



Calculus for ML

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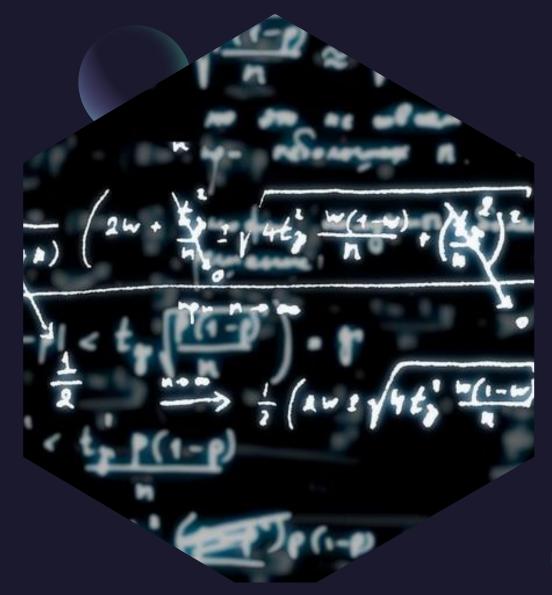
Agenda

- Motivation
- Limits
- When doesn't limits exist?
- Limits and continuity
- From limits to differentiation
- Numerical differentiation
- Differentiation Rules
- Partial derivative
- Chain Rule

- Gradient
- Beyond gradient
- Optimization
- Optimization and the learning problem
- Gradient Ascent for maximizing
- Gradient Descent for minimizing
- Gradient Ascent vs Gradient Descent
- The effect of learning rate η

Motivation

- Calculus, is not an isolated mathematical field.
- Calculus is the engine that powers the machines with the ability to learn and adapt.
- Calculus provide a set of tools for optimizing our machine learning models.
- When ever you train ML model you probably are doing a lot of derivatives in the background.





- Where would you reach if you kept following this way?
- The answer doesn't mean you've fully reached it, and you may never get there, but you're getting as close as possible
- You can think of it as Zooming \bigcirc a picture $\boxed{\mathbb{Z}}$, the more you zoom the more you see more details, until you reach a point you can't zoom any more, this would be limit of zooming the image, further zooming won't change the image.
- Example, consider a function f(x) = 2x, As x gets closer to 3, 2x would get closer to 6, the $\lim_{x \to 3} f(x) = 6$
- You won't always end with a finite number as a limit, for some functions you the limit may be infinity ∞ , for example $\lim_{x\to 0^+}(\frac{1}{x})=\infty$, try inputting (0.1, 0.01, 0.001,...).



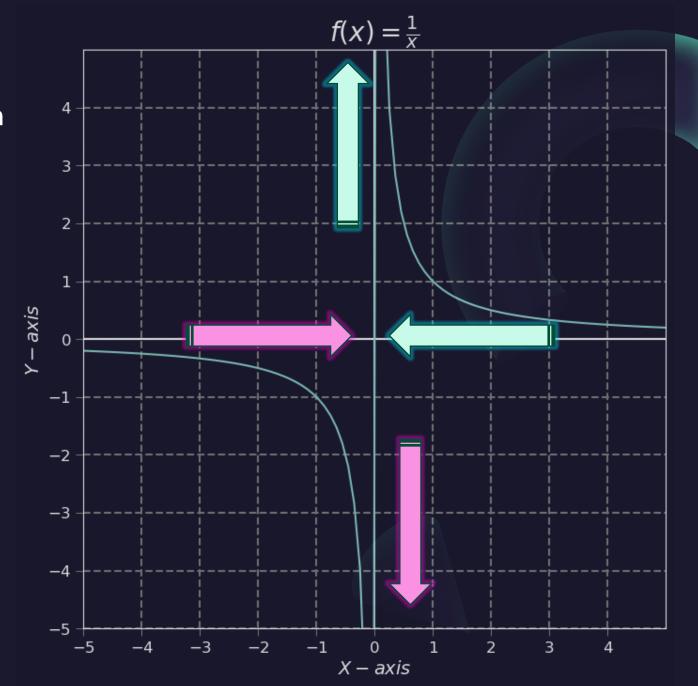
• You won't always end with a finite number as a limit, for some functions you the limit may be infinity ∞ , for example $\lim_{x\to 0^+}(\frac{1}{x})=\infty$, try inputting (0.1,0.01,0.001,...).

f(0.1)	f(0.01)	f(0.001)	f(0.0001)	f(0.00001)		f(0.000001)
10	100	1000	10000	100000	?	1000000

- How many zeros can you add before you reach zero? (you try not to reach)
- You can add infinity zeros so that the output of the function is going towards infinity.
- $\lim_{x\to c} f(x) = L$, the limit of f as x approaches c equals L, this mean the value (output) of the function can be made arbitrarily close to L by choosing x sufficiently close to c.

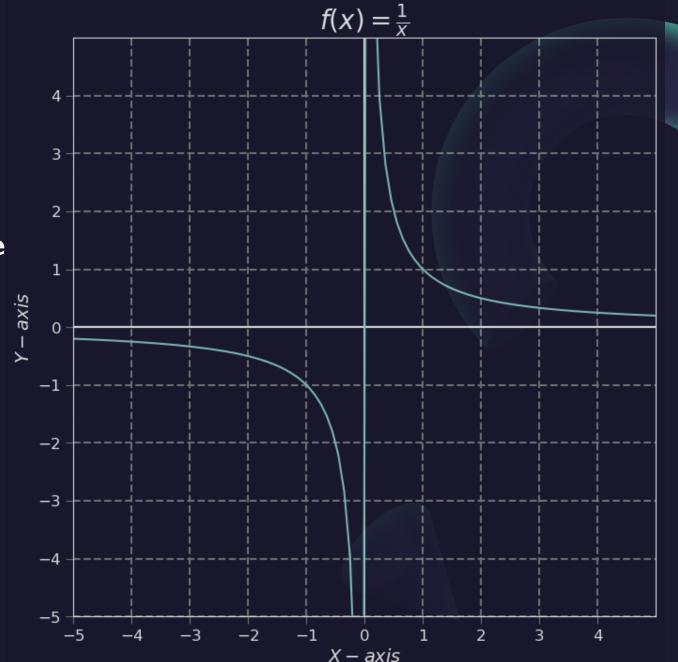


- Till now we treated this function from the positive side only, but it has two parts.
- When we inputted numbers that are close to zero in positive side it goes to infinity.
- Let's input number that are closer to zero but for the negative part of the function.
- For the negative part of this function it would go to negative infinity.





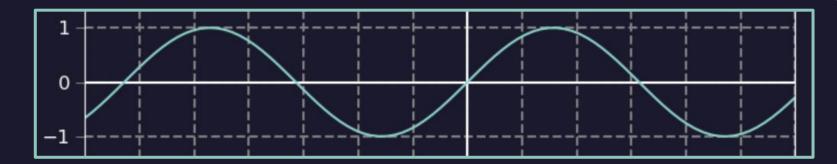
- $\lim_{x\to 0^+} (\frac{1}{x}) = \infty$ for the positive side
- $\lim_{x\to 0^-} (\frac{1}{x}) = -\infty$ for the negative side
- What is the limit $\lim_{x\to 0} (\frac{1}{x}) = ?$
- This <u>limit doesn't exist</u> for this function as the two parts of the functions are not approaching the same value.





When doesn't limits exist?

- A limit doesn't exist if:
- The function behaves different from left and right.
- If the function oscillate between several values like (sin) and (cos)



- That only mean that the overall function like sin or cos doesn't converge to a single number, it oscillate between I and -I.
- This mean that the limit of the sin function as x approach infinity doesn't exist, but if x approach another value say a, the limit in this case would exist (equals sin(a))



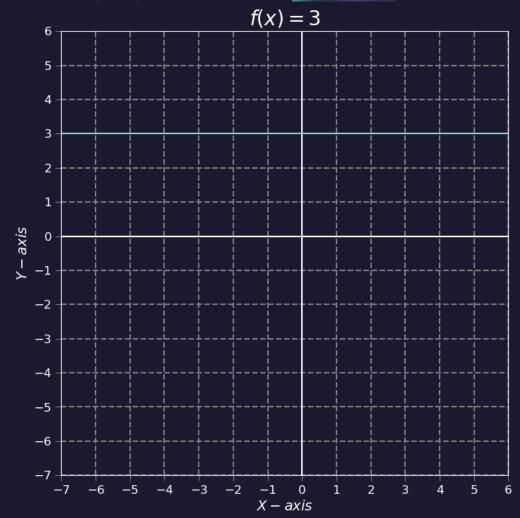
Limits and continuity

- We can use the limits to decide if a function is conditions, that mean all inputs have possible outputs (defined everywhere).
- Function f(x) is continuous if it satisfy three conditions.
- Function f(a) is defined for all values of a.
- $\lim_{x\to\infty} f(x)$ exist, the function should approach the same value from both sides.
- $\lim_{x\to a} f(x) = a$, the limit and the actual value of the function should be the same.



- The derivative (differentiation) of a function $f'(x) = \lim_{h \to 0} \frac{f(x+h) f(x)}{h}$
- Let's start by a simple function f(x) = 3 constant function.
- f(x) = 3 is given but f(x + h) what is the value of h, it would be value that approach zero, it doesn't matter for this case as this function is a constant.

$$\lim_{h\to 0} \frac{f(x+h) - f(x)}{h} = \frac{3-3}{h} = \frac{0}{h} = 0$$





$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

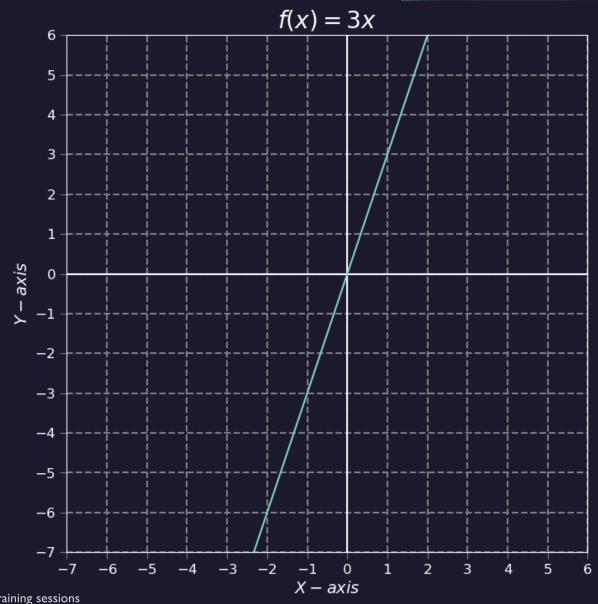
• function f(x) = 3x constant function.

$$\lim_{h\to 0}\frac{3(x+h)-3x}{h}$$

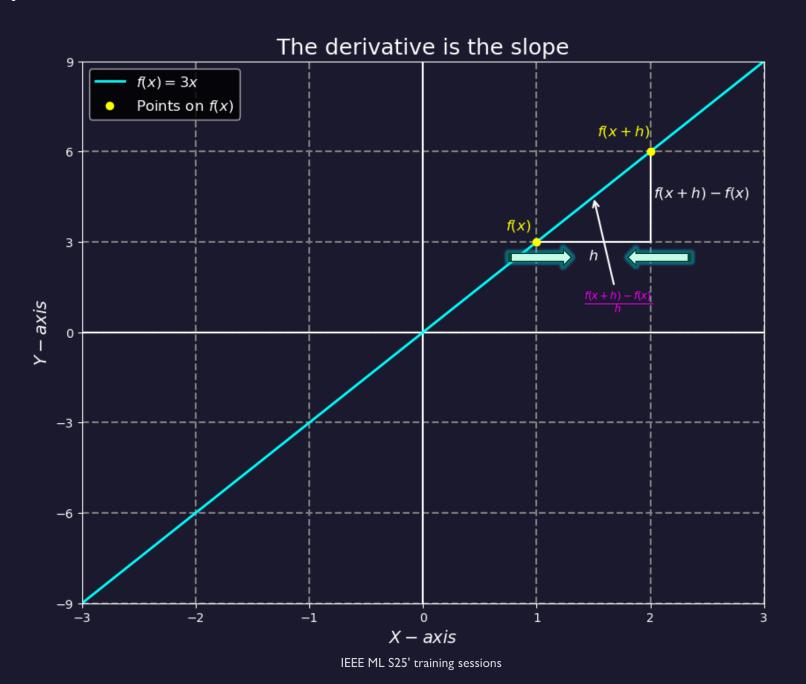
$$= \lim_{h\to 0} \frac{3x + 3h - 3x}{h}$$

$$=\lim_{h\to 0}\frac{3h}{h}=3$$

• Derivative is the rate of change (difference) between the output of two inputs for the function these inputs are spaced by h.







$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

- We are trying to get the rate of change between two outputs.
- *h* is the distance between the inputs that produced these two outputs.
- h is a value that approach zero but would never be a zero.
- That is why the derivative is the slope.



$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

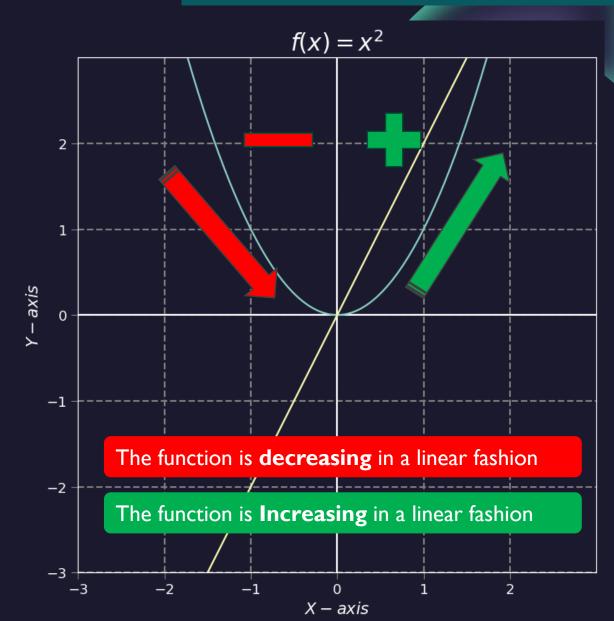
• function $f(x) = x^2$ quadratic equation.

$$\lim_{h \to 0} \frac{(x+h)^2 - x^2}{h}$$

$$= \lim_{h \to 0} \frac{x^2 + 2xh + h^2 - x^2}{h}$$

$$= \lim_{h \to 0} \frac{2xh + h^2}{h} = \frac{h(2x+h)}{h}$$

$$\frac{\mathbf{d}f(x)}{\mathbf{d}x} = \lim_{h \to 0} 2x + h = 2x$$

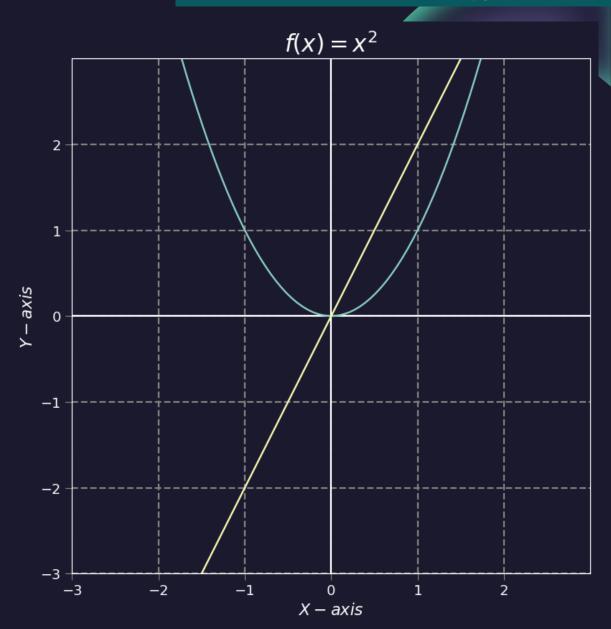




$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$

• function $f(x) = x^2$ quadratic equation.

```
6.009999999999849
x = 3
                          6.000999999999479
def f(x): # x^2 -> 2x
                          6.000100000012054
                          6.000009999951316
    return x**2
h 1 = 0.01
h_2 = 0.001
h_3 = 0.0001
h_4 = 0.00001
print((f(x+h_1) - f(x)) / h_1)
print( (f(x+h_2) - f(x)) / h_2 )
print( (f(x+h_3) - f(x)) / h_3 )
print( (f(x+h_4) - f(x)) / h_4 )
```





```
f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}
```

- This formula has an issue when handled to a computer.
- Computer represent numbers with finite precision (bits), when h is very small, f(x + h) and f(x) can become very close in value.
- <u>Subtracting two nearly equal values</u> leads to <u>catastrophic cancellation</u>, significant digits are lost, and the result is prune to round-offs errors.
- We can use something called Machine Epsilon $\epsilon_{machine} = (2.22 \times 10^{-16})$ which is smallest meaningful increment you can add to 1 without it being lost due to precision limitation.



$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

• Machine Epsilon $\epsilon_{machine} = (2.22 \times 10^{-16})$ we can find it in NumPy.

```
epsilon_machine = np.finfo(float).eps
```



• Let's check the definition, it's the smallest number we can add to one in the floating-point system.

- There are 4 types of errors that can interrupt our results and ruing it due to the limitations of machine representation of numbers.
 - Round-off error: computer can't represent numbers like π which has infinity digits.
 - Truncation error: the error when computers (or we) approximate numbers.
 - Underflow/ overflow: it's decreasing / growing beyond the representation capabilities.



$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

- The first 2 errors may be ignorable at first, but they can **accumulate** causing more issues.
- Round-off error, computers use fixed number of bits to store real numbers
 - When you try to represent a number with more precision than the computer can handle, it rounds the number to fit into the available space.
 - This rounding process introduces small differences between the real number and its computer representation.
- **Truncation error**, Truncation error arises because you're cutting off part of the calculation to make the problem solvable.
 - This what happen in our derivative law, so we use a limited precision h.
- How these Errors affect our derivative law?



$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

- How these Errors affect our derivative law?
- The difference f(x + h) f(x) can be smaller than the Machine Epsilon $\epsilon_{machine}$.
- When this happen, the computer might round the difference to zero or very small value, causing the derivative approximation to be incorrect (Round-off error).
- The result of the division $\frac{f(x+h)-f(x)}{h}$ may be truncated if h is too small. (Truncation error)
- Truncation error scale with h and at very small h, truncation error becomes negligible.
- Round-off error scale with $\frac{1}{h}$ and at very small h, round-off error dominates.
- So there is a trade-off, so we would use the square root of $\epsilon_{machine}$ as the h.



```
# Machine epsilon for double-precision floats
                                                     Forward Difference Approximation: 6.0
                                                     Expected Derivative: 6
epsilon machine = np.finfo(float).eps
# Optimal h
h optimal = np.sqrt(epsilon machine)
# Forward difference method
forward\_diff = (f(x + h\_optimal) - f(x)) / h\_optimal
# Print the result
print(f"Forward Difference Approximation: {forward_diff}")
print(f"Expected Derivative: \{2 * x\}") # Analytical derivative of x^2 is 2x
```



$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

• We can **reduce** the error also by modifying the law, this variation is called **symmetric difference formula.**

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x-h)}{2h}$$

• This f(x+h) - f(x-h) this produce less error (truncation) but aren't immune to representational errors.

```
x = 3
def f(x): # x^2 -> 2x
return x**2
6.217248937900877
6.128431095930864
h_5 = 0.0000000000000001
print((f(x+h_5) - f(x)) / h_5)
print((f(x+h_5)-f(x-h_5))/ (2*h_5))
```

Differentiation Rules

- Constant rule: If f(x) = C, where C is a constant then f'(x) = 0
 - f(x) = 6 then f'(x) = 0
- Power rule: If $f(x) = x^n$, where n is a constant then f'(x) = n. x^{n-1}
 - $f(x) = x^4$ then $f'(x) = 4x^3$
- Constant Multiple rule: If $f(x) = C \cdot g(x)$, where C is a constant then $f'(x) = C \cdot g'(x)$
 - $f(x) = 3x^4$ then $f'(x) = 12x^3$
- Sum rule : If f(x) = g(x) + h(x), then f'(x) = g'(x) + h'(x)
 - $f(x) = 3x^4 + 4x$ then $f'(x) = 12x^3 + 4$
- Product rule : If $f(x) = g(x) \cdot h(x)$, then $f'(x) = g'(x) \cdot h(x) + h'(x) \cdot g(x)$
 - f(x) = (x-2)(x+3) then f'(x) = (1)(x+3) + (1)(x-2) = 2x + 1

Differentiation Rules

- Quotient rule : If $f(x) = \frac{g(x)}{h(x)}$, then $f'(x) = \frac{g'(x)h(x)-h'(x)g(x)}{h(x)^2}$
 - $f(x) = \frac{x^2}{x+1}$ then $f'(x) = \frac{2x(x+1)-1x^2}{(x+1)^2}$
- Exponential functions: If $f(x) = e^x$, then $f'(x) = e^x$
- If $f(x) = a^x$, where C is a constant then, $f'(x) = a^x \ln(a)$
 - If $f(x) = 2^x$ then $f'(x) = 2^x \ln(2)$
- Logarithmic functions: If f(x) = ln(x), then $f'(x) = \frac{1}{x}$
- If $f(x) = log_a(x)$, where a is a constant then $f'(x) = \frac{1}{xln(a)}$
 - If $f(x) = log_a(2x^2 + 4x)$, then $f'(x) = \frac{4x+4}{(2x^2+4x)ln(a)}$

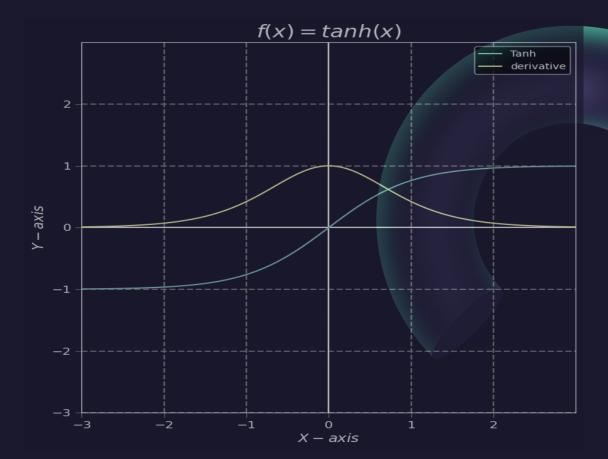


Differentiation Rules

•
$$\frac{d}{dx}(\sin(x)) = \cos(x)$$

•
$$\frac{d}{dx}(\cos(x)) = -\sin(x)$$

•
$$\frac{d}{dx}(tan(x)) = \sec^2(x)$$



•
$$\frac{d}{dx}(tanh(x)) = \frac{d}{dx}(\frac{\sinh(x)}{\cosh(x)}) = 1 - \tanh^2(x) = \operatorname{sech}^2(x)$$

Remember that the range of the output for the trigonometric functions is between -I
and I.



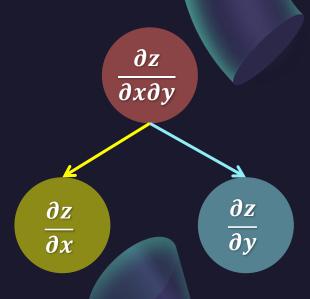
- Partial derivative of a function of several variables is its derivative with respect to one of those variables, with the other held constant.
 - Notation $\frac{\partial f}{\partial x}$

•
$$z = f(x, y) = x^2 + y^2$$

• $\frac{\partial z}{\partial x} = 2x + \frac{\partial}{\partial x}(y^2) = 2x + 0 = 2x$

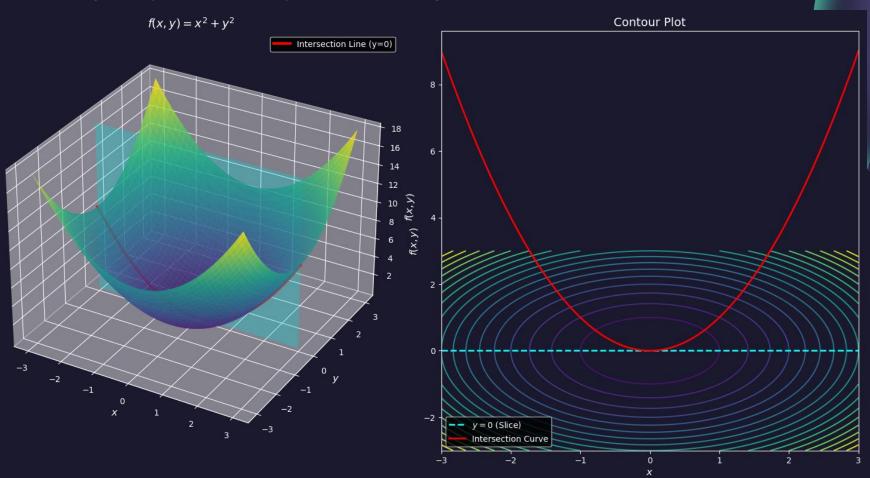
•
$$\frac{\partial z}{\partial y} = \frac{\partial}{\partial y}(x^2) + 2y = 0 + 2y = 2y$$

•
$$\frac{\partial z}{\partial x \partial y} = \frac{\partial z}{\partial x} + \frac{\partial z}{\partial y}$$





• When you set y=0 (as we are considering it constant), you are fixing one variable in the function z=f(x,y) reducing it to single variable function $f(x,y)=x^2+y^2=x^2, \rightarrow f(x,0)=x^2$

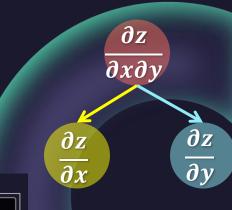


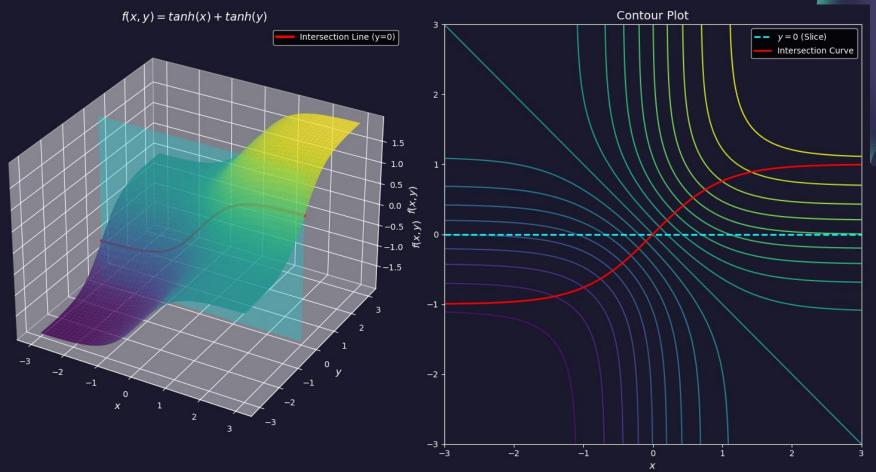
 $\partial x \partial y$

 $\frac{\partial z}{\partial x}$



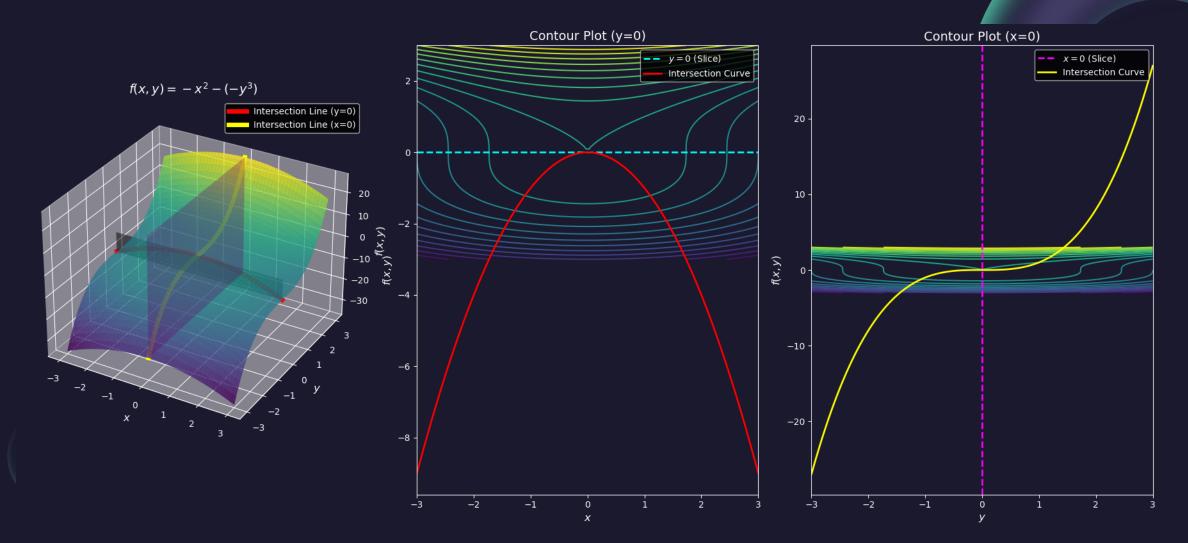
• Another example on the function f(x, y) = tanh(x) + tanh(y)





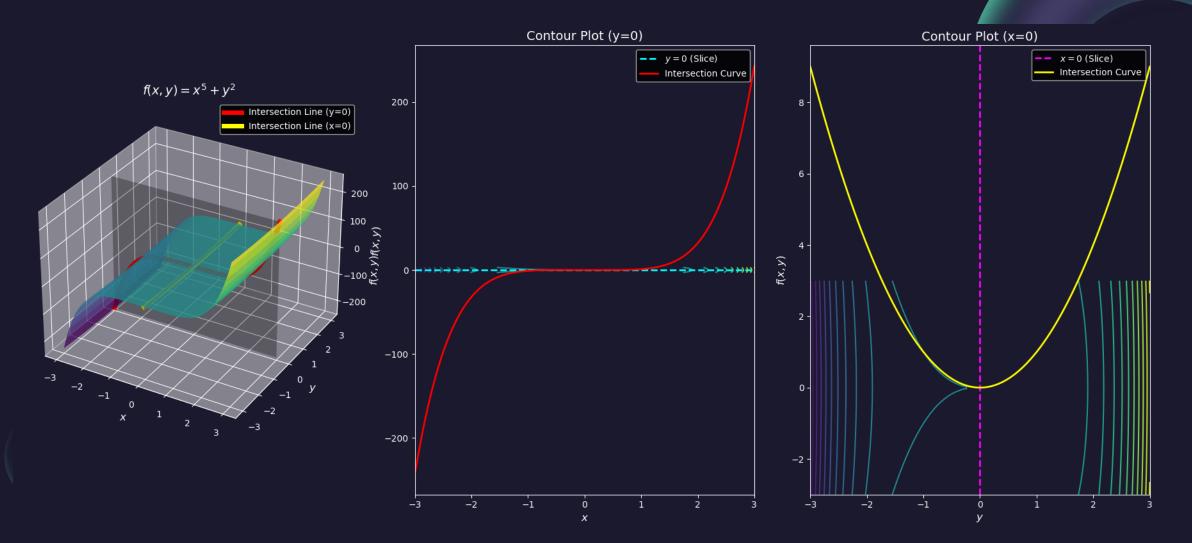


• Another example on the function $f(x, y) = -x^2 - (-y^3)$





• Another example on the function $f(x, y) = x^5 + y^2$



Chain Rule

- Chain rule is a formula that express the derivative of the composition of two differentiable functions f and g in terms of the derivatives of f and g.
 - h(x) = f(g(x))
 - h'(x) = f'(g(x))g'(x) another notation $\frac{d}{dx}[f(g(x))] = \frac{df}{dg} * \frac{dg}{dx}$
- h(x) = sin(3x), the outer function f(u) = sin(u), the inner function g(x) = 3x
 - $\frac{d}{dx}[sin(3x)] = \frac{d}{du}[sin(u)] * \frac{d}{dx}[3x] = cos(u) * 3 = cos(3x) * 3$
- The chain rule arise from the existence of chain of dependencies between some functions, x depends on y and y depends on z and so on.
- Let's expand our notation, if we have a composition of many functions

$$f_1(f_2(...f_n(x)))$$
, the derivative is $\frac{d}{dx}[f_1(f_2(...f_n(x)))] = \frac{d}{df_1} * \frac{df_1}{df_2} * \cdots * \frac{df_{n-1}}{df_n}$

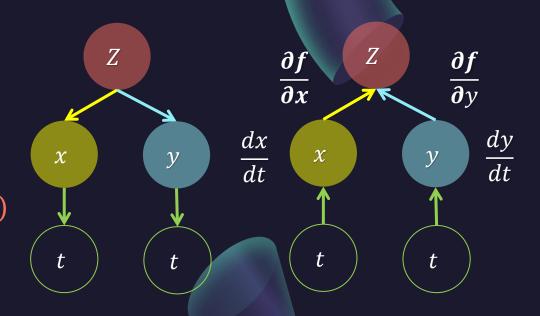


Chain Rule

- Calculate $\frac{dz}{dt}$ given the following functions, express the final output in terms of t
 - $z = f(x, y) = x^2 3xy + 2y^2$
 - $x = x(t) = 3 \sin(2t)$
 - $y = y(t) = 4 \cos(2t)$

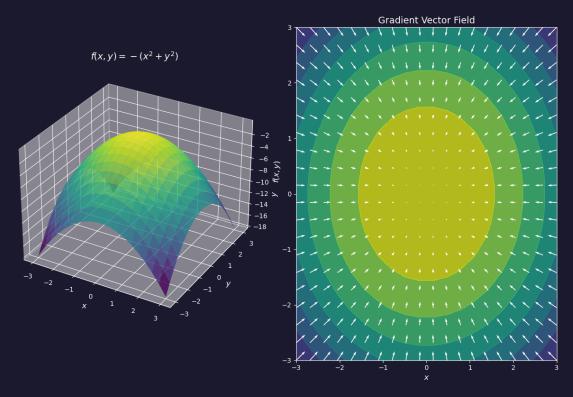
$$\frac{dz}{dt} = \frac{\partial f}{\partial x} \frac{dx}{dt} + \frac{\partial f}{\partial y} \frac{dy}{dt}$$

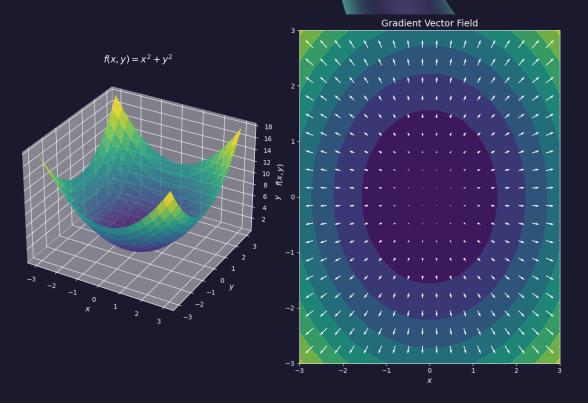
$$\frac{dz}{dt} = (2x - 3y)(6\cos 2t) + (-3x + 4y)(-8\sin 2t)$$
$$= -64\sin 4t - 72\cos t 4t$$





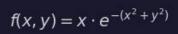
- The gradient of a scaler function f(x, y) is a vector field that points in the <u>direction of</u> the greatest rate of change of f, for a function f(x, y) the gradient is defined as:
 - $\nabla f(x,y) = (\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y})$ vector of partial derivatives.

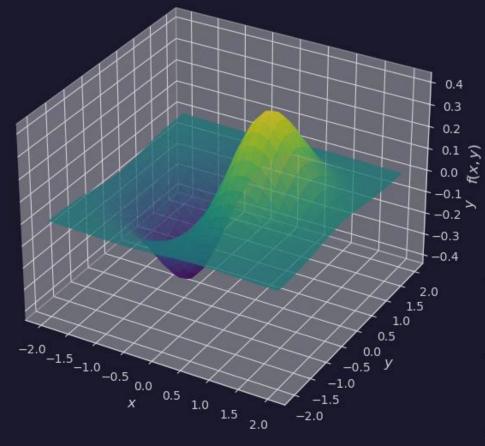


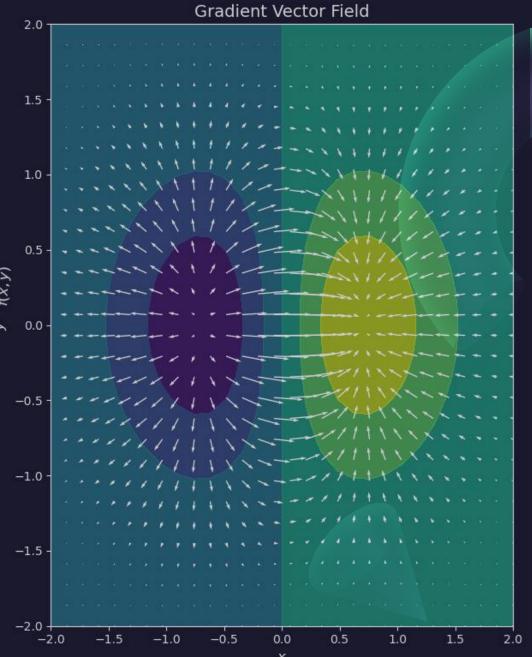


IEEE ML S25' training sessions











$$f(x, y, z) = 2x + 3y^{2} - sin(z)$$

$$\nabla f(x, y, z) = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}\right)$$

$$\nabla f(x, y, z) = \left(2, 6y, -cos(z)\right)$$

- We can write the gradient as a row vector or column vector.
- To generalize the definition, for a function f(x, y, ...), the gradient ∇f is a vector that point towards the direction of the steepest increase of f.

•
$$\nabla f(x, y, ...) = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, ...\right)$$

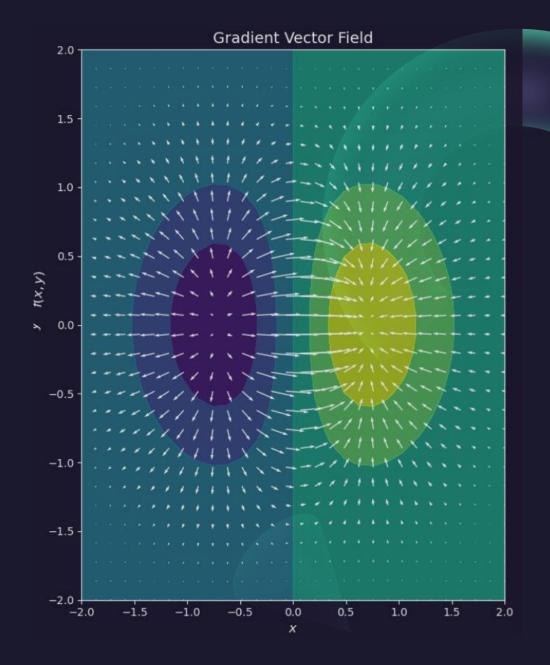
- Since the gradient is a vector, it has a direction and a magnitude represented by the arrows we plotted in the vector field.
- These vectors represent the steepest ascent, and the magnitude tell us how fast the function increase in that direction.



 How we know the direction of the arrow (gradient vector at specific point)?

• The direction is
$$\theta = tan^{-1} \begin{pmatrix} \frac{\partial f}{\partial y} \\ \frac{\partial f}{\partial x} \end{pmatrix}$$

• The magnitude is $\| \nabla f \| = \sqrt{\sum_{i=1}^n \left(\frac{\partial f}{\partial x_i} \right)^2}$





Beyond gradient

- Jacobian matrix of vector valued function of several variables is the matrix of its all fist-order partial derivatives.
- If we have a function $f: \mathbb{R}^n \to \mathbb{R}^m$, the Jacobian matrix $J \in \mathbb{R}^{n \times m}$ is defined as:

$$J_{i,j} = \frac{\partial}{\partial x_i} f(x)_i$$

$$J_{i,j} = \frac{\partial}{\partial x_j} f(x)_i = \begin{bmatrix} \frac{\partial f}{\partial x_1} \dots \frac{\partial f}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \nabla^{\mathrm{T}} f_1 \\ \vdots \\ \nabla^{\mathrm{T}} f_m \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \dots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \dots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

• $\nabla^{\mathrm{T}} f_i$ is the transpose of (row vector) of the gradient of the $i - \mathrm{th}$ component.



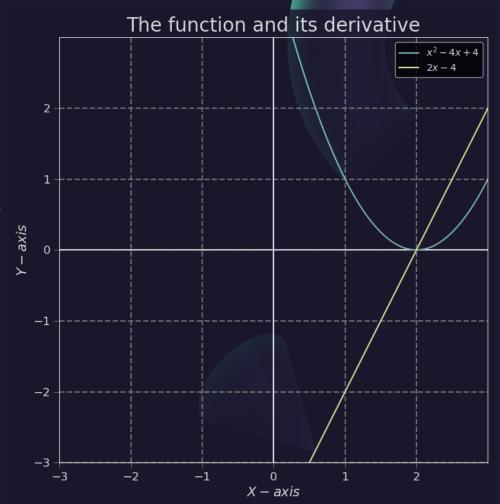
Optimization

- Optimization is the selection of the best element, with regards to some criteria, from a set of available alternatives.
- Optimization problem consist of maximizing or minimizing a real function by systematically choosing input values from within allowed set and computing the value of the function.
- How it this related to machine learning and calculus?
- In ML the model has some parameters (elements) we need to select the best that maximize its performance and minimizing its mistakes.
- What makes ML special is the use of data to approximate some function using the parameters that minimize the Error and maximize its accuracy.



Optimization

- Derivative can be a good tool for finding the maximum or minimum values based on finding the points where the slope is zero, we call them critical points.
- $f(x) = x^2 4x + 4$, the derivative (slope) f'(x) = 2x - 4, when the slope would equal zero?
- f'(x) = 2x 4, the question is when f'(x) = 0
 - 2x 4 = 0
 - $x = \frac{4}{2} = 2$
- For ML we are searching for a function, and we don't have the perfect function to minimize directly.





Optimization and the learning problem

- In machine learning we try to minimize the error, and to minimize it we need to measure it.
- By the nature of the learning problem, you don't have all the possible errors to represent as a function, so how we know the error?
- We can know or measure the error at some point using the training data.
- Error function is a way to quantify the error by comparing our model outputs to the data points we have.
- We have unknown function to learn and error function that is known only when we have a function and data points to compare to, this would enforce use to learn iteratively in most cases.



Gradient Ascent for maximizing

- Do you remember how the vector field of the gradient was pointing to the maxima points?
- We would <u>maximize</u> this function $f(x) = -(x^2 4x + 4)$, its derivative is f'(x) = -(2x 4)
- In the initial step we would guess a value for x let's say 0
- We would update the value of x using this formula $x_{new} = x_{old} + \eta f'(x_{old})$
 - η is the step size (learning rate), how much we want to go in this direction.
- This algorithm work with iterative approach so we can set number of steps (iteration) also the size of the step η in each iteration.
 - For simplicity we would simulate 5 iterations.
 - $\eta = 0.4$

$x_{new} = x_{old} + \eta f'(x_{old})$

Gradient Ascent for maximizing

• Step I

•
$$x_{new} = x_{old} + \eta f'(x_{old})$$

•
$$x_{new} = 0 + 0.4 (-(2(0) - 4))$$

•
$$x_{new} = 1.6$$

• Step 2

•
$$x_{new} = 1.6 + 0.4 (-(2(1.6) - 4))$$

•
$$x_{new} = 1.92$$

• Step 3

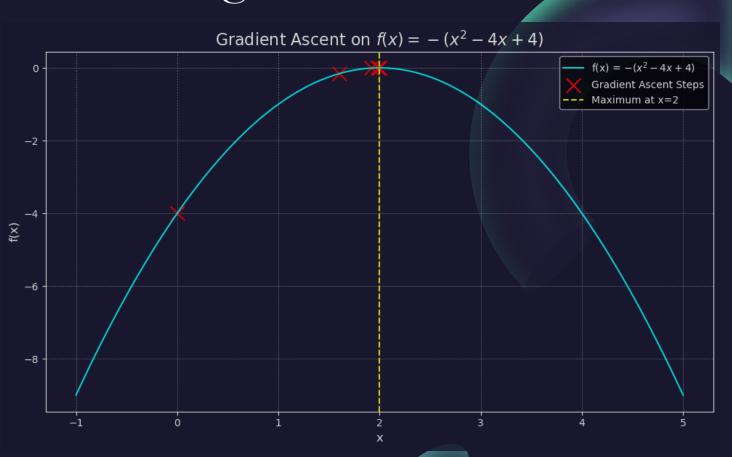
•
$$x_{new} = 1.92 + 0.4 (-(2(1.92) - 4))$$

•
$$x_{new} = 1.984$$

• Step 4

•
$$x_{new} = 1.984 + 0.4 (-(2(1.984) - 4))$$

•
$$x_{new} = 1.9968$$



• Step 5

•
$$x_{new} = 1.9968 + 0.4 (-(2(1.9968) - 4))$$

•
$$x_{new} = 1.99936$$



Gradient Descent for minimizing

- We would minimize this function $f(x) = x^2 4x + 4$, its derivative is f'(x) = 2x 4
- In the initial step we would guess a value for x let's say 0
- We would update the value of x using this formula $x_{new} = x_{old} \eta f'(x_{old})$
 - η is the step size (learning rate), how much we want to go in this direction.
- This algorithm work with iterative approach so we can set number of steps (iteration) also the size of the step η in each iteration.
 - For simplicity we would simulate 5 iterations.
 - $\eta = 0.4$
- Notice the we are going in the negative direction of the gradient (derivative) to minimize the function.

$x_{new} = x_{old} - \eta f'(x_{old})$

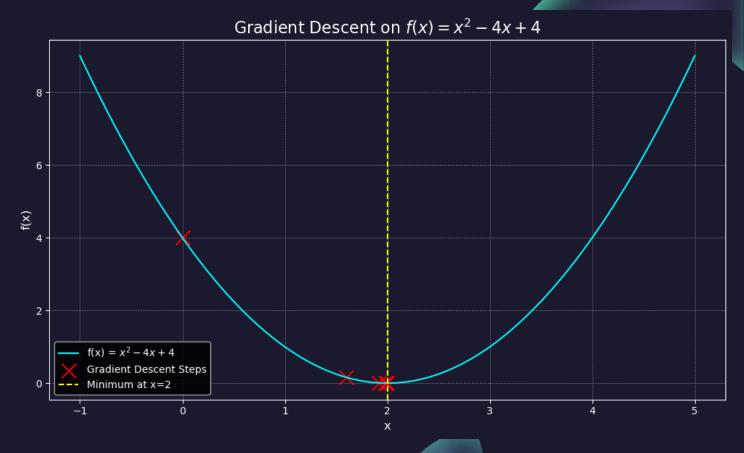
Gradient Descent for minimizing

• Step I

•
$$x_{new} = x_{old} - \eta f'(x_{old})$$

•
$$x_{new} = 0 - 0.4(2(0) - 4)$$

- $x_{new} = 1.6$
- Step 2
 - $x_{new} = 1.6 0.4 (2(1.6) 4)$
 - $x_{new} = 1.92$
- Step 3
 - $x_{new} = 1.92 0.4(2(1.92) 4)$
 - $x_{new} = 1.984$
- Step 4
 - $x_{new} = 1.984 0.4(2(1.984) 4)$
 - $x_{new} = 1.9968$



- Step 5
 - $x_{new} = 1.9968 0.4(2(1.9968) 4)$
 - $x_{new} = 1.99936$



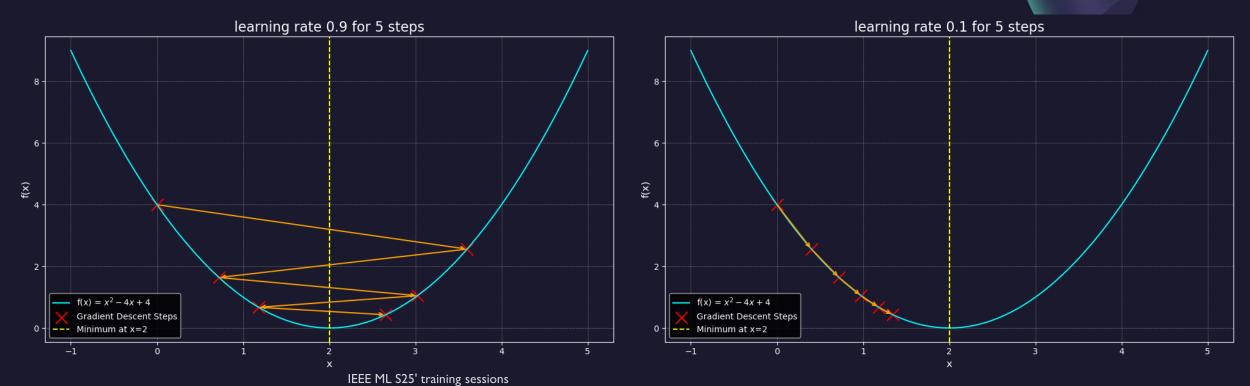
Gradient Ascent 🚺 vs Gradient Descent 🖳

Aspect	Gradient Descent	Gradient Ascent
Objective	Minimize a function	Maximize a function
Direction	Negative gradient	Positive gradient
Formula	$x_{new} = x_{old} - \eta f'(x_{old})$	$x_{new} = x_{old} + \eta f'(x_{old})$
in ML	Used to minimize the loss function.	Used to maximize the reward function in reinforcement learning.



The effect of learning rate η

- Learning rate (step size) is a critical parameter in gradient ascent/descent.
- We need to make the learning rate high so we can reach the best point in fewer steps.
- But if we made η a very large number we may miss our goal, too small number is bad also.



See w

- https://youtu.be/TglD4Y6ImQk?si=uLiClQDrSdXOB7oQ (7h of Limits problems, if you want to practice)
- https://home.iitk.ac.in/~pranab/ESO208/rajesh/03-04/Errors.pdf (Types of Errors ____)
- https://zingale.github.io/comp_astro_tutorial/basics/floating-point/numerical_error.html (Types of Errors ___)
- https://web.engr.oregonstate.edu/~webbky/ESC440_files/Section%201%20Roundoff%20and%20Truncation%20Error.pdf
- https://en.wikipedia.org/wiki/Round-off_erro
- https://youtu.be/03Lg60MTSdM?si=edZqtyywFMtlJNyD
- https://kapilcaet.wordpress.com/wp-content/uploads/2015/01/unit-4-round-off-and-truncation-errors.pdf
- https://en.wikipedia.org/wiki/Differentiation_rules
- https://www.khanacademy.org/math/multivariable-calculus/thinking-about-multivariable-function/ways-to-represent-multivariable-functions/a/contour-maps