10-301/601: Introduction to Machine Learning Lecture 8 – Optimization for Machine Learning

Henry Chai & Matt Gormley

9/26/22

Q & A:

The Perceptron mistake bound is so strange, how exactly did we end up with R/γ^2?

- Definitely a fair question: while the proof of the Perceptron mistake bound isn't too complicated, it's also not strictly speaking relevant to the content of our course.
- That being said, Matt has graciously agreed to put together a short (optional) video going through the proof; if you're interested, you can find it here, in our Panopto folder.

Front Matter

- Announcements:
  - HW3 released 9/21, due 9/28 at 11:59 PM
    - **Only two grace days allowed on HW3**
    - HW3 exit poll has also been released: you have until one week from the due date to complete it
  - Exam 1 on 10/4 (one week from tomorrow!) from 6:30 PM - 8:30 PM
    - If you have a conflict, you must complete the Exam conflict form by 9/27 (tomorrow!) at 1 PM

Exam 1 Logistics

- Location & Seats: You all will be split across multiple (large) rooms.
  - Everyone will have an assigned seat
  - Please watch Piazza carefully for more details
  - If you have exam accommodations through ODR, they will be proctoring your exam on our behalf; **you are responsible for submitting the exam proctoring request through your student portal.**

Exam 1 Logistics

- Format of questions:
  - Multiple choice
  - True / False (with justification)
  - Derivations
  - Short answers
  - Drawing & Interpreting figures
  - Implementing algorithms on paper
- No electronic devices (you won’t need them!)
- You are allowed to bring one letter-size sheet of notes; you can put *whatever* you want on *both sides*

Exam 1 Topics

- Covered material: Lectures 1 – 7
  - Foundations
    - Probability, Linear Algebra, Geometry, Calculus
    - Optimization
  - Important Concepts
    - Overfitting
    - Model selection / Hyperparameter optimization
  - Decision Trees
  - k-NN
  - Perceptron
  - Regression
    - Decision Tree and k-NN Regression
    - Linear Regression

Exam 1 Preparation

- Attend the midterm review lecture (right now!)
- Review the exam practice problems (released 9/22 on the course website, under Coursework)
- Review HWs 1 - 3
- Consider whether you have achieved the “learning objectives” for each lecture / section
- Write your one-page cheat sheet (back and front)

Exam 1 Tips

- Solve the easy problems first
- If a problem seems extremely complicated, you might be missing something
- If you make an assumption, write it down
- Don't leave any answer blank
    - If you look at a question and don't know the answer:
        - just start trying things
        - consider multiple approaches
        - imagine arguing for some answer and see if you like it

Practice Problem 1a: Decision Trees

Consider the problem of predicting whether the university will be closed on a particular day. We will assume that the factors which decide this are whether there is a snowstorm, whether it is a weekend or an official holiday. Suppose we have the training examples described in the Table 5.2.

Snowstorm	Holiday	Weekend	Closed
T	T	F	F
T	T	F	T
F	T	F	F
T	T	F	F
F	F	F	F
F	F	F	T
T	F	F	T
F	F	F	T

Table 1: Training examples for decision tree

- What would be the effect of the “Weekend” attribute on the decision tree if we made it the root node? Explain your answer in terms of mutual information

Practice Problem 1b: Decision Trees

Consider the problem of predicting whether the university will be closed on a particular day. We will assume that the factors which decide this are whether there is a snowstorm, whether it is a weekend or an official holiday. Suppose we have the training examples described in the Table 5.2.

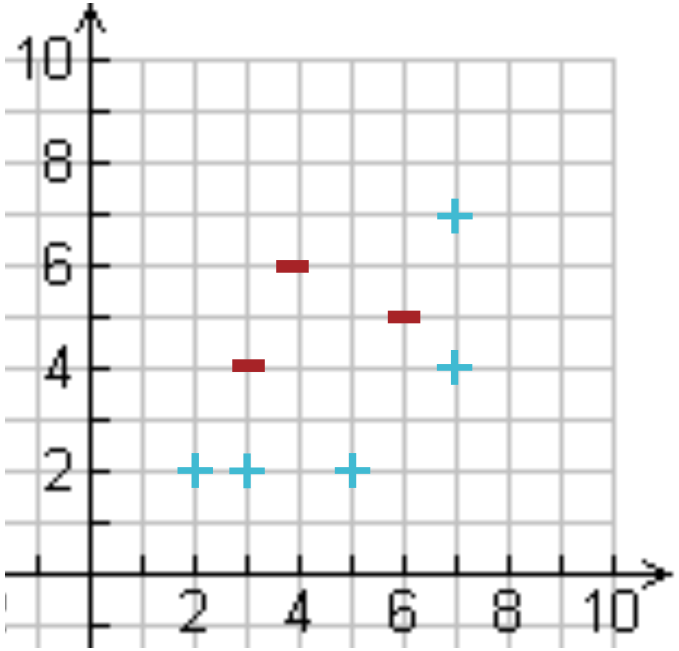
Snowstorm	Holiday	Weekend	Closed
T	T	F	F
T	T	F	T
F	T	F	F
T	T	F	F
F	F	F	F
F	F	F	T
T	F	F	T
F	F	F	T

Table 1: Training examples for decision tree

- Which attribute would we split on first if we used mutual information as the splitting criterion? You may use $\log_2\left(\frac{3}{4}\right) = -0.4$ and $\log_2\left(\frac{1}{4}\right) = -2$

Practice Problem 2: k-NN

- Consider the dataset below:



- What is the leave-one-out cross-validation error for a 1-NN model using the Euclidean distance?

Practice Problem 3: Perceptron

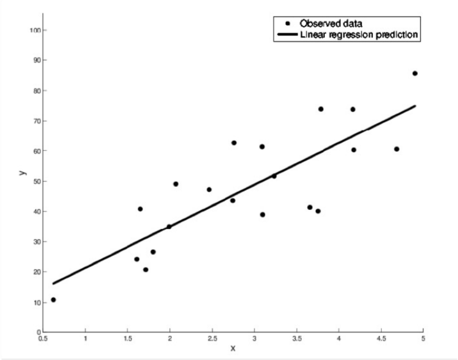
- True or False: Consider two datasets $\mathcal{D}_1 = \left\{\left(\boldsymbol{x}_1^{(1)}, y_1^{(1)}\right), \left(\boldsymbol{x}_1^{(2)}, y_1^{(2)}\right), \dots, \left(\boldsymbol{x}_1^{(N_1)}, y_1^{(N_1)}\right)\right\}$ and $\mathcal{D}_2 = \left\{\left(\boldsymbol{x}_2^{(1)}, y_2^{(1)}\right), \left(\boldsymbol{x}_2^{(2)}, y_2^{(2)}\right), \dots, \left(\boldsymbol{x}_2^{(N_2)}, y_2^{(N_2)}\right)\right\}$ where $\boldsymbol{x}_1^{(i)} \in \mathbb{R}^{d_1}$ and $\boldsymbol{x}_2^{(i)} \in \mathbb{R}^{d_2}$. Suppose $N_1 > N_2$ and $d_1 > d_2$. The maximum number of mistakes the Perceptron learning algorithm will make on $\mathcal{D}_1$ is higher than the maximum number of mistakes it will make on $\mathcal{D}_2$.

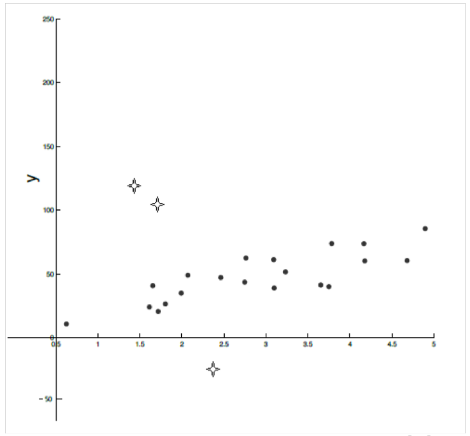
Poll Question 1

- True or False: Consider two datasets $\mathcal{D}_1 = \left\{\left(\boldsymbol{x}_1^{(1)}, y_1^{(1)}\right), \left(\boldsymbol{x}_1^{(2)}, y_1^{(2)}\right), \dots, \left(\boldsymbol{x}_1^{(N_1)}, y_1^{(N_1)}\right)\right\}$ and $\mathcal{D}_2 = \left\{\left(\boldsymbol{x}_2^{(1)}, y_2^{(1)}\right), \left(\boldsymbol{x}_2^{(2)}, y_2^{(2)}\right), \dots, \left(\boldsymbol{x}_2^{(N_2)}, y_2^{(N_2)}\right)\right\}$ where $\boldsymbol{x}_1^{(i)} \in \mathbb{R}^{d_1}$ and $\boldsymbol{x}_2^{(i)} \in \mathbb{R}^{d_2}$. Suppose $N_1 > N_2$ and $d_1 > d_2$. The maximum number of mistakes the Perceptron learning algorithm will make on $\mathcal{D}_1$ is higher than the maximum number of mistakes it will make on $\mathcal{D}_2$.
  - True
  - False
  - True and False **(TOXIC)**

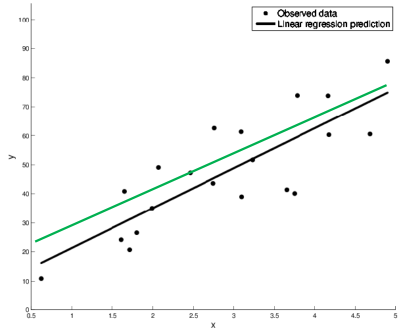
Practice Problem 4a: Linear Regression

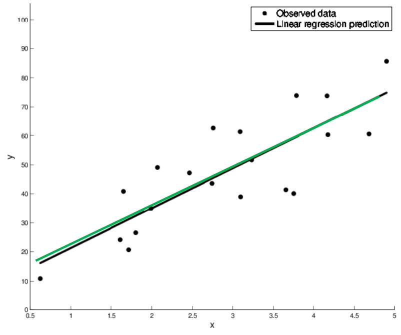
Consider the dataset plotted in the figure below along with the line learned by linear regression.

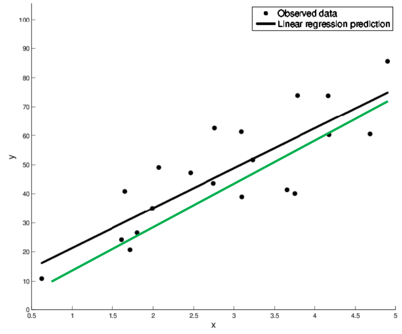




Now suppose we slightly alter the dataset in different ways: for each new dataset, select the option below that best approximates the new line linear regression would learn

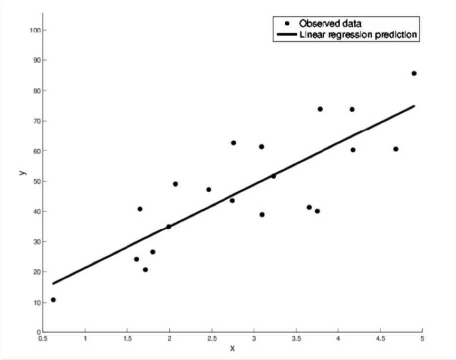


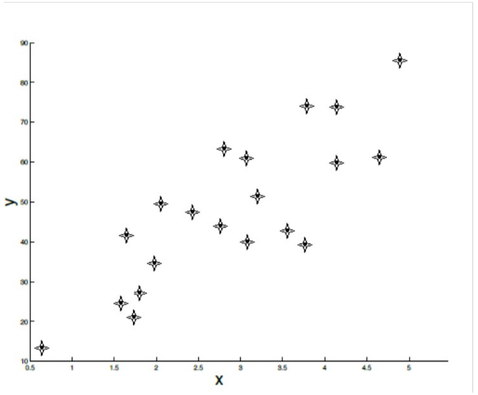




Practice Problem 4b: Linear Regression

Consider the dataset plotted in the figure below along with the line learned by linear regression.





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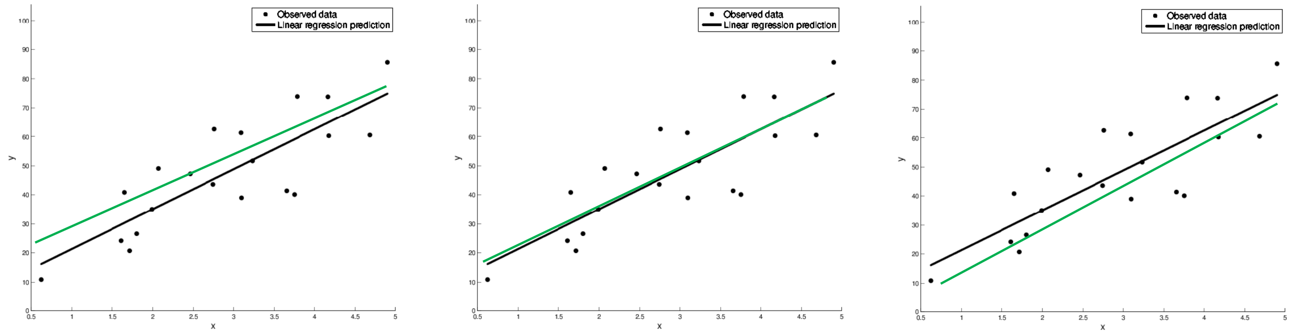
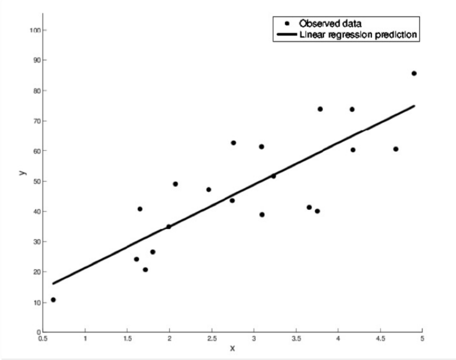
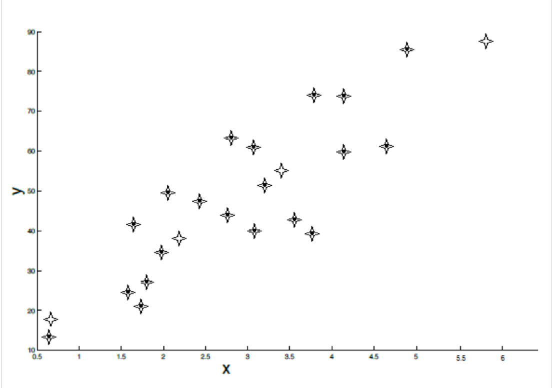


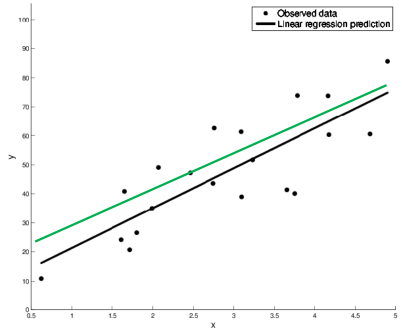
Practice Problem 4c: Linear Regression

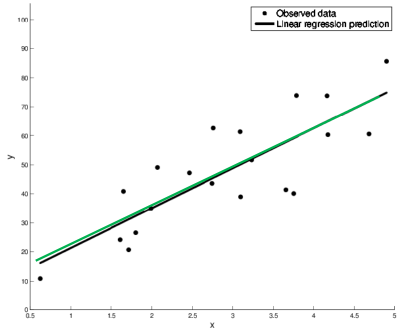
Consider the dataset plotted in the figure below along with the line learned by linear regression.

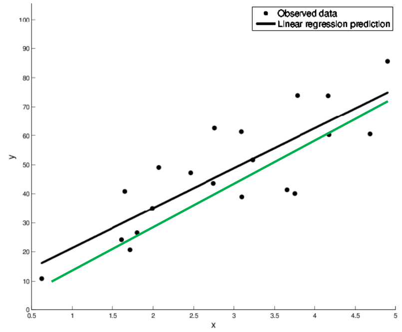




Now suppose we slightly alter the dataset in different ways: for each new dataset, select the option below that best approximates the new line linear regression would learn







Poll Question 2

What questions do you have?

Recall: Gradient Descent for Linear Regression

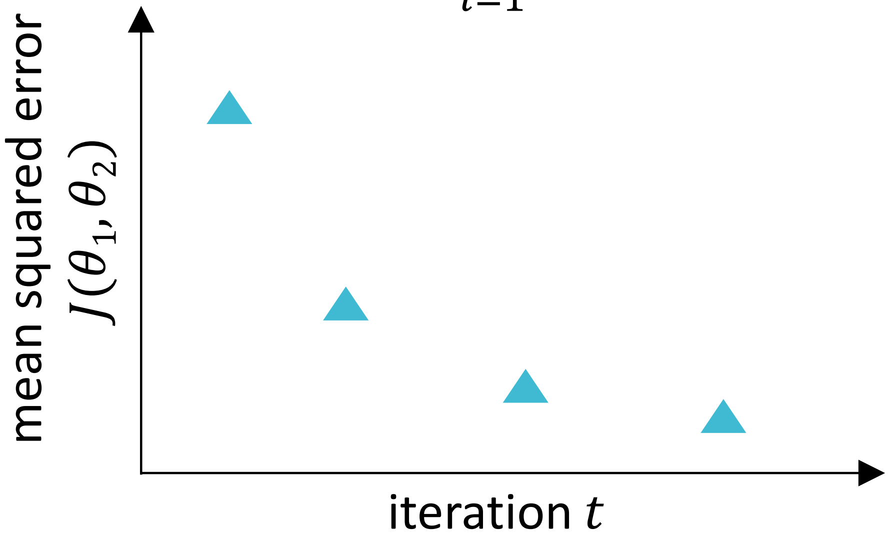
- Gradient descent for linear regression repeatedly takes steps opposite the gradient of the objective function

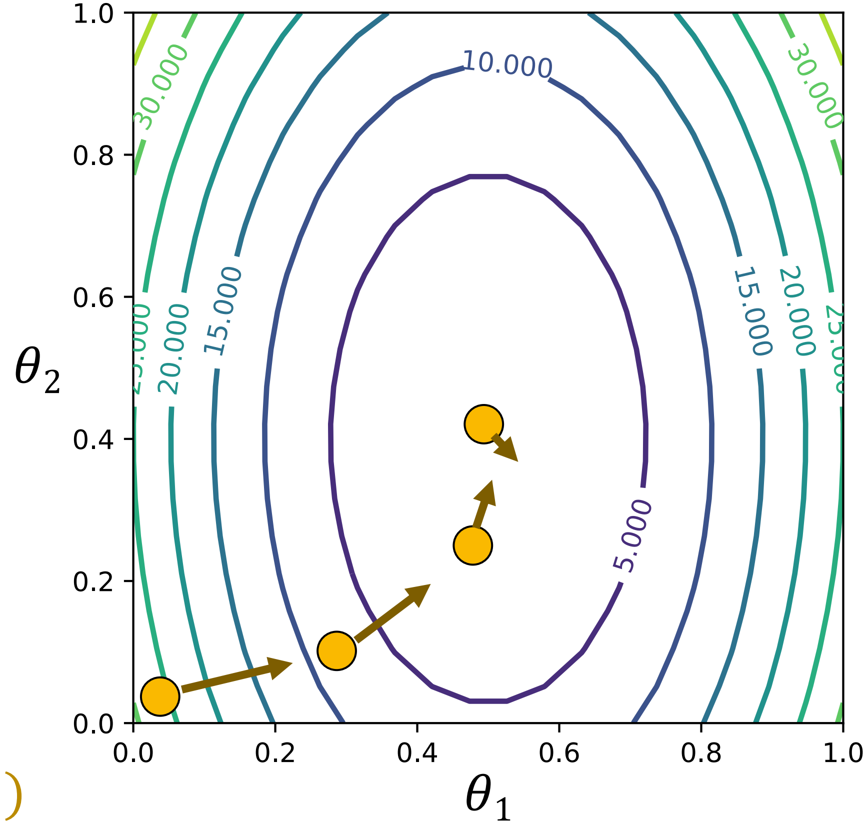
Algorithm 1 GD for Linear Regression

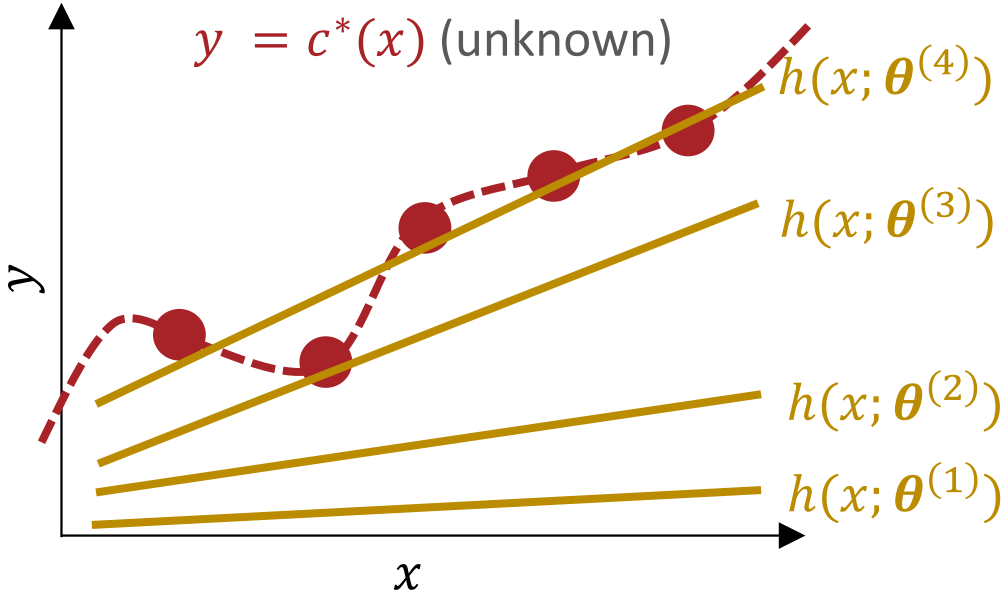
1: **procedure** GDLR($\mathcal{D}$, $\boldsymbol{\theta}^{(0)}$)
2: $\quad\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$ ▷ Initialize parameters
3: $\quad$**while** not converged **do**
4: $\quad\quad\mathbf{g} \leftarrow \sum_{i=1}^{N} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) \mathbf{x}^{(i)}$ ▷ Compute gradient
5: $\quad\quad\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \gamma \mathbf{g}$ ▷ Update parameters
6: $\quad$**return** $\boldsymbol{\theta}$

Recall: Gradient Descent for Linear Regression

$$J(\theta_1, \theta_2) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T \boldsymbol{x}^{(i)}\right)^2$$







t	θ_1	θ_2	$J(\theta_1, \theta_2)$
1	0.01	0.02	25.2
2	0.30	0.12	8.7
3	0.51	0.30	1.5
4	0.59	0.43	0.2

Why Gradient Descent for Linear Regression?

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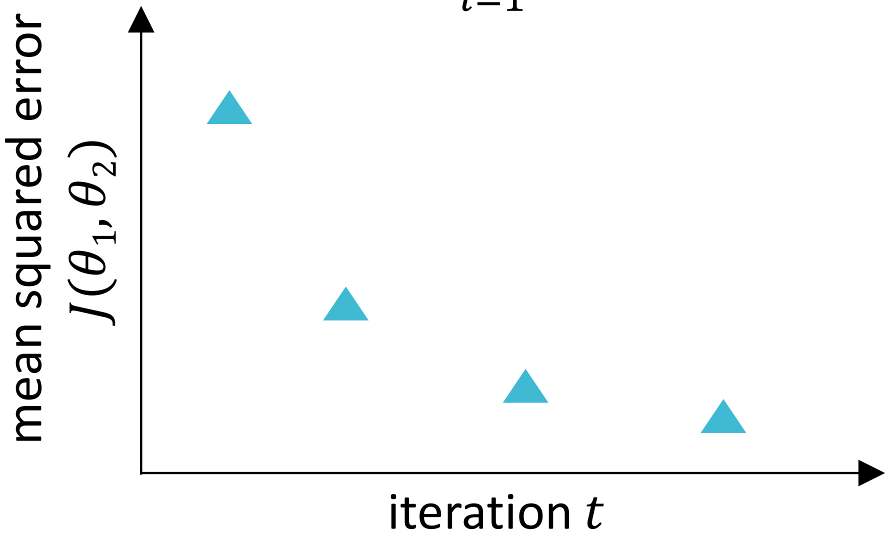

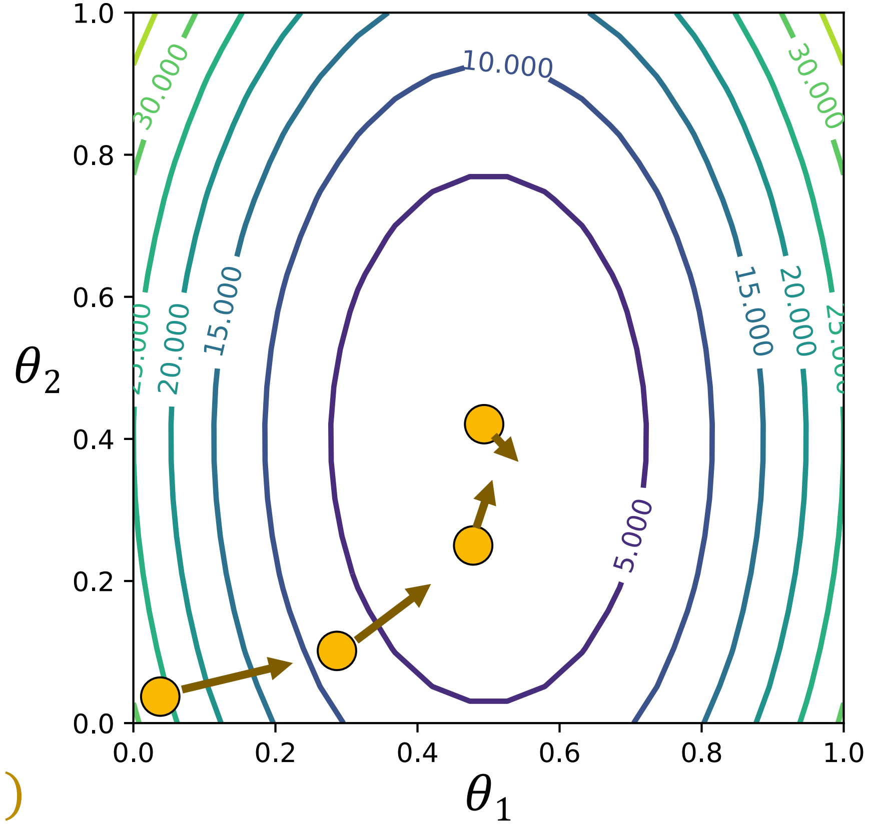

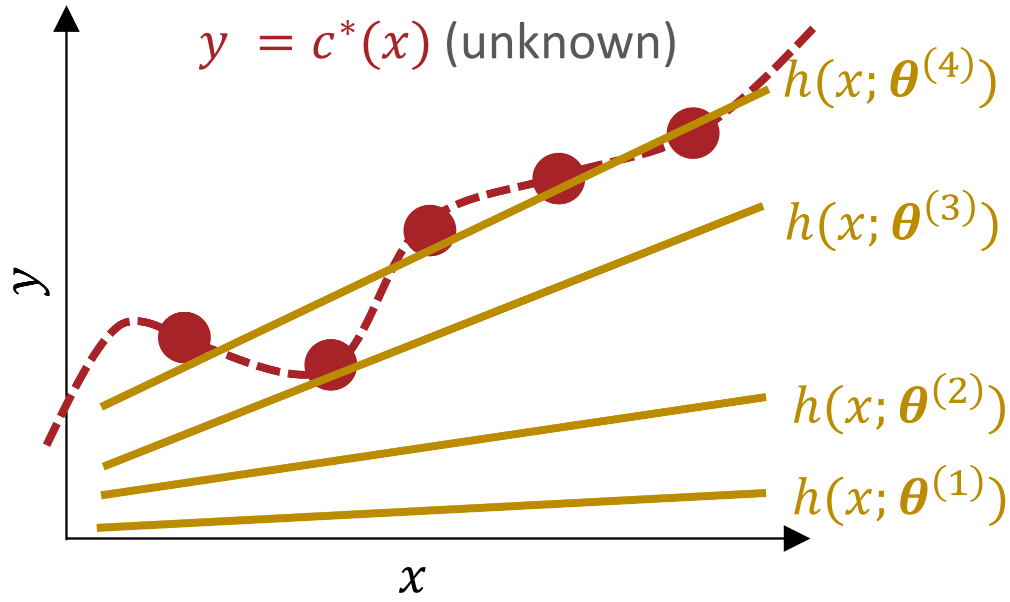

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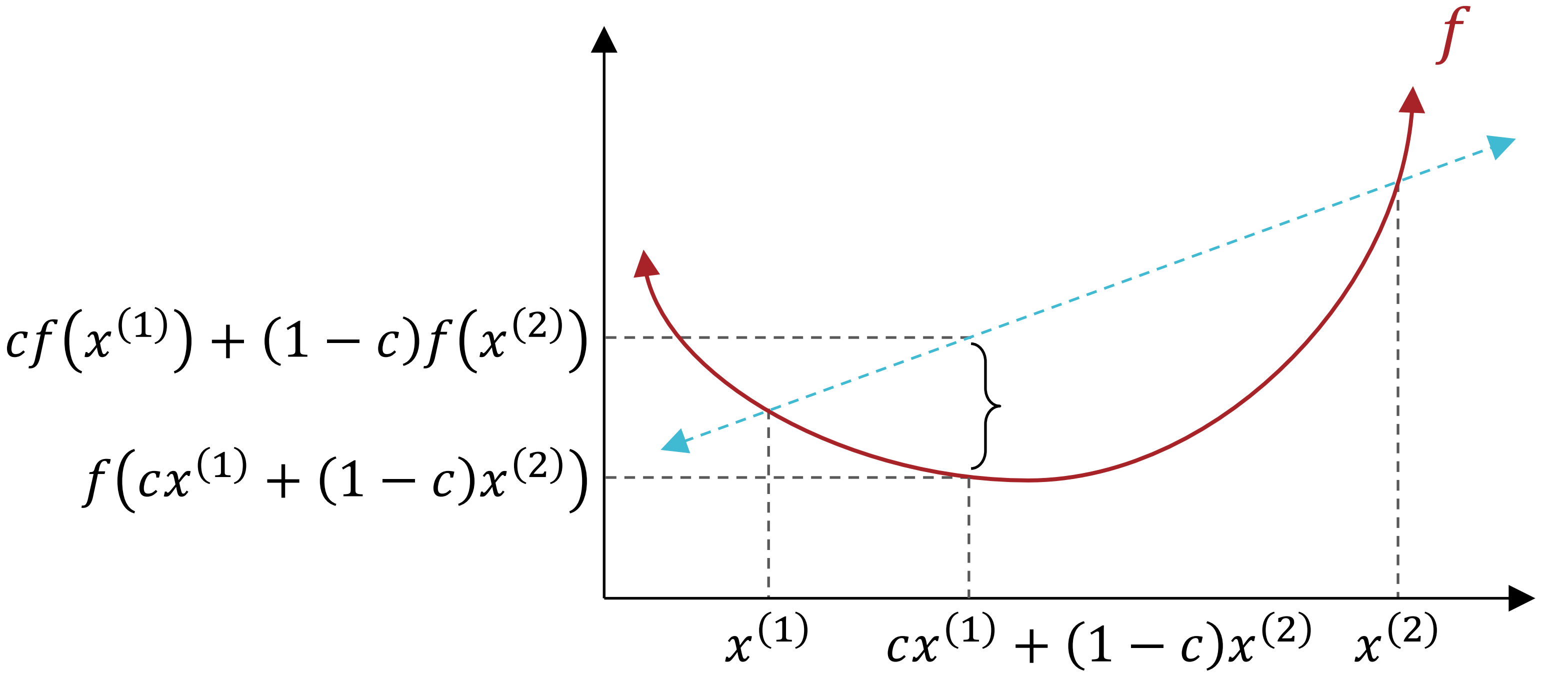
Convexity

- A function $f: \mathbb{R}^D \to \mathbb{R}$ is convex if

  $\forall\, \boldsymbol{x}^{(1)} \in \mathbb{R}^D, \boldsymbol{x}^{(2)} \in \mathbb{R}^D$ and $0 \leq c \leq 1$

  $$f\left(c\boldsymbol{x}^{(1)} + (1-c)\boldsymbol{x}^{(2)}\right) \leq cf\left(\boldsymbol{x}^{(1)}\right) + (1-c)f\left(\boldsymbol{x}^{(2)}\right)$$



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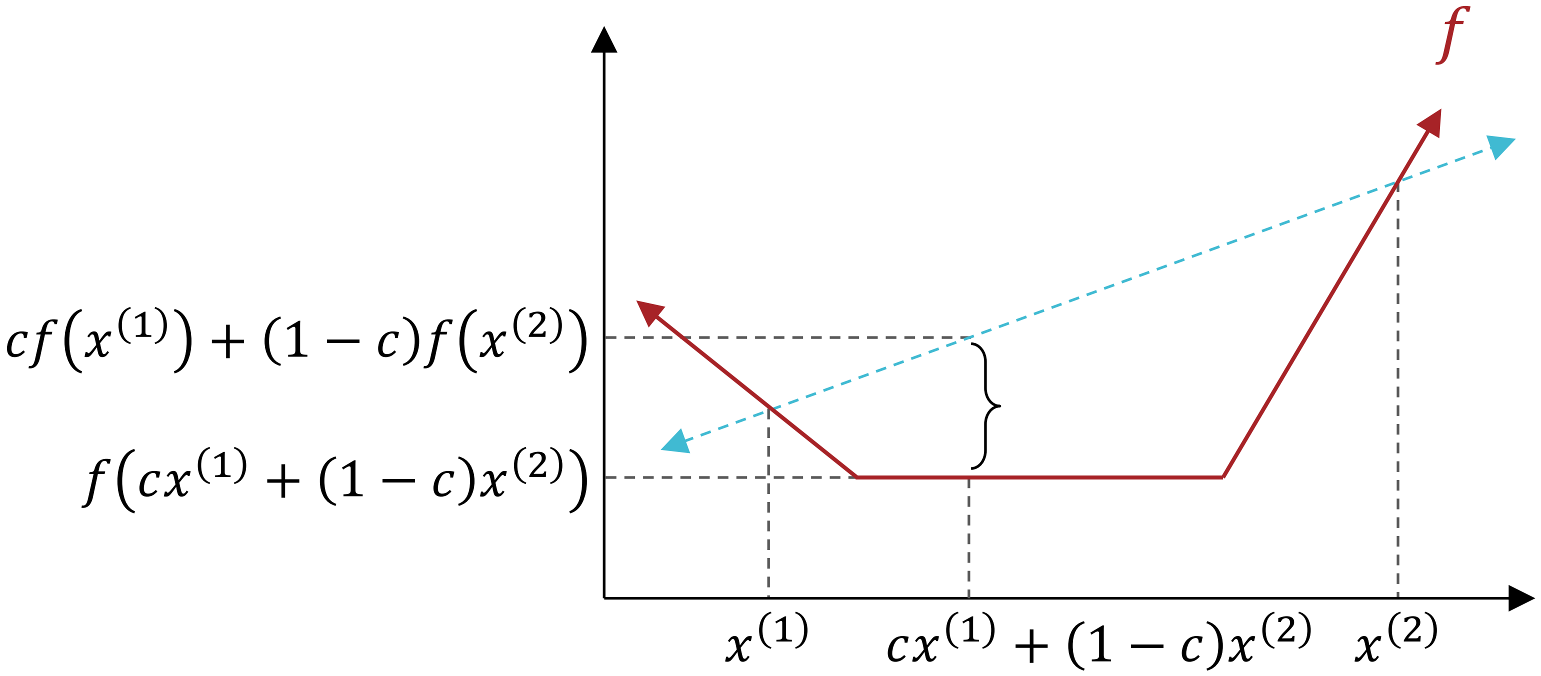
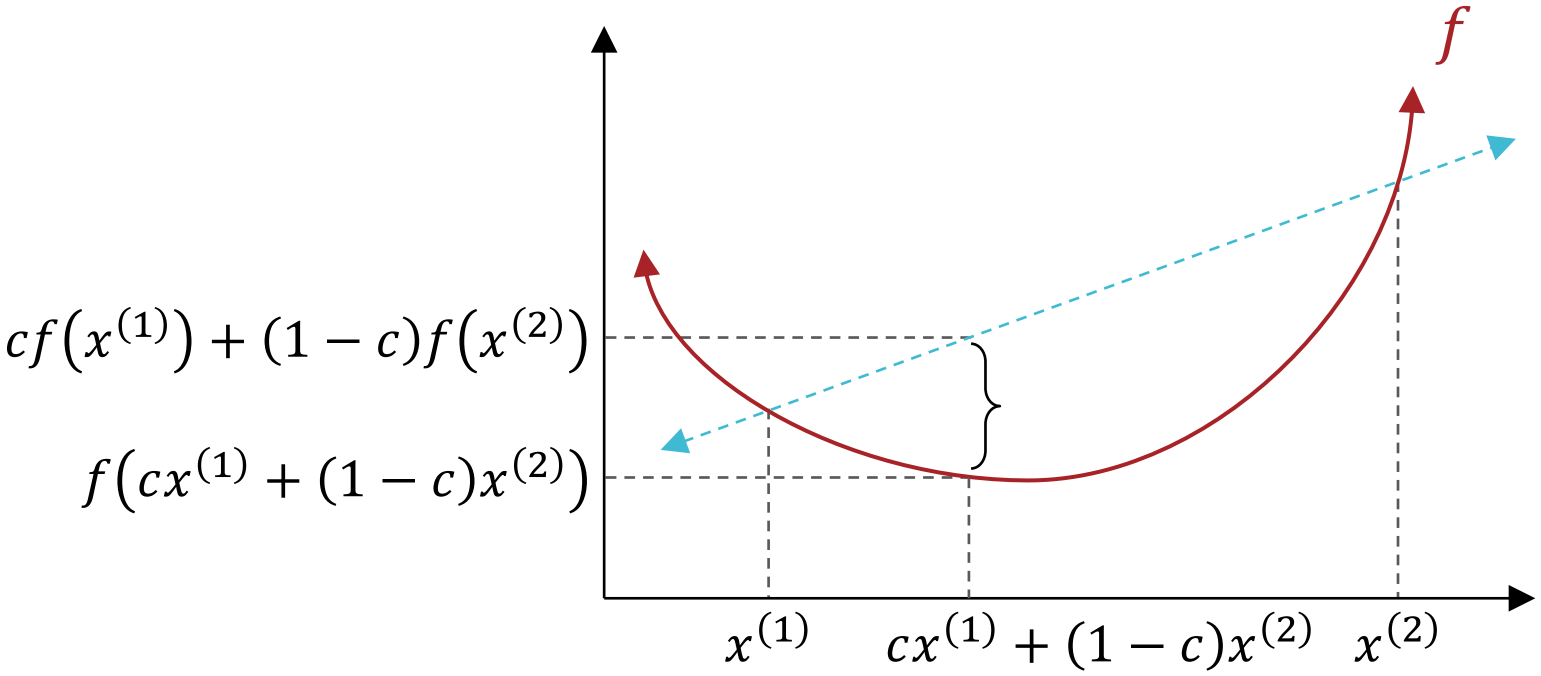


Convexity

- A function $f: \mathbb{R}^D \rightarrow \mathbb{R}$ is *strictly* convex if $\forall\ \boldsymbol{x}^{(1)} \in \mathbb{R}^D, \boldsymbol{x}^{(2)} \in \mathbb{R}^D$ and $0 < c < 1$

$$f\left(c\boldsymbol{x}^{(1)} + (1-c)\boldsymbol{x}^{(2)}\right) < cf\left(\boldsymbol{x}^{(1)}\right) + (1-c)f\left(\boldsymbol{x}^{(2)}\right)$$



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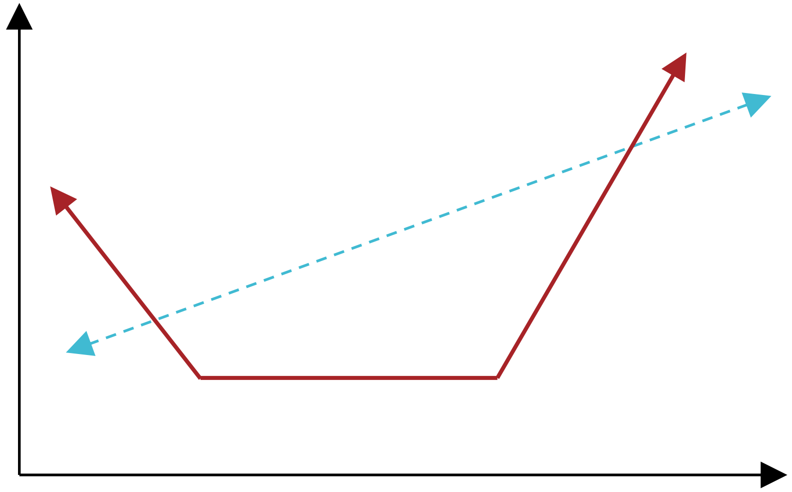
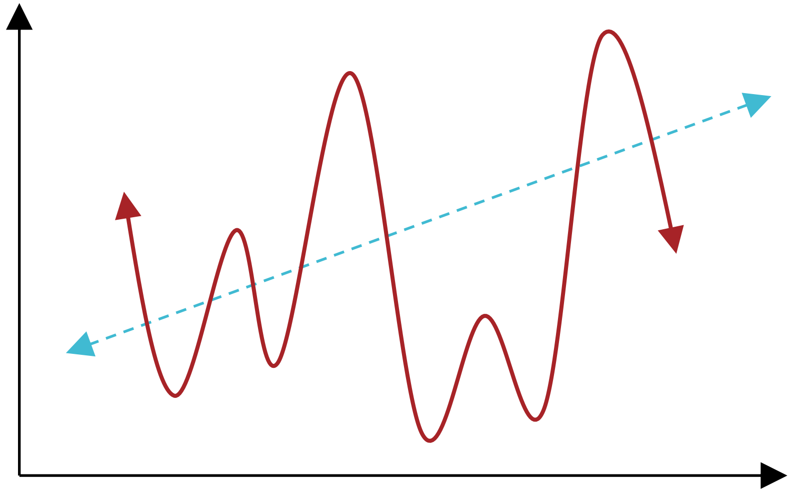
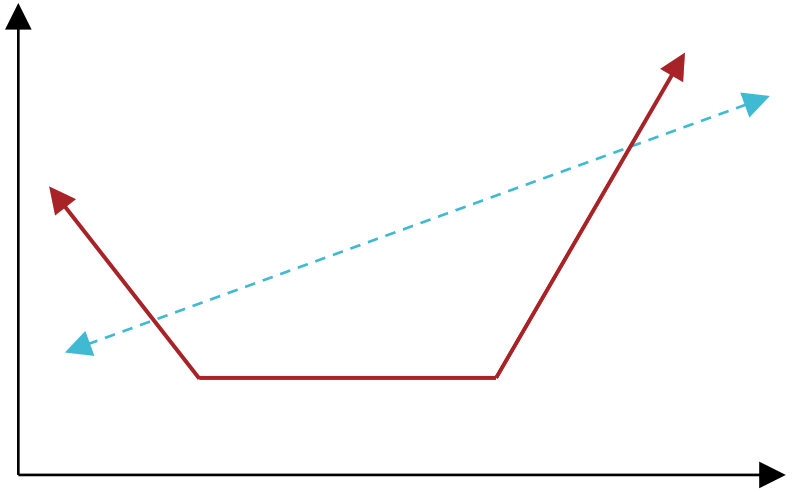


Convex functions



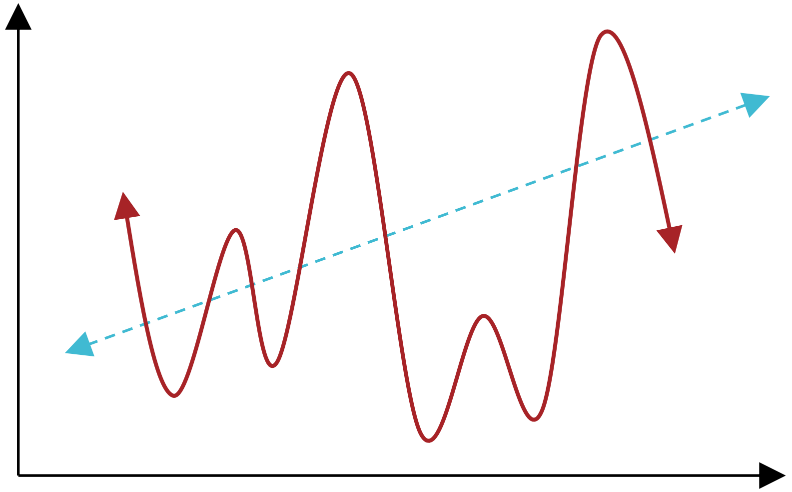
Non-convex functions

Convexity



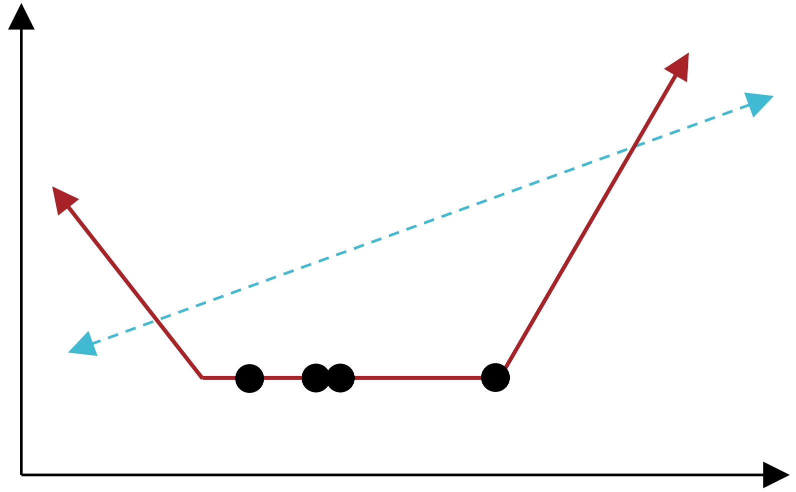
Given a function $f : \mathbb{R}^D \to \mathbb{R}$

- $\boldsymbol{x}^*$ is a global minimum iff $f(\boldsymbol{x}^*) \leq f(\boldsymbol{x})\ \forall\ \boldsymbol{x} \in \mathbb{R}^D$



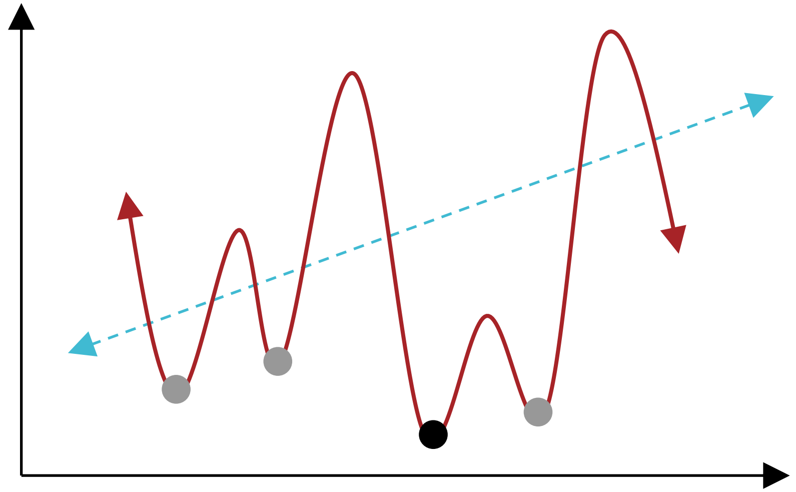
- $\boldsymbol{x}^*$ is a local minimum iff $\exists\ \epsilon$ s.t. $f(\boldsymbol{x}^*) \leq f(\boldsymbol{x})\ \forall$ $\boldsymbol{x}$ s.t. $\|\boldsymbol{x} - \boldsymbol{x}^*\|_2 < \epsilon$

Convexity



Convex functions:

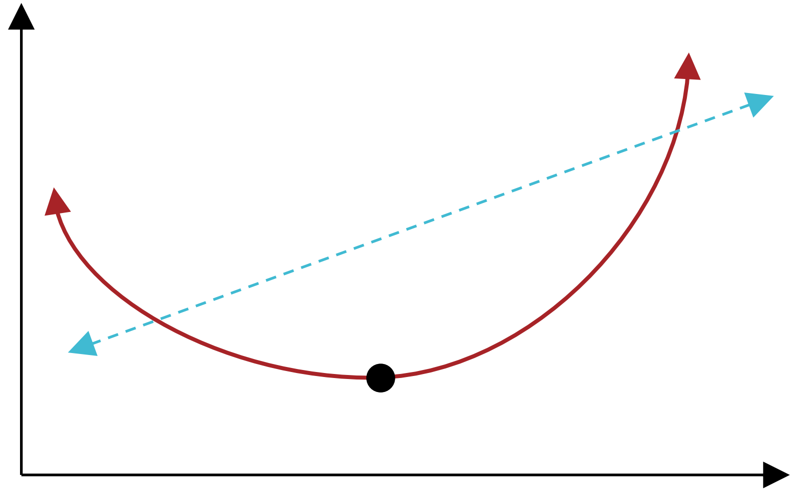
Each local minimum is a global minimum!



Non-convex functions:

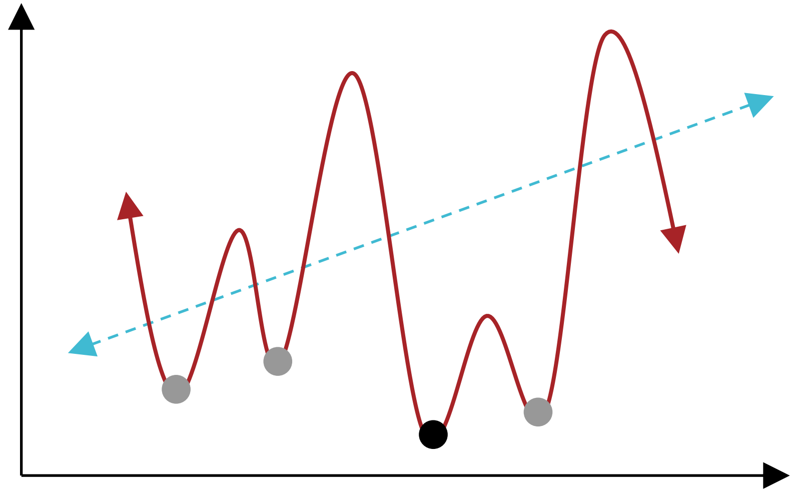
A local minimum may or may not be a global minimum…

Convexity



Strictly convex functions:

There exists a unique global minimum!



Non-convex functions:

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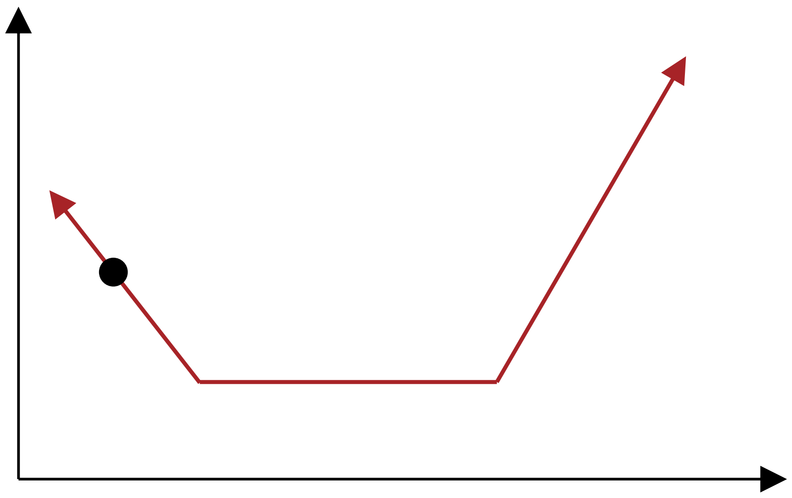
Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
  - Works great if the objective function is convex!



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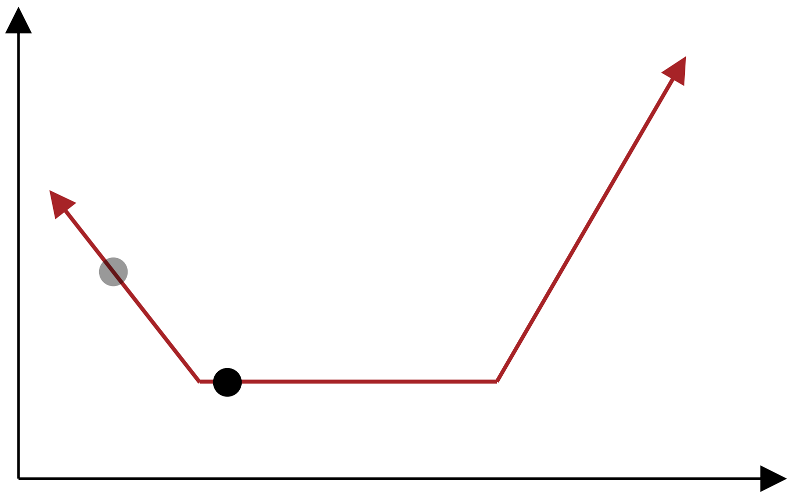

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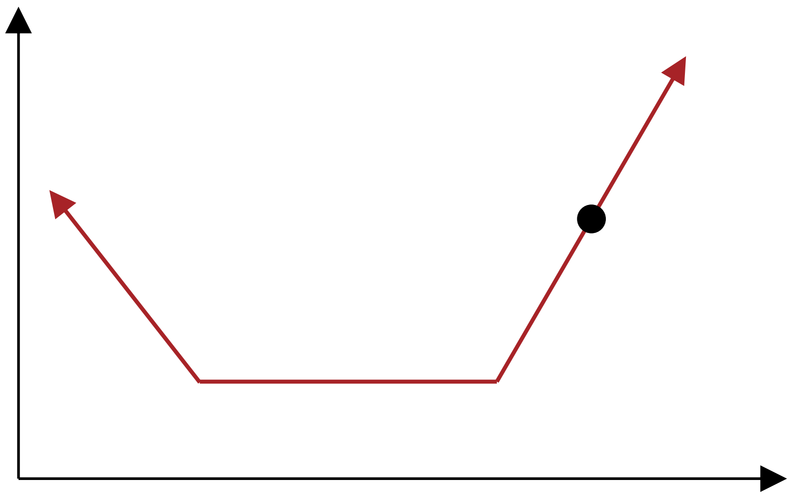

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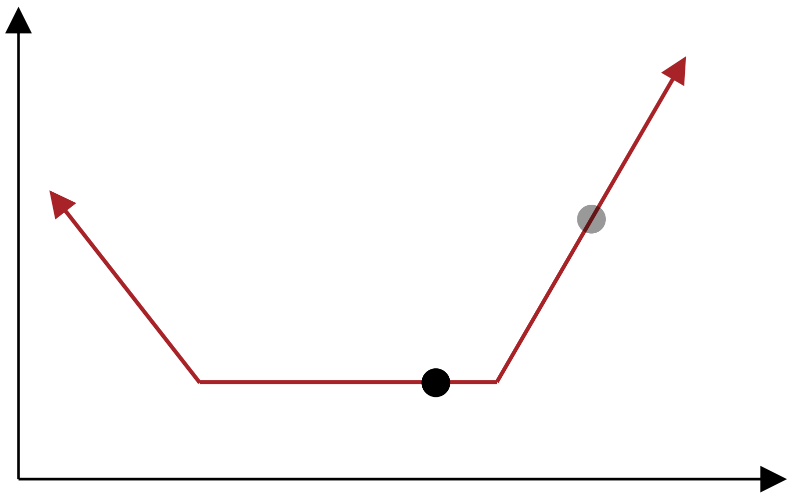

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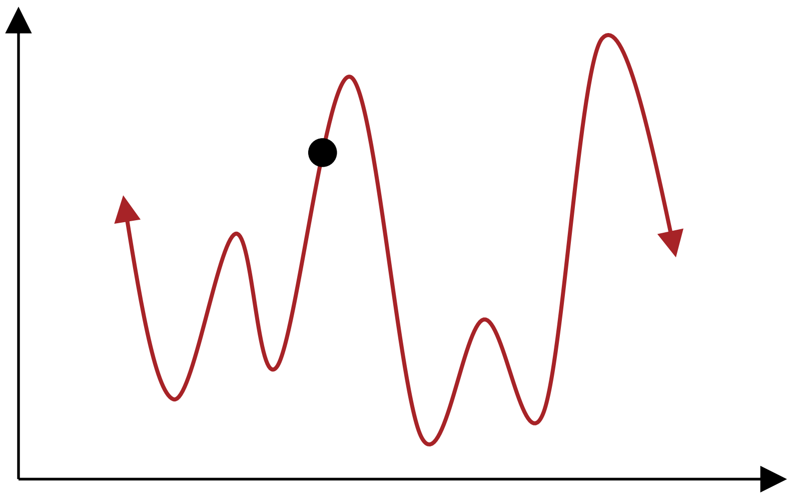

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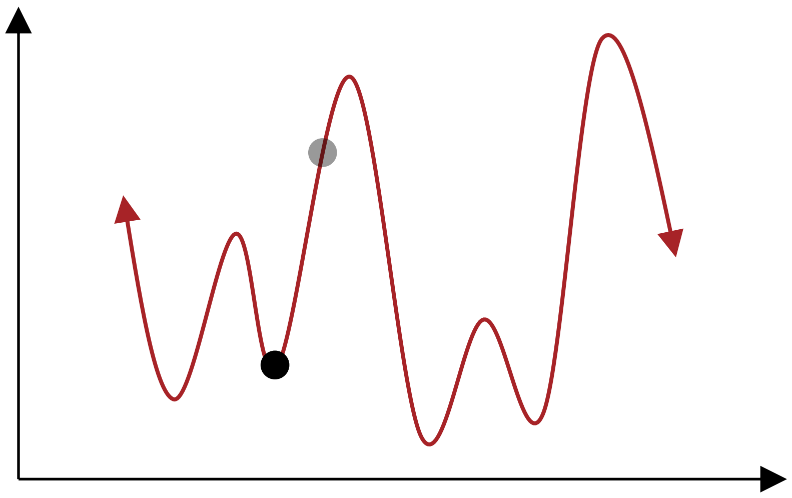

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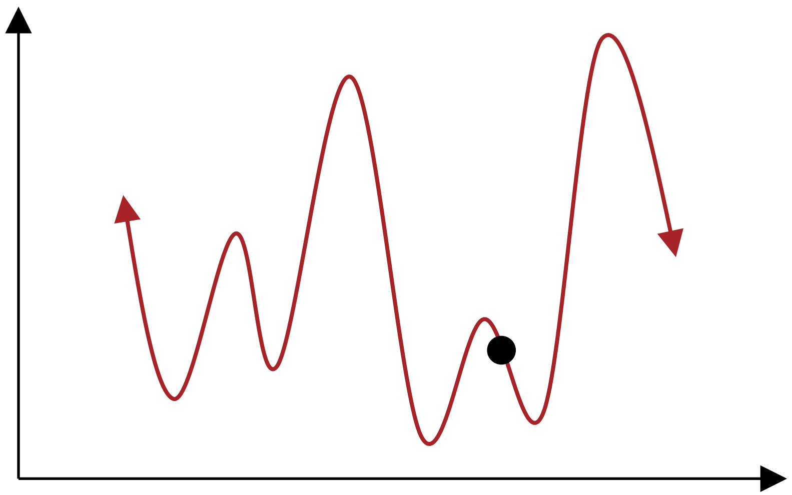

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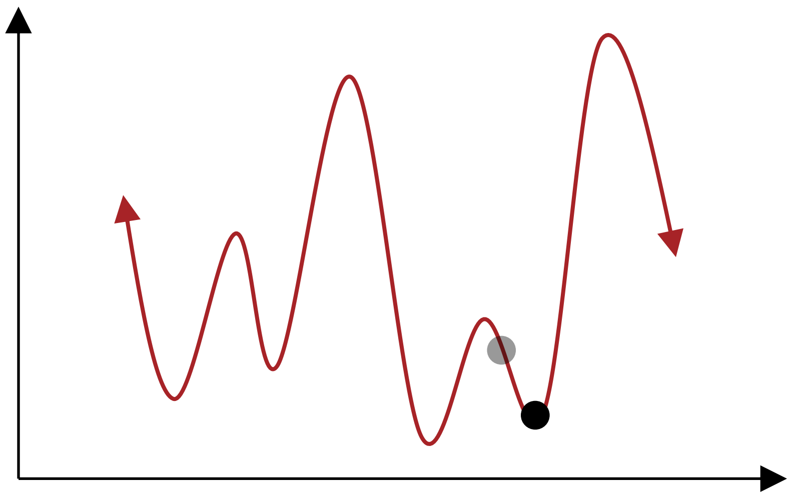
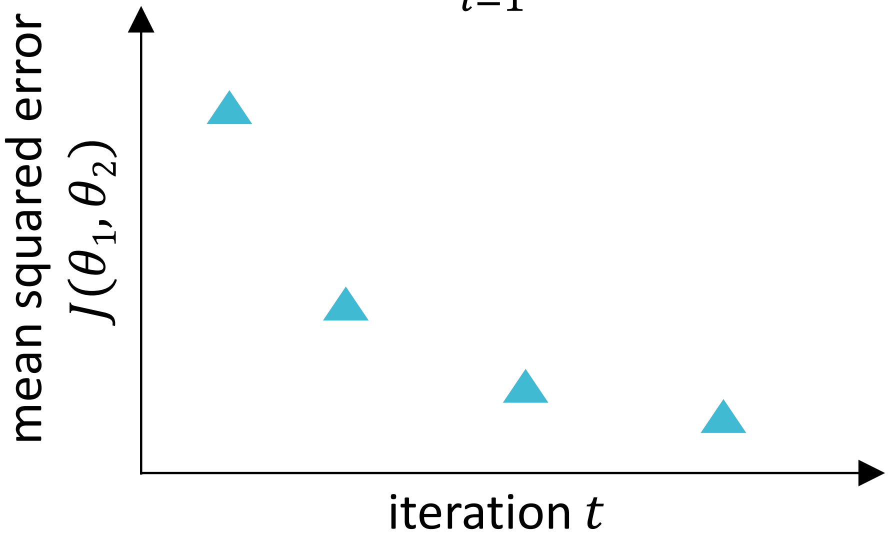
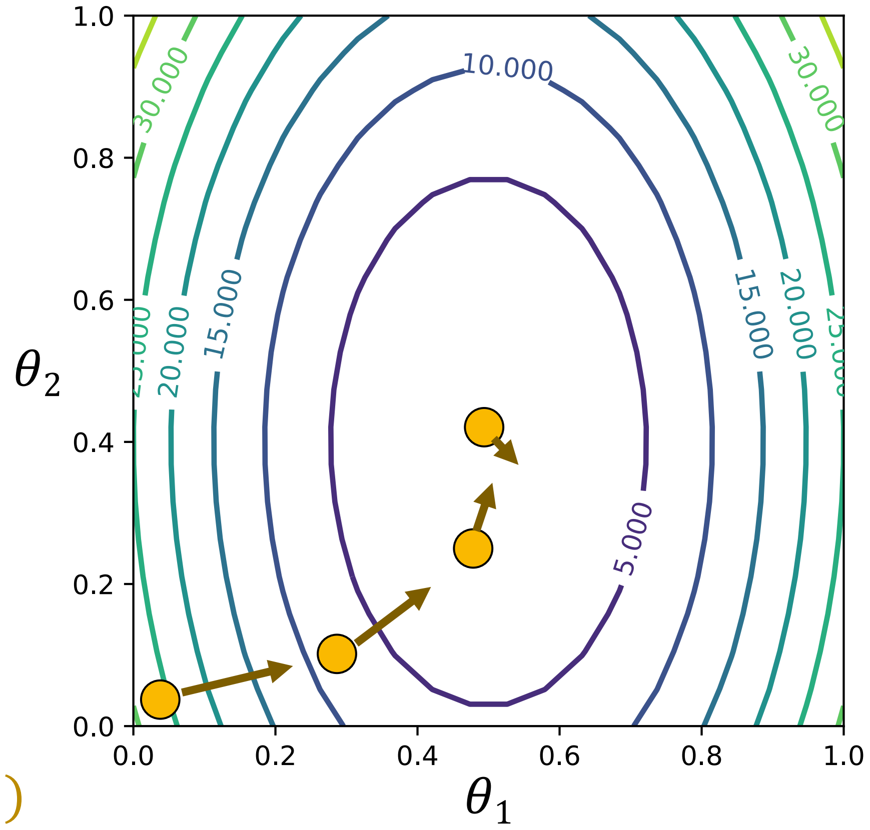
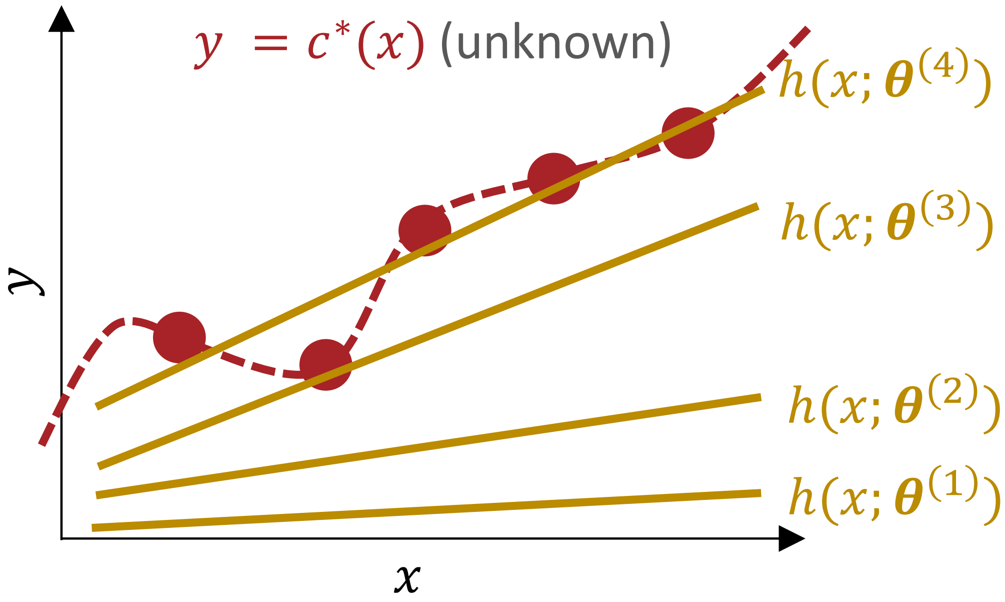


Why Gradient Descent for Linear Regression?

$$J(\theta_1, \theta_2) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T \boldsymbol{x}^{(i)}\right)^2$$







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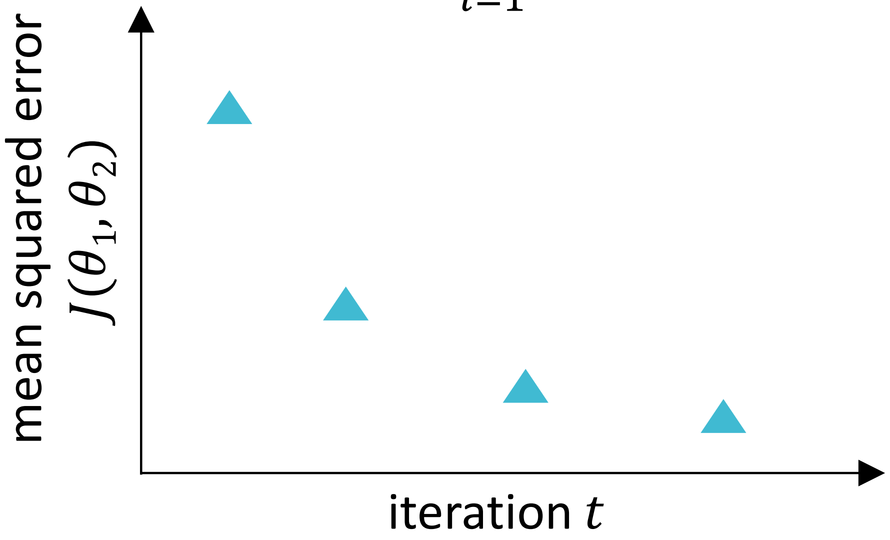
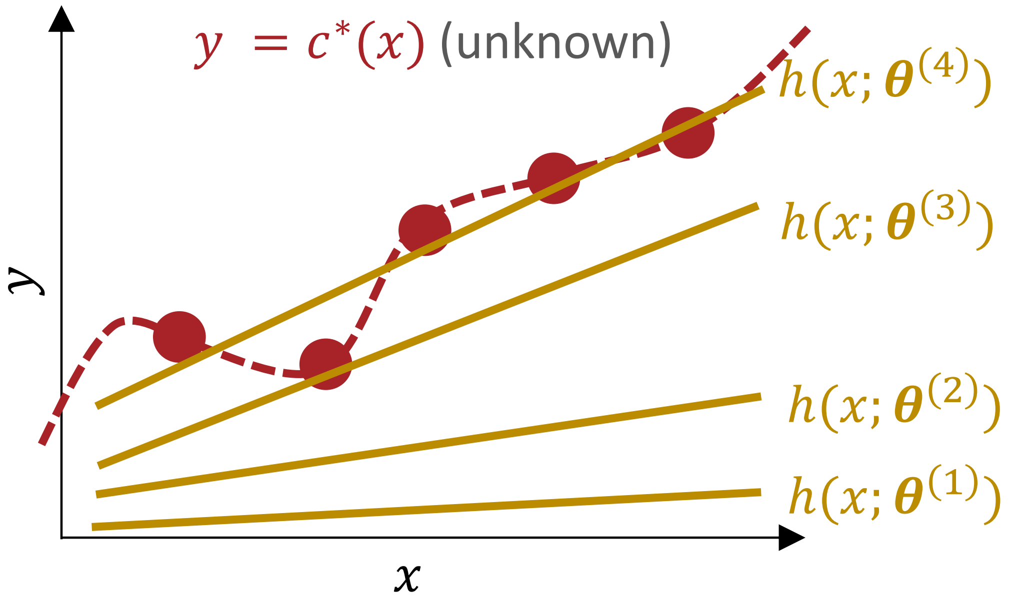
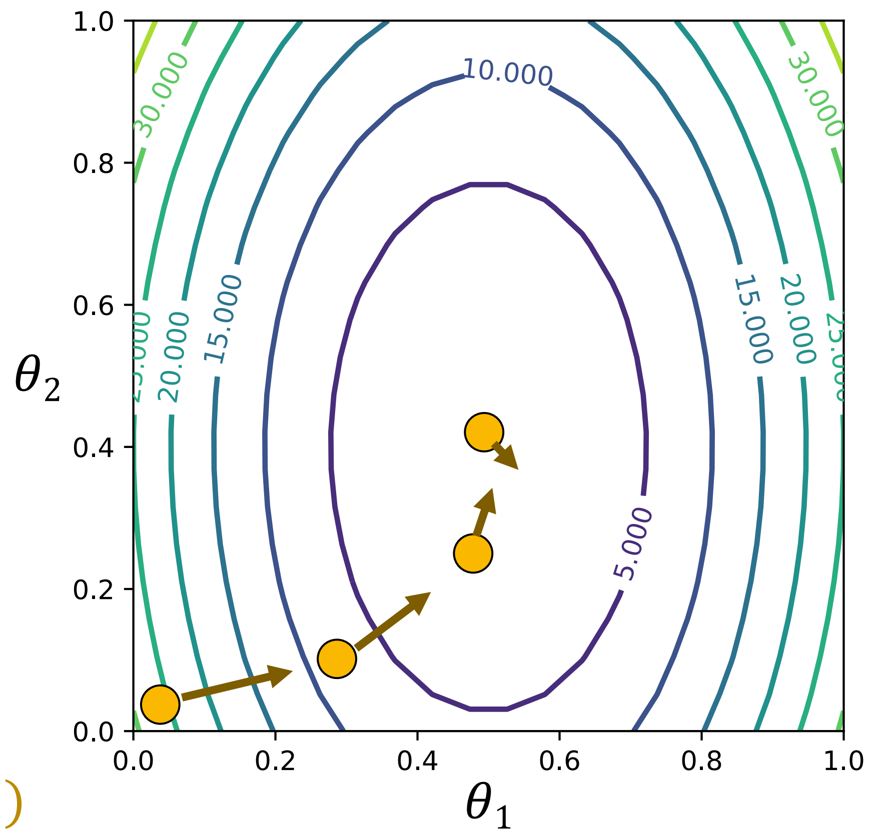
The mean squared error is convex (but not always strictly convex)

$$J(\theta_1, \theta_2) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T \boldsymbol{x}^{(i)}\right)^2$$





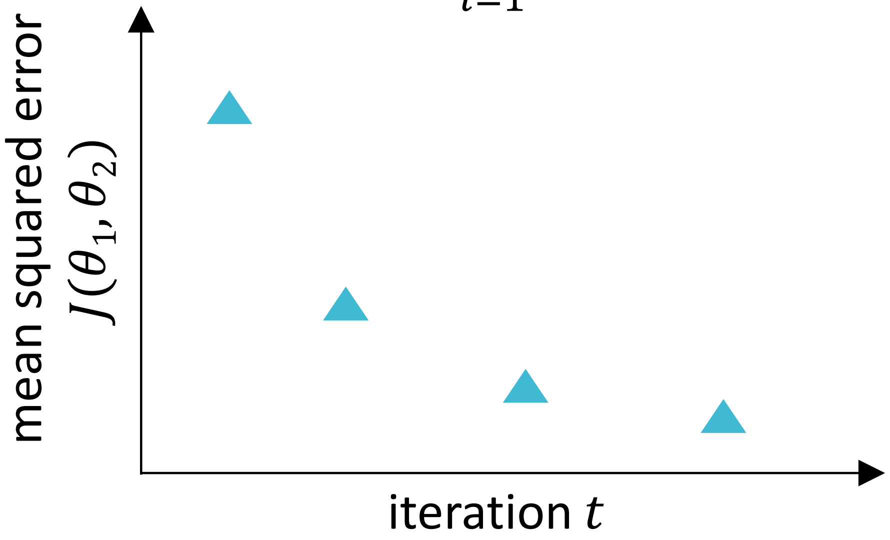


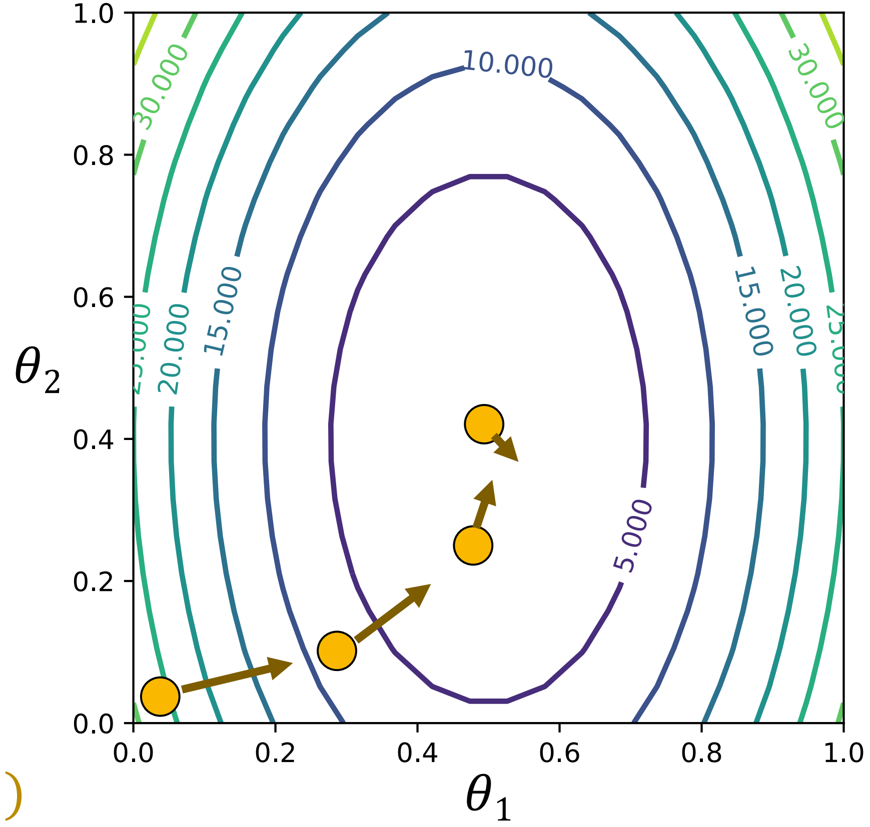
t	θ_1	θ_2	$J(\theta_1, \theta_2)$
1	0.01	0.02	25.2
2	0.30	0.12	8.7
3	0.51	0.30	1.5
4	0.59	0.43	0.2

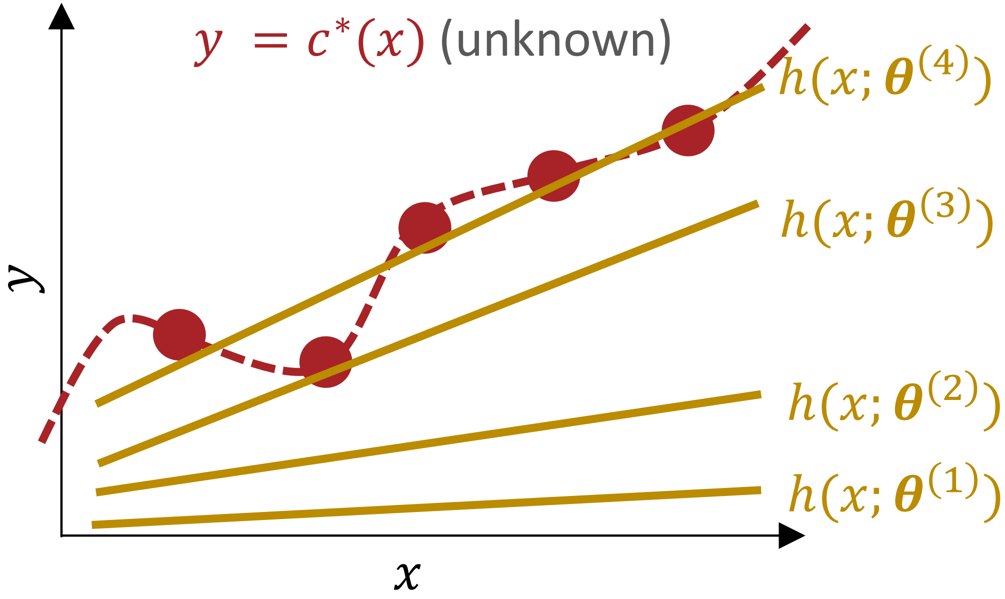
Okay, fine but couldn't we do something simpler?

Yes! (sometimes)

$$J(\theta_1, \theta_2) = \frac{1}{N} \sum_{i=1}^{N} \left(y^{(i)} - \boldsymbol{\theta}^T \boldsymbol{x}^{(i)} \right)^2$$







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Closed Form Optimization

- Idea: find the *critical points* of the objective function, specifically the ones where $\nabla J(\theta) = \mathbf{0}$ (the vector of all zeros), and check if any of them are local minima

- Notation: given training data $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(n)}, y^{(n)}\right)\right\}_{n=1}^{N}$

  - $X = \begin{bmatrix} 1 & \boldsymbol{x}^{(1)^T} \\ 1 & \boldsymbol{x}^{(2)^T} \\ \vdots & \vdots \\ 1 & \boldsymbol{x}^{(N)^T} \end{bmatrix} = \begin{bmatrix} 1 & x_1^{(1)} & \cdots & x_D^{(1)} \\ 1 & x_1^{(2)} & \cdots & x_D^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(N)} & \cdots & x_D^{(N)} \end{bmatrix} \in \mathbb{R}^{N \times D+1}$

    is the *design matrix*

  - $\boldsymbol{y} = \left[y^{(1)}, \dots, y^{(N)}\right]^T \in \mathbb{R}^N$ is the *target vector*

Minimizing the Mean Squared Error

$$J(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{2}\left(y^{(i)} - \boldsymbol{\theta}^T\boldsymbol{x}^{(i)}\right)^2 = \frac{1}{2N}\sum_{i=1}^{N}\left(\boldsymbol{x}^{(i)^T}\boldsymbol{\theta} - y^{(i)}\right)^2$$

$$= \frac{1}{2N}(X\theta - \boldsymbol{y})^T(X\theta - \boldsymbol{y})$$

$$= \frac{1}{2N}(\boldsymbol{\theta}^T X^T X\boldsymbol{\theta} - 2\boldsymbol{\theta}^T X^T\boldsymbol{y} + \boldsymbol{y}^T\boldsymbol{y})$$

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = \frac{1}{2N}(2X^T X\boldsymbol{\theta} - 2X^T\boldsymbol{y})$$

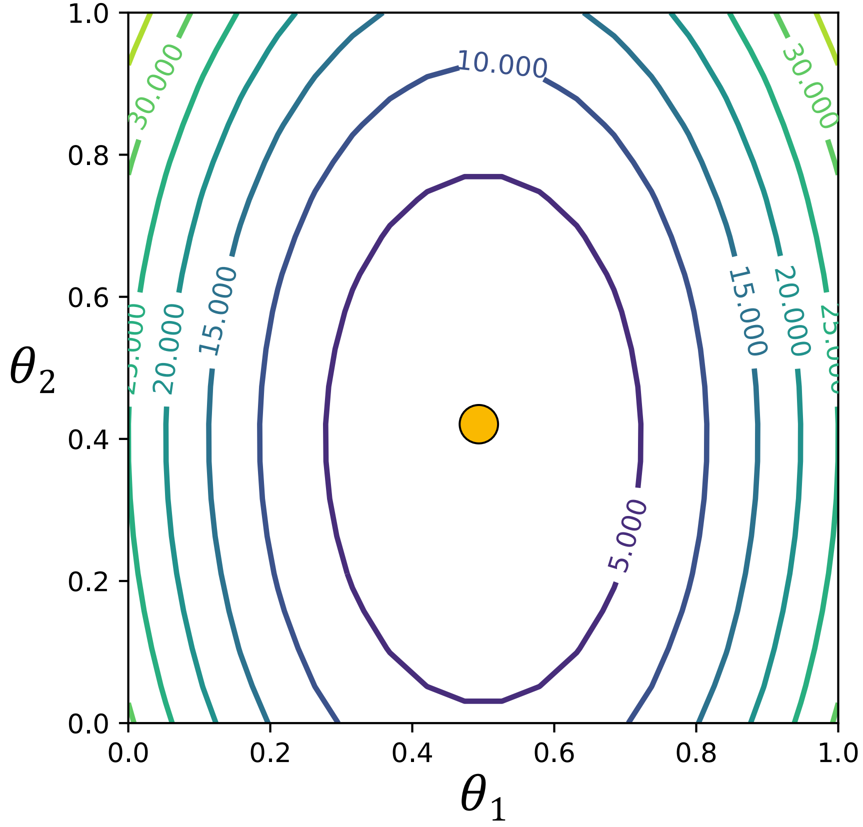
$$\nabla_{\boldsymbol{\theta}} J(\widehat{\boldsymbol{\theta}}) = \frac{1}{2N}\left(2X^T X\widehat{\boldsymbol{\theta}} - 2X^T\boldsymbol{y}\right) = 0$$

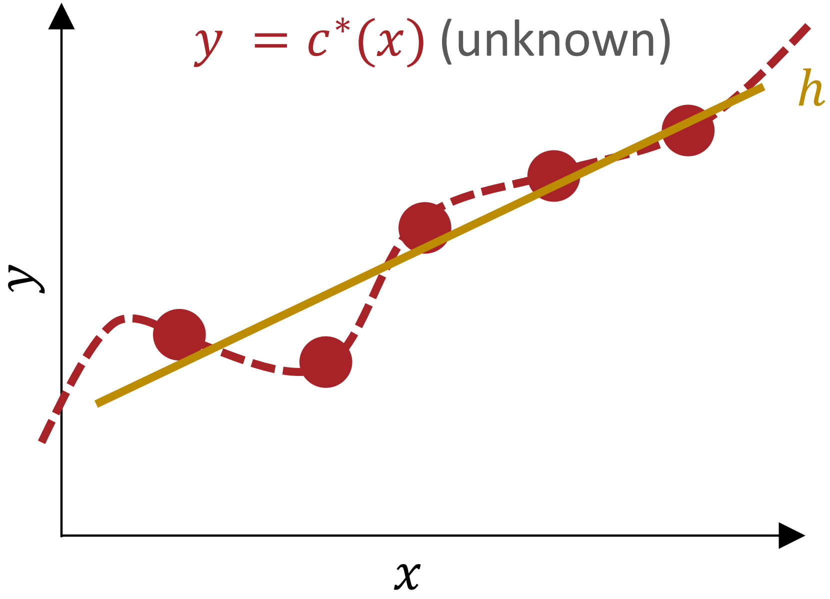
$$\rightarrow X^T X\widehat{\boldsymbol{\theta}} = X^T\boldsymbol{y}$$

$$\rightarrow \widehat{\boldsymbol{\theta}} = (X^T X)^{-1}X^T\boldsymbol{y}$$

Closed Form Optimization

$$\hat{\boldsymbol{\theta}} = (X^T X)^{-1} X^T \boldsymbol{y}$$





t	θ_1	θ_2	$J(\theta_1, \theta_2)$
1	0.59	0.43	0.2

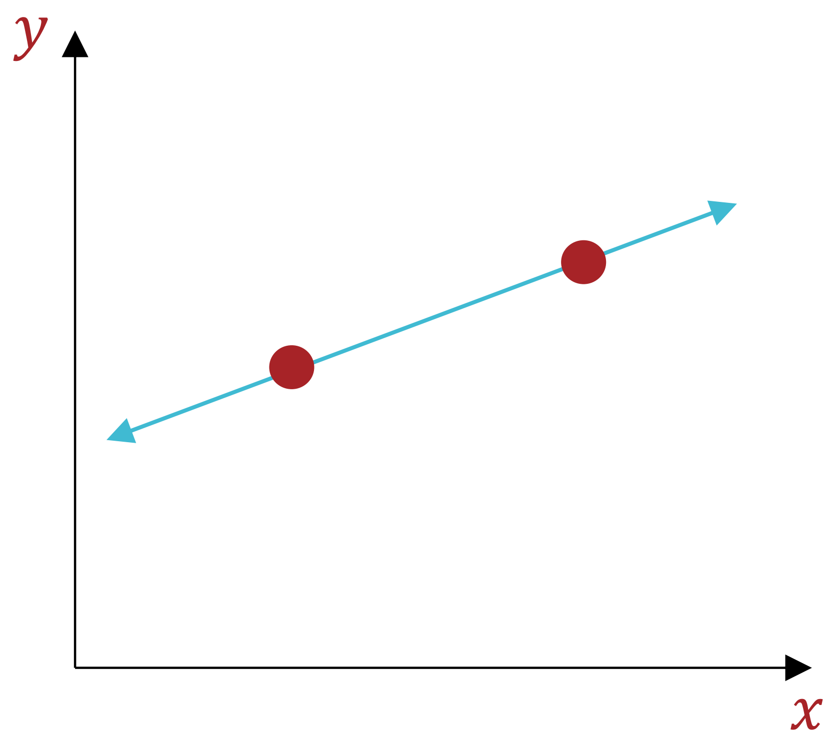
Closed Form Solution

$$\hat{\boldsymbol{\theta}} = (X^T X)^{-1} X^T \boldsymbol{y}$$

1. Is $X^T X$ invertible?
   - When $N \gg D + 1$, $X^T X$ is (almost always) full rank and therefore, invertible!
   - If $X^T X$ is not invertible (occurs when one of the features is a linear combination of the others) then there are either 0 or infinitely many solutions!
2. If so, how computationally expensive is inverting $X^T X$?

Linear Regression: Uniqueness

- Consider a 1D linear regression model trained to minimize the mean squared error: how many optimal solutions (i.e., sets of parameters θ) are there for the given dataset?



Linear Regression: Uniqueness

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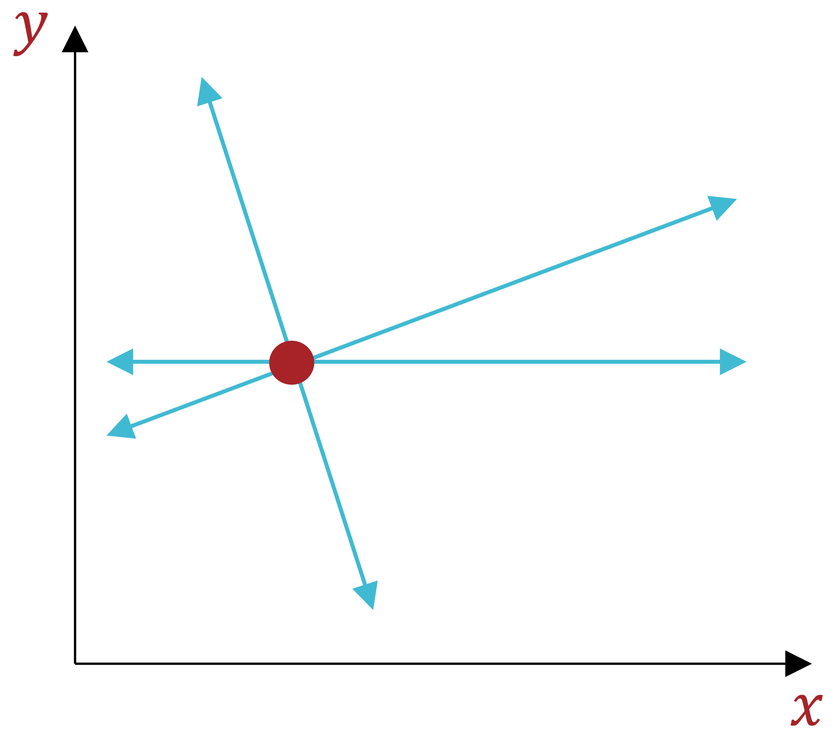

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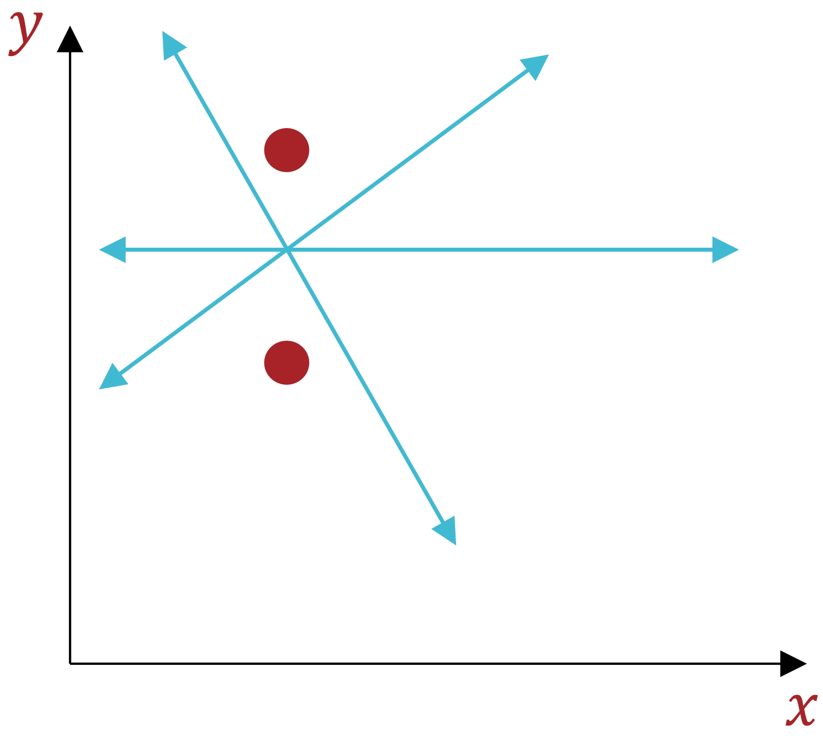
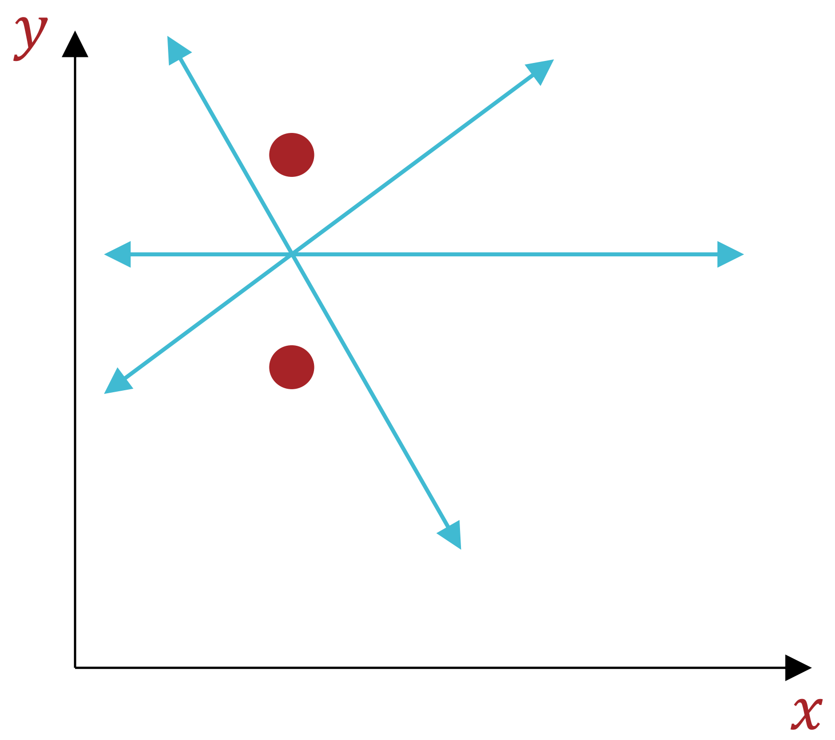


Poll Question 3

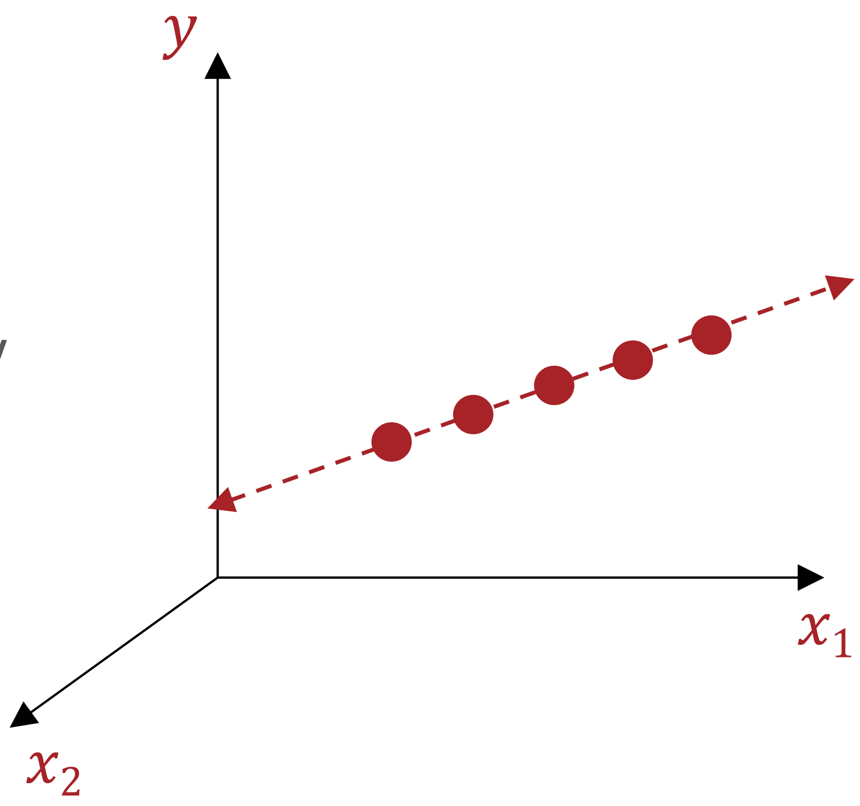
- Consider a 1D linear regression model trained to minimize the mean squared error: how many optimal solutions (i.e., sets of parameters θ) are there for the given dataset?



A. -1 **(TOXIC)** B. 0 C. 1 D. 2 E. ∞

Linear Regression: Uniqueness

- Consider a 2D linear regression model trained to minimize the mean squared error: how many optimal solutions (i.e., sets of parameters θ) are there for the given dataset?



Linear Regression: Uniqueness

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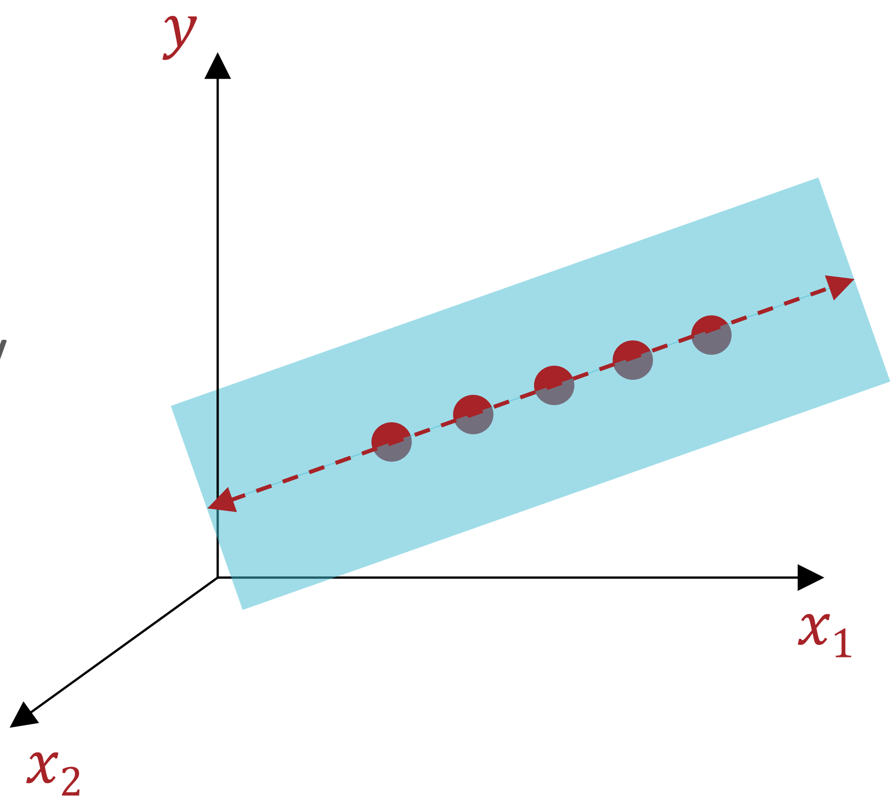

Linear Regression: Uniqueness

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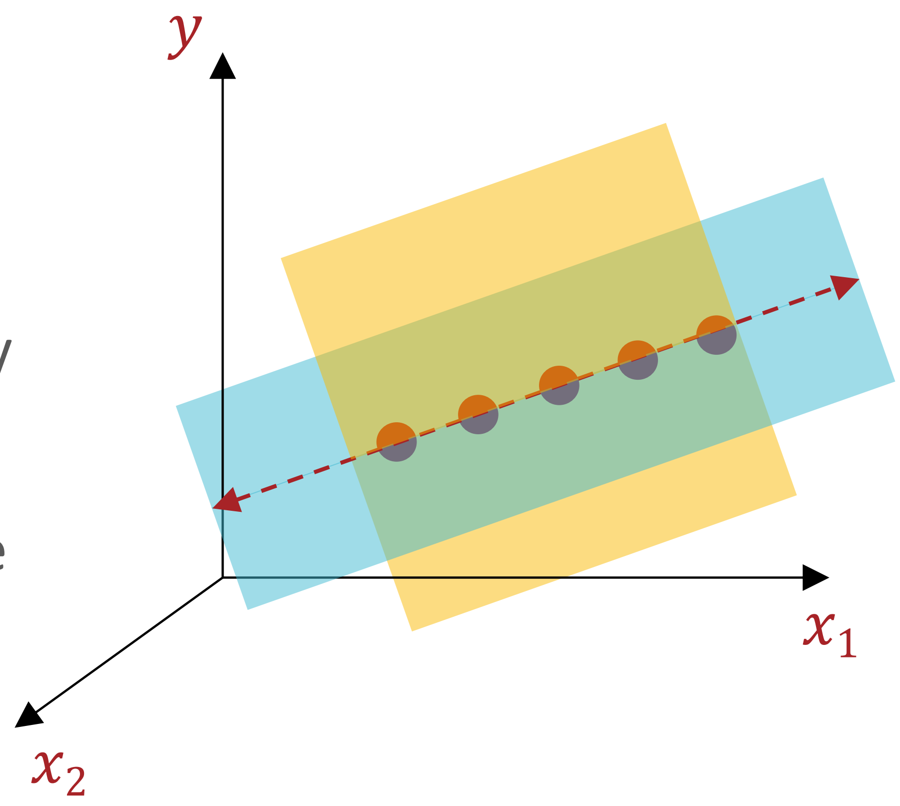

Closed Form Solution

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1. Is $X^T X$ invertible?
   - When $N \gg D + 1$, $X^T X$ is (almost always) full rank and therefore, invertible!
   - If $X^T X$ is not invertible (occurs when one of the features is a linear combination of the others) then there are either 0 or infinitely many solutions
2. If so, how computationally expensive is inverting $X^T X$?
   - $X^T X \in \mathbb{R}^{D+1 \times D+1}$ so inverting $X^T X$ takes $O(D^3)$ time…
     - Computing $X^T X$ takes $O(ND^2)$ time
   - Can use gradient descent to (potentially) speed things up when N and D are large!

Linear Regression Learning Objectives

You should be able to…

- Design k-NN Regression and Decision Tree Regression
- Implement learning for Linear Regression using gradient descent or closed form optimization
- Choose a Linear Regression optimization technique that is appropriate for a particular dataset by analyzing the tradeoff of computational complexity vs. convergence speed
- Identify situations where least squares regression has exactly one solution or infinitely many solutions