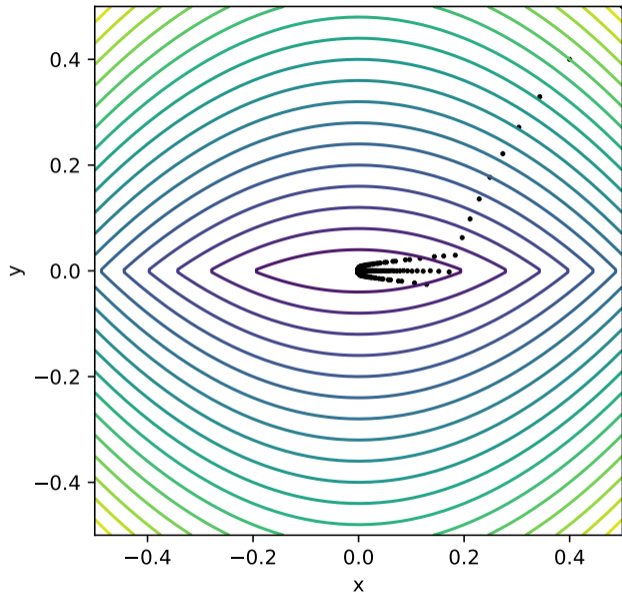


Problem

- ▶ 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.



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 $\vec{z}^{(t)}$.

DSC 140A

Probabilistic Modeling & Machine Learning

Lecture 5 | Part 3

Minimizing Risk w.r.t. Absolute Loss

Absolute Loss

- ▶ The **absolute loss** is a natural first choice for regression.
- ▶ The empirical risk becomes:

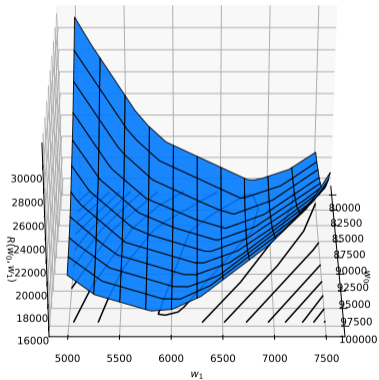
$$\begin{aligned} R_{\text{abs}}(\vec{w}) &= \frac{1}{n} \sum_{i=1}^n |H(\vec{x}^{(i)}) - y_i| \\ &= \frac{1}{n} \sum_{i=1}^n |\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) - y_i| \end{aligned}$$

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



Regression with Absolute Loss

- ▶ We were stuck before.
 - ▶ This risk is **not differentiable**.
- ▶ **Now:** we can minimize the risk with respect to the absolute loss using **subgradient descent**.

Subgradient of Empirical Risk

- ▶ We need a **subgradient** of the empirical risk with respect to the absolute loss.
- ▶ **Useful fact:** the subgradient of a sum is the sum of the subgradients.¹
- ▶ So it suffices to find a subgradient of the loss function:

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

¹At least, for convex functions.

Subgradient of the Absolute Loss

- ▶ We need a subgradient of the absolute loss.

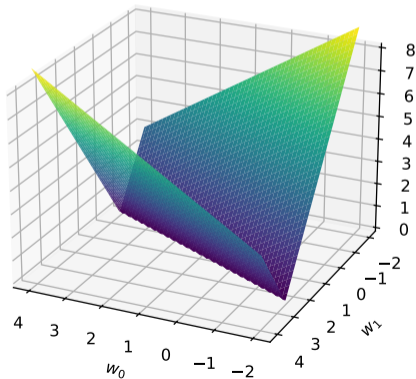
$$\ell_{\text{abs}}(\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}), y_i) = |\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) - y_i|$$

- ▶ An equivalent piecewise definition:

$$\ell_{\text{abs}}(\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}), y_i) = \begin{cases} \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) - y_i, & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) > y_i, \\ y_i - \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}), & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) < y_i, \\ 0, & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) = y_i. \end{cases}$$

The Absolute Loss

- ▶ Gradient exists except at $\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) = y_i$.
 - ▶ Here, we need a subgradient.



Exercise

What is the gradient when $\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) > y_i$? What about when $\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) < y_i$?

$$\ell_{\text{abs}}(\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}), y_i) = \begin{cases} \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) - y_i, & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) > y_i, \\ y_i - \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}), & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) < y_i, \\ 0, & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) = y_i. \end{cases}$$

Subgradient of the Absolute Loss

$$\ell_{\text{abs}}(\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}), y_i) = |\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) - y_i|$$

If $\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) > y_i$:

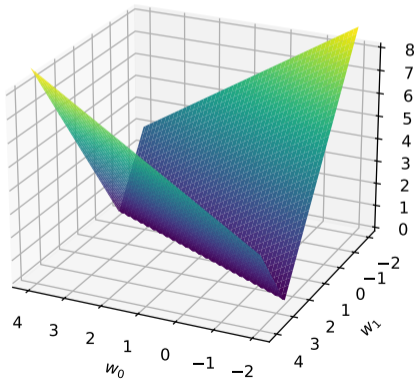
- ▶ Loss is $\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) - y_i$.
- ▶ Gradient is $\text{Aug}(\vec{x}^{(i)})$.

If $\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) < y_i$:

- ▶ Loss is $y_i - \vec{w} \cdot \text{Aug}(\vec{x}^{(i)})$.
- ▶ Gradient is $-\text{Aug}(\vec{x}^{(i)})$.

Subgradient of the Absolute Loss

- ▶ The zero vector works as a subgradient.



Subgradient of the Absolute Loss

- ▶ Our subgradient of the absolute loss:

$$s(\vec{w}; \vec{x}^{(i)}, y_i) = \begin{cases} \text{Aug}(\vec{x}^{(i)}), & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) > y_i, \\ -\text{Aug}(\vec{x}^{(i)}), & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) < y_i, \\ \vec{0}, & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) = y_i. \end{cases}$$

Minimizing the Absolute Loss

- ▶ The subgradient of the empirical risk is the average of the subgradients of the loss:

subgrad. of $R(\vec{w})$

$$= \frac{1}{n} \sum_{i=1}^n s(\vec{w}, \vec{x}^{(i)}, y_i)$$

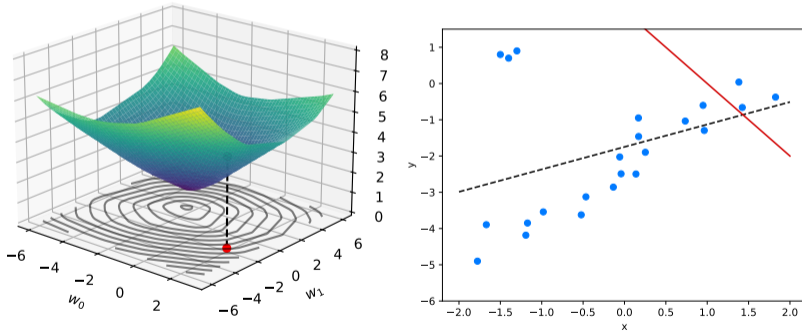
$$= \frac{1}{n} \sum_{i=1}^n \begin{cases} \text{Aug}(\vec{x}^{(i)}), & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) > y_i, \\ -\text{Aug}(\vec{x}^{(i)}), & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) < y_i, \\ \vec{0}, & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) = y_i. \end{cases}$$

Subgradient Descent

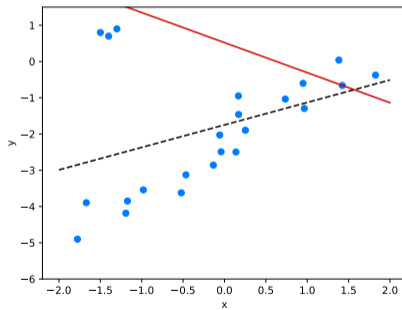
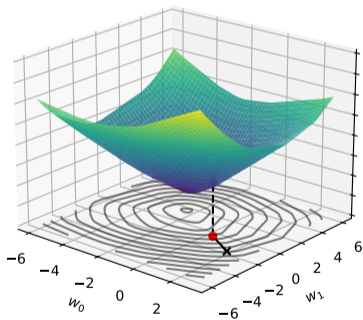
- ▶ We minimize the empirical risk with respect to the absolute loss using subgradient descent.
- ▶ Pick an initial $\vec{w}^{(0)}$, a decreasing learning rate schedule $\eta(t) > 0$.
- ▶ Until convergence, repeat:
 - ▶ Update

$$\vec{w}^{(t+1)} = \vec{w}^{(t)} - \eta(t) \times \frac{1}{n} \sum_{i=1}^n \begin{cases} \text{Aug}(\vec{x}^{(i)}), & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) > y_i, \\ -\text{Aug}(\vec{x}^{(i)}), & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) < y_i, \\ \vec{0}, & \text{if } \vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) = y_i. \end{cases}$$

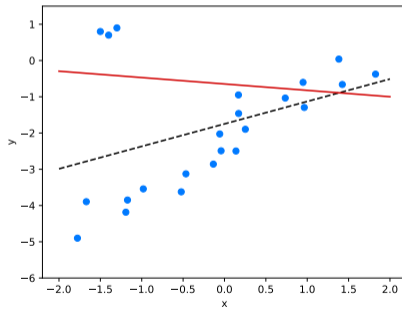
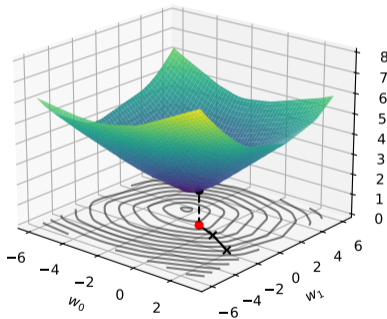
Example



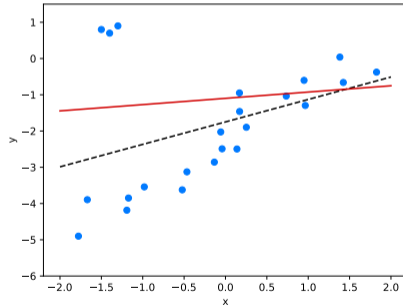
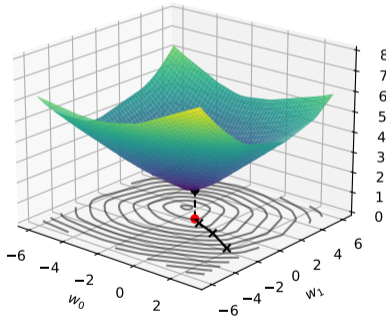
Example



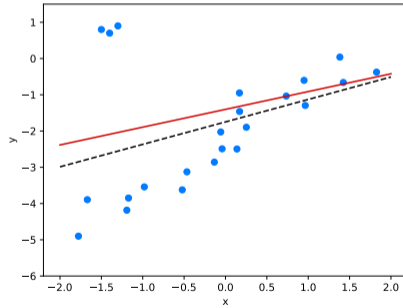
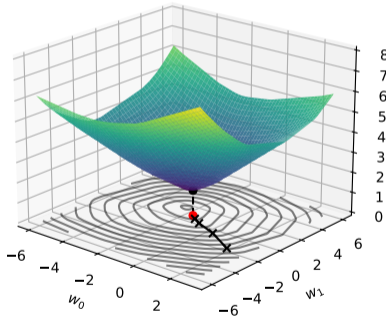
Example



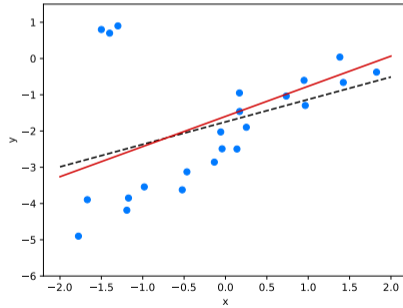
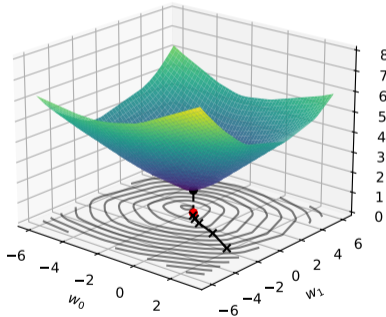
Example



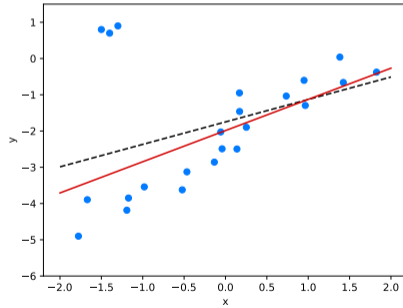
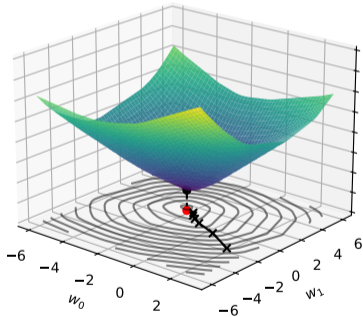
Example



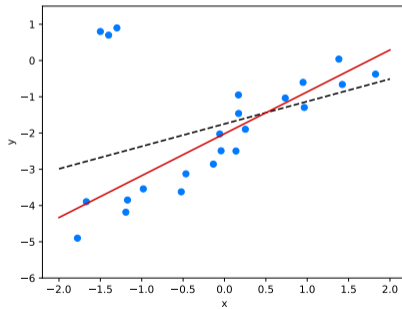
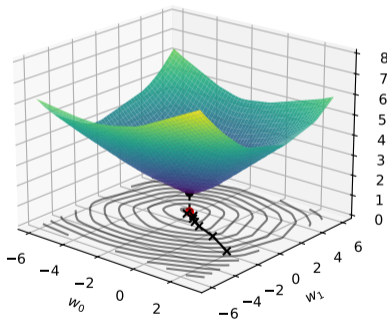
Example



Example



Example



In Practice

- ▶ We've minimized the risk with respect to the absolute loss.
- ▶ This approach has different names:
 - ▶ Quantile regression, median regression
 - ▶ Minimum Absolute Deviations (MAD)
- ▶ Solvable by (S)GD, or as a **linear program**.

DSC 140A

Probabilistic Modeling & Machine Learning

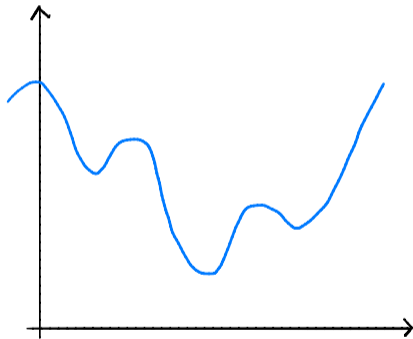
Lecture 5 | Part 4

Convexity

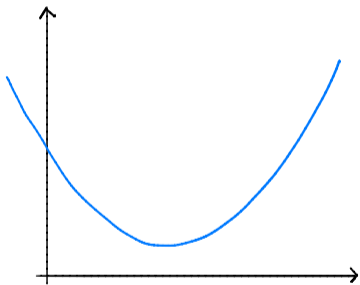
Question

- ▶ When is gradient descent guaranteed to work?

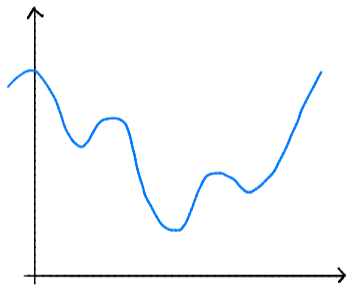
Not here...



Convex Functions



Convex



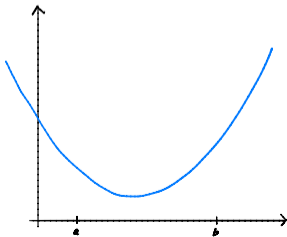
Non-convex

Convexity: Definition

- ▶ f is **convex** if for **every** a, b the line segment between

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

does not go below the plot of f .

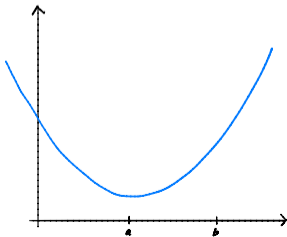


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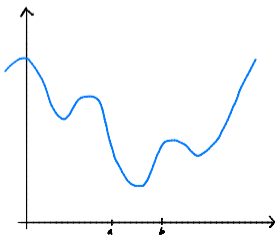


Convexity: Definition

- ▶ f is **convex** if for **every** a, b the line segment between

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

does not go below the plot of f .

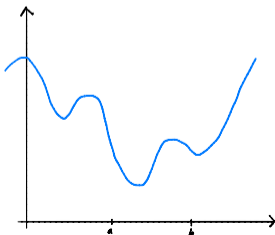


Convexity: Definition

- ▶ f is **convex** if for **every** a, b the line segment between

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

does not go below the plot of f .



Other Terms

- ▶ If a function is not convex, it is **non-convex**.
- ▶ **Strictly convex**: the line lies strictly above curve.
- ▶ **Concave**: the line lies on or below curve.

Exercise

True or False: a convex function must have a unique global minimum.

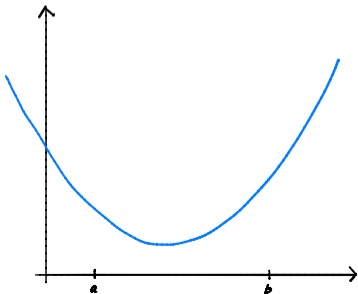
True or False: a local minimum of a convex function is always a global minimum.

True or False: a *strictly* convex function must have a unique global minimum.

Convexity: Formal Definition

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

$$(1 - t)f(a) + tf(b) \geq f((1 - t)a + tb).$$

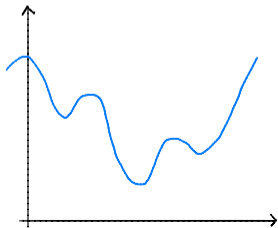
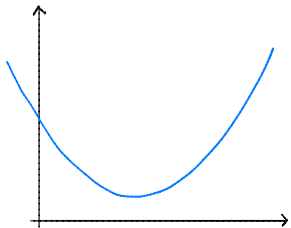


Exercise

Using the definition, is $f(x) = |x|$ convex?

Another View: Second Derivatives

- ▶ If $\frac{d^2f}{dx^2}(x) \geq 0$ for all x , then f is convex.
- ▶ Example: $f(x) = x^4$ is convex.
- ▶ **Warning!** Only works if f is twice differentiable!

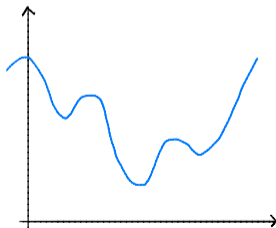
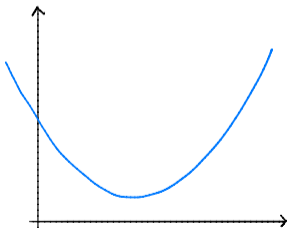


Another View: Second Derivatives

- ▶ “Best” straight line at x_0 :
 - ▶ $f_1(x) = f(x_0) + f'(x_0) \cdot (x - x_0)$
- ▶ “Best” parabola at x_0 :
 - ▶ $f_2(x) = f(x_0) + f'(x_0) \cdot (x - x_0) + \frac{1}{2}f''(x_0) \cdot (x - x_0)^2$
 - ▶ Possibilities: upward-facing, downward-facing, flat.

Convexity and Parabolas

- ▶ Convex if for **every** x_0 , parabola is upward-facing (or flat).
 - ▶ That is, $f''(x_0) \geq 0$.



Proving Convexity Using Properties

Suppose that $f(x)$ and $g(x)$ are convex. Then:

- ▶ $w_1 f(x) + w_2 g(x)$ is convex, provided $w_1, w_2 \geq 0$
 - ▶ Example: $3x^2 + |x|$ is convex
- ▶ $g(f(x))$ is convex, provided g is non-decreasing.
 - ▶ Example: e^{x^2} is convex
- ▶ $\max\{f(x), g(x)\}$ is convex
 - ▶ Example: $\begin{cases} 0, & x < 0 \\ x, & x \geq 0 \end{cases}$ is convex

Note!

- ▶ These properties are useful for proving convexity for functions of **one variable**.
- ▶ Some of them will not generalize to higher dimensions.

Convexity and Gradient Descent

- ▶ Convex functions are (relatively) easy to optimize.
- ▶ **Theorem:** if $f(x)$ is convex and “not too steep”² then (stochastic) (sub)gradient descent converges to a **global optimum** of f provided that the step size is small enough³

²Technically, c -Lipschitz

³step size related to steepness, should decrease like $1/\sqrt{\text{step \#}}$.

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Probabilistic Modeling & Machine Learning

Lecture 5 | Part 5

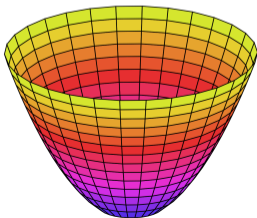
Convexity in Many Dimensions

Convexity: Definition

- ▶ $f(\vec{x})$ is **convex** if for **every** \vec{a}, \vec{b} the line segment between

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

does not go below the plot of f .



Convexity: Formal Definition

- ▶ A function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is **convex** if for every choice of $\vec{a}, \vec{b} \in \mathbb{R}^d$ and $t \in [0, 1]$:

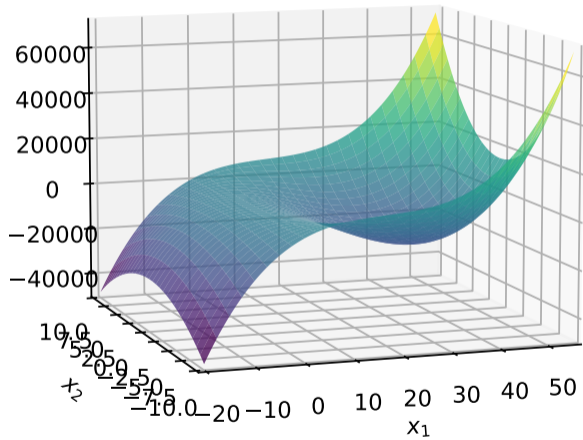
$$(1 - t)f(\vec{a}) + tf(\vec{b}) \geq f((1 - t)\vec{a} + t\vec{b}).$$

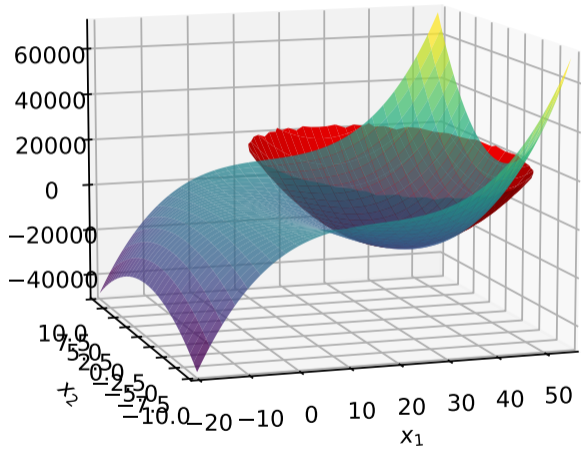
The Second Derivative Test

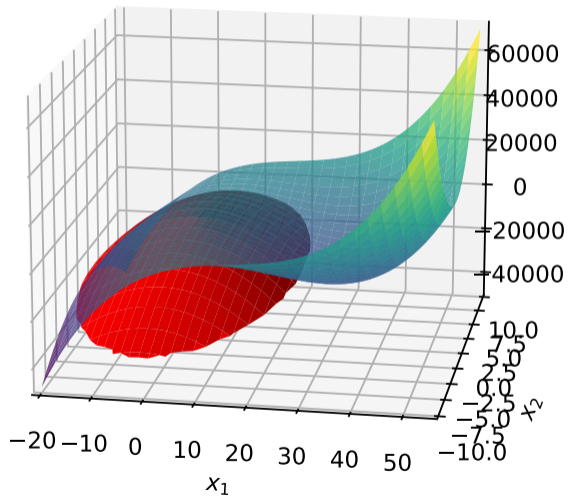
- ▶ For 1-dimensions functions:
 - ▶ convex if second derivative ≥ 0 .
- ▶ For d -dimensional functions:
 - ▶ convex if ???

Second Derivatives in d -Dimensions

- ▶ In 2-dimensions, there are 4 second derivatives:
 - ▶ $\frac{\partial^2 f}{\partial x_1^2}, \frac{\partial^2 f}{\partial x_2^2}, \frac{\partial^2 f}{\partial x_1 x_2}, \frac{\partial^2 f}{\partial x_2 x_1}$
- ▶ In d -dimensions, there are d^2 :
 - ▶ $\frac{\partial^2 f}{\partial x_i \partial x_j}$ for all i, j .
- ▶ The second derivatives describe the curvature of a paraboloid approximating f .







The Hessian Matrix

- ▶ Create the **Hessian** matrix of second derivatives:
- ▶ For $f : \mathbb{R}^2 \rightarrow \mathbb{R}$:

$$H(\vec{X}) = \begin{pmatrix} \frac{\partial f^2}{\partial x_1^2}(\vec{X}) & \frac{\partial f^2}{\partial x_1 x_2}(\vec{X}) \\ \frac{\partial f^2}{\partial x_2 x_1}(\vec{X}) & \frac{\partial f^2}{\partial x_2^2}(\vec{X}) \end{pmatrix}$$

In General

- If $f : \mathbb{R}^d \rightarrow \mathbb{R}$, the **Hessian** at \vec{x} is:

$$H(\vec{x}) = \begin{pmatrix} \frac{\partial f^2}{\partial x_1^2}(\vec{x}) & \frac{\partial f^2}{\partial x_1 x_2}(\vec{x}) & \dots & \frac{\partial f^2}{\partial x_1 x_d}(\vec{x}) \\ \frac{\partial f^2}{\partial x_2 x_1}(\vec{x}) & \frac{\partial f^2}{\partial x_2^2}(\vec{x}) & \dots & \frac{\partial f^2}{\partial x_2 x_d}(\vec{x}) \\ \dots & \dots & \dots & \dots \\ \frac{\partial f^2}{\partial x_d x_1}(\vec{x}) & \frac{\partial f^2}{\partial x_d^2}(\vec{x}) & \dots & \frac{\partial f^2}{\partial x_d^2}(\vec{x}) \end{pmatrix}$$

Second Derivative Test

- ▶ A function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is **convex** if for any $\vec{x} \in \mathbb{R}^d$, all **eigenvalues** of the Hessian matrix $H(\vec{x})$ are ≥ 0 .

For This Class...

- ▶ You will not need to compute eigenvalues “by hand”...
- ▶ Unless the matrix is diagonal.
 - ▶ In which case, the eigenvalues are the diagonal entries.

Example

- ▶ The eigenvalues of this matrix are 5, 2, and 1.

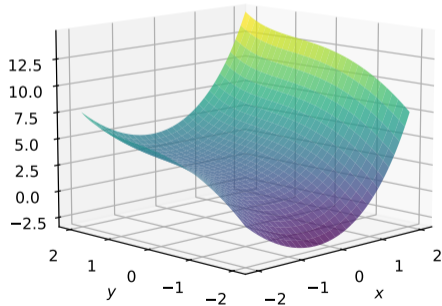
$$\begin{pmatrix} 5 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Exercise

Is $f(x, y) = e^x + e^y + x^2 - y^2$ convex?

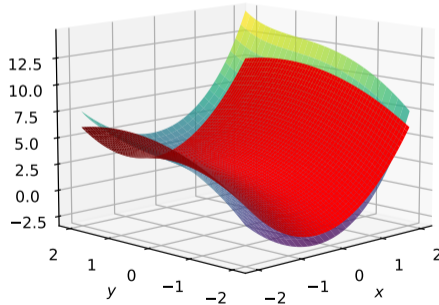
No

- ▶ The Hessian at $(0,0)$ has a negative eigenvalue.



No

- ▶ The Hessian at $(0,0)$ has a negative eigenvalue.



Exercise

Is $f(\vec{w}) = \|\vec{w}\|^2$ convex?

Note

- ▶ The second derivative test only works if f is twice differentiable.
- ▶ A function can be convex without having a second derivative.

Properties

- ▶ We can often prove convexity using properties.
- ▶ Two useful properties:
 - ▶ Sums of convex functions are convex.
 - ▶ Affine compositions of convex functions are convex.

Sums of Convex Functions

- ▶ Suppose that $f(\vec{x})$ and $g(\vec{x})$ are convex. Then $w_1 f(\vec{x}) + w_2 g(\vec{x})$ is convex, provided $w_1, w_2 \geq 0$.

Affine Composition

- ▶ Suppose that $f(x)$ is convex. Let A be a matrix, and \vec{x} and \vec{b} be vectors. Then

$$g(\vec{x}) = f(A\vec{x} + \vec{b})$$

is convex as a function of \vec{x} .

- ▶ **Remember:** a vector is a matrix with one column/row.
- ▶ Useful!

Exercise

Consider the function

$$f(\vec{w}) = (\vec{x} \cdot \vec{w} - y)^2$$

Is this function convex as a function of \vec{w} ?

DSC 140A

Probabilistic Modeling & Machine Learning

Lecture 5 | Part 6

Convex Loss Functions

Empirical Risk Minimization (ERM)

- ▶ Step 1: choose a **hypothesis class**
 - ▶ We've chosen linear predictors, $H(\vec{x}) = \text{Aug}(\vec{x}) \cdot \vec{w}$.
- ▶ Step 2: choose a **loss function**
- ▶ Step 3: find \vec{w} minimizing **empirical risk**
 - ▶ Some choices of loss function make this **easier**.

Convexity and Gradient Descent

- ▶ Convex functions are (relatively) easy to optimize.
- ▶ **Theorem:** if $f(x)$ is convex and “not too steep”⁴ then (stochastic) (sub)gradient descent converges to a **global optimum** of f provided that the step size is small enough⁵.

⁴Technically, c -Lipschitz

⁵step size related to steepness, should decrease like $1/\sqrt{\text{step \#}}$

Convex Loss

- ▶ **Recall:** sums of convex functions are convex.
- ▶ **Implication:** if loss function is convex as a function of \vec{w} , so is the empirical risk, $R(\vec{w})$

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

- ▶ **Takeaway:** Convex losses make ERM **easier**.

Example: Square Loss

- ▶ Recall the square loss for a linear predictor:

$$\ell_{\text{sq}}(\text{Aug}(\vec{x}) \cdot \vec{w}, y) = (\text{Aug}(\vec{x}) \cdot \vec{w} - y)^2$$

- ▶ This is **convex** as a function of \vec{w} .
- ▶ **Proof:** a few slides ago.

Example: Absolute Loss

- ▶ Recall the absolute loss for a linear predictor:

$$\ell_{\text{abs}}(\text{Aug}(\vec{x}) \cdot \vec{w}, y) = |\text{Aug}(\vec{x}) \cdot \vec{w} - y|$$

- ▶ This is **convex** as a function of \vec{w} .

Linear Predictors

- ▶ It's also important that we've chosen linear predictors.
- ▶ A loss that is **convex** in \vec{w} for linear $H_1(x)$ may be **non-convex** for non-linear $H_2(x)$.
- ▶ Example: square loss.
 - ▶ If $H_1(x) = w_0 + w_1x$, then $(w_0 + w_1x - y)^2$ is **convex**.
 - ▶ If $H_2(x) = w_0 e^{w_1x}$, then $(w_0 e^{w_1x} - y)^2$ is **non-convex**.

Summary

- ▶ By combining 1) linear predictors and 2) a convex loss function, we make ERM **easier**.
- ▶ **Many** machine learning algorithms are linear predictors with convex loss functions.
 - ▶ As we'll see...

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Probabilistic Modeling & Machine Learning

Lecture 5 | Part 7

Appendix: From Theory to Practice

Gradient Descent

- ▶ We've spent three lectures on **gradient descent**.
- ▶ A powerful optimization algorithm.
- ▶ In practice, we use extensions of (stochastic) gradient descent.

Extensions of SGD

- ▶ Newton's method
 - ▶ Second order optimization, using the Hessian.
 - ▶ Can converge in fewer steps.
 - ▶ But the Hessian is **expensive** to compute.

- ▶ Adagrad, RMSprop, Adam
 - ▶ SGD with adaptive learning rates.
 - ▶ Used heavily in training of deep neural networks.

Non-Convex Optimization

- ▶ So far, we've only seen convex risks.
- ▶ But there's an important class of machine learning algorithms that have **non-convex** risks.
- ▶ **Namely:** deep neural networks.

Empirical Risk Minimization (ERM)

- ▶ Step 1: choose a **hypothesis class**
 - ▶ **Deep neural networks.**
- ▶ Step 2: choose a **loss function**
- ▶ Step 3: find \vec{w} minimizing **empirical risk**

Deep Learning

- ▶ A **deep neural network** is a prediction function $H(\vec{x}; \vec{w})$ composed of many layers.
- ▶ Typically, H is not linear in \vec{w} .
- ▶ The risk becomes highly **non-convex**.
 - ▶ Even, for example, the square loss.
- ▶ How do we minimize the empirical risk?

Answer: SGD

- ▶ We use **stochastic gradient descent** (and extensions).
 - ▶ Even though the empirical risk is **non-convex**.
 - ▶ The optimization problem becomes much harder.
- ▶ SGD may not find a global minimum of the risk.
- ▶ But often finds a “**good enough**” local minimum.

Next Time

- ▶ Linear classification.