# DSC 140A

## Probabilistic Modeling & Machine Learning

Lecture 5 | 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**
  - In case of linear predictors, equivalent to finding $\vec{w}$.

# Minimizing Empirical Risk

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

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

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

# 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**.

# Last Time

We addressed 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 outstanding questions:

1. How do we minimize the risk with respect to the **absolute loss**?
2. When is gradient descent **guaranteed** to work?

# DSC 140A

Probabilistic Modeling & Machine Learning

Lecture 5 | Part 2

## Minimizing Risk w.r.t. Absolute Loss

# Regression with Absolute Loss

- The risk with respect to the absolute loss:

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

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

# 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:

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

[1] At least, for convex functions.

# Subgradient of the Absolute Loss

- We need a subgradient of the absolute loss.

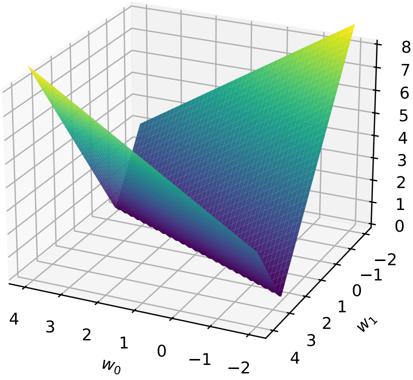
$$\ell_{\text{abs}}(\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}), y_i) = |\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) - y_i|$$

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

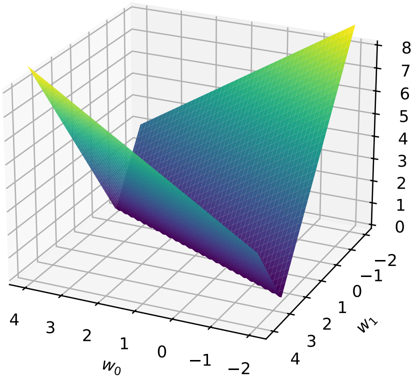
- Loss is $\vec{w} \cdot \text{Aug}(\vec{x}^{(i)}) - y_i$.
- Gradient is $\text{Aug}(\vec{x}^{(i)})$.

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:

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

# Minimizing the Absolute Loss

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

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

# Subgradient Descent

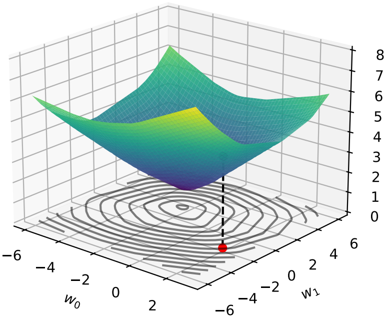
- We minimize the empirical risk with respect to the absolute loss using subgradient descent.

- Pick an initial $\vec{w}^{(0)}$, a decreasing learning rate schedule $\eta(t) > 0$.

- Until convergence, repeat:
  - Update

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

# Example



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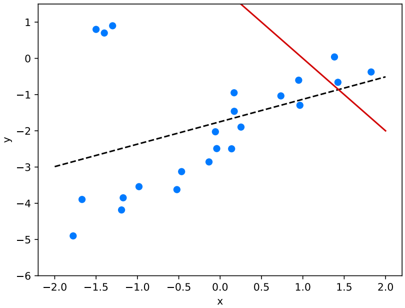

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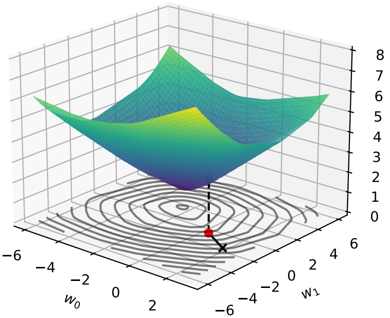


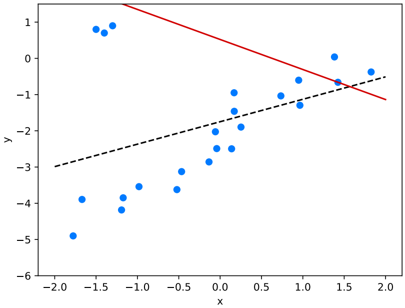

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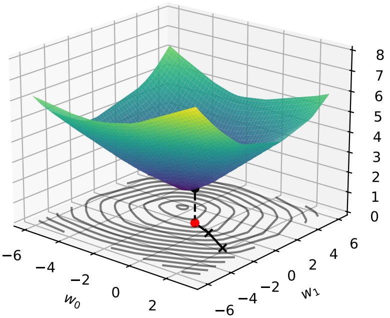

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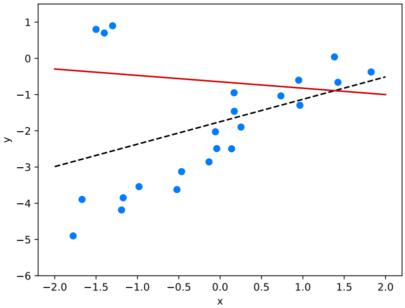

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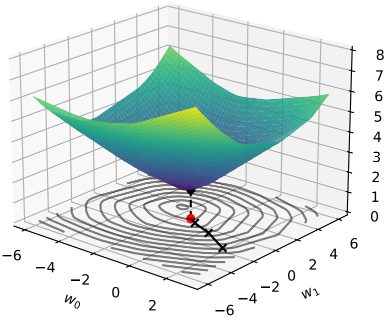


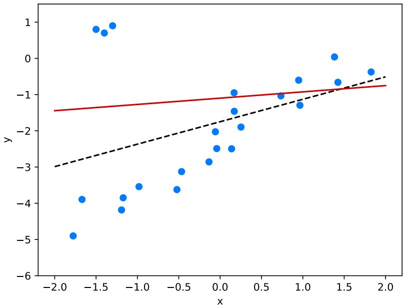

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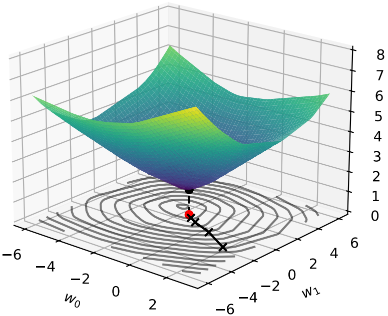

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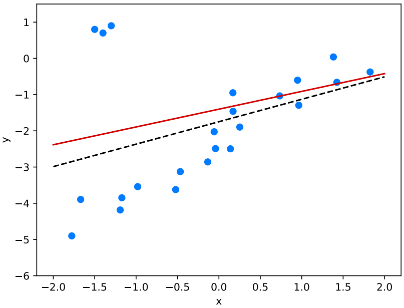

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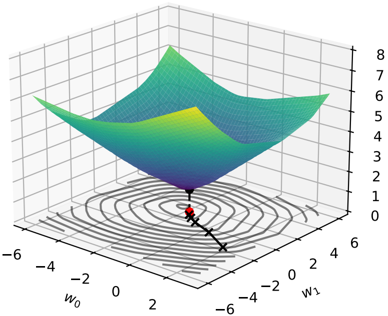

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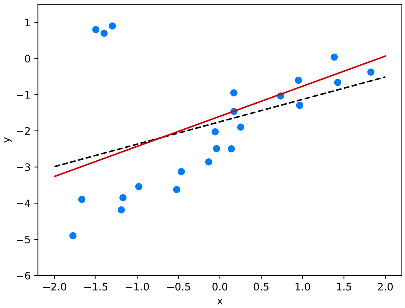

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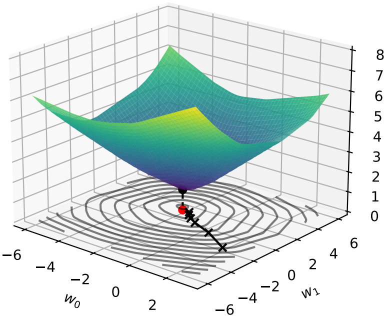

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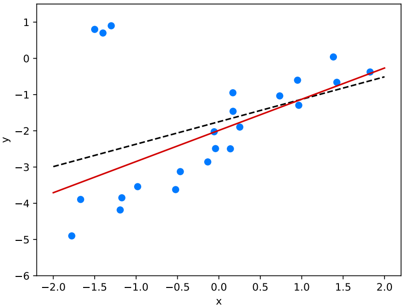

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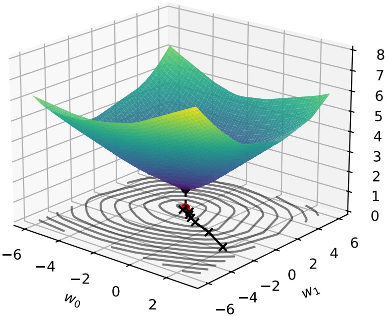
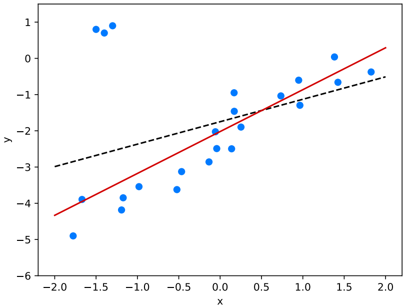


# In Practice

- 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

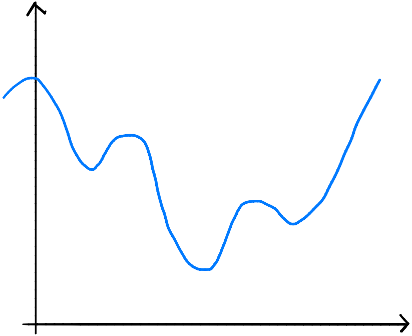
Lecture 5 | Part 3

## Convexity

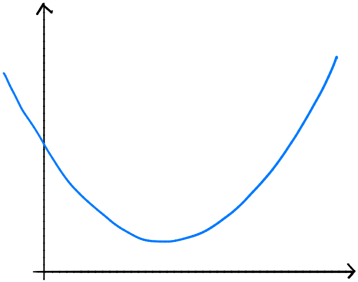
# Question

- When is gradient descent guaranteed to work?

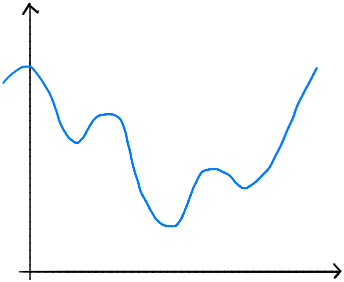
# Not here...



# Convex Functions



Convex



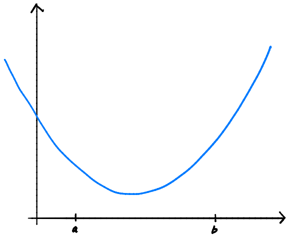
Non-convex

# Convexity: Definition

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

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

does not go below the plot of $f$.



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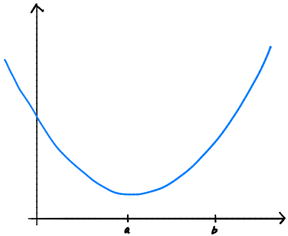

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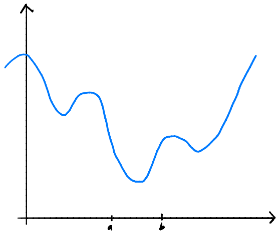

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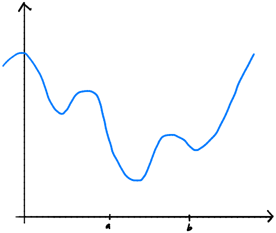


# Other Terms

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

## Exercise

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

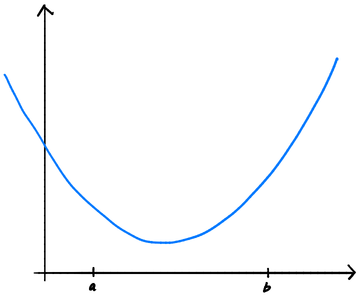
**True** or **False**: a local minimum of a convex function is always a global minimum.

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

# Convexity: Formal Definition

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

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

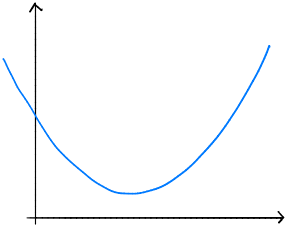


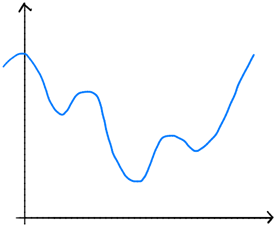
## Exercise

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

# Another View: Second Derivatives

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



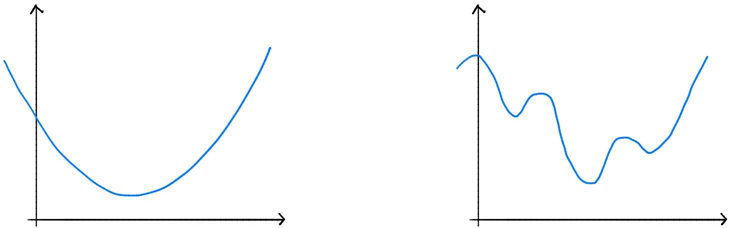


# Another View: Second Derivatives

- "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: $\begin{cases} 0, & \text{x} < 0 \\ x, & \text{x} \geq 0 \end{cases}$ 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 enough[3]

[2] Technically, $c$-Lipschitz

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

# DSC 140A

## Probabilistic Modeling & Machine Learning

Lecture 5 | Part 4

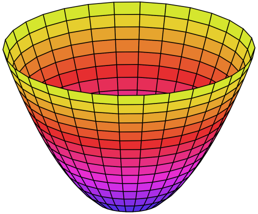
## Convexity in Many Dimensions

# Convexity: Definition

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

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

does not go below the plot of $f$.



# Convexity: Formal Definition

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

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

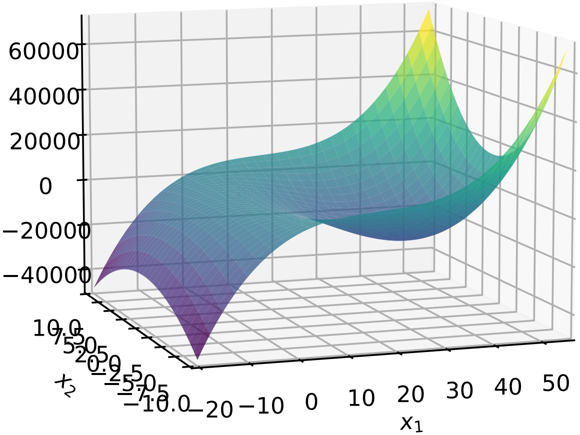
# The Second Derivative Test

- For 1-dimensions functions:
  - convex if second derivative $\geq 0$.

- For $d$-dimensional functions:
  - convex if ???

# Second Derivatives in $d$-Dimensions

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



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−2.5
−5.0
−7.5
−10.0
$x_2$
−20
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0
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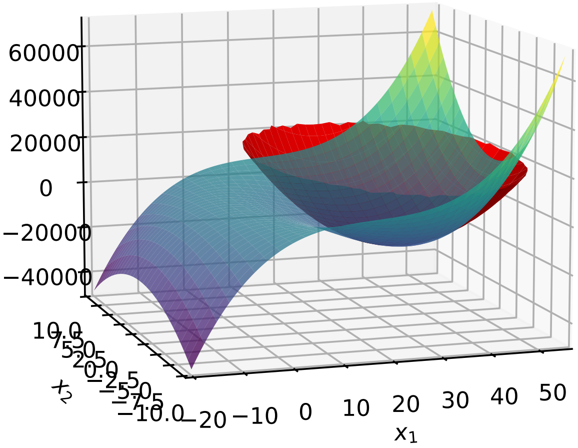
20
30
40
50
$x_1$


60000
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$x_2$
−20
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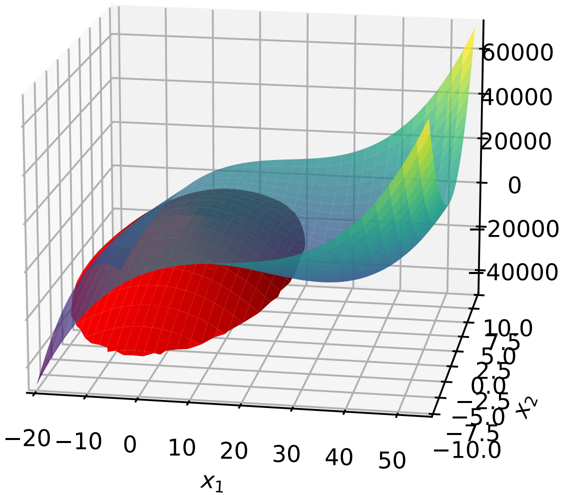
$x_1$



60000
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−5.0
−7.5
−10.0
$x_2$
−20
−10
0
10
20
30
40
50
$x_1$

# The Hessian Matrix

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

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

# In General

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

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

# Second Derivative Test

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

# 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.

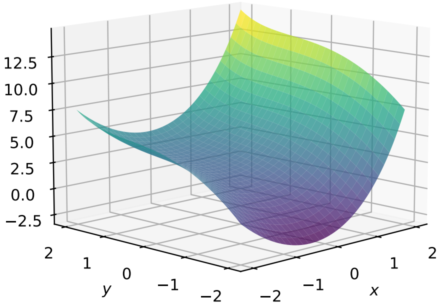
$$\begin{pmatrix} 5 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

**Exercise**

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

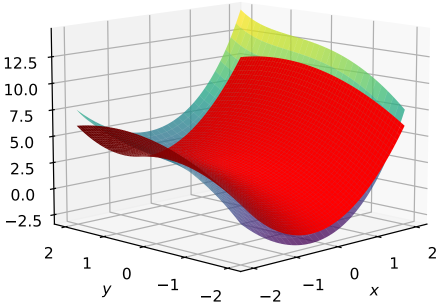
# No

- 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 5

## 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 enough[5].

[4] Technically, $c$-Lipschitz

[5] step 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 $H_1(x) = w_0 + w_1 x$, then $(w_0 + w_1 x - y)^2$ is **convex**.
  - If $H_2(x) = w_0 e^{w_1 x}$, then $(w_0 e^{w_1 x} - y)^2$ 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...

# DSC 140A

Probabilistic Modeling & Machine Learning

Lecture 5 | Part 6

## 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.