https://introml.mit.edu/

6.390 Intro to Machine Learning

Lecture 3: Gradient Descent Methods

Shen Shen

Sept 13, 2024

(some slides adapted from Tamara Broderick)

- Lecture pages have centralized resources

https://introml.mit.edu/fall24/lectures/lec02

- Lecture recordings might be used for edX or beyond; pick a seat outside the camera/mic zone if you do not wish to participate.
- Next Friday Sept 20, lecture will still be held at 12pm in 45-230, and live-streamed; But, it's a student holiday, attendance *ultra* not expected but *always* appreciated 😉

Outline

- Recap, motivation for gradient descent methods
- Gradient descent algorithm (GD)
  - The gradient vector
  - GD algorithm
  - Gradient decent properties
    - convex functions, local vs global min
- Stochastic gradient descent (SGD)
  - SGD algorithm and setup
  - GD vs SGD comparison

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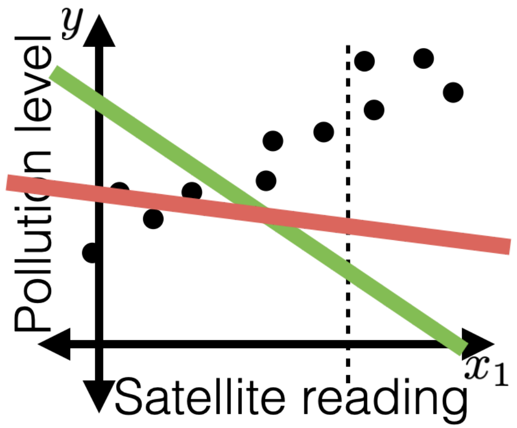
Recall

$$\frac{1}{n}\sum_{i=1}^{n} L(h(x^{(i)};\Theta), y^{(i)}) + \lambda R(\Theta)$$

- A general ML approach
  - Collect data
  - Choose hypothesis class, hyperparameter, loss function
  - Train (optimize for) "good" hypothesis by minimizing loss.



- Limitations of a closed-form solution for objective minimizer
  - Don't always have closed-form solutions. (Recall, half-pipe cases.)
  - Ridge came to the rescue, but we don't always have such "savior".
  - Even when closed-form solutions exist, can be expensive to compute (recall, lab2, Q2.8)
- Want a more general, efficient way! (=> GD methods today)

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Gradient

For $f : \mathbb{R}^m \to \mathbb{R}$, its ***gradient*** $\nabla f : \mathbb{R}^m \to \mathbb{R}^m$ is defined at the point $p = (x_1, \ldots, x_m)$ in m-dimensional space as the vector

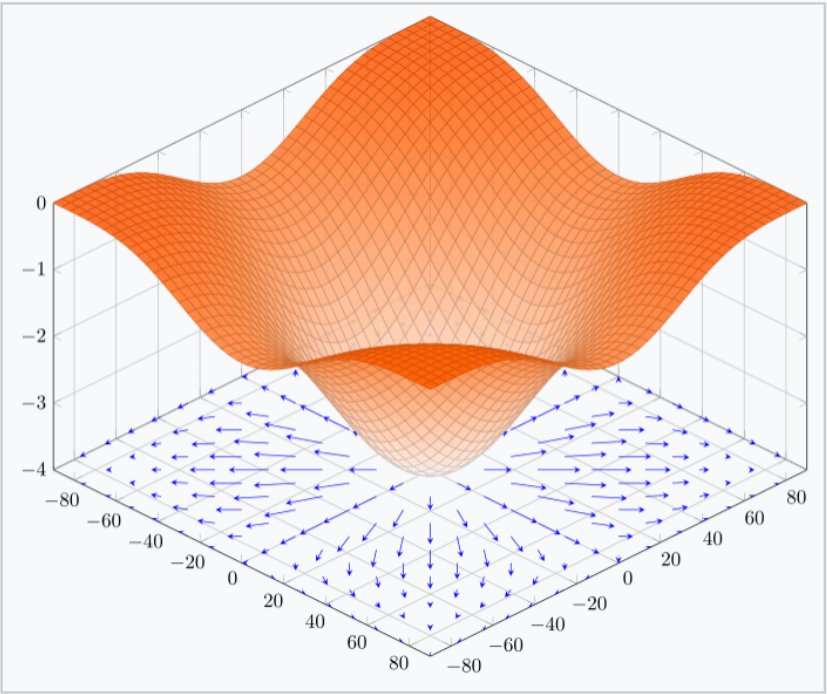
$$\nabla f(p) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(p) \\ \vdots \\ \frac{\partial f}{\partial x_m}(p) \end{bmatrix}$$

1. Generalizes 1-dimensional derivatives.
2. By construction, always has the same dimensionality as the function input.

(Aside: sometimes, the gradient doesn't exist, or doesn't behave nicely, as we'll see later in this course. For today, we have well-defined, nice, gradients.)

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

one cute example:



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

another example

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

a gradient can be the (symbolic) function

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

or,

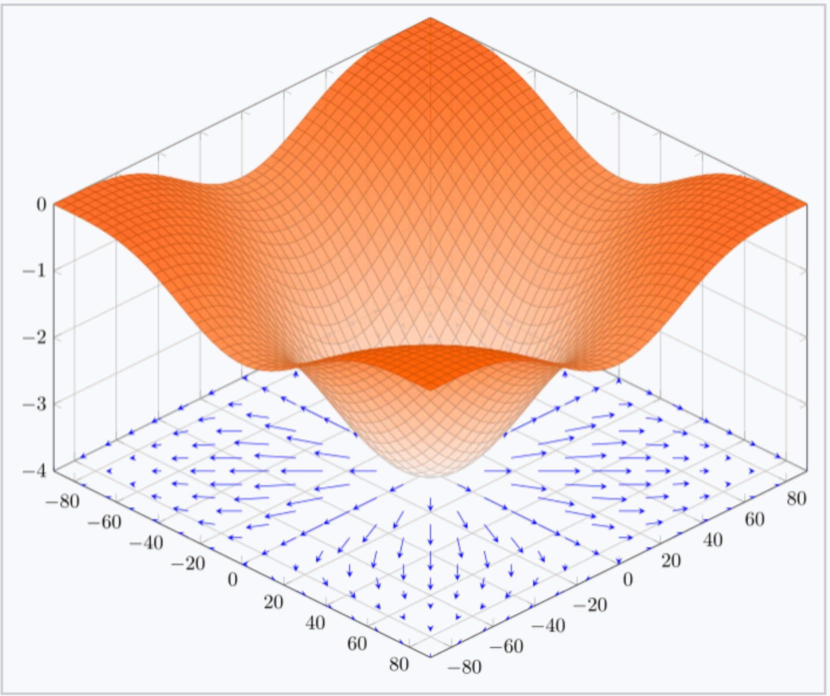
we can also evaluate the gradient function at a point and get (numerical) gradient vectors

$$\nabla f(3, 2, 1) = \begin{bmatrix} 6 \\ 12 \\ 1 \end{bmatrix}$$

exactly like how derivative can be both a function and a number.

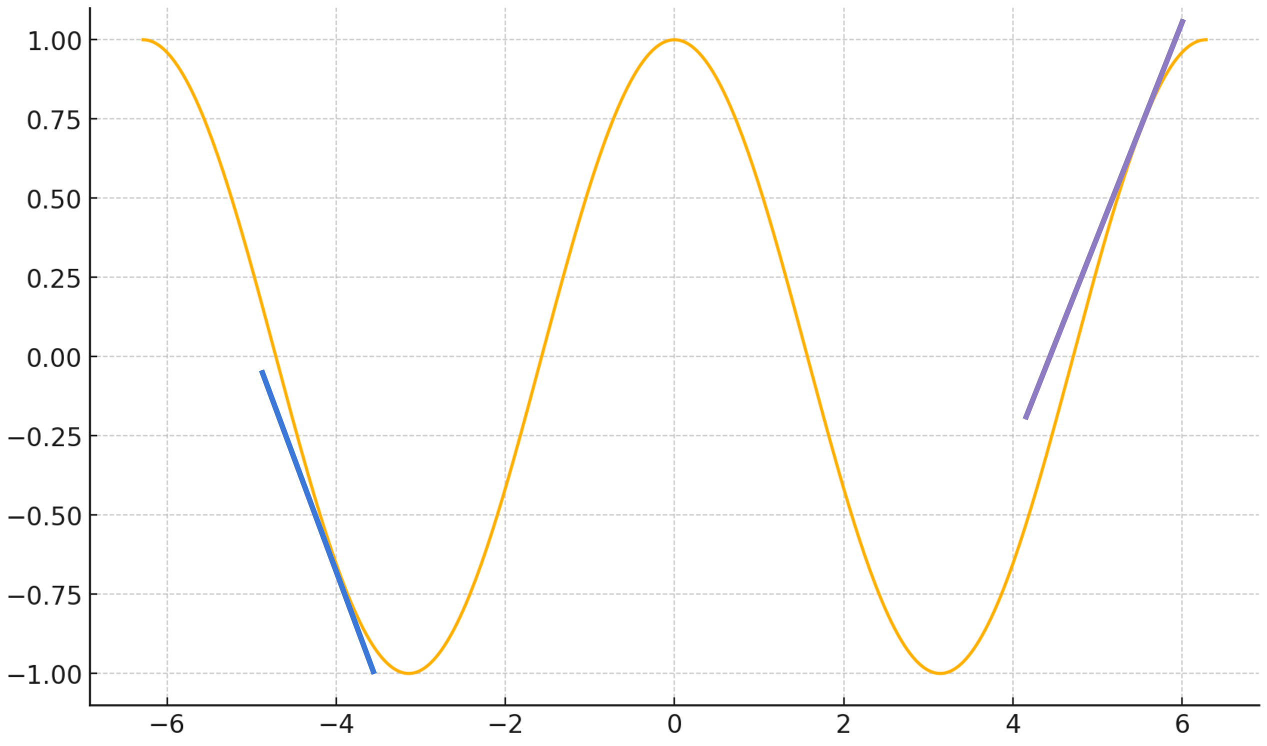
$$\nabla f(p) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(p) \\ \vdots \\ \frac{\partial f}{\partial x_m}(p) \end{bmatrix}$$

3. the gradient points in the direction of the (steepest) increase in the function value.



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

$$\frac{d}{dx}\cos(x)\Big|_{x=5} = -\sin(5) \approx 0.9589$$



$$\frac{d}{dx}\cos(x)\Big|_{x=-4} = -\sin(-4) \approx -0.7568$$

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hyperparameters — initial guess of parameters — learning rate, aka, step size — precision

Gradient-Descent($\Theta_{\text{init}}, \eta, f, \nabla_{\Theta} f, \epsilon$)

    Initialize $\Theta^{(0)} = \Theta_{\text{init}}$

    Initialize t = 0

    repeat

        t = t + 1

        $\Theta^{(t)} = \Theta^{(t-1)} - \eta \nabla_{\Theta} f(\Theta^{(t-1)})$

    until $\left| f(\Theta^{(t)}) - f(\Theta^{(t-1)}) \right| < \epsilon$

    Return $\Theta^{(t)}$

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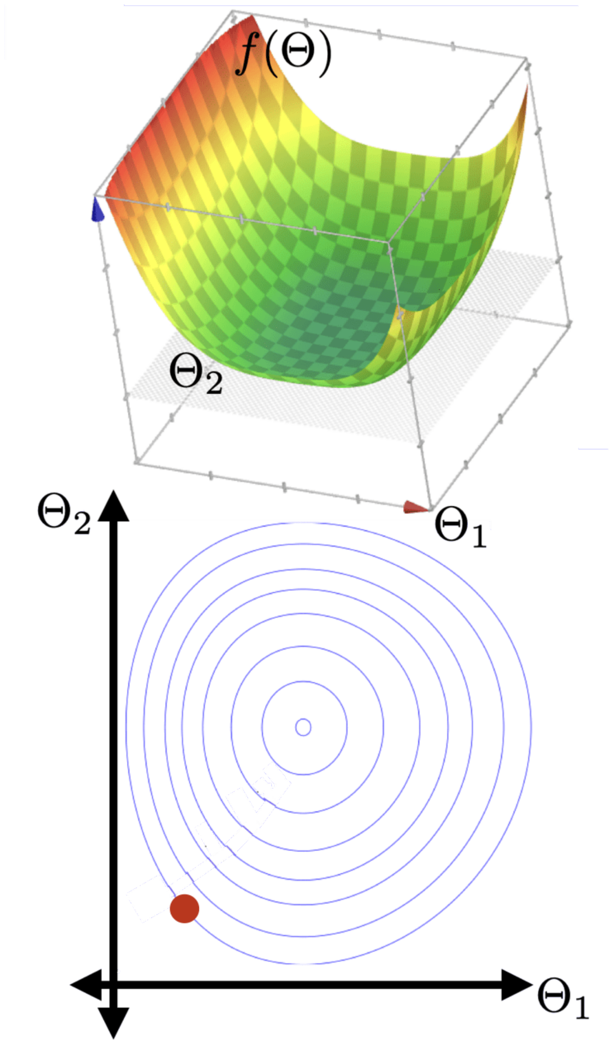

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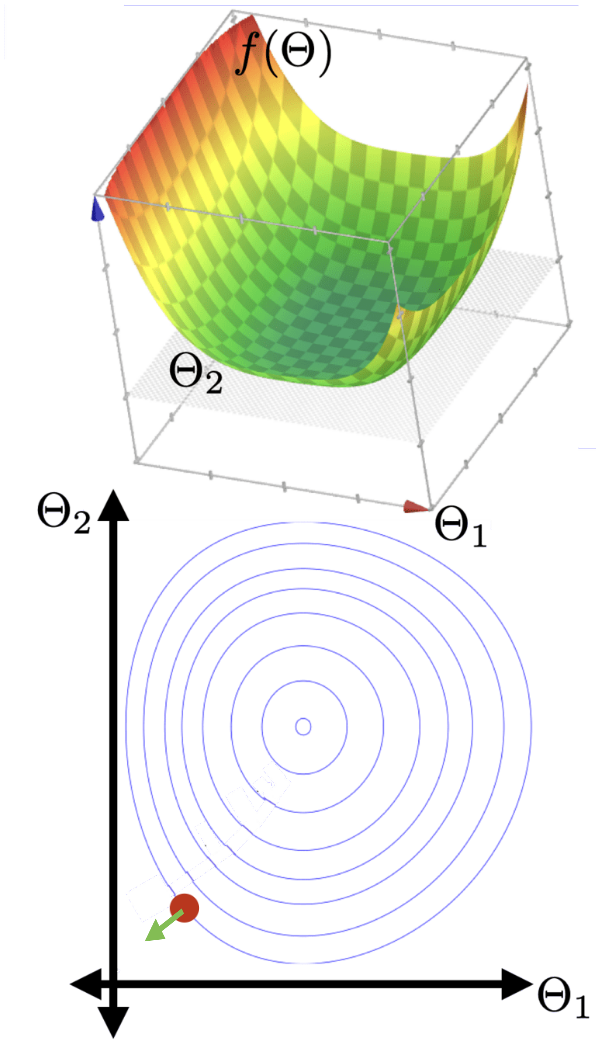

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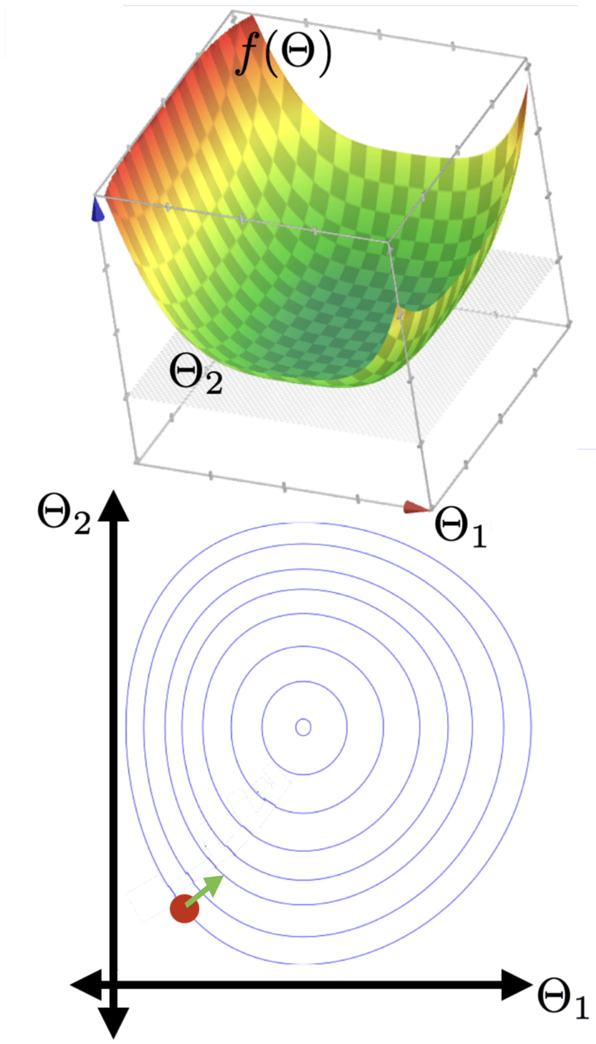

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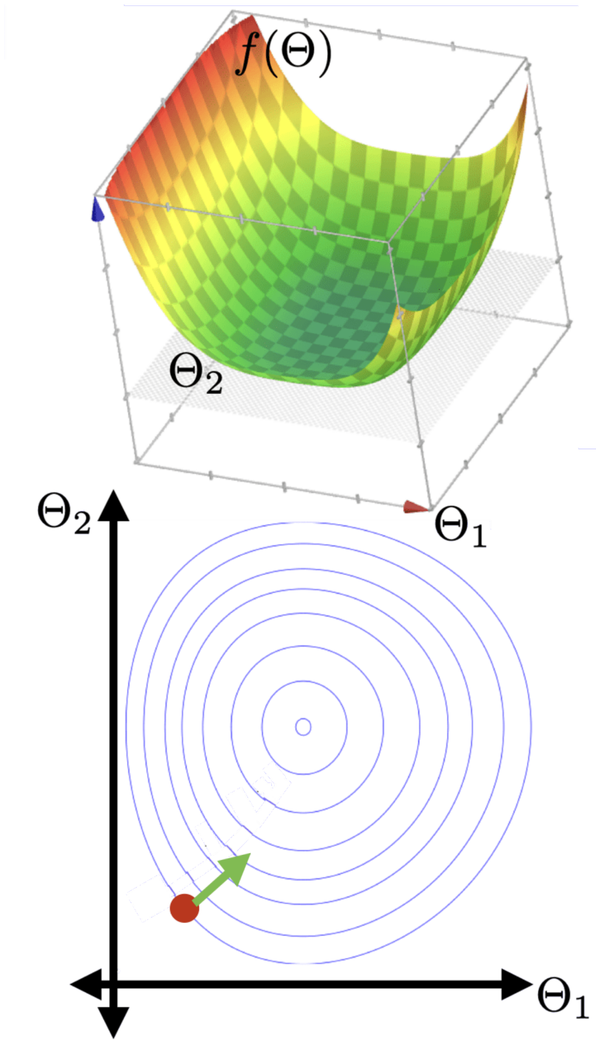

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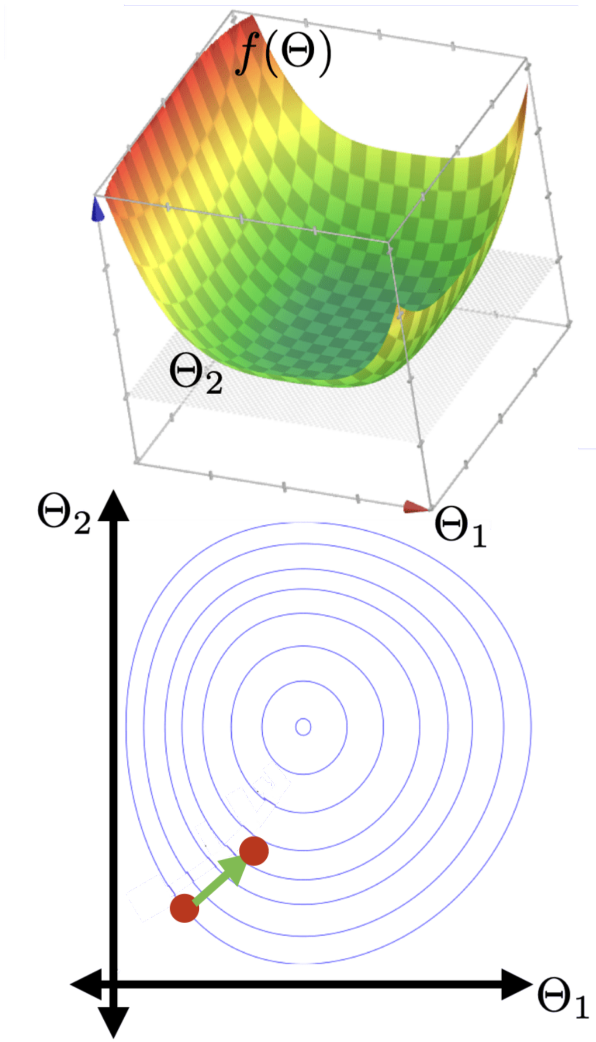

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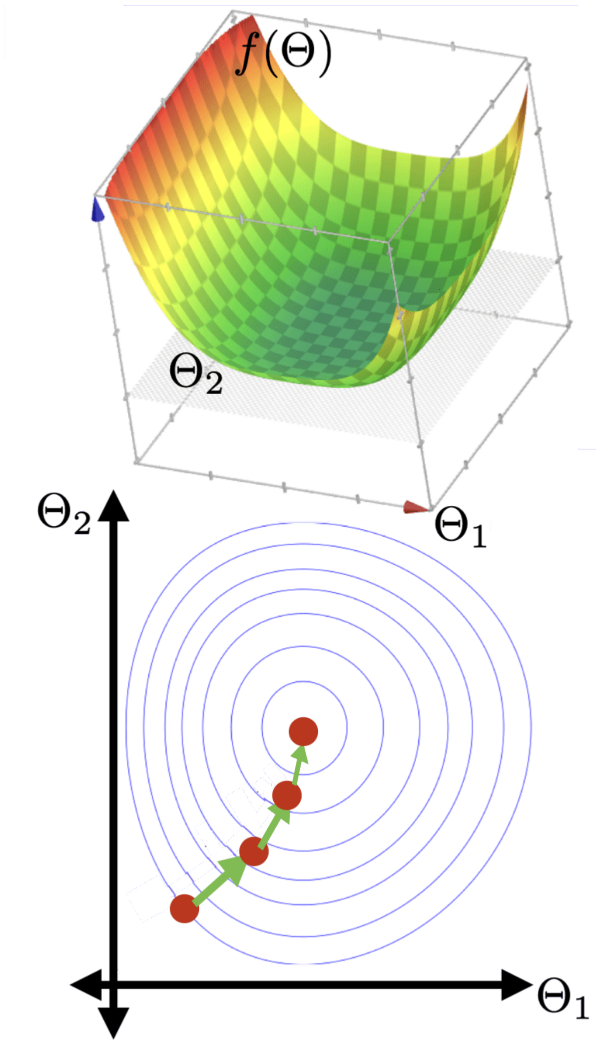

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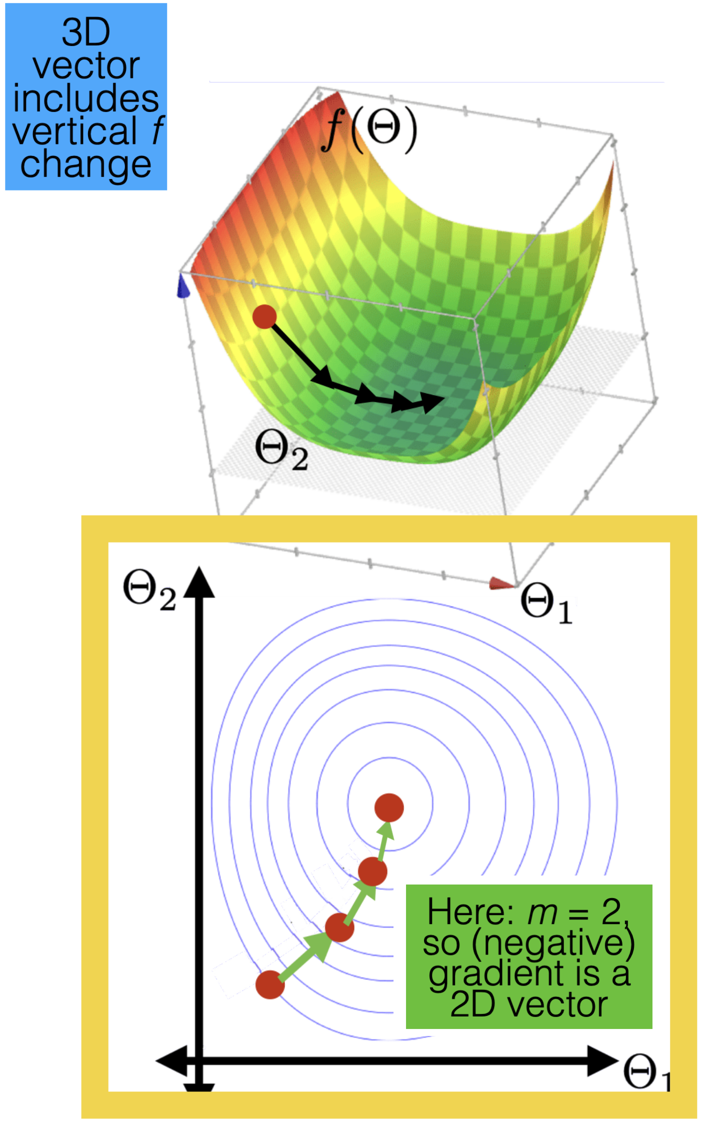
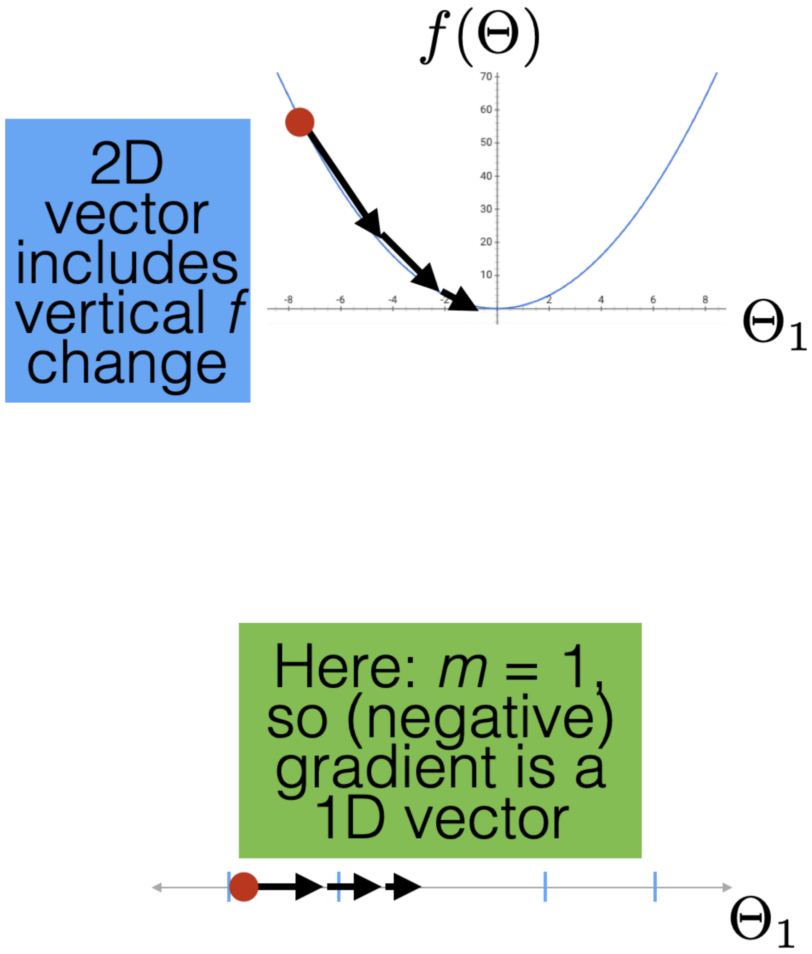
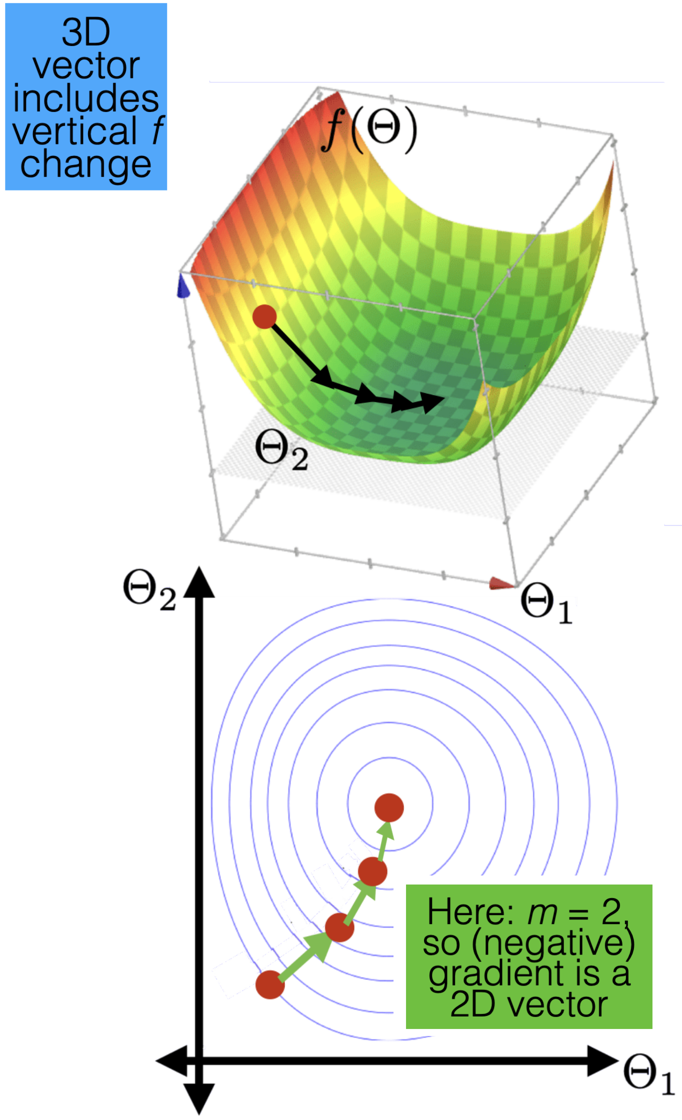




2D vector includes vertical f change
f(Θ)
Θ1
Here: m = 1, so (negative) gradient is a 1D vector
Θ1



3D vector includes vertical f change
f(Θ)
Θ2
Θ1
Θ2
Here: m = 2, so (negative) gradient is a 2D vector
Θ1

Gradient-Descent($\Theta_{\text{init}}, \eta, f, \nabla_\Theta f, \epsilon$)

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  repeat

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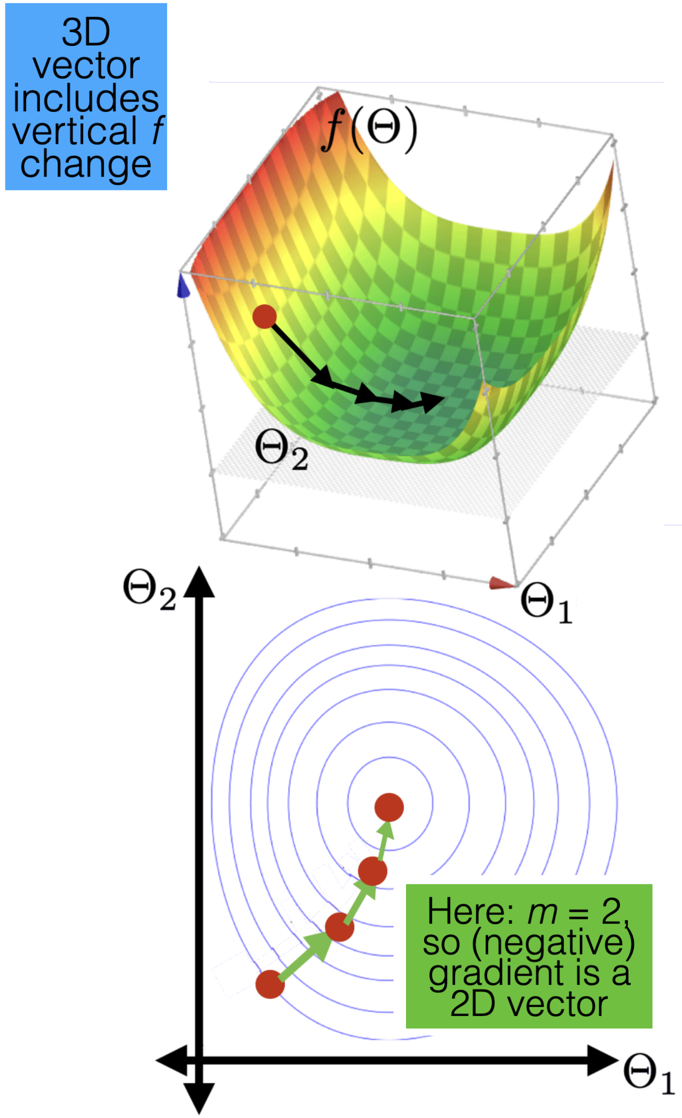


Q: if this condition is satisfied, what does it imply?

A: the gradient at the current parameter is almost zero.

1 `Gradient-Descent(` $\Theta_{\text{init}}, \eta, f, \nabla_\Theta f, \epsilon$ `)`

2   `Initialize` $\Theta^{(0)} = \Theta_{\text{init}}$

3   `Initialize t = 0`

4   **`repeat`**

5   `t = t + 1`

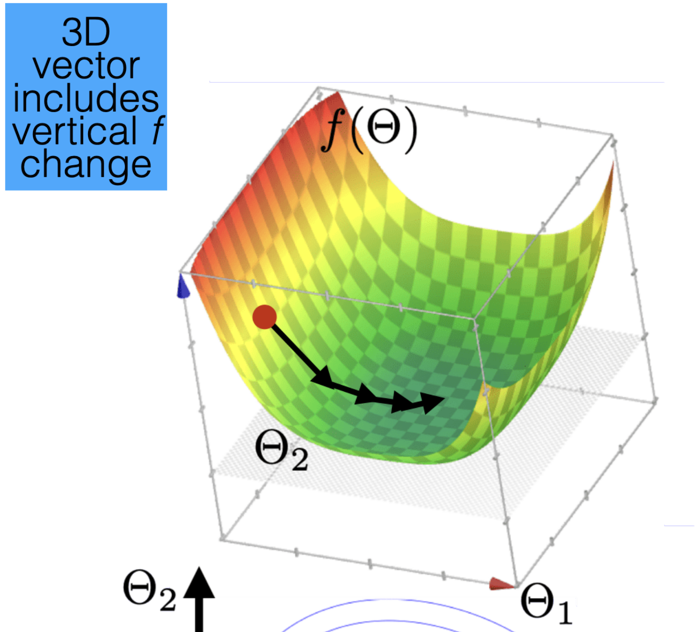
6     $\Theta^{(t)} = \Theta^{(t-1)} - \eta \nabla_\Theta f(\Theta^{(t-1)})$

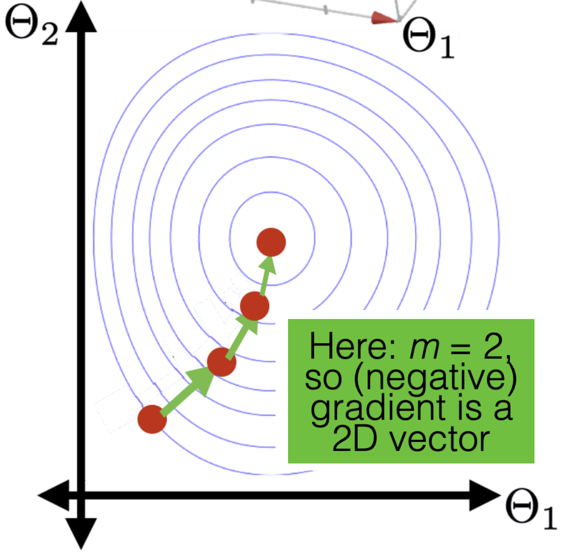
7   **`until`** $\left| f(\Theta^{(t)}) - f(\Theta^{(t-1)}) \right| < \epsilon$

8   **`Return`** $\Theta^{(t)}$

Other possible stopping criteria for line 7:

- Parameter norm change between iteration $\left\| \Theta^{(t)} - \Theta^{(t-1)} \right\| < \epsilon$
- Gradient norm close to zero $\left\| \nabla_\Theta f \left(\Theta^{(t)} \right) \right\| < \epsilon$
- Max number of iterations T





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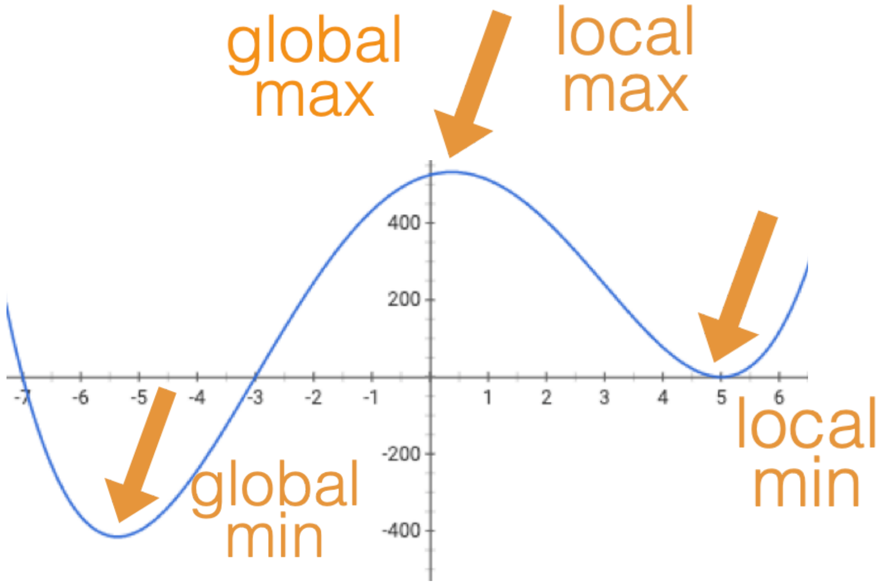
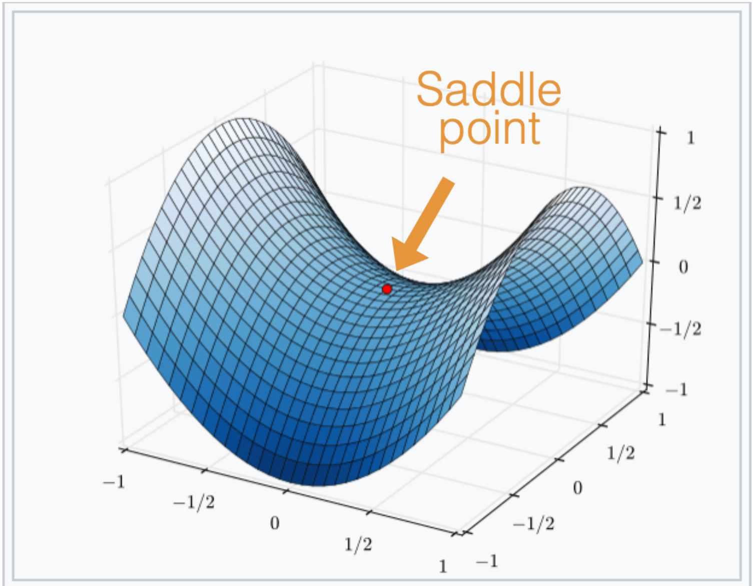
When minimizing a function, we'd hope to get to a global minimizer

$$\Rightarrow$$

At a global minimizer $\quad$ the gradient vector is the zero vector

$$\not\Leftarrow$$





When minimizing a function, we'd hope to get to a global minimizer

At a global minimizer $\Longleftarrow \begin{cases} \text{the gradient vector is the zero vector} \\ \text{the function is a convex function} \end{cases}$

A function f is ***convex***

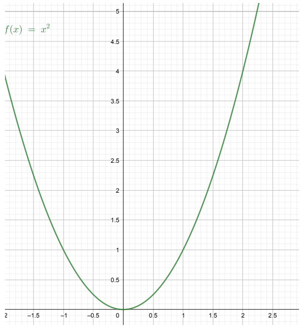
if any line segment connecting two points of the graph of f lies above or on the graph.

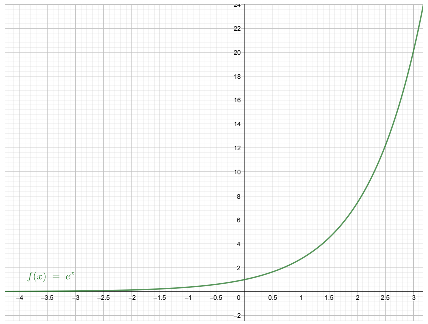
- (f is concave if $-f$ is convex.)
- (one can say a lot about optimization convergence for convex functions.)

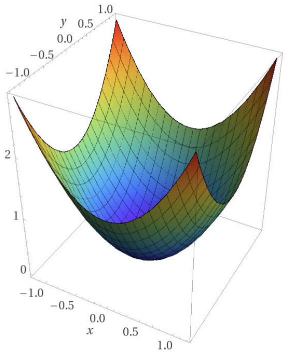
https://shenshen.mit.edu/demos/convex.html

Some examples

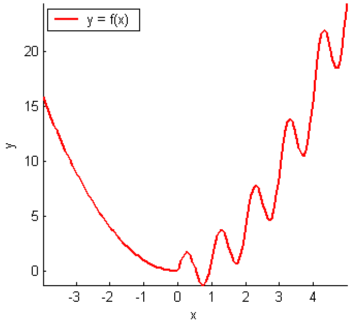
Convex functions

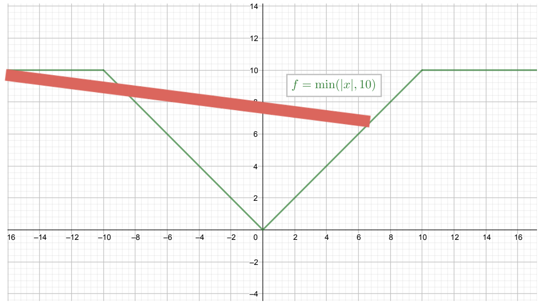


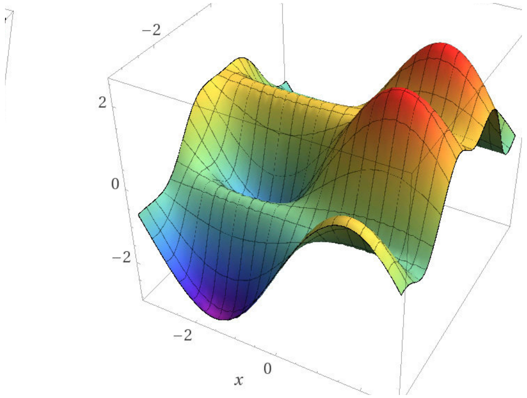




Non-convex functions







Gradient Descent Performance

- Assumptions:
  - f is sufficiently "smooth"
  - f has at least one global minimum
  - Run the algorithm long enough
  - η is sufficiently small
  - f is convex
- Conclusion:
  - Gradient descent will return a parameter value within $\tilde{\epsilon}$ of a global minimum (for any chosen $\tilde{\epsilon} > 0$)

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

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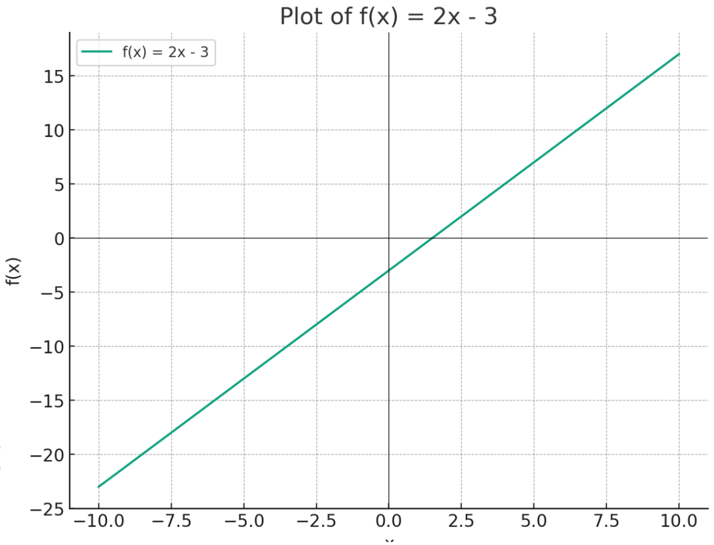
if violated:

may not terminate/no minimum to converge to



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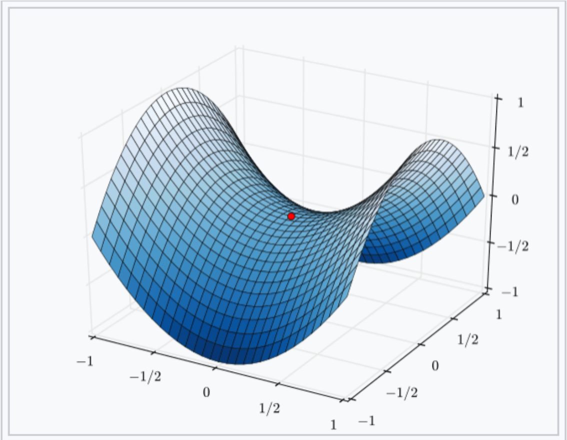
if violated:

see demo on next slide, also lab/recitation/hw https://shenshen.mit.edu/demos/gd.html

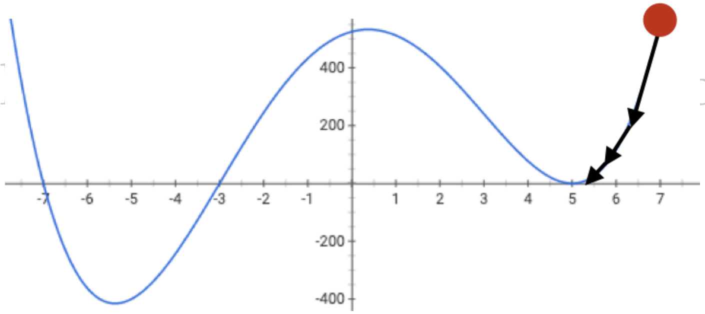
Gradient descent performance

- Assumptions:
  - f is sufficiently "smooth"
  - f has at least one global minimum
  - Run the algorithm sufficiently "long"
  - η is sufficiently small
  - f is convex

if violated, may get stuck at a saddle point



or a local minimum



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Gradient of an ML objective

In general,

- An ML objective function is a finite sum

$$f(\Theta) = \frac{1}{n}\sum_{i=1}^{n} f_i(\Theta)$$

- The gradient of an ML objective :

$$\nabla f(\Theta) = \nabla(\frac{1}{n}\sum_{i=1}^{n} f_i(\Theta)) = \frac{1}{n}\sum_{i=1}^{n} \nabla f_i(\Theta)$$

👆

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

For instance,

- the MSE of a linear hypothesis:

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

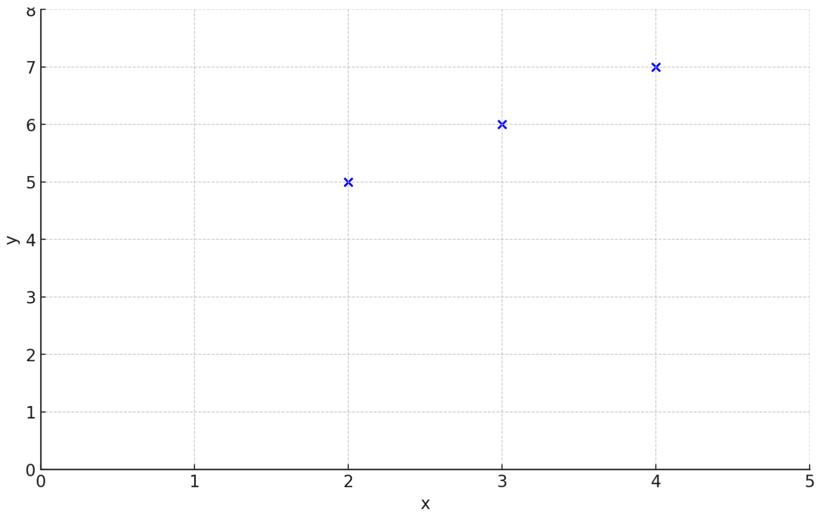
- and its gradient w.r.t. θ:

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

Concrete example

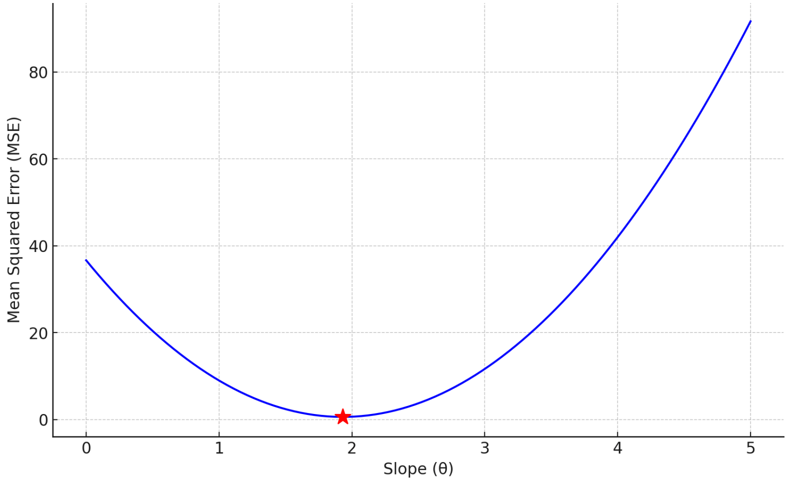
Three data points:

{(2,5), (3,6), (4,7)}



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

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



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

First data point's "pull"

Second data point 's "pull"

Third data point's "pull"

Stochastic gradient descent

```
Gradient-Descent( Θ_init, η, f, ∇_Θ f, ε )
  Initialize Θ^(0) = Θ_init
  Initialize t = 0
  repeat
    t = t + 1
    Θ^(t) = Θ^(t-1) − η ∇_Θ f(Θ^(t-1))
  until |f(Θ^(t)) − f(Θ^(t-1))| < ε
  Return Θ^(t)
```

```
Stochastic
Gradient-Descent( Θ_init, η, f, ∇_Θ f, ε )
  Initialize Θ^(0) = Θ_init
  Initialize t = 0
  repeat
    t = t + 1
    randomly select i from {1,…,n}
    Θ^(t) = Θ^(t-1) − η(t) ∇_Θ f_i(Θ^(t-1))
  until |f(Θ^(t)) − f(Θ^(t-1))| < ε
  Return Θ^(t)
```

$$\nabla f(\Theta) = \frac{1}{n}\sum_{i=1}^{n} \nabla f_i(\Theta) \approx \nabla f_i(\Theta)$$

for a randomly picked data point i

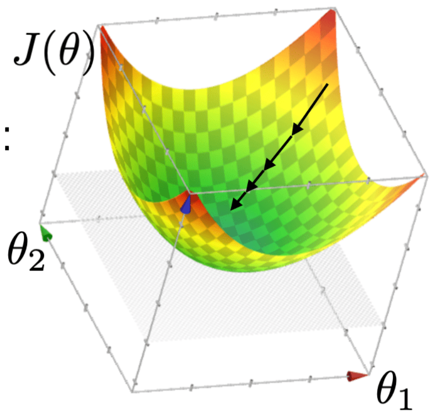
Stochastic gradient descent performance

- Assumptions:
  - f is sufficiently "smooth"
  - f has at least one global minimum
  - Run the algorithm long enough
  - η is sufficiently small and **satisfies additional "scheduling" condition**
  - f is convex

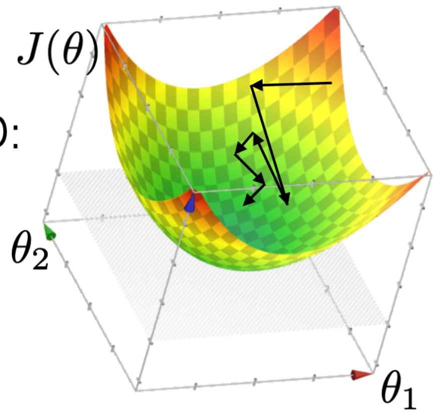
$\sum_{t=1}^{\infty} \eta(t) = \infty$ and $\sum_{t=1}^{\infty} \eta(t)^2 < \infty$

- Conclusion:
  - **Stochastic** gradient descent will return a parameter value within $\tilde{\epsilon}$ of a global minimum **with probability 1** (for any chosen $\tilde{\epsilon} > 0$)

- GD:

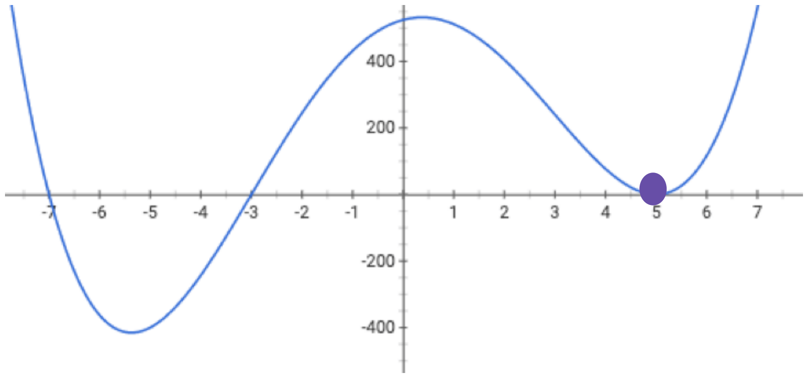


- SGD:



Compared with GD, SGD

is more "random"



may get us out of a local min

$$\nabla f(\Theta) = \frac{1}{n}\sum_{i=1}^{n} \nabla f_i(\Theta) \approx \nabla f_i(\Theta)$$

is more efficient

Summary

- Most ML methods can be formulated as optimization problems.
- We won't always be able to solve optimization problems analytically (in closed-form).
- We won't always be able to solve (for a global optimum) efficiently.
- We can still use numerical algorithms to good effect. Lots of sophisticated ones available.
- Introduce the idea of gradient descent in 1D: only two directions! But magnitude of step is important.
- In higher dimensions the direction is very important as well as magnitude.
- GD, under appropriate conditions (most notably, when objective function is convex), can guarantee convergence to a global minimum.
- SGD: approximated GD, more efficient, more random, and less guarantees.

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

We'd love to hear your thoughts.

Thanks!