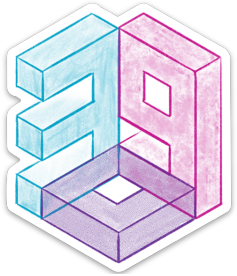


https://introml.mit.edu/

6.390 Intro to Machine Learning

Lecture 3: Gradient Descent Methods

Shen Shen

Sept 18, 2025

11am, Room 10-250

Interactive Slides and Lecture Recording

Logistics

1. There is a student in our class who needs copies of class notes as an approved accommodation. If you're interested in serving as a paid note taker, please reach out to DAS, at 617-253-1674 or das-student@mit.edu.

2. **Midterm 1: October 8, 730pm-9pm**. It covers all the materials up to and including week 4 (linear classification). If you need to take the conflict or accommodation exam, please get in touch with us at 6.390-personal@mit.edu by **Sept 24**.

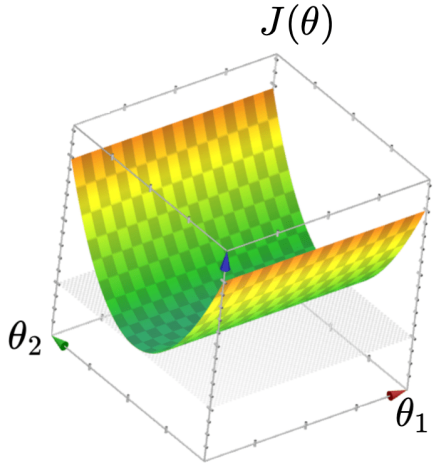
3. Heads-up: Midterm 2 is November 12, 730pm-9pm. Final is December 15, 9am-12pm.

More details on introML homepage

Outline

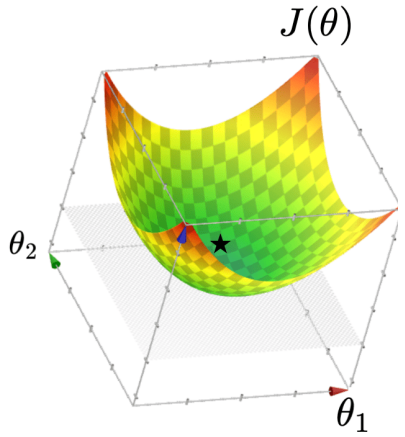
- Gradient descent (GD)
  - The gradient vector
  - GD algorithm
  - Gradient decent properties
- Stochastic gradient descent (SGD)
  - SGD algorithm and setup
  - SGD vs. GD

`Recall:`



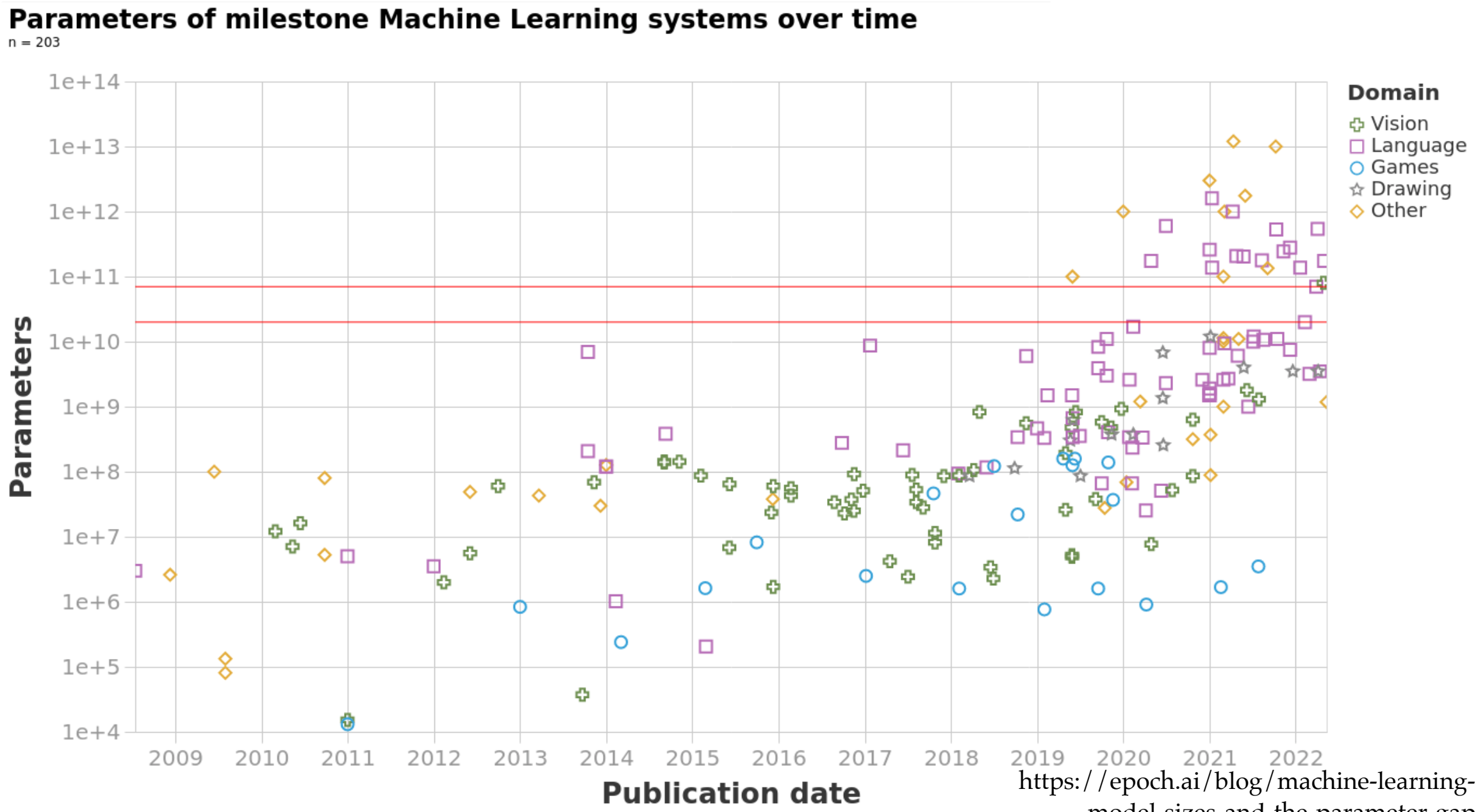
When X is not full column rank

- $J(\theta)$ has a "flat" bottom, like a half pipe
- This 👉 formula is not well-defined
- Infinitely many optimal hyperplanes
- No way yet to obtain an optimal parameter



Typically, X is full column rank

- $J(\theta)$ "curves up" everywhere
- $\theta^* = \left(X^\top X\right)^{-1} X^\top Y$
- θ^* gives the unique optimal hyperplane
- θ^* can be costly to compute (lab2, Q2.7)



https://epoch.ai/blog/machine-learning-model-sizes-and-the-parameter-gap

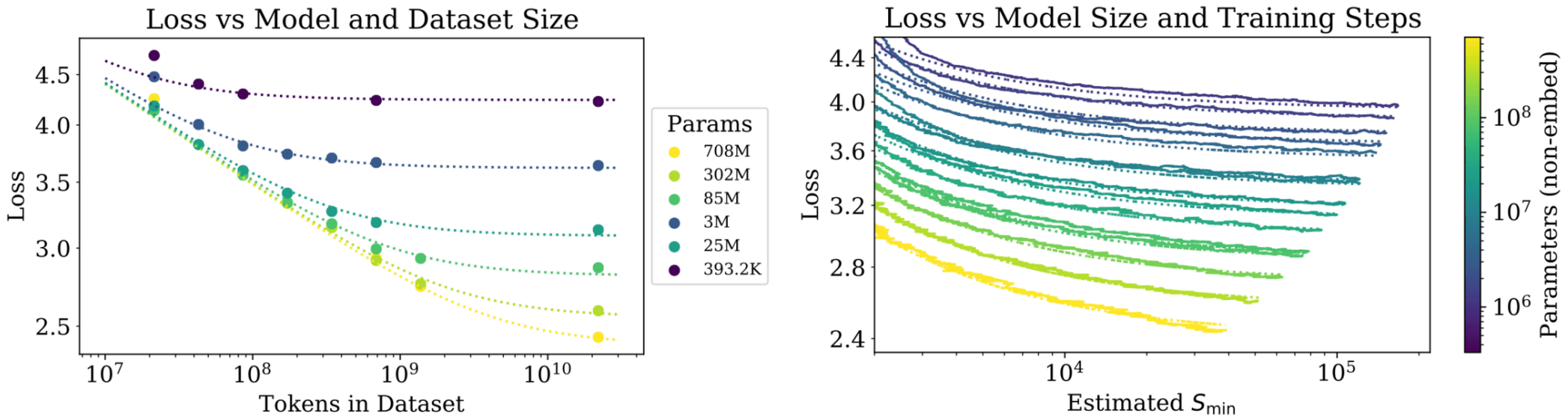


Figure 4 **Left**: The early-stopped test loss $L(N, D)$ varies predictably with the dataset size D and model size N according to Equation (1.5). **Right**: After an initial transient period, learning curves for all model sizes N can be fit with Equation (1.6), which is parameterized in terms of S_{min}, the number of steps when training at large batch size (details in Section 5.1).

https://arxiv.org/pdf/2001.08361

https://losslandscape.com/gallery/

In the real world,

- the number of parameters is huge
- the number of training data points is huge
- hypothesis class is typically highly nonlinear
- loss function is rarely as simple as squared error

Need a more **efficient** and **general** algorithm to train
=> gradient descent methods

Outline

- Gradient descent algorithm (GD)
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  - GD algorithm
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- Stochastic gradient descent (SGD)
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For $f : \mathbb{R}^m \to \mathbb{R}$, its ***gradient*** $\nabla f : \mathbb{R}^m \to \mathbb{R}^m$ is defined at the point $p = (x_1, \ldots, x_m)$ as:

$$\nabla f(p) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(p) \\ \vdots \\ \frac{\partial f}{\partial x_m}(p) \end{bmatrix}$$

1. The gradient generalizes the concept of a derivative to multiple dimensions.
2. By construction, the gradient's dimensionality always matches the function input.

Sometimes the gradient is undefined or ill-behaved, but today it is well-behaved.

3. The gradient can be symbolic or numerical.

example: $f(x, y, z) = x^2 + y^3 + z$

$$\nabla f(p) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(p) \\ \vdots \\ \frac{\partial f}{\partial x_m}(p) \end{bmatrix}$$

its *symbolic* gradient:

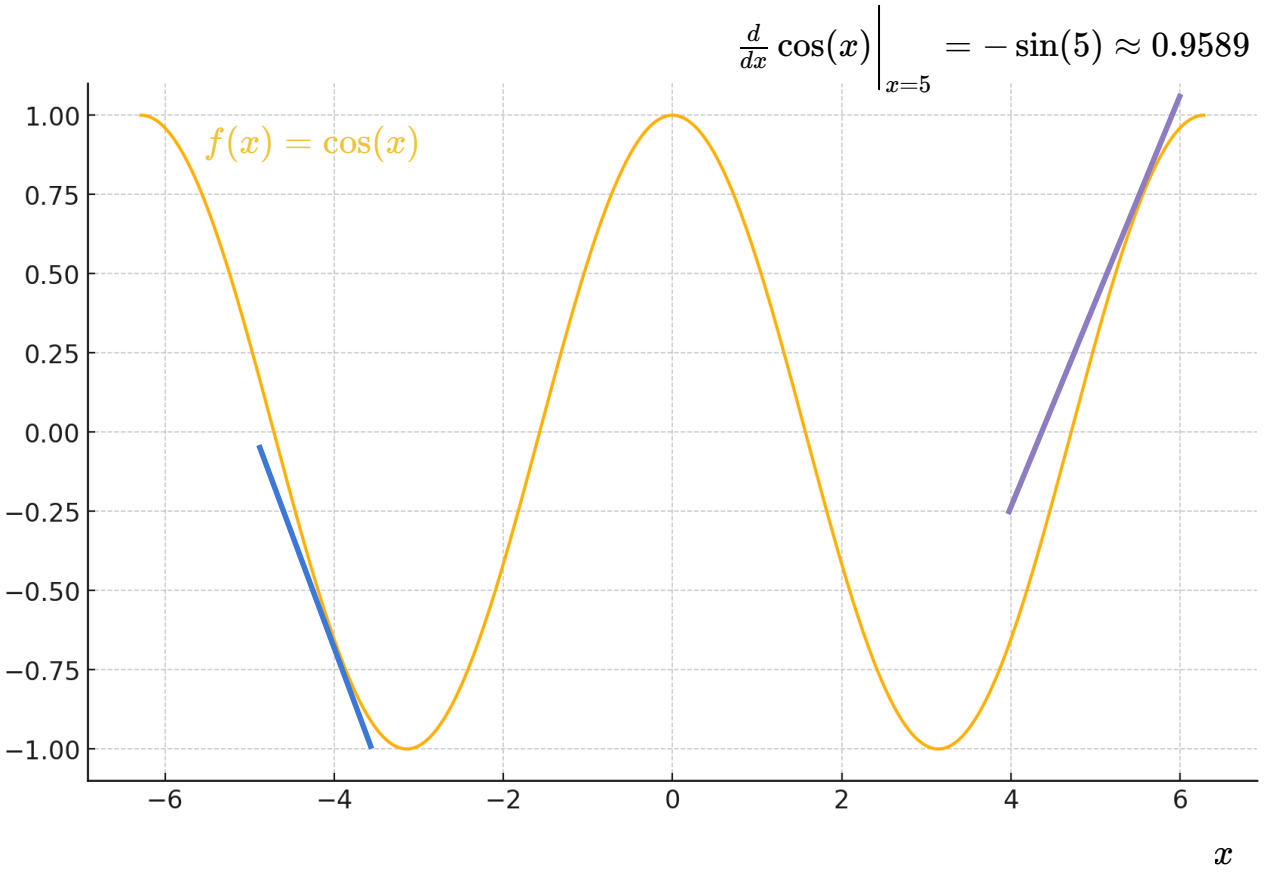
$$\nabla f(x, y, z) = \begin{bmatrix} 2x \\ 3y^2 \\ 1 \end{bmatrix}$$

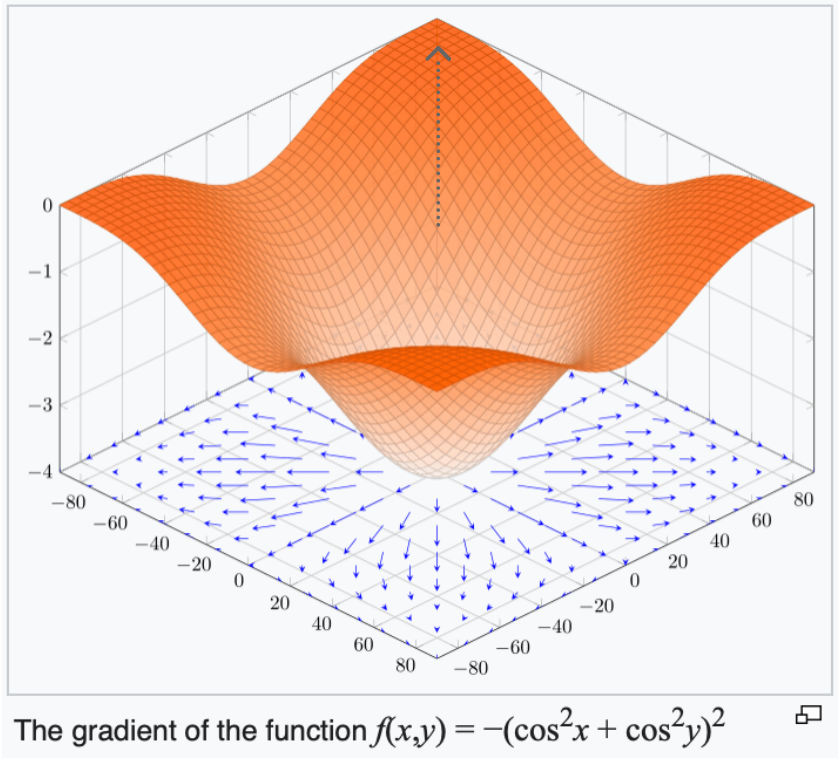
evaluating the symbolic gradient at a point gives a *numerical* gradient:

$$\nabla f(3, 2, 1) = \nabla f(x, y, z)\Big|_{(x,y,z)=(3,2,1)} = \begin{bmatrix} 6 \\ 12 \\ 1 \end{bmatrix}$$

just like a derivative can be a function or a number.

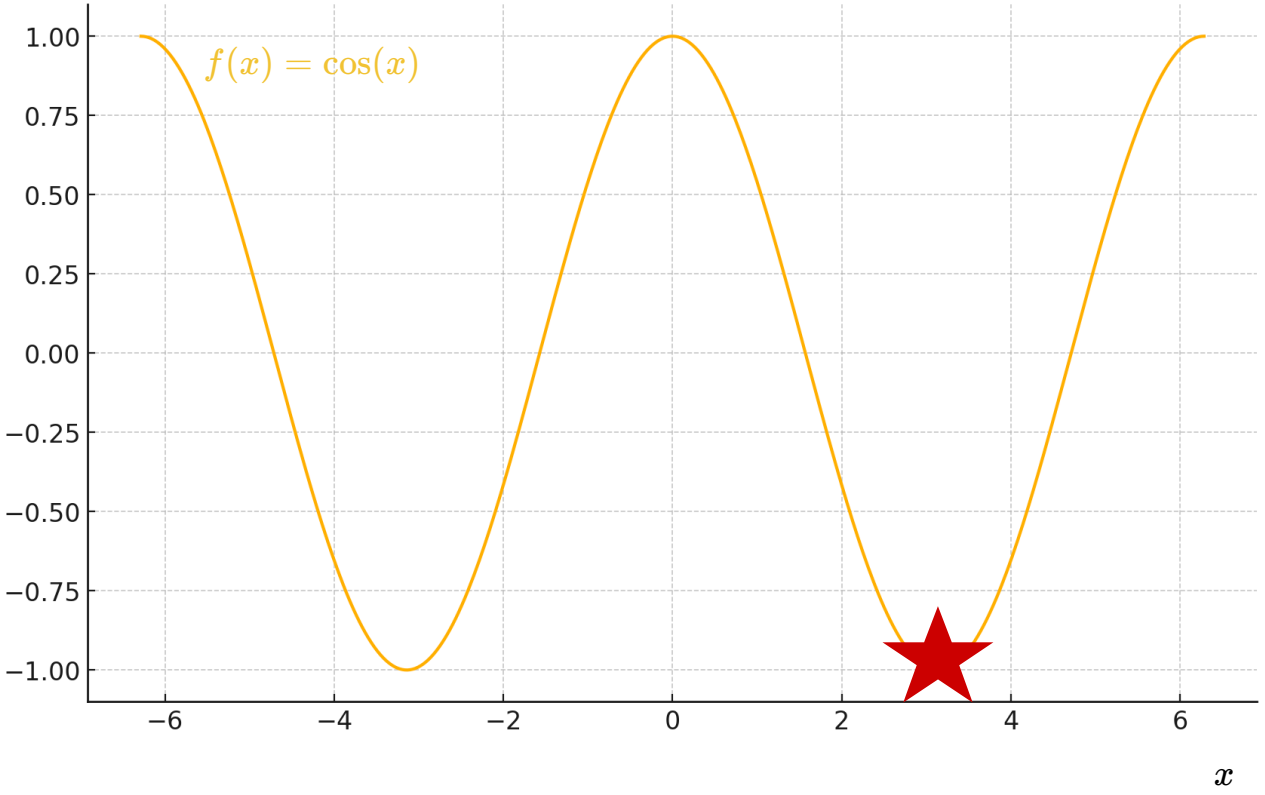
4. The gradient points in the direction of the (steepest) *increase* in the function value.

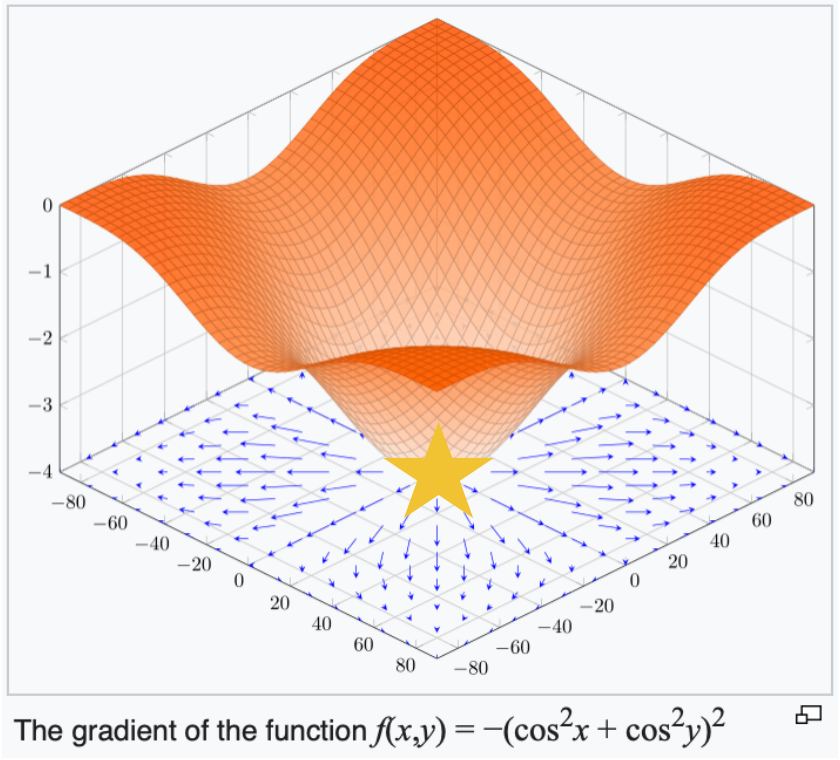




The gradient of the function $f(x,y) = -(\cos^2 x + \cos^2 y)^2$

5. The gradient at the function minimizer is *necessarily* zero.





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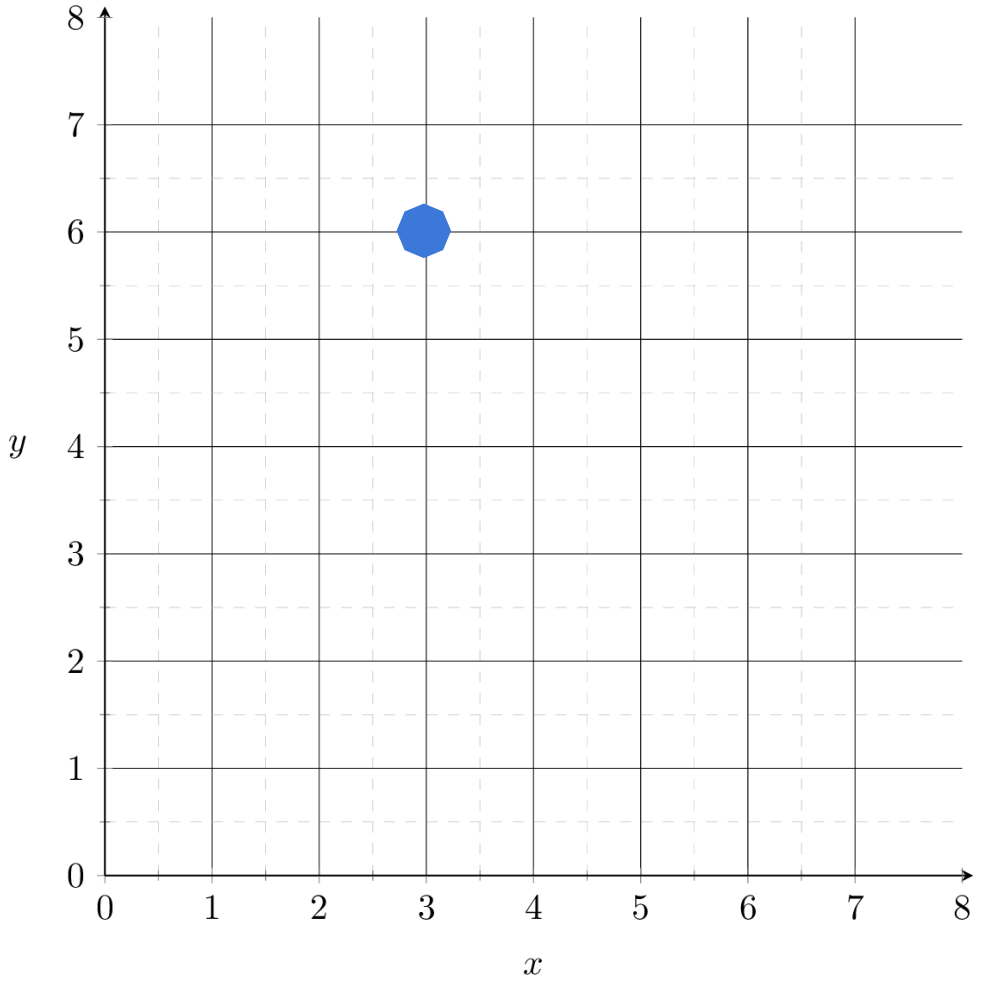
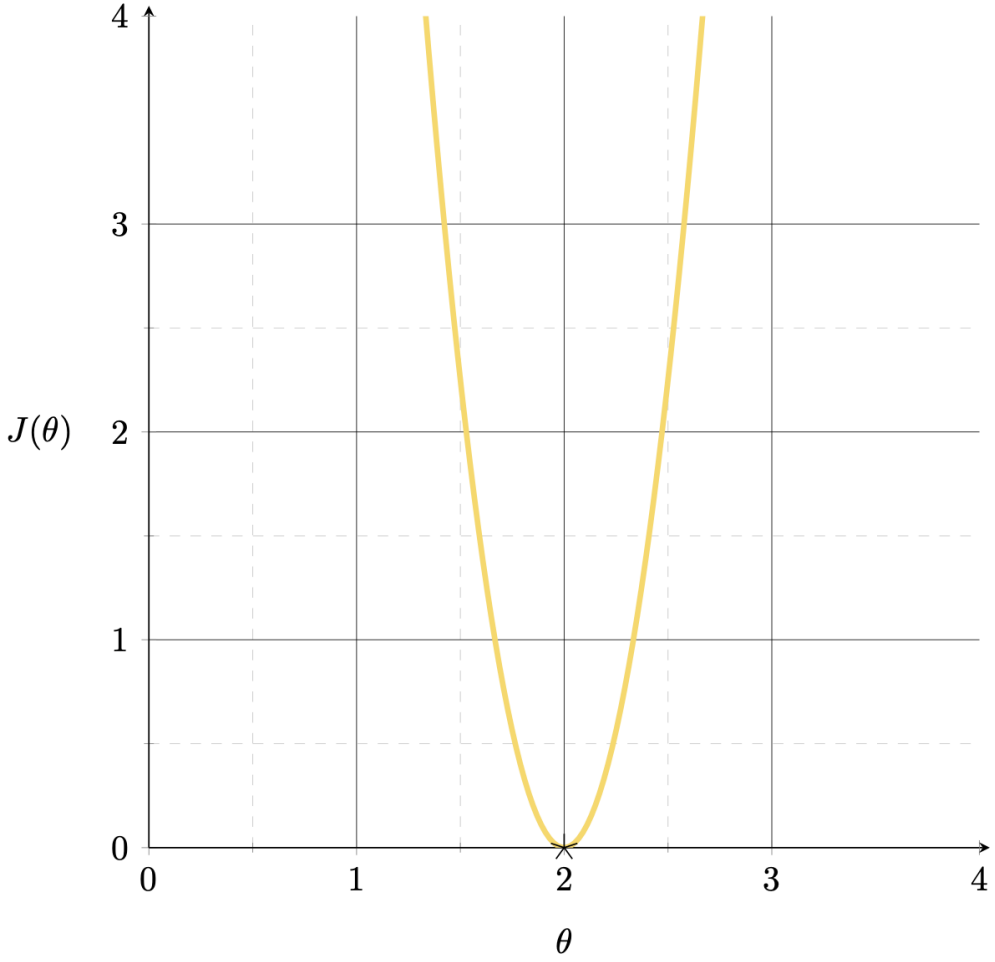
A single training data point

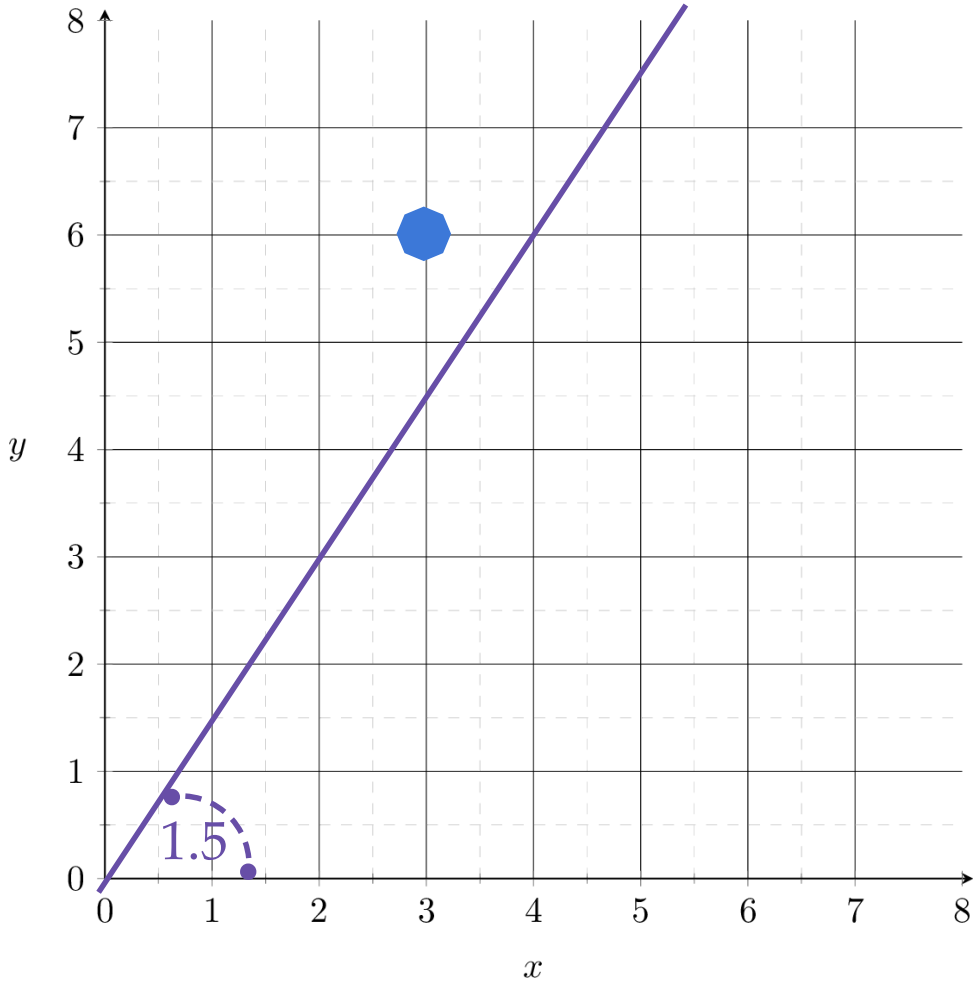
$(x, y) = (3, 6)$



Want to fit a line (without offset) to minimize the MSE: $J(\theta) = (3\theta - 6)^2$

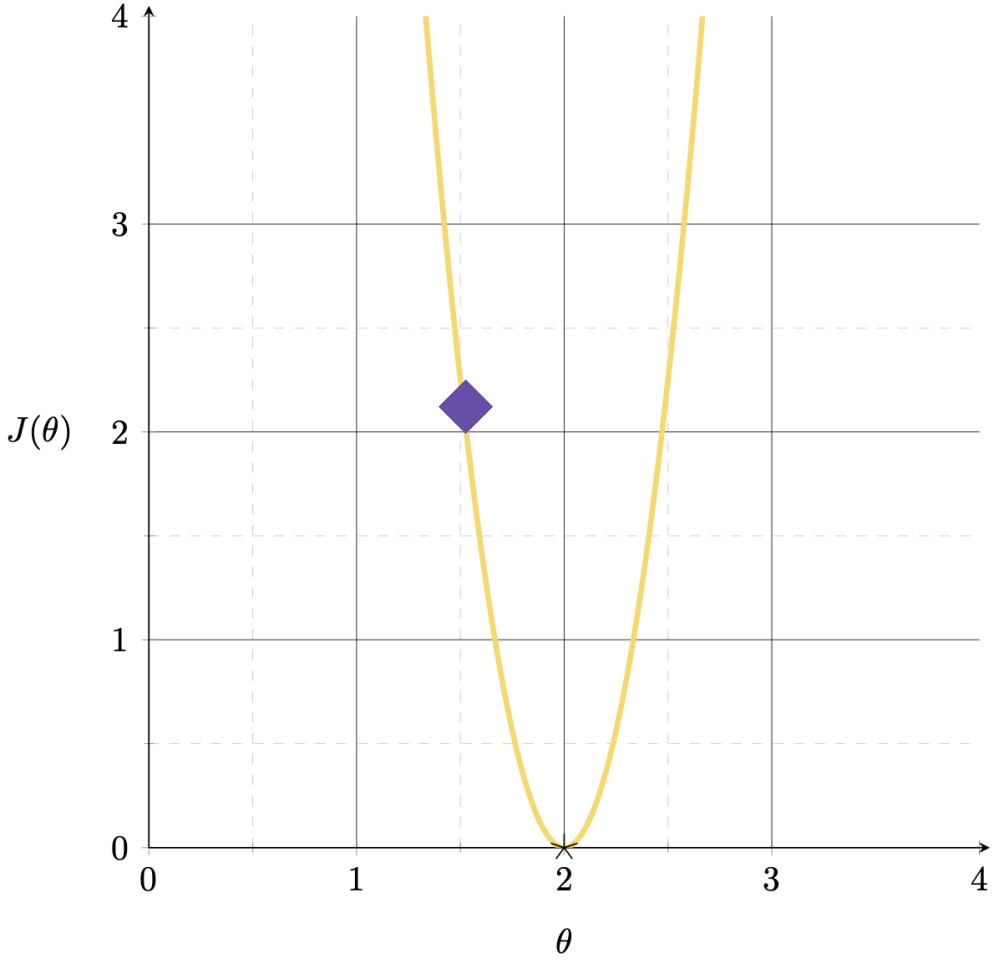


Suppose we fit a line $y = 1.5x$



MSE could get better.

How to formalize this?



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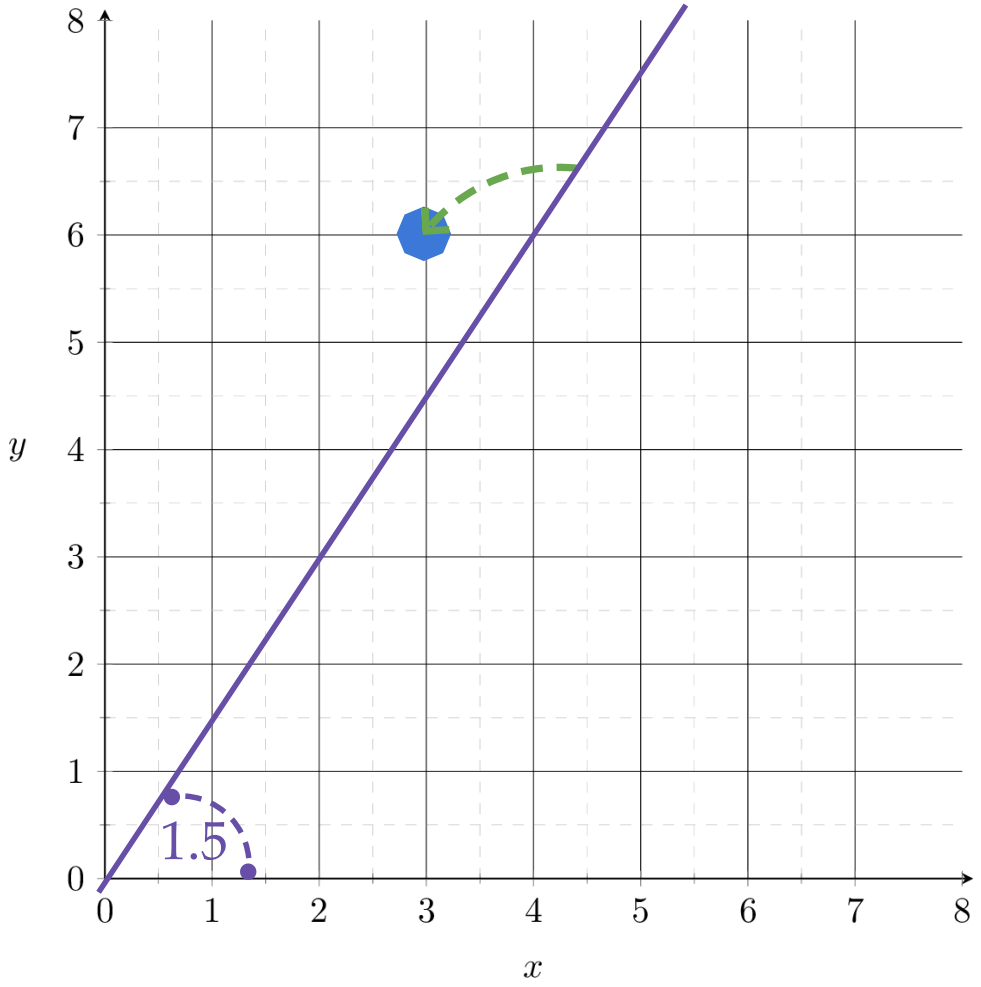
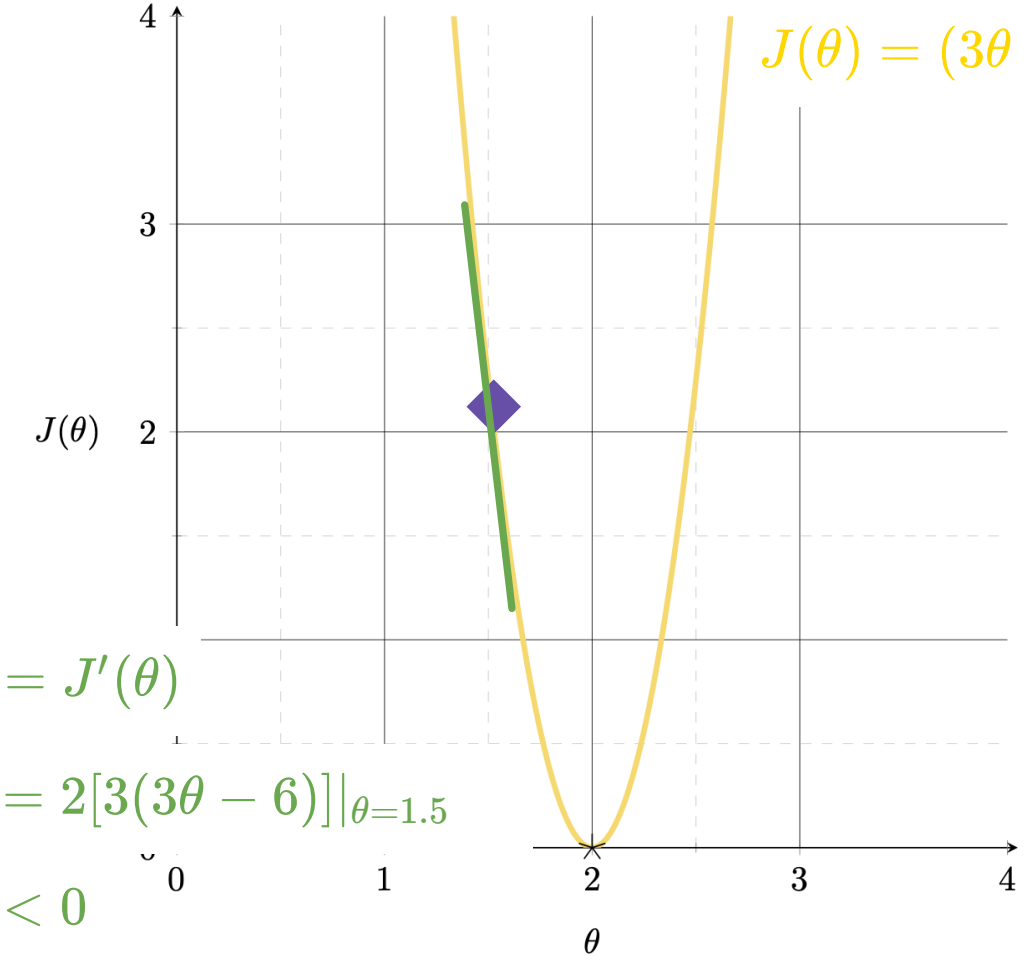


MSE could get better. How to?

Leveraging the gradient.

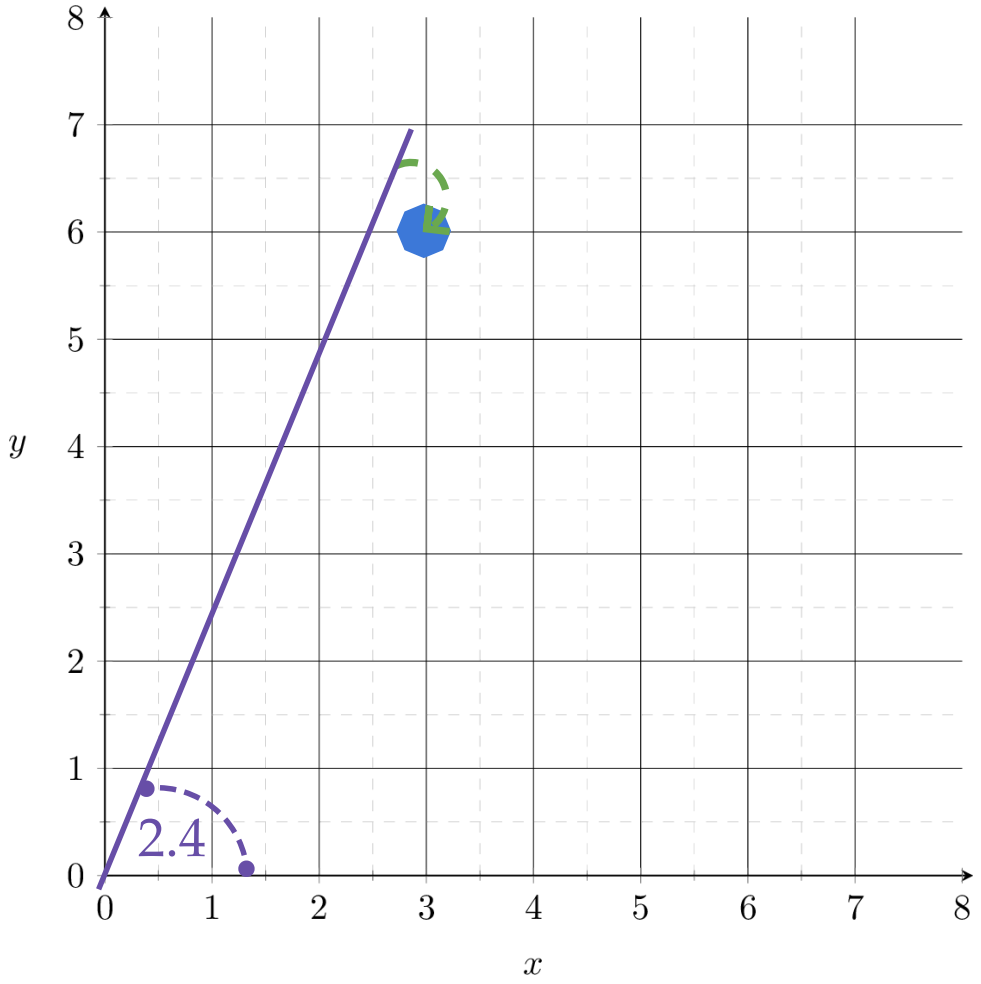


$$\nabla_\theta J = J'(\theta)$$

$$= 2[3(3\theta - 6)]|_{\theta=1.5}$$

$$< 0$$

Suppose we fit a line $y = 2.4x$



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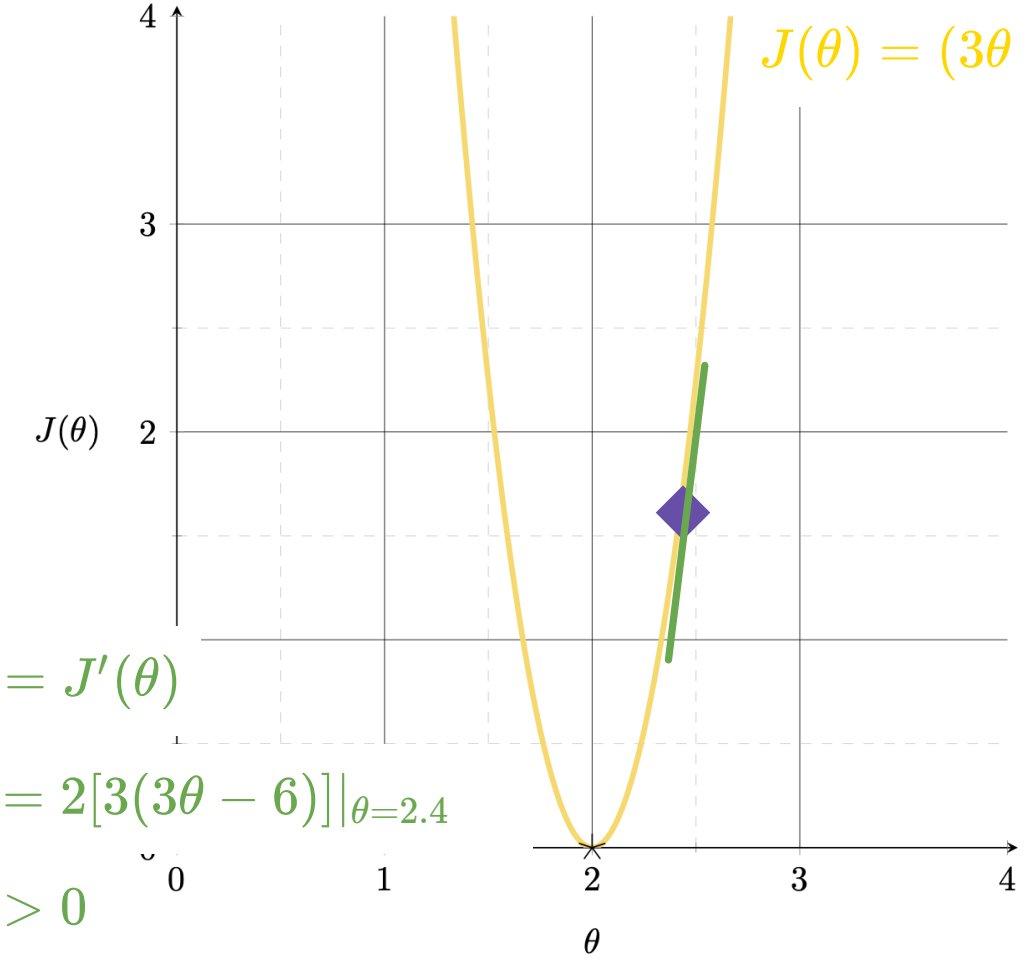

$$\nabla_\theta J = J'(\theta)$$

$$= 2[3(3\theta - 6)]|_{\theta=2.4}$$

$$> 0$$

initial guess

hyperparameters of parameters learning rate precision

Algorithm 1 Gradient Descent($\theta_{\text{init}}, \eta, J, \nabla_\theta J, \epsilon$)

1: Initialize $\theta^{(0)} = \theta_{\text{init}}$
2: Initialize $t = 0$
3: **repeat**
4: $\quad t = t + 1$
5: $\quad \theta^{(t)} = \theta^{(t-1)} - \eta \nabla_\theta J(\theta^{(t-1)})$
6: **until** $\left| J(\theta^{(t)}) - J(\theta^{(t-1)}) \right| < \epsilon$
7: **return** $\theta^{(t)}$

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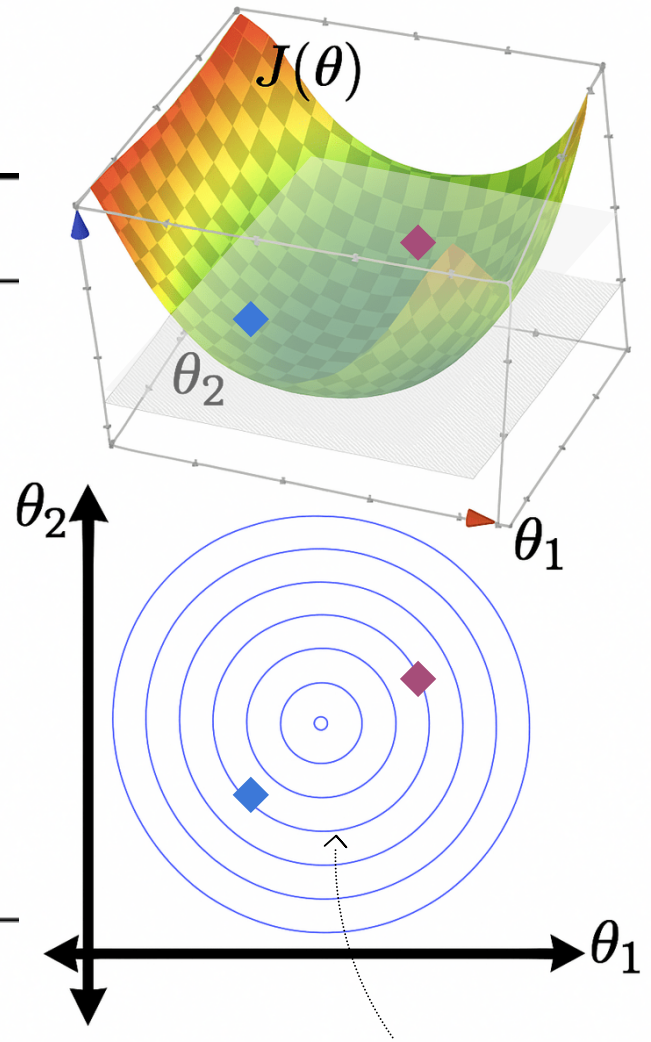

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repeat
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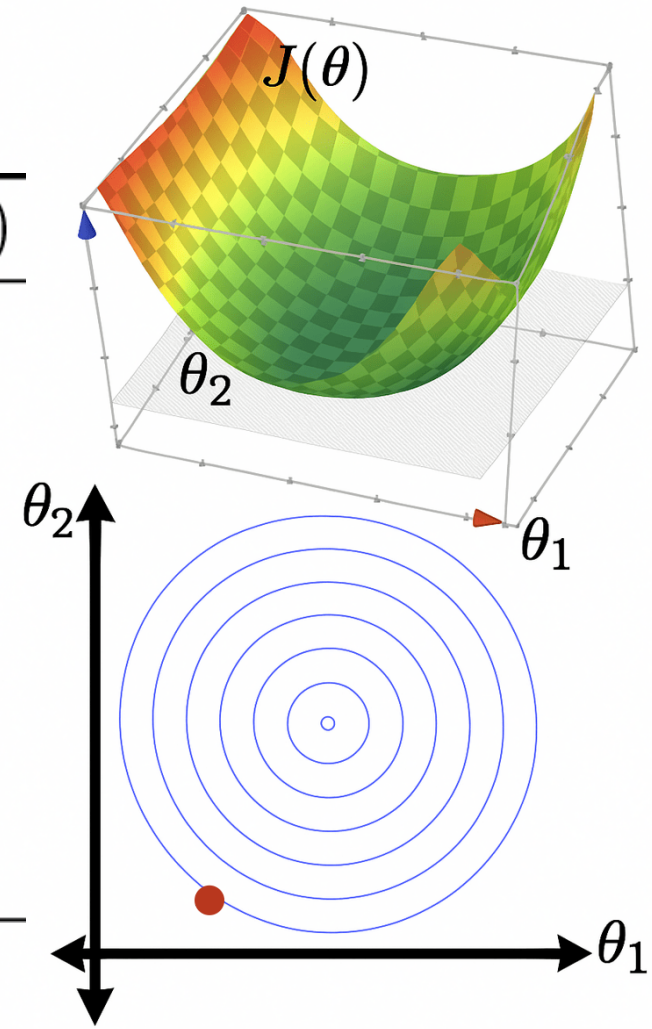

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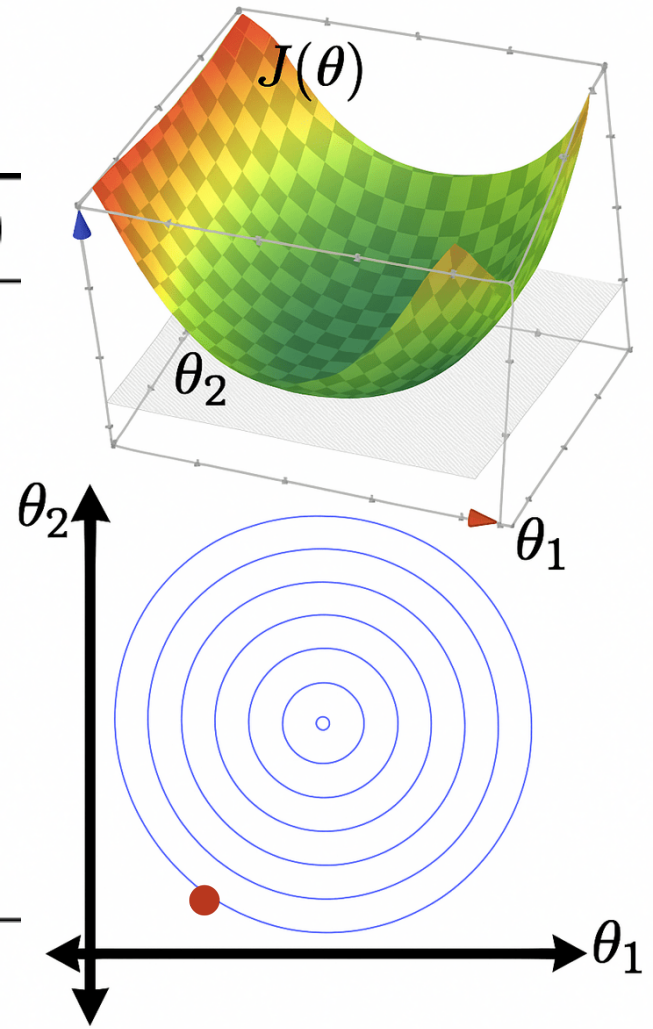
iteration counter



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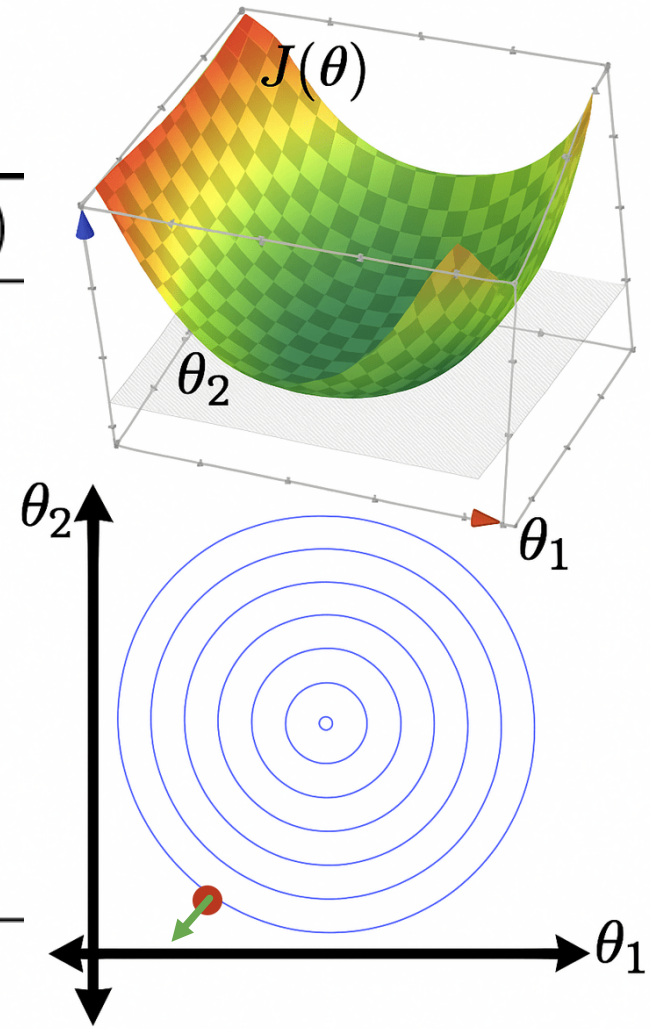

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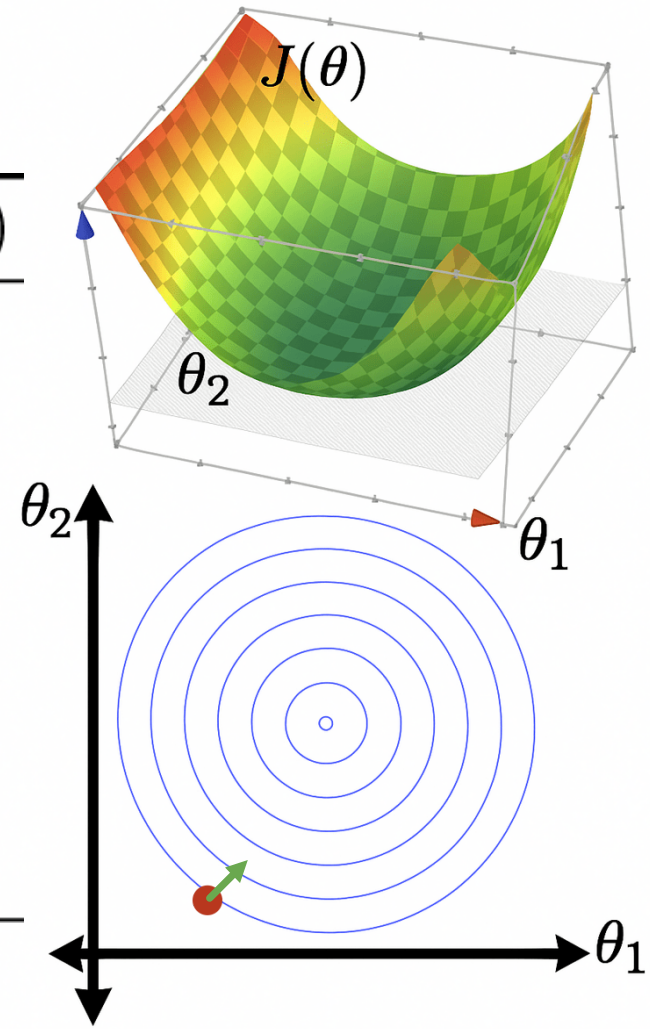

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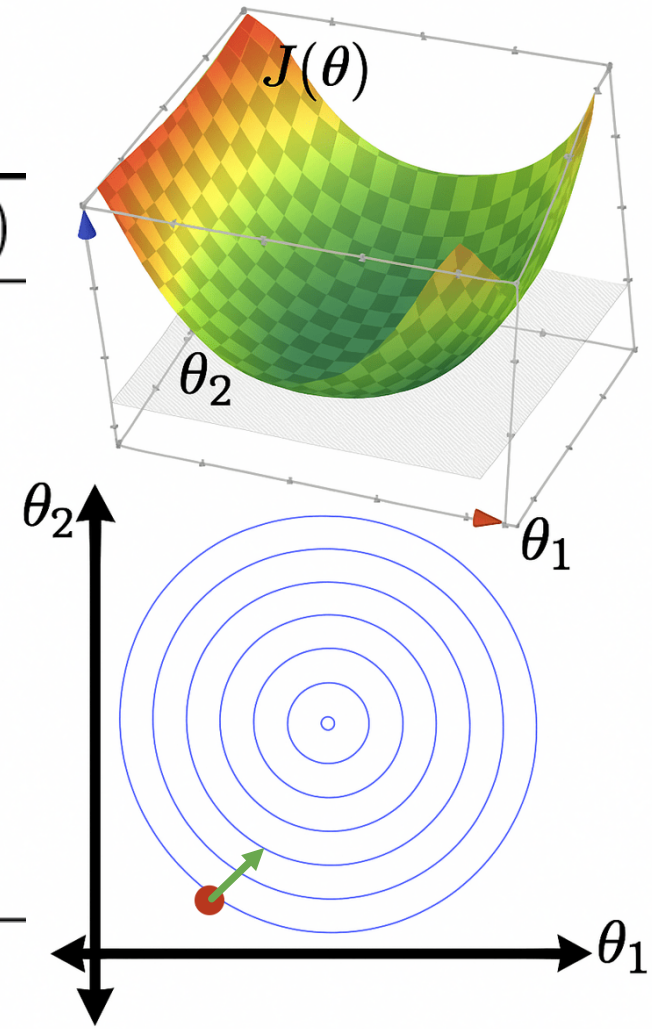

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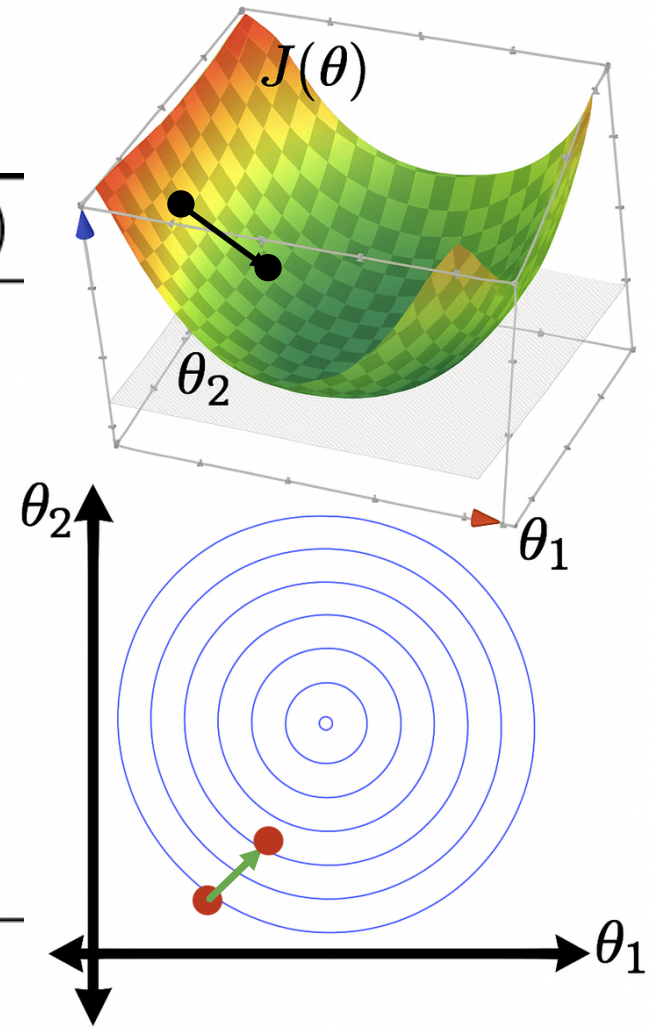

- What does this 3d vector ↘ represent? anything in the psuedocode?

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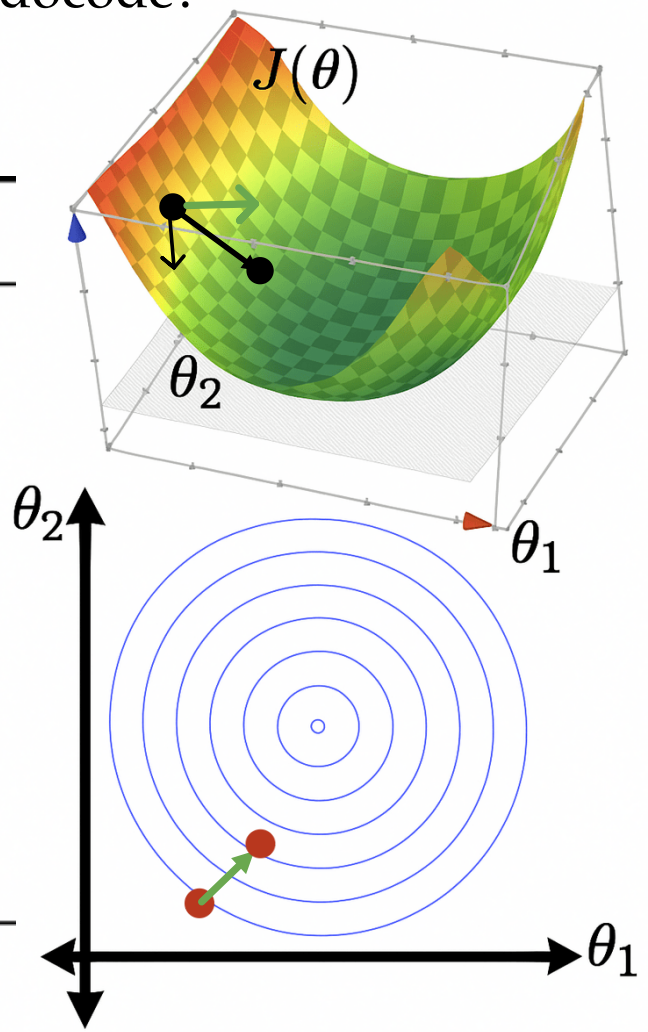

- What does this 2d vector ↗ represent? anything in the psuedocode?

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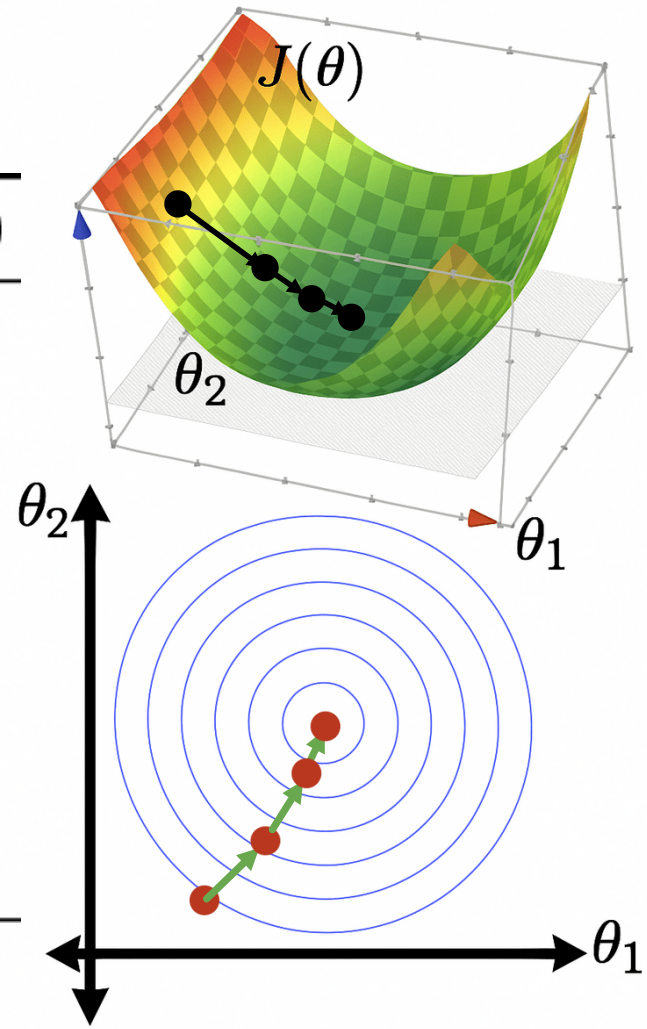

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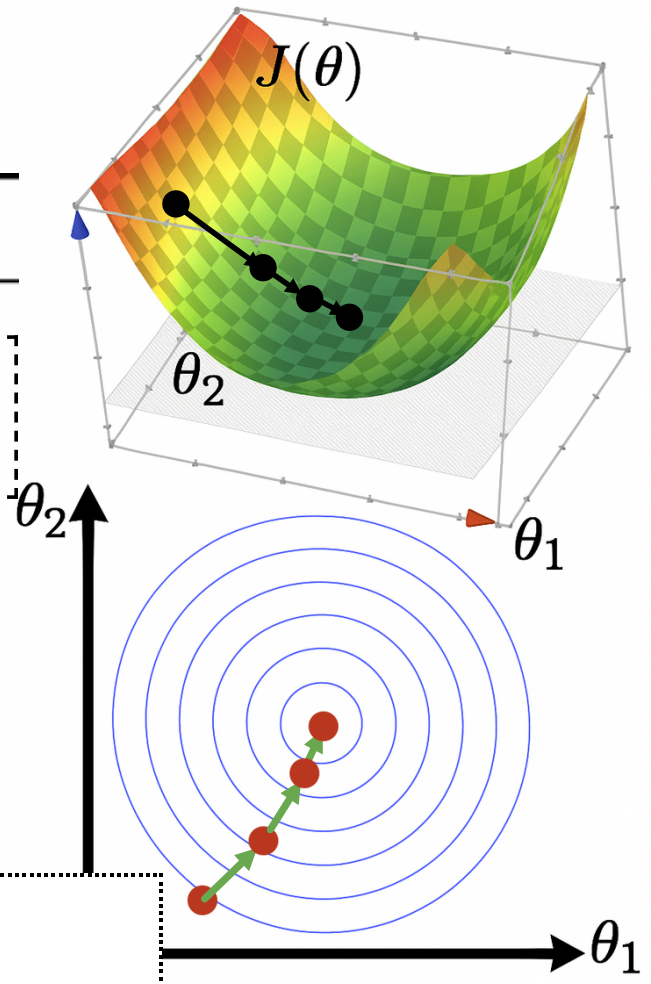
objective improvement is nearly zero.



Other possible stopping criterion for line 6:

- Small parameter change: $\|\theta^{(t)} - \theta^{(t-1)}\| < \epsilon$, or
- Small gradient norm: $\|\nabla_\theta J(\theta^{(t-1)})\| < \epsilon$

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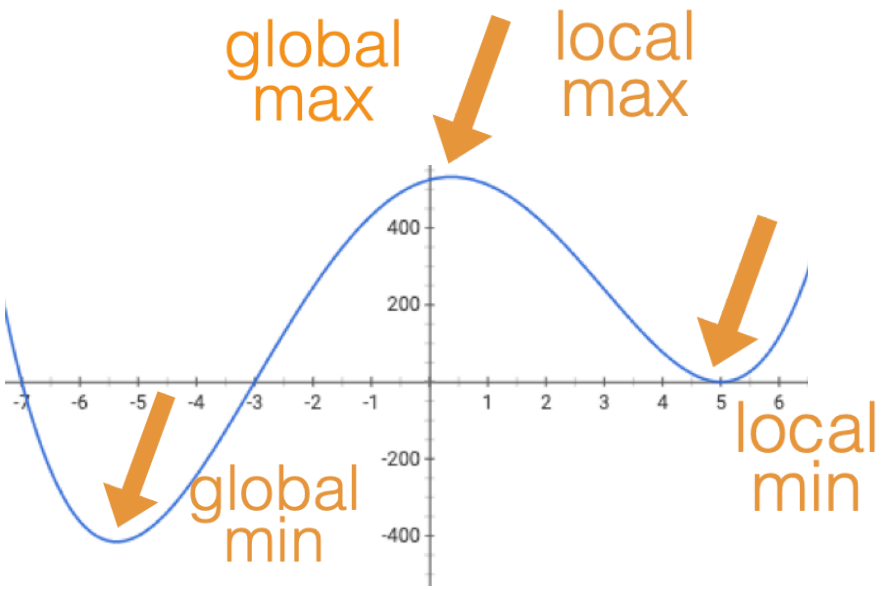
When minimizing a function, we aim for a global minimizer.

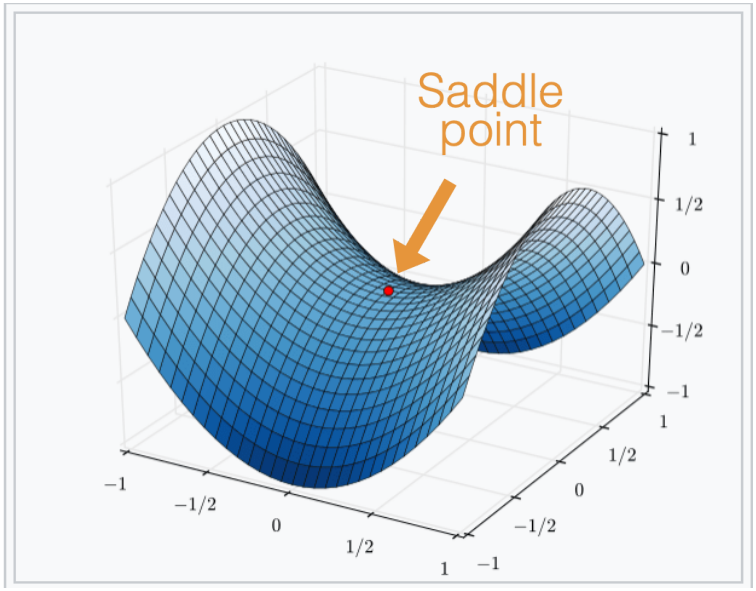
$\Rightarrow$

At a global minimizer the gradient vector is zero

gradient descent can achieve this (to arbitrary precision)

$\not\Leftarrow$





When minimizing a function, we aim for a global minimizer.

At a global minimizer $\Leftarrow$ { the gradient vector is zero ; the objective function is convex

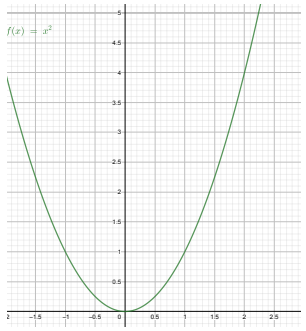
A function f is ***convex*** if any line segment connecting two points of the graph of f lies above or on the graph.

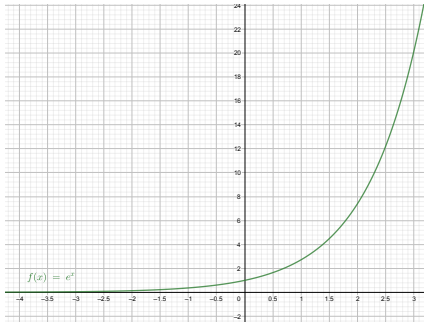
- f is concave if $-f$ is convex.
- Convex functions are the largest well-understood class of functions where optimization theory guarantees convergence and efficiency

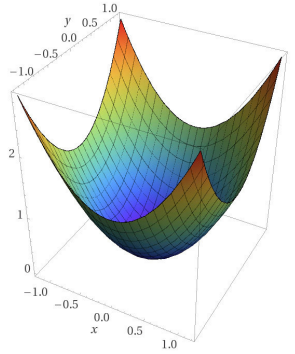
https://shenshen.mit.edu/demos/convex.html

Some examples

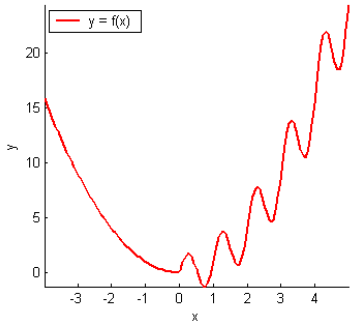
Convex functions

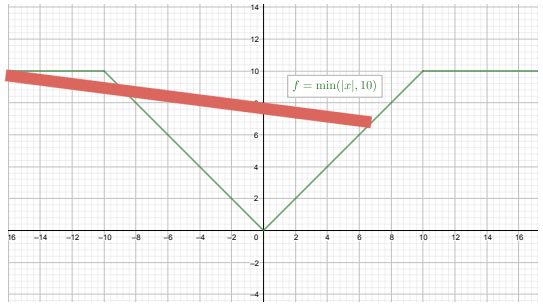


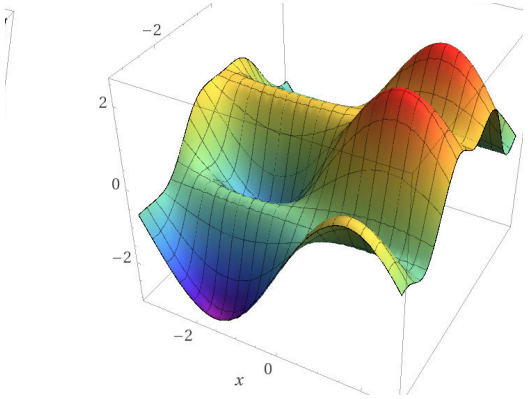




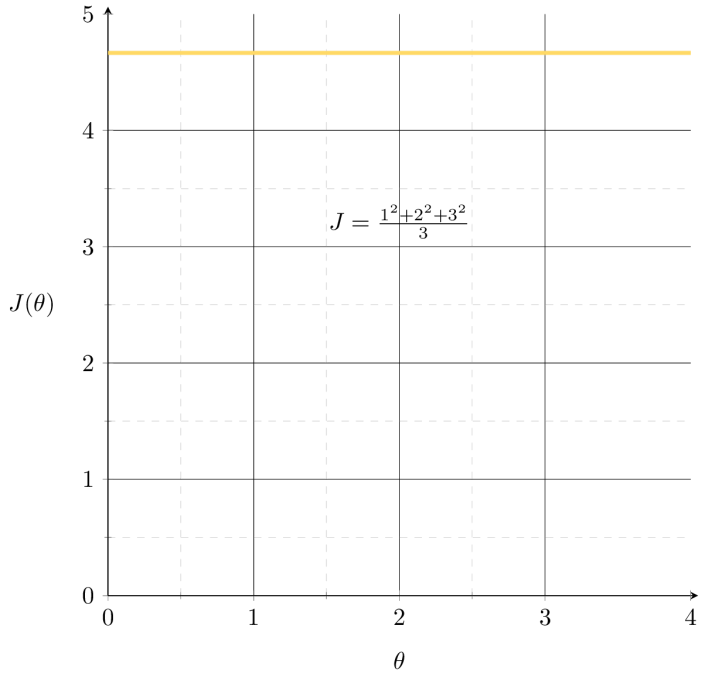
Non-convex functions

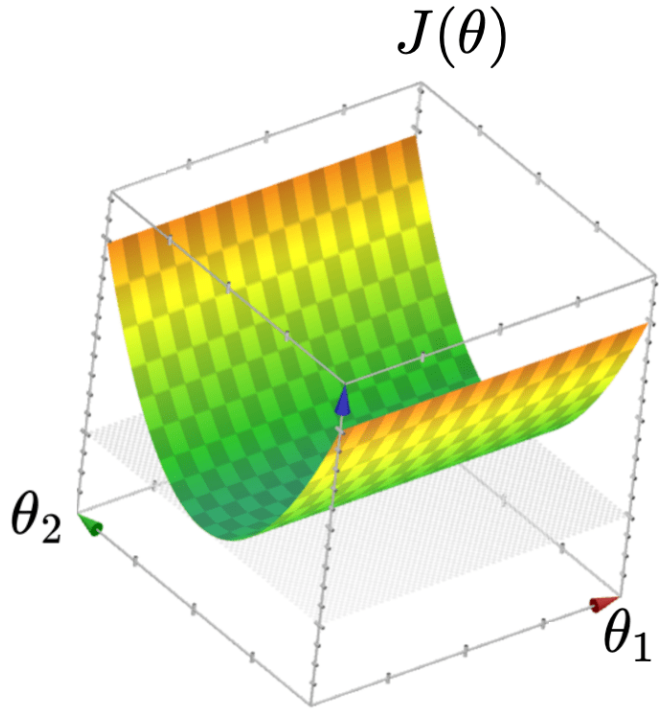


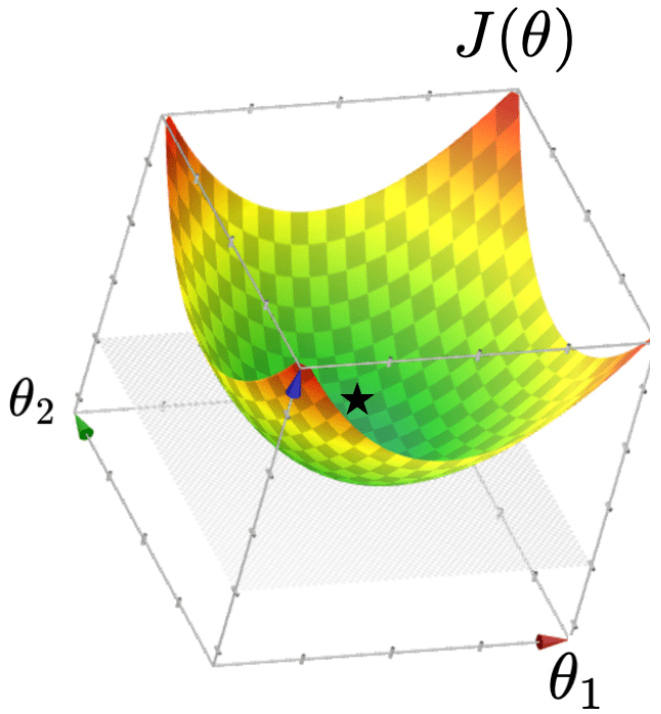




- MSE: $J(\theta) = \frac{1}{n}(X\theta - Y)^\top (X\theta - Y)$ is always convex



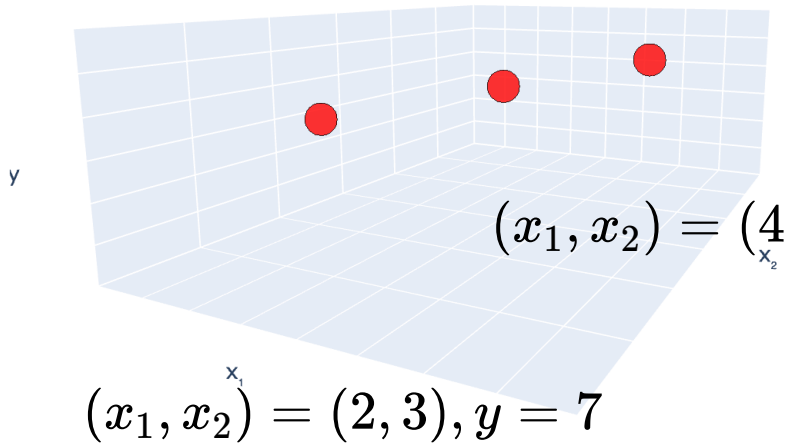




convexity is why we can claim the point whose gradient is zero is a global minimizer.

case (c) training data set again

$(x_1, x_2) = (6, 9), y = 9$



$(x_1, x_2) = (4, 6), y = 8$

$(x_1, x_2) = (2, 3), y = 7$

- Ridge objective with $\lambda > 0$ is always (strongly) convex

convexity is why we can claim the point whose gradient is zero is a global minimizer.

Gradient Descent Performance

- Assumptions:
  - f is sufficiently "smooth"
  - f is convex
  - f has at least one global minimum
  - Run gradient descent for sufficient iterations
  - η is sufficiently small
- Conclusion:
  - Gradient descent converges arbitrarily close to a global minimizer of f.

Gradient Descent Performance

- Assumptions:
  - f is sufficiently "smooth"
  - f is convex
  - f has at least one global minimum
  - Run gradient descent for sufficient iterations
  - η is sufficiently small

if violated, may not have gradient, can't run gradient descent

- Conclusion:
  - Gradient descent converges arbitrarily close to a global minimizer of f.

Gradient Descent Performance

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  - f is convex
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  - Run gradient descent for sufficient iterations
  - η is sufficiently small
- Conclusion:
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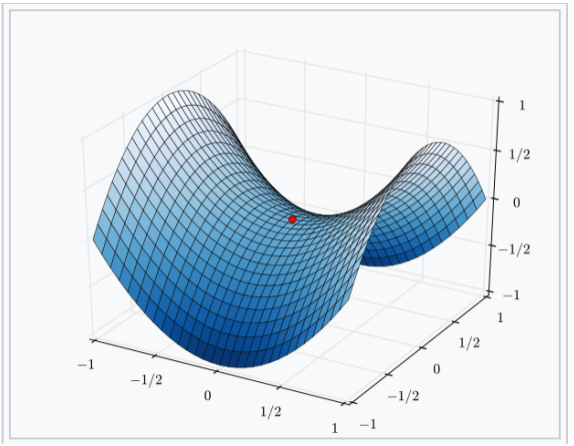
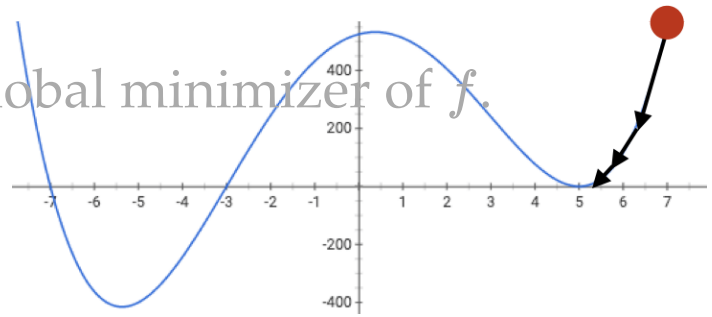
if violated, may get stuck at a saddle point



or a local minimum



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  - η is sufficiently small
- Conclusion:
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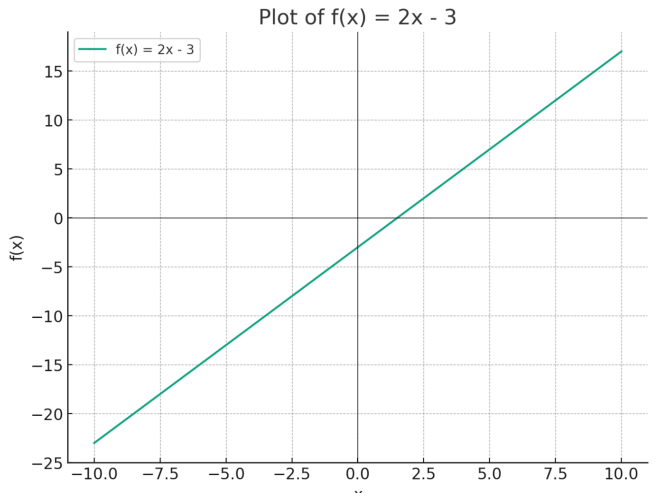
if violated:

may not terminate/no minimum to converge to



Gradient Descent Performance

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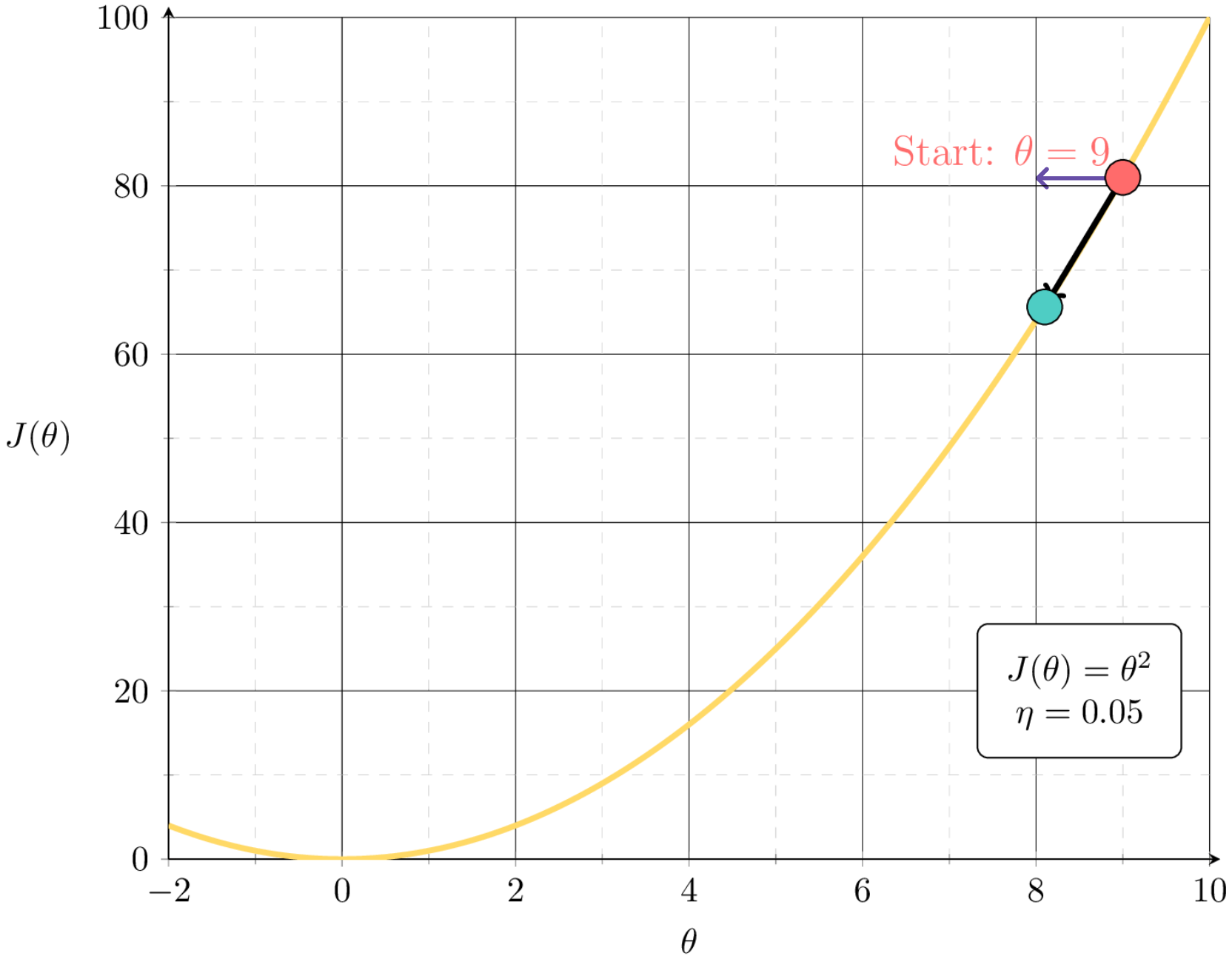
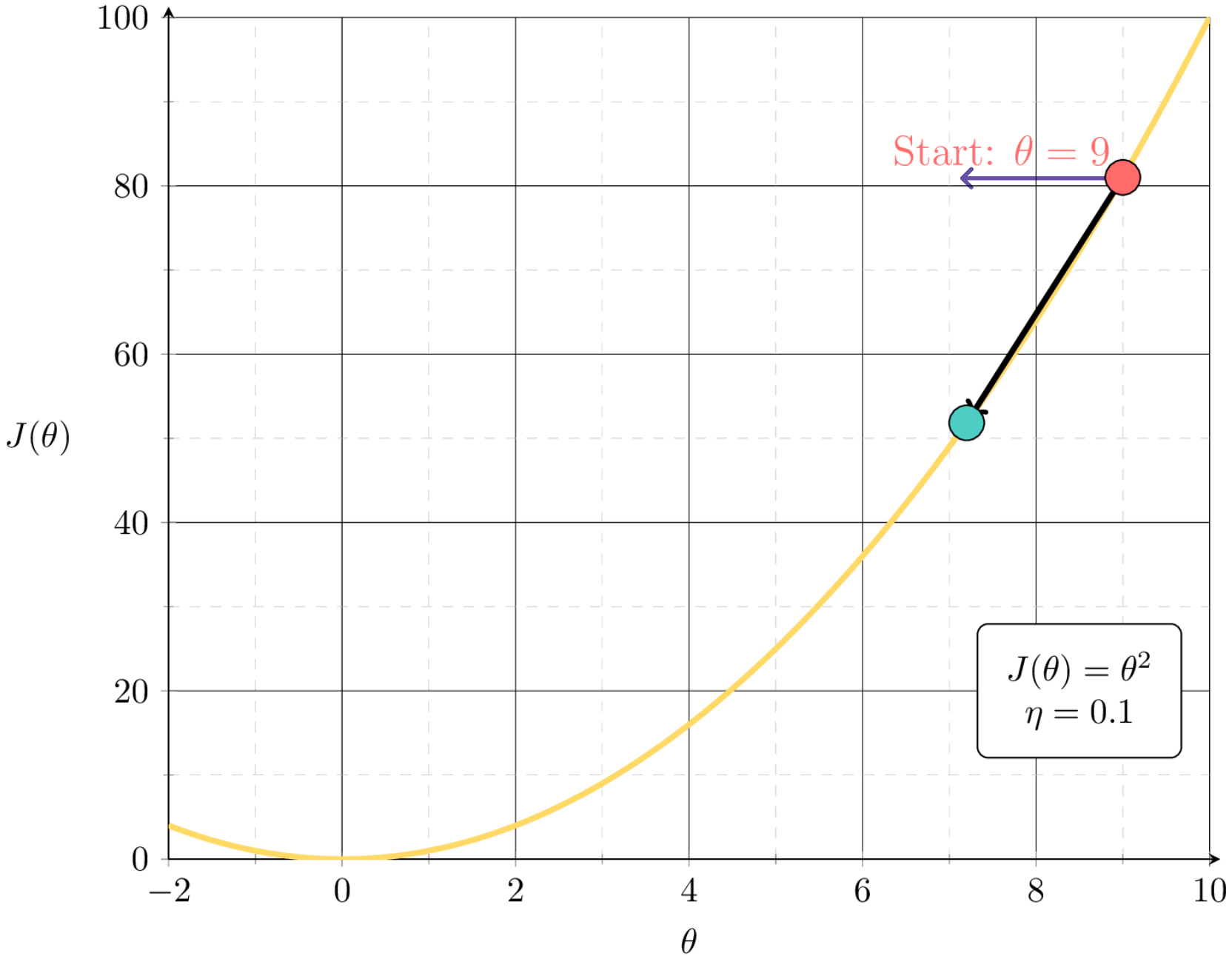
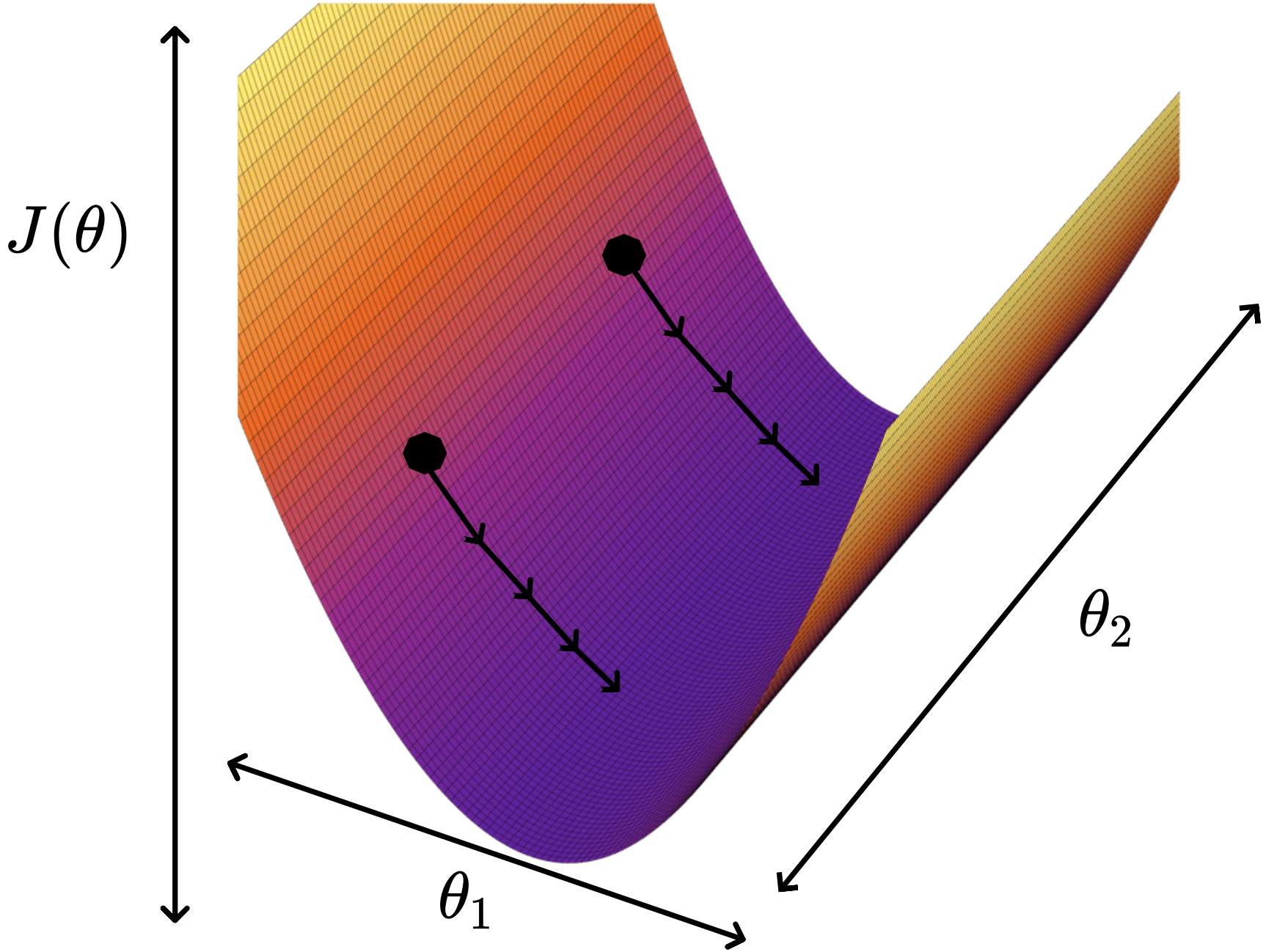
if violated:

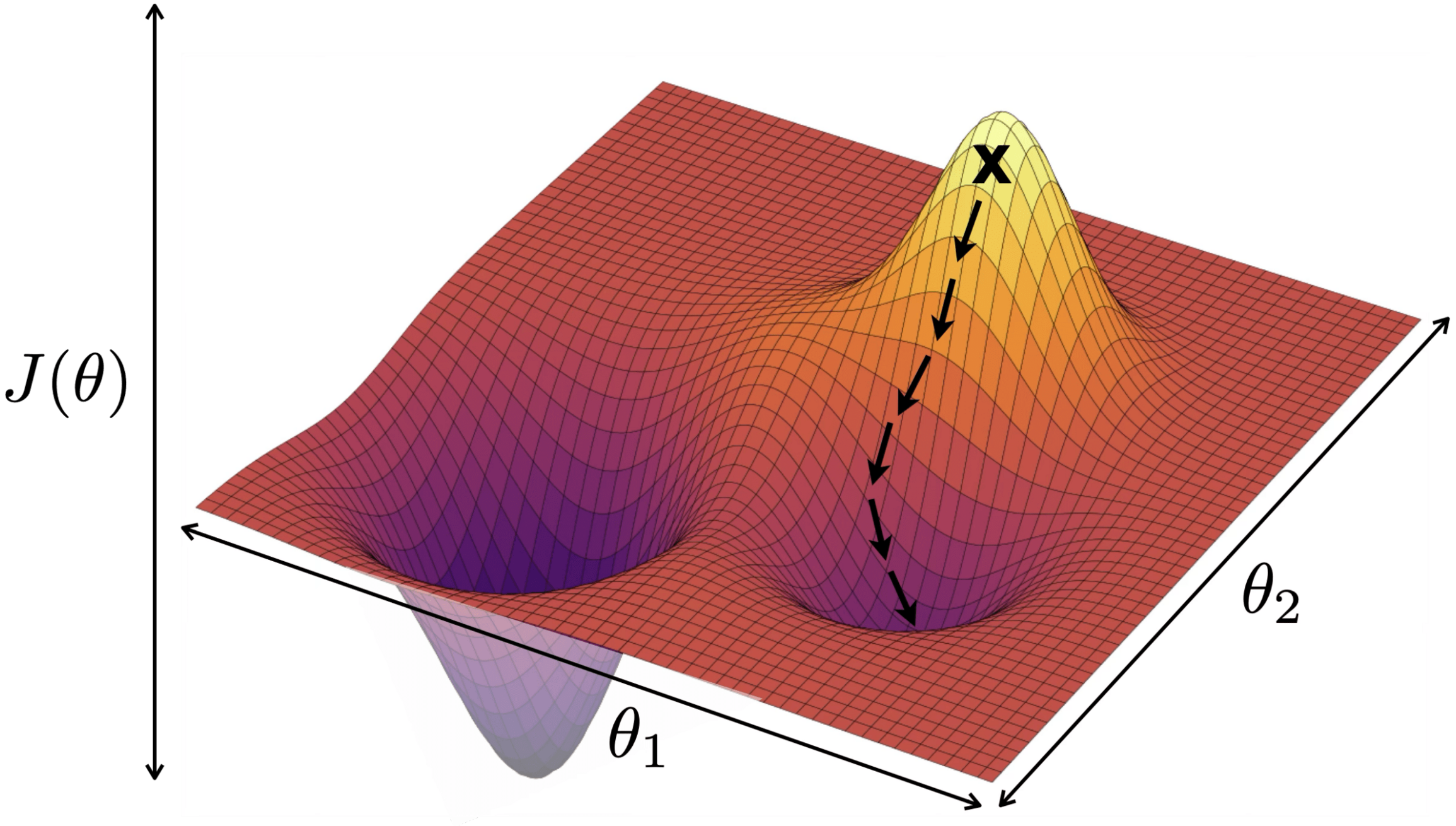
see demo on next slide, also lab/hw


100
80
60
40
20
0
$J(\theta)$
−2
0
2
4
6
8
10
θ
Start: $\theta = 9$
$J(\theta) = \theta^2$
$\eta = 0.05$


100
80
60
40
20
0
$J(\theta)$
−2
0
2
4
6
8
10
θ
Start: $\theta = 9$
$J(\theta) = \theta^2$
$\eta = 0.1$

https://shenshen.mit.edu/demos/gd.html


$J(\theta)$
θ_1
θ_2

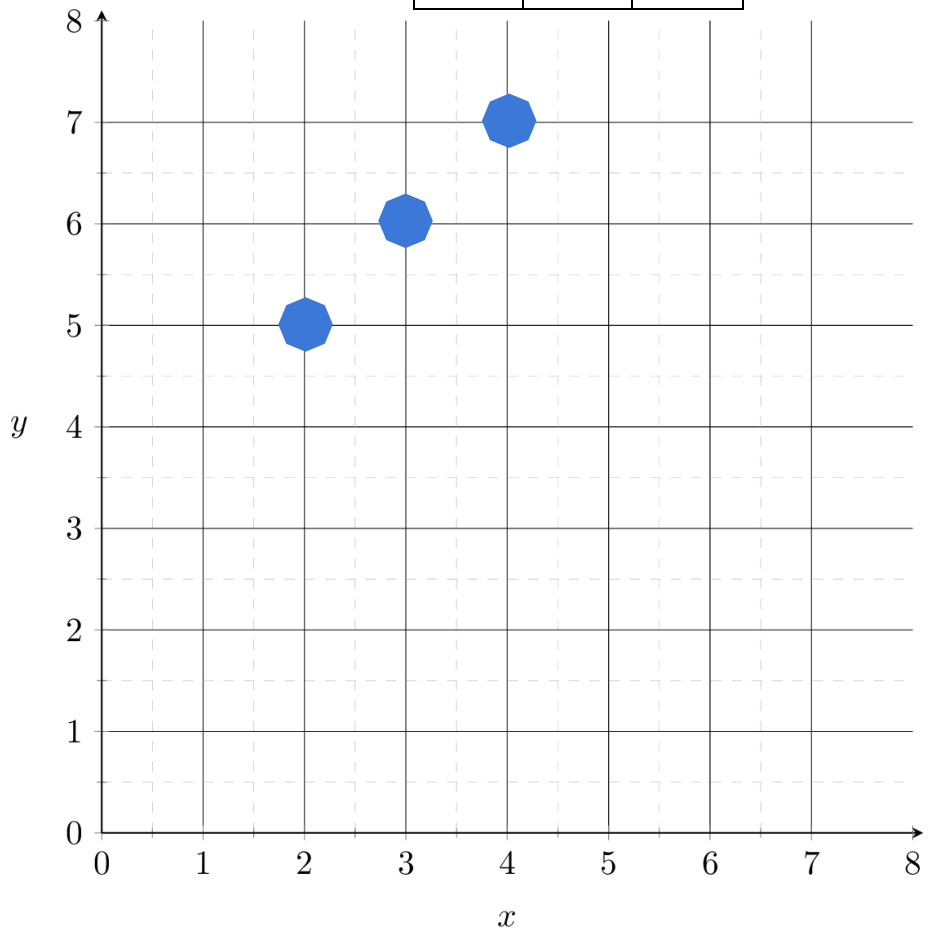

$J(\theta)$
x
θ_1
θ_2

Outline

- Gradient descent algorithm (GD)
  - The gradient vector
  - GD algorithm
  - Gradient decent properties
- Stochastic gradient descent (SGD)
  - SGD algorithm and setup
  - SGD vs. GD

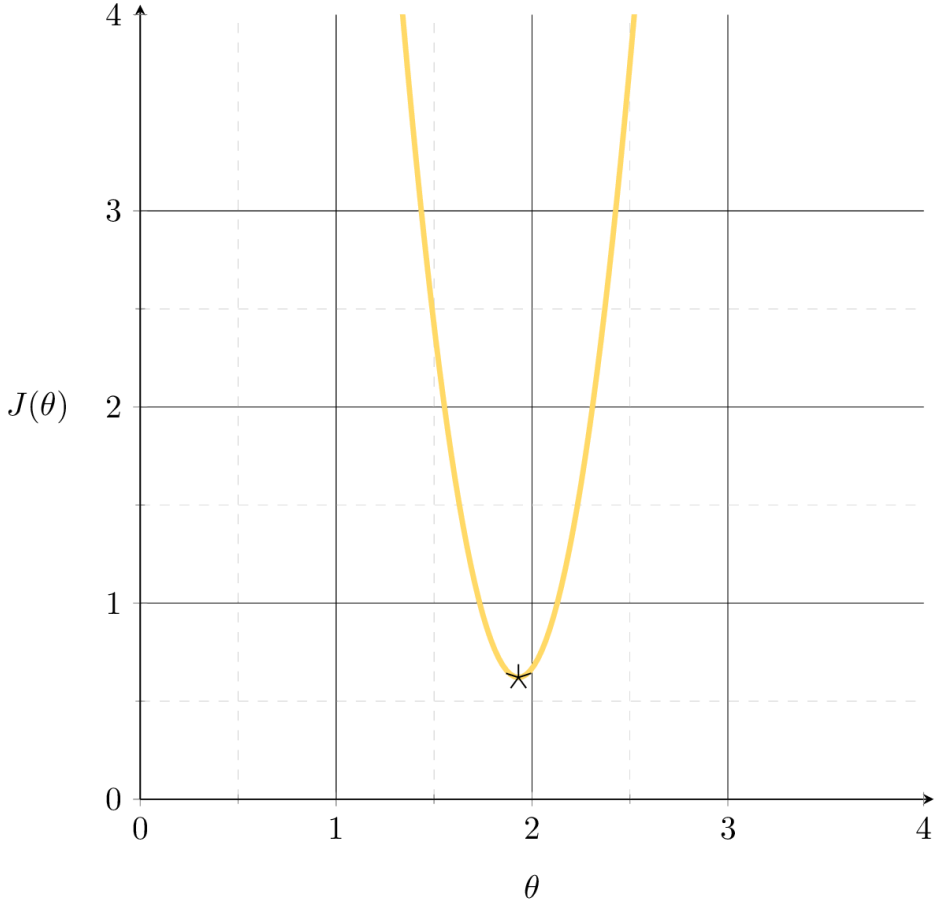
training data

	x	y
p1	2	5
p2	3	6
p3	4	7



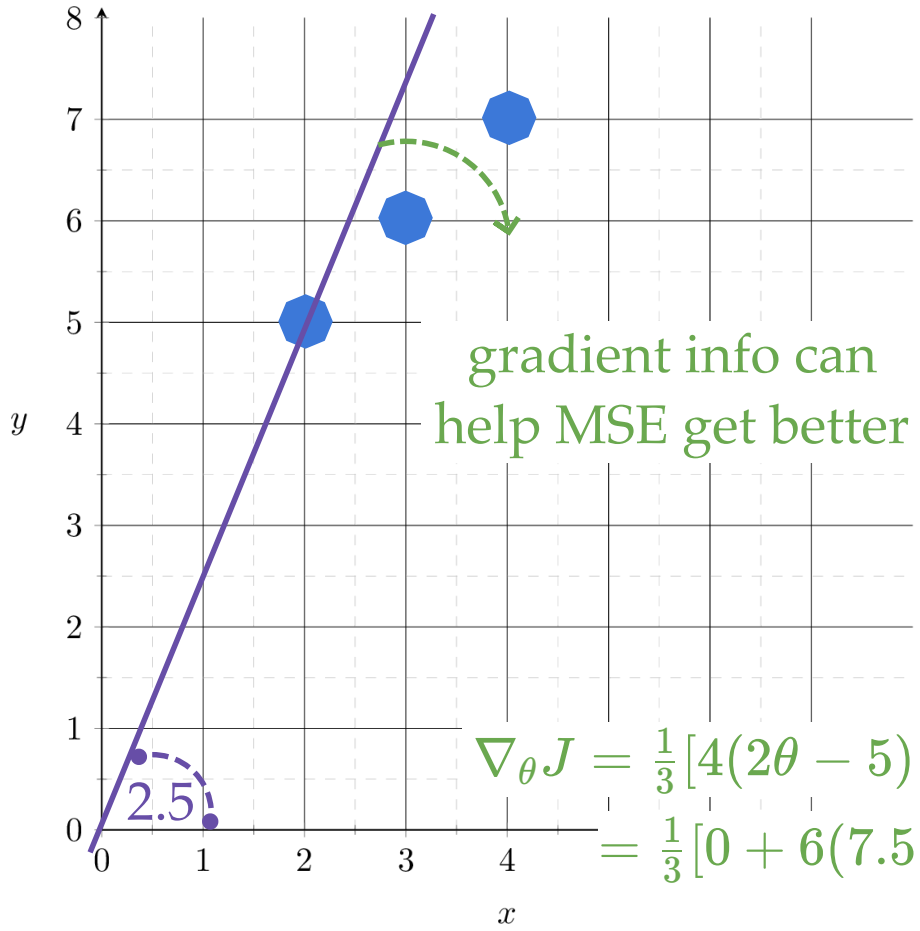
Fit a line (without offset) to the dataset, the MSE:

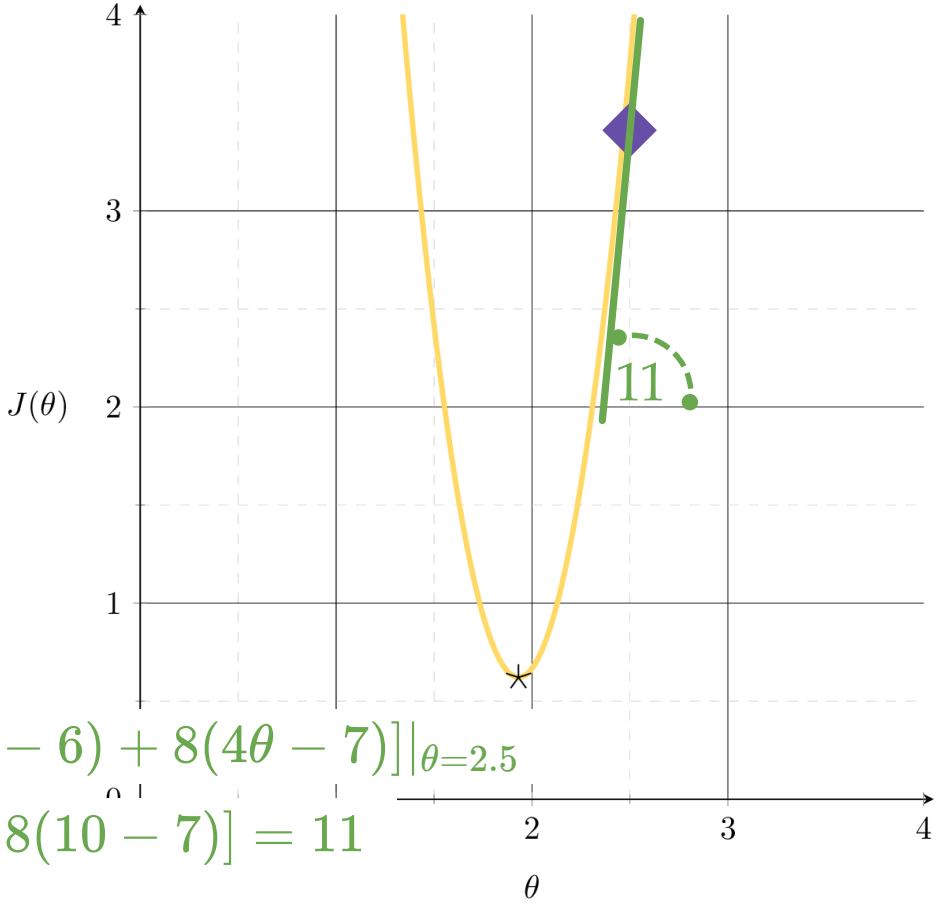
$$J(\theta) = \frac{1}{3}\left[(2\theta - 5)^2 + (3\theta - 6)^2 + (4\theta - 7)^2\right]$$



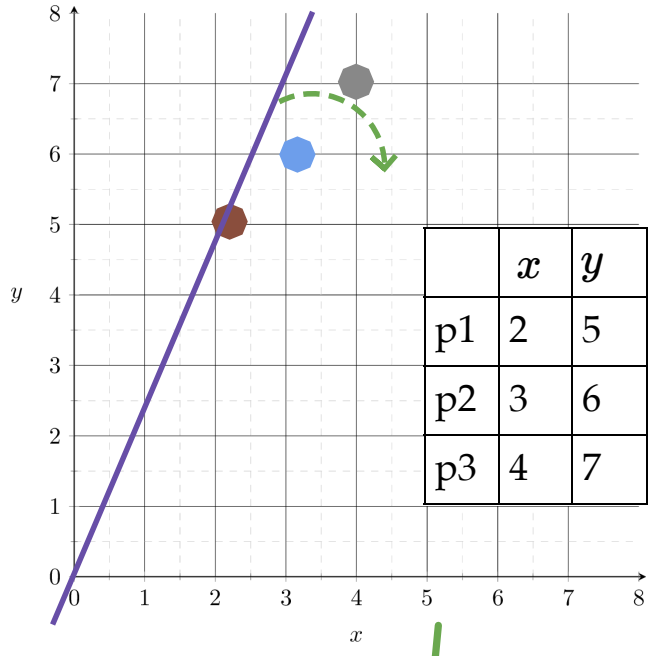
Suppose we fit a line $y = 2.5x$

$$J(\theta) = \frac{1}{3}\left[(2\theta - 5)^2 + (3\theta - 6)^2 + (4\theta - 7)^2\right]$$





$$\nabla_\theta J = \frac{1}{3}[4(2\theta - 5) + 6(3\theta - 6) + 8(4\theta - 7)]|_{\theta=2.5}$$
$$= \frac{1}{3}[0 + 6(7.5 - 6) + 8(10 - 7)] = 11$$



	x	y
p1	2	5
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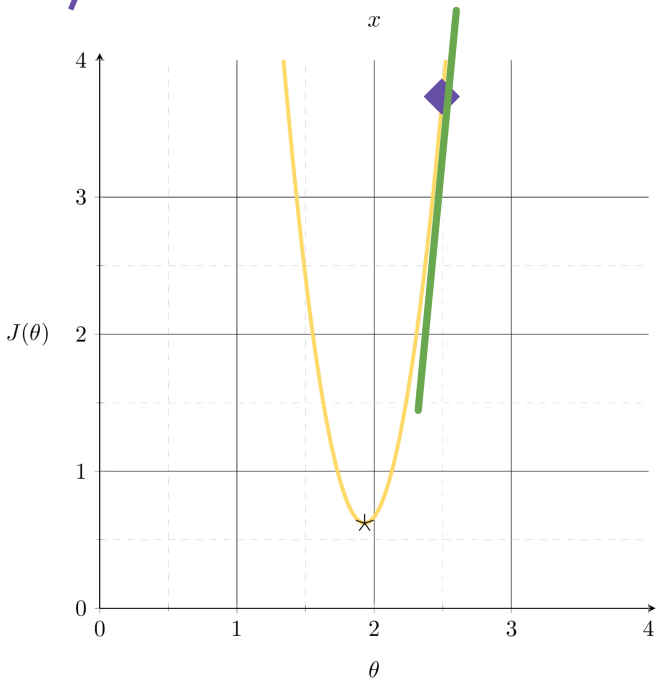
p3	4	7



- the MSE of a linear hypothesis:

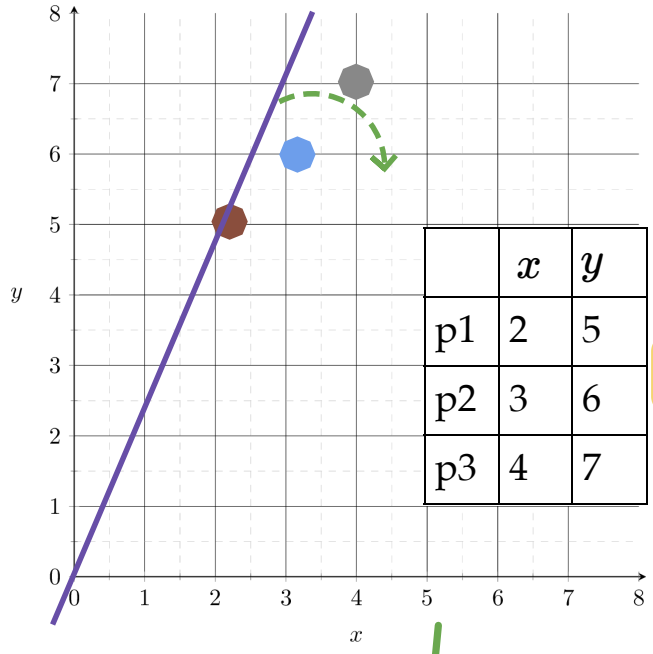
$$J(\theta) = \frac{1}{3}\left[(2\theta - 5)^2 + (3\theta - 6)^2 + (4\theta - 7)^2\right]$$

$$= \frac{1}{3}\left[\quad J_1 \quad + \quad J_2 \quad + \; J_3\;\right]$$

- and its gradient w.r.t. θ:

$$\nabla_\theta J = \frac{1}{3}\left[4(2\theta - 5) + 6(3\theta - 6) + 8(4\theta - 7)\right]$$

$$= \frac{1}{3}\left[\; \nabla_\theta J_1 \; + \; \nabla_\theta J_2 \; + \; \nabla_\theta J_3 \quad\right]$$



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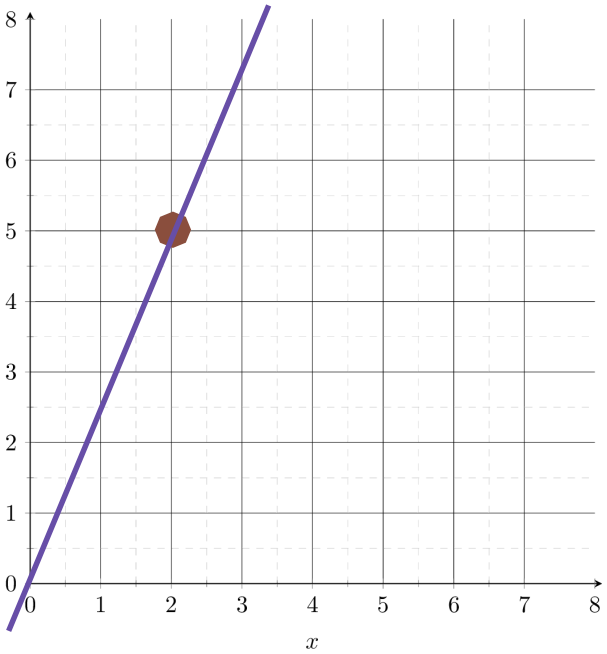

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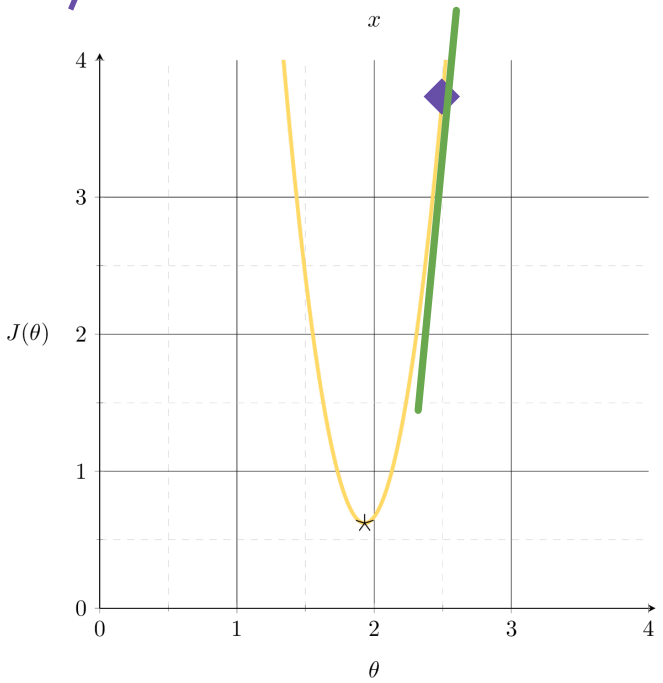

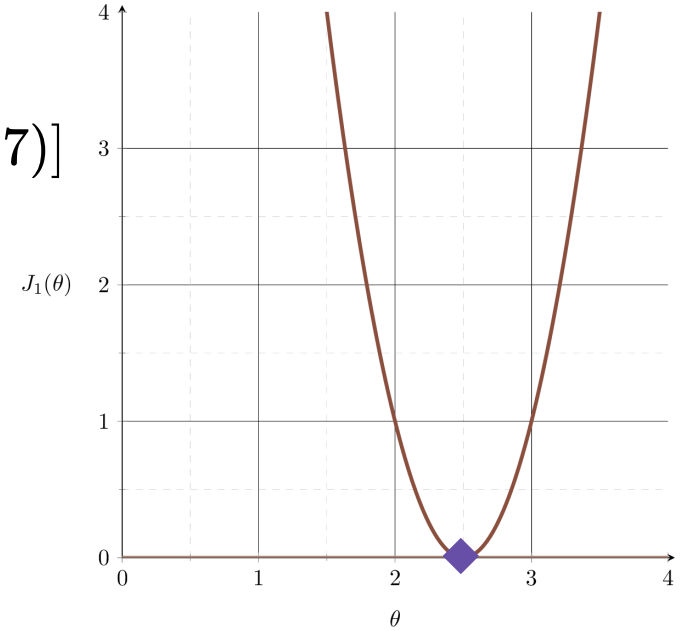

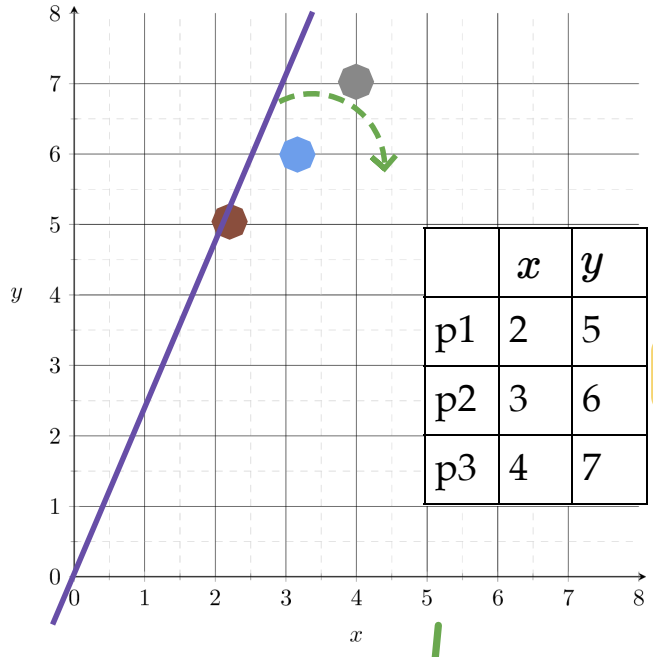

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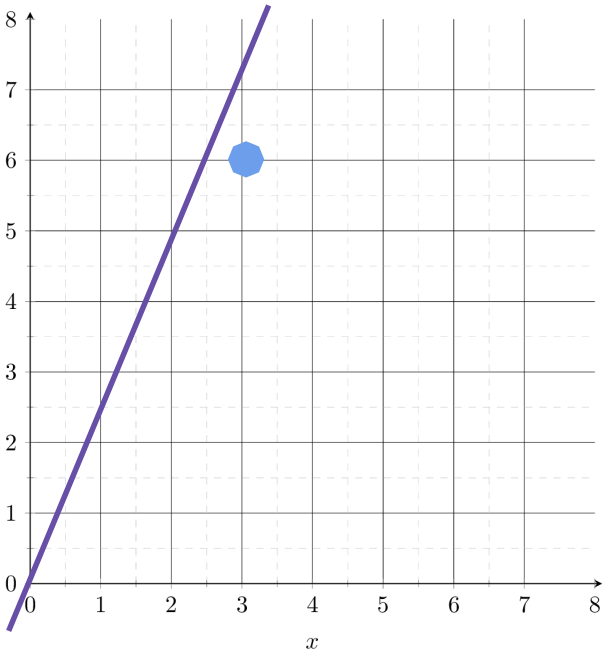

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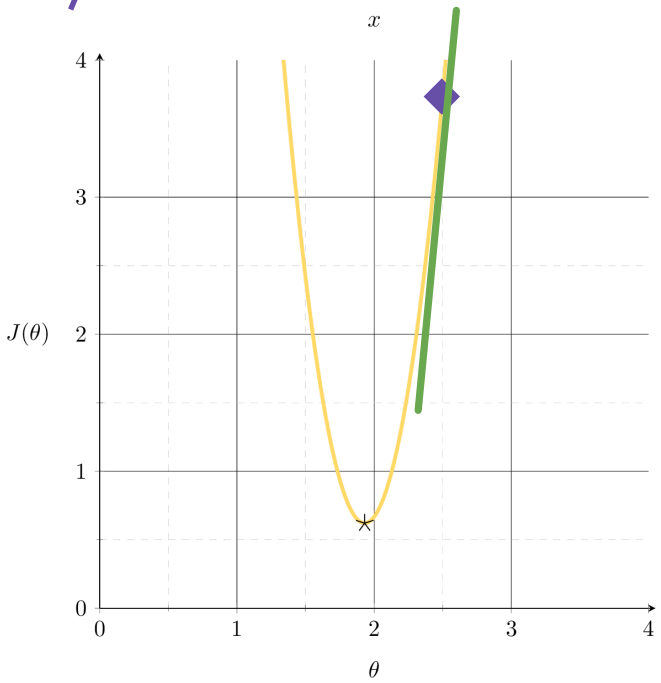
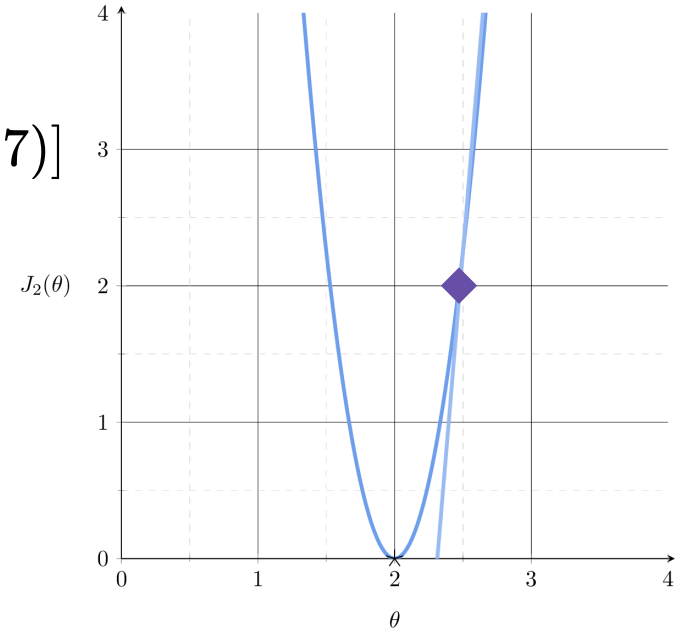
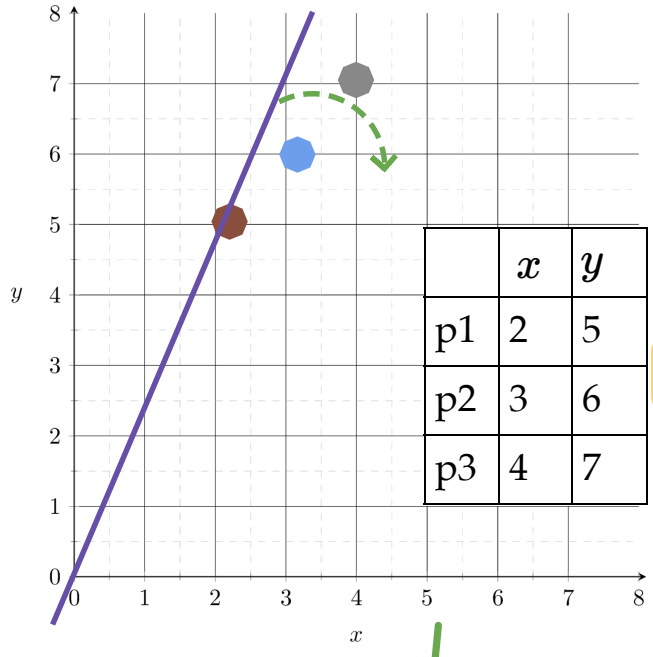
$$= \frac{1}{3}\left[\quad \nabla_\theta J_1 \quad + \quad \nabla_\theta J_2 \quad + \quad \nabla_\theta J_3 \quad\right]$$







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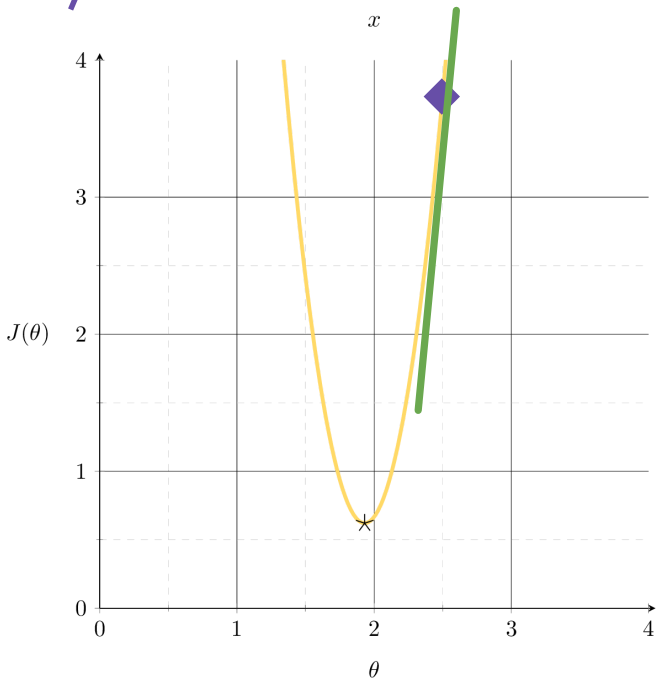
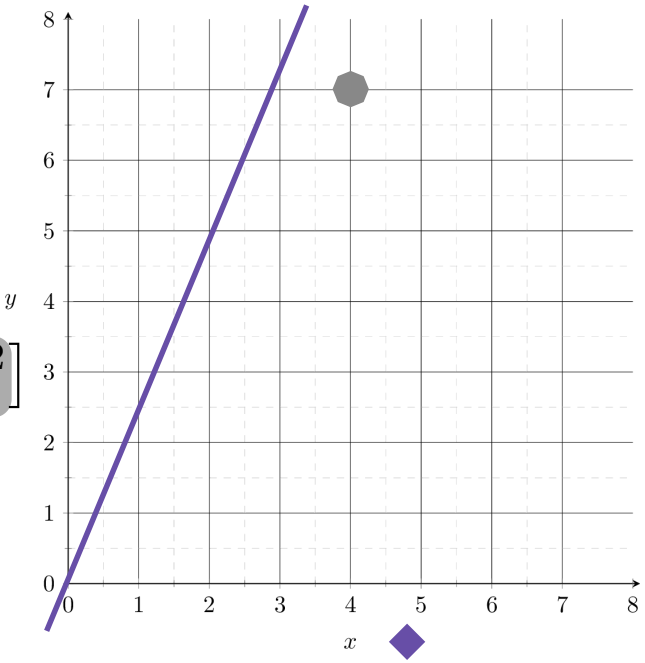
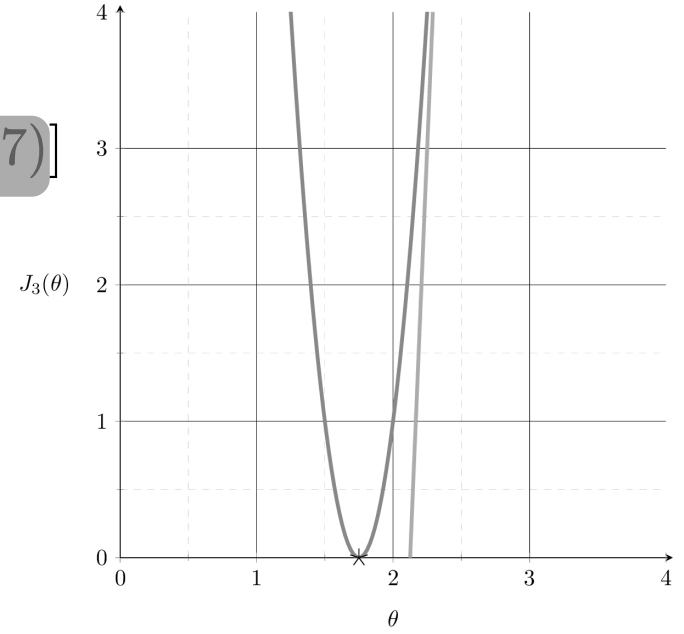






Gradient of an ML objective

Using our example data set,

- the MSE of a linear hypothesis:

$$J(\theta) = \tfrac{1}{3}\left[(2\theta - 5)^2 + (3\theta - 6)^2 + (4\theta - 7)^2\right]$$

- and its gradient w.r.t. θ:

$$\nabla_\theta J = \tfrac{1}{3}[4(2\theta - 5) + 6(3\theta - 6) + 8(4\theta - 7)]$$

Using any dataset,

- the MSE of a linear hypothesis:

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

- and its gradient w.r.t. θ:

$$\nabla_\theta J(\theta) = \frac{1}{n}\sum_{i=1}^{n} 2\left(\theta^\top x^{(i)} - y^{(i)}\right) x^{(i)}$$

Gradient of an ML objective

- the MSE of a linear hypothesis:

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

- and its gradient w.r.t. θ:

$$\nabla_\theta J(\theta) = \frac{1}{n}\sum_{i=1}^{n} 2\left(\theta^\top x^{(i)} - y^{(i)}\right) x^{(i)}$$

In general,

- An ML objective function is a finite sum

$$J(\theta) = \frac{1}{n}\sum_{i=1}^{n} J_i(\theta)$$

- and its gradient w.r.t. θ:

$$\nabla_\theta J(\theta) = \nabla\left(\frac{1}{n}\sum_{i=1}^{n} J_i(\theta)\right) = \frac{1}{n}\sum_{i=1}^{n} \nabla_\theta J_i(\theta)$$

👆

👋 (gradient of the sum) = (sum of the gradient)

Gradient of an ML objective

In general,

- An ML objective function is a finite sum

$$J(\theta) = \frac{1}{n}\sum_{i=1}^{n} J_i(\theta)$$

loss incurred on a single i^{th} data point

- and its gradient w.r.t. θ:

$$\nabla_\theta J(\theta) = \nabla_\theta\left(\frac{1}{n}\sum_{i=1}^{n} J_i(\theta)\right) = \frac{1}{n}\sum_{i=1}^{n} \nabla_\theta J_i(\theta)$$

need to add n of these, each $\nabla_\theta J_i(\theta) \in \mathbb{R}^d$

gradient info from a single i^{th} data point's loss

Costly in practice!

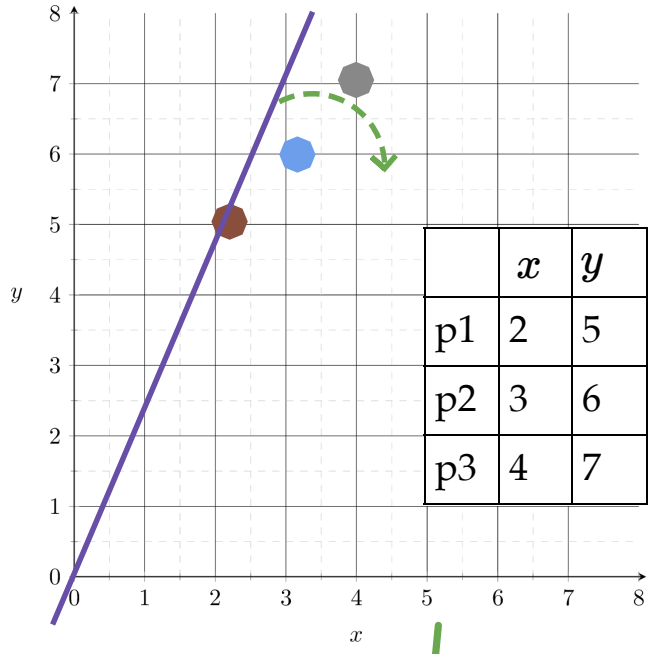
Algorithm 1 Gradient Descent$(\theta_{\text{init}}, \eta, J, \nabla_\theta J, \epsilon)$

Initialize $\theta^{(0)} = \theta_{\text{init}}$
Initialize $t = 0$
repeat
  $t = t + 1$
  $\theta^{(t)} = \theta^{(t-1)} - \eta \nabla_\theta J(\theta^{(t-1)})$
until $\left|J(\theta^{(t)}) - J(\theta^{(t-1)})\right| < \epsilon$
return $\theta^{(t)}$

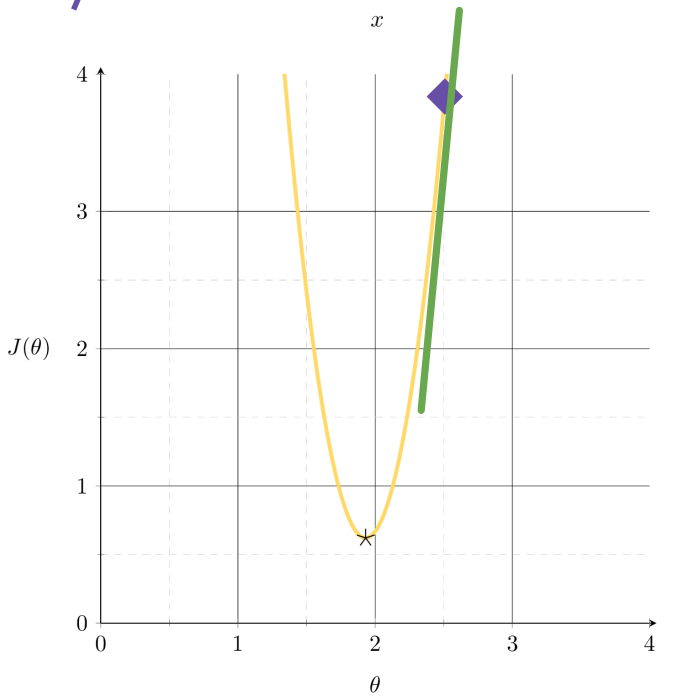
Algorithm 2 Stochastic Gradient Descent$(\theta_{\text{init}}, \eta, J, \nabla_\theta J, \epsilon)$

Initialize $\theta^{(0)} = \theta_{\text{init}}$
Initialize $t = 0$
repeat
  $t = t + 1$
  $i =$ randomly sample from $\{1, \ldots, n\}$
  $\theta^{(t)} = \theta^{(t-1)} - \eta \nabla_\theta J_i(\theta^{(t-1)})$
until $\left|J(\theta^{(t)}) - J(\theta^{(t-1)})\right| < \epsilon$
return $\theta^{(t)}$

$$\nabla_\theta J(\theta) = \frac{1}{n} \sum_{i=1}^{n} \nabla_\theta J_i(\theta) \approx \nabla_\theta J_i(\theta)$$



	x	y
p1	2	5
p2	3	6
p3	4	7



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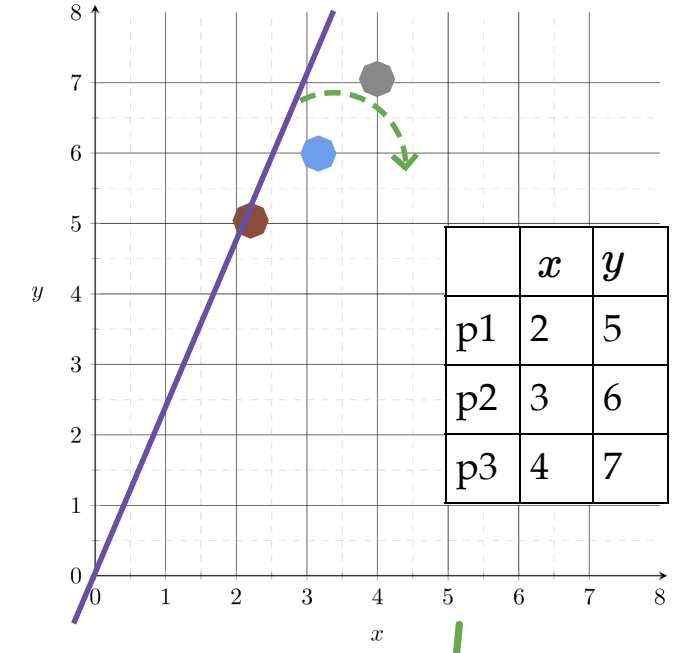

	x	y
p1	2	5
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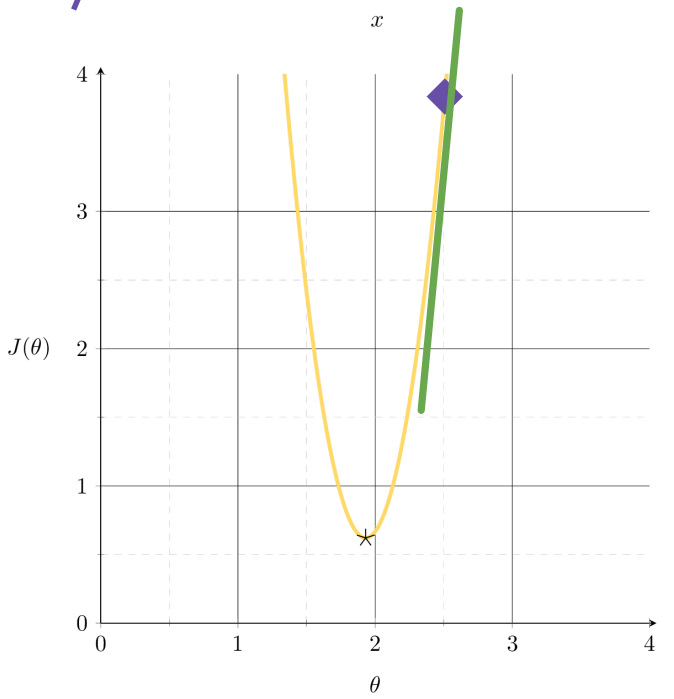
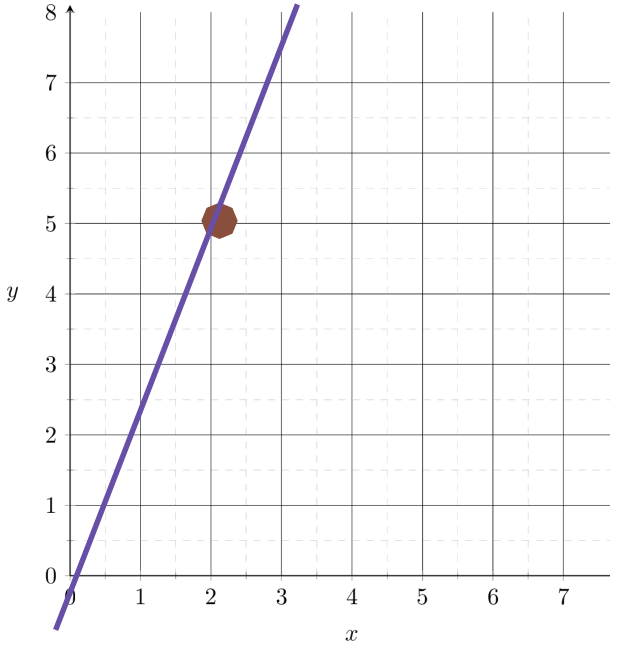
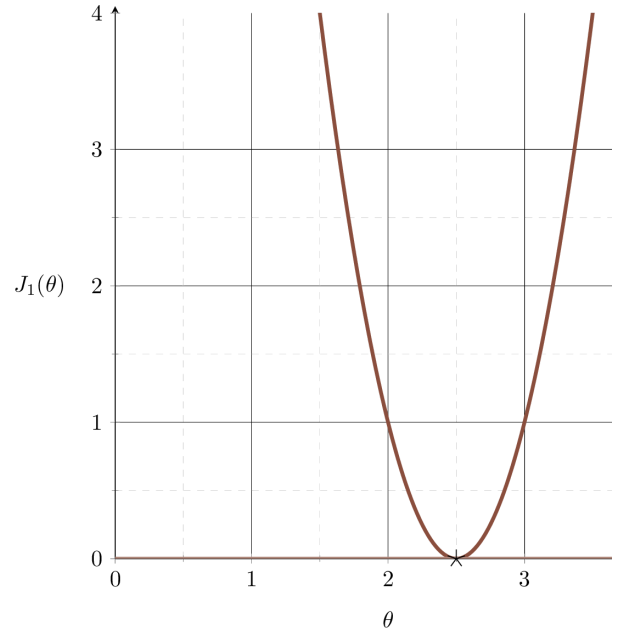
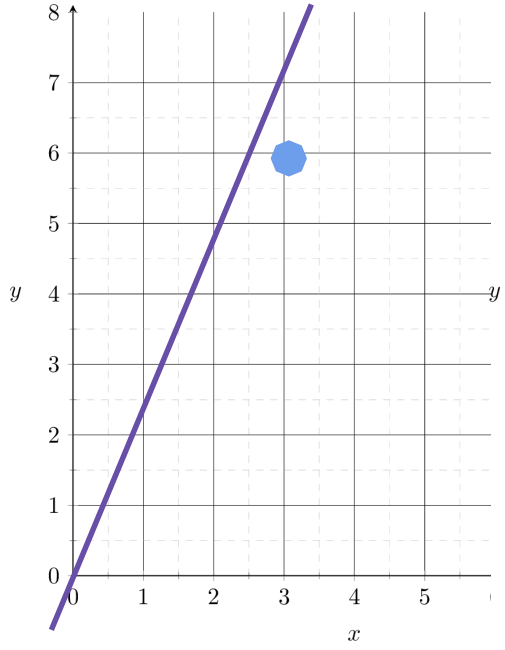
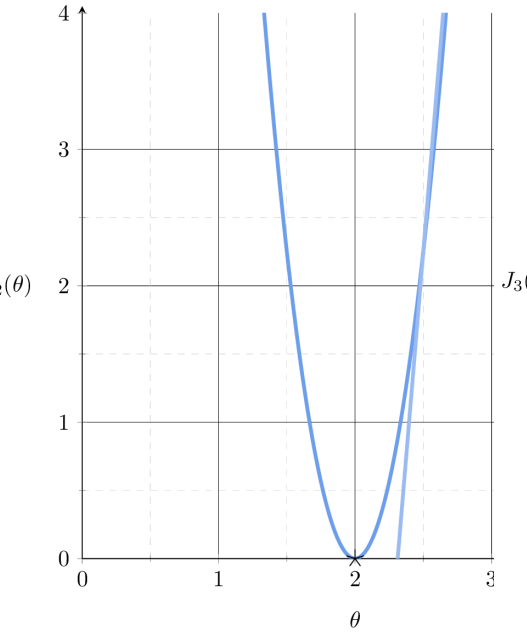
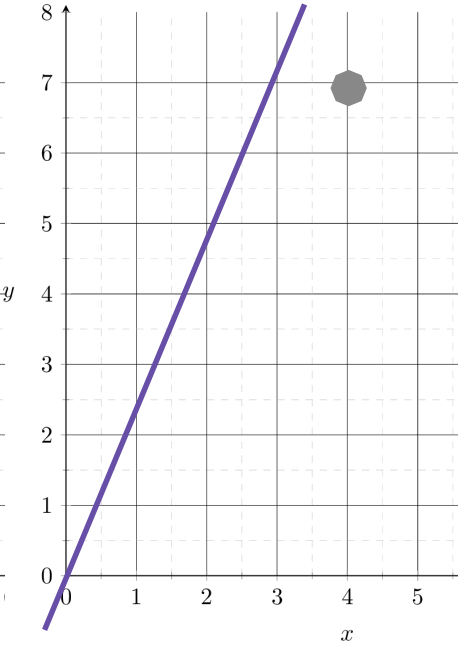


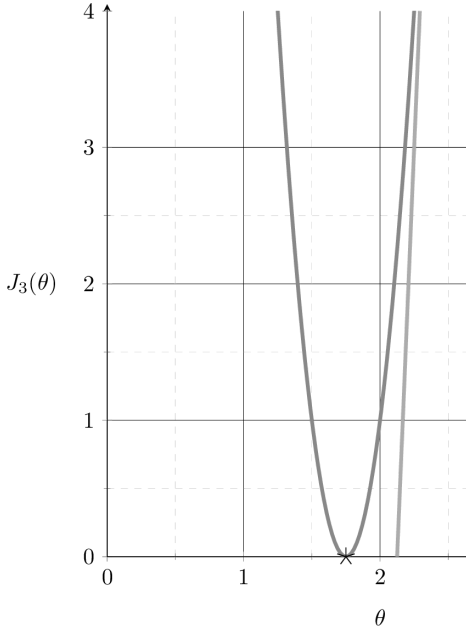






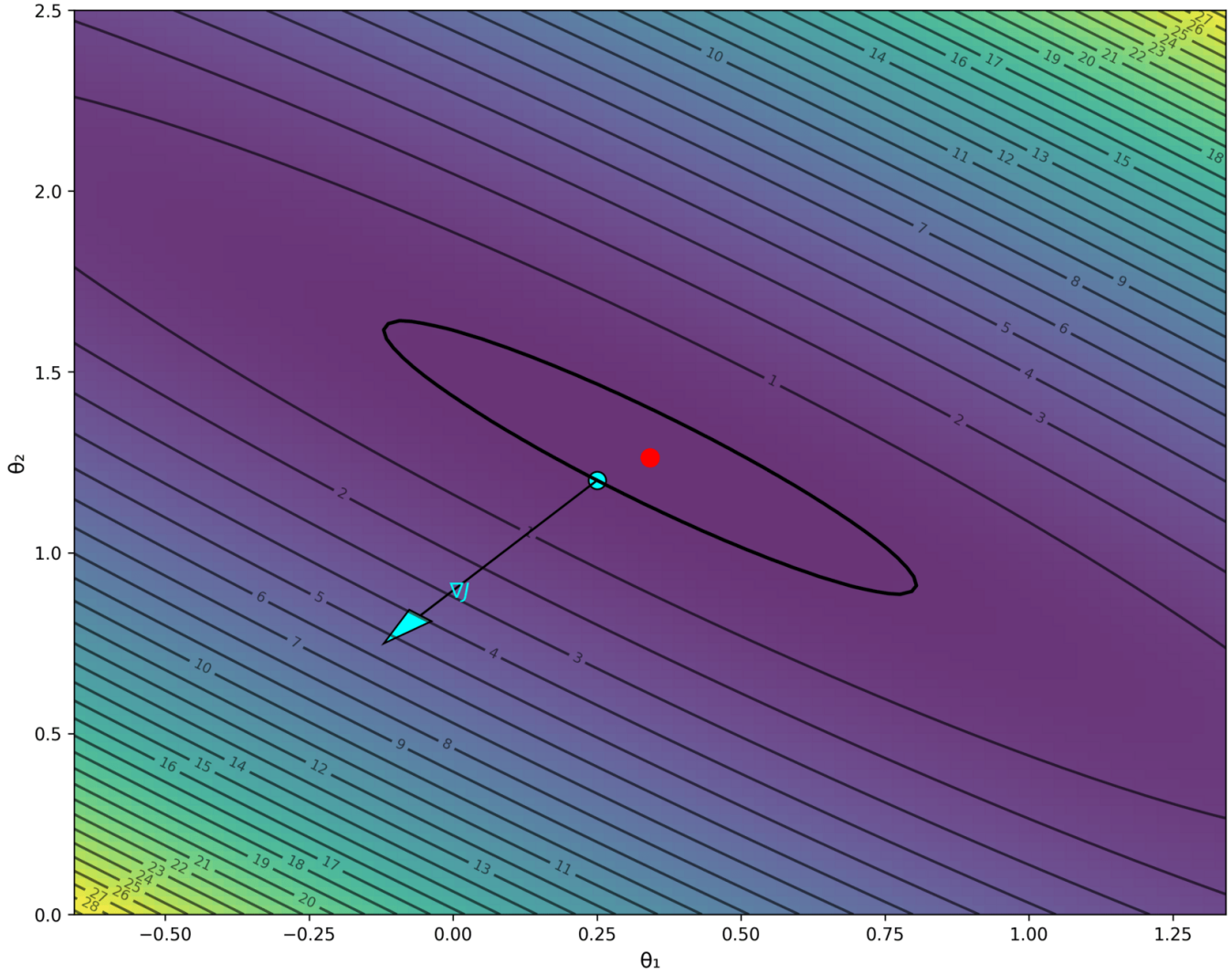






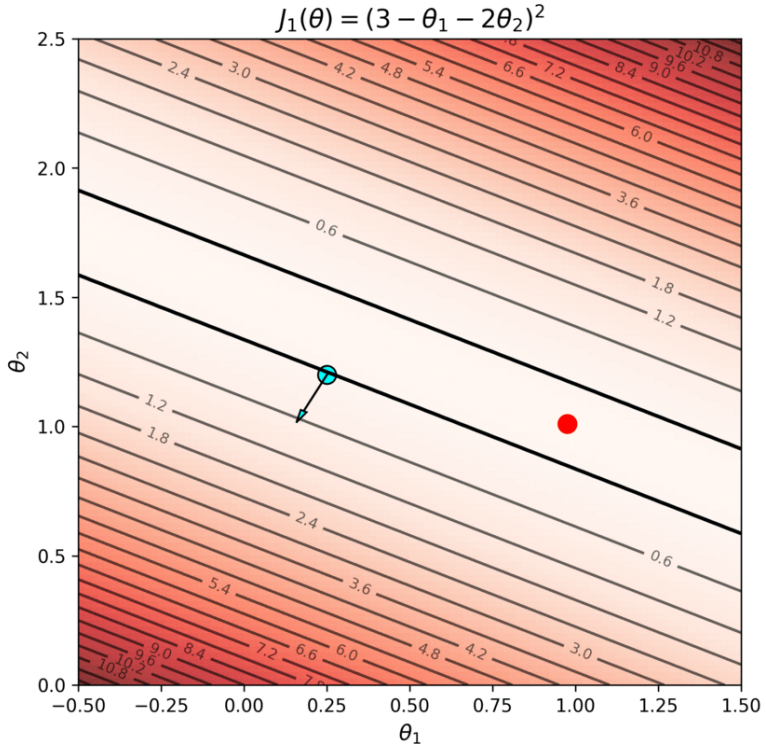
	x1	x2	y
p1	1	2	3
p2	2	1	2
p3	3	4	6

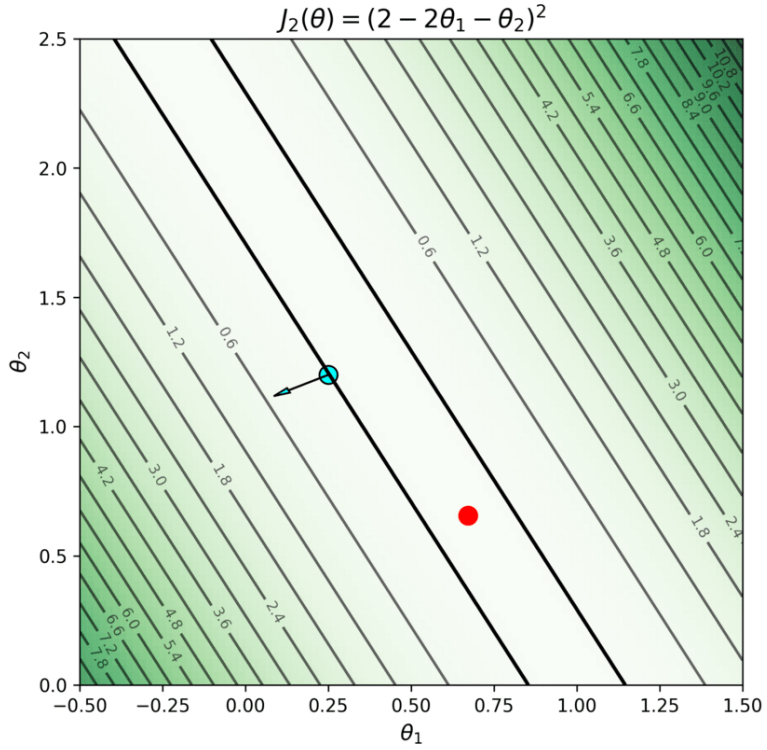
$$J(\theta) = \frac{1}{3}\left[(3 - \theta_1 - 2\theta_2)^2 + (2 - 2\theta_1 - \theta_2)^2 + (6 - 3\theta_1 - 4\theta_2)^2\right]$$

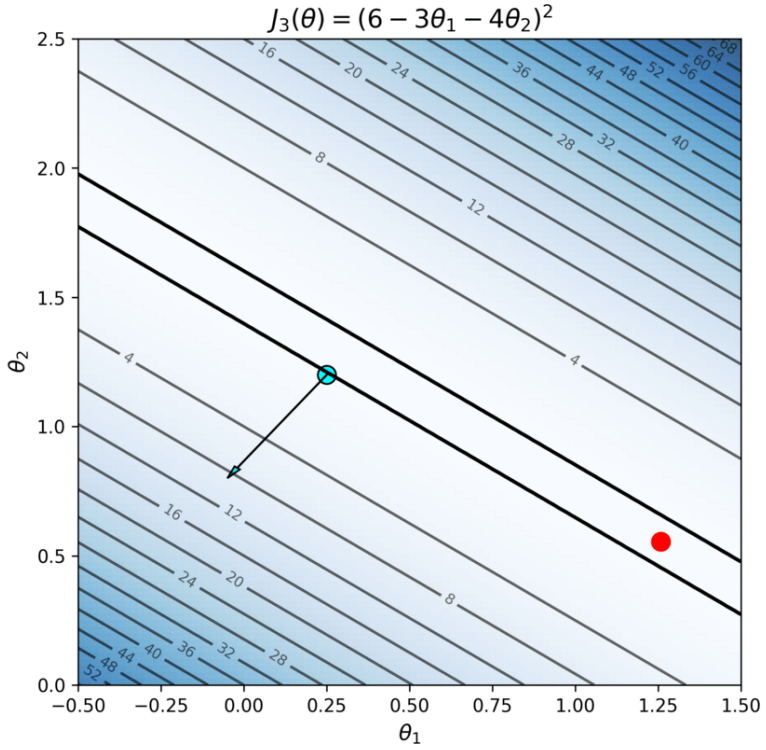


	x1	x2	y
p1	1	2	3
p2	2	1	2
p3	3	4	6

$$J(\theta) = \frac{1}{3}\left[(3-\theta_1-2\theta_2)^2 + (2-2\theta_1-\theta_2)^2 + (6-3\theta_1-4\theta_2)^2\right]$$







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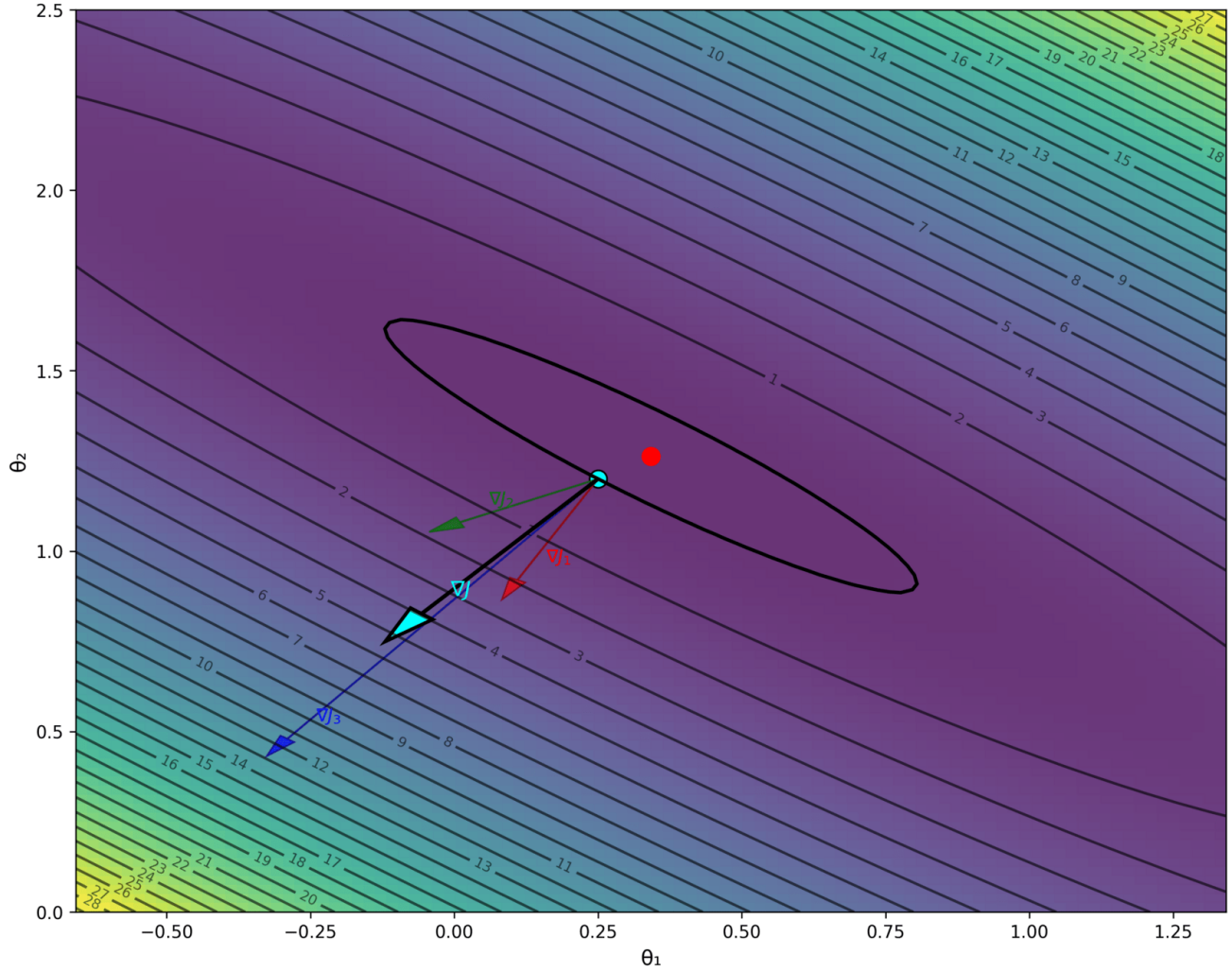
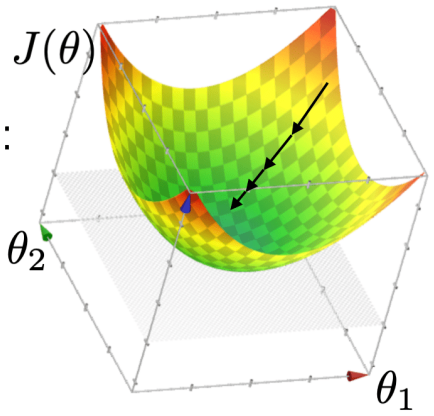


Compared with GD, SGD:

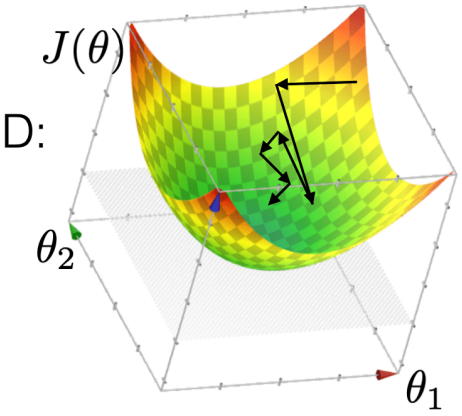
$$\nabla_\theta J(\theta) = \frac{1}{n}\sum_{i=1}^{n} \nabla_\theta J_i(\theta) \approx \nabla_\theta J_i(\theta)$$

is more efficient

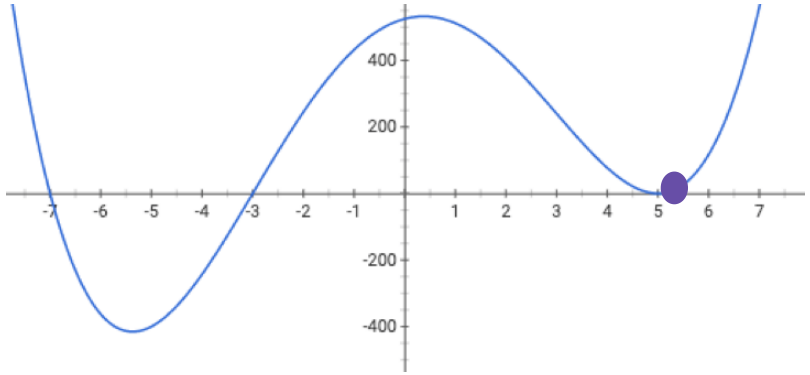
- GD:



- SGD:



is much more "random"



may get us out of a local min

Stochastic gradient descent performance

- Assumptions:
  - f is sufficiently "smooth"
  - f is convex
  - f has at least one global minimum
  - Run gradient descent for sufficient iterations
  - η is sufficiently small and satisfies additional "scheduling" condition
- Conclusion:

$$\sum_{t=1}^{\infty} \eta(t) = \infty \text{ and } \sum_{t=1}^{\infty} \eta(t)^2 < \infty$$

  - Stochastic gradient descent converges arbitrarily close to a global minimum of f with probability 1.

Algorithm 3 Mini-batch Gradient Descent$(\theta_{\text{init}}, \eta, b, J, \nabla_\theta J, \epsilon)$

1: Initialize $\theta^{(0)} = \theta_{\text{init}}$
2: Initialize $t = 0$
3: **repeat**
4: $\quad t = t + 1$
5: $\quad B =$ random mini-batch of size b from $\{1, \ldots, n\}$
6: $\quad \theta^{(t)} = \theta^{(t-1)} - \eta \nabla_\theta J_B(\theta^{(t-1)})$
7: **until** $\left|J(\theta^{(t)}) - J(\theta^{(t-1)})\right| < \epsilon$
8: **return** $\theta^{(t)}$

batch size

SGD

$\nabla_\theta J_i(\theta)$

mini-batch GD

$$\frac{1}{b}\sum_{i=1}^{b} \nabla_\theta J_i(\theta)$$

GD

$$\frac{1}{n}\sum_{i=1}^{n} \nabla_\theta J_i(\theta) = \nabla_\theta J(\theta)$$

🥰more accurate gradient estimate

🥰stronger theoretical guarantee

🥺higher cost per parameter update

Summary

- Most ML methods can be formulated as optimization problems. We won't always be able to solve optimization problems analytically (in closed-form) nor efficiently.
- We can still use numerical algorithms to good effect. Lots of sophisticated ones available. Gradient descent is one of the simplest.
- The GD algorithm, iterative algorithm, keeps applying the parameter update rule.
- Under appropriate conditions (most notably, when objective function is convex, and when learning rate is small enough), GD can guarantee convergence to a global minimum.
- SGD is approximated GD, it uses a single data point to approximate the entire data set, it's more efficient, more random, and less guarantees.
- mini-batch GD is a middle ground between GD and SGD.

https://docs.google.com/forms/d/e/1FAIpQLScj9i83AI8TuhWDZXSjiWzX6gZpnPugjGsH-i3RdrBCtF-opg/viewform?embedded=true

We'd love to hear
your thoughts.

Thanks!