



Calculus for ML

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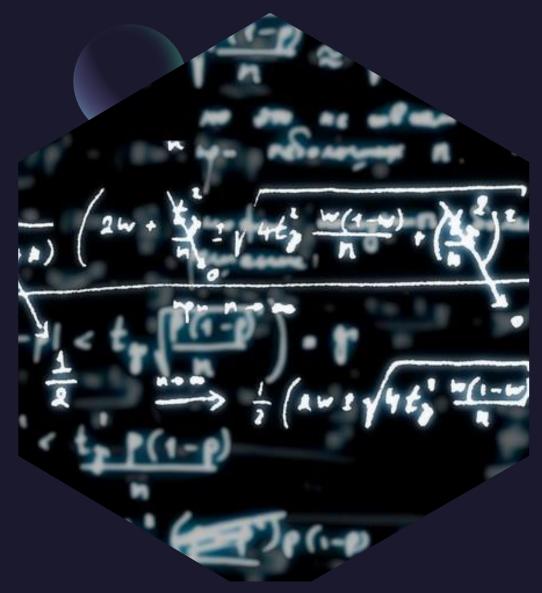
Agenda

- 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, ...).



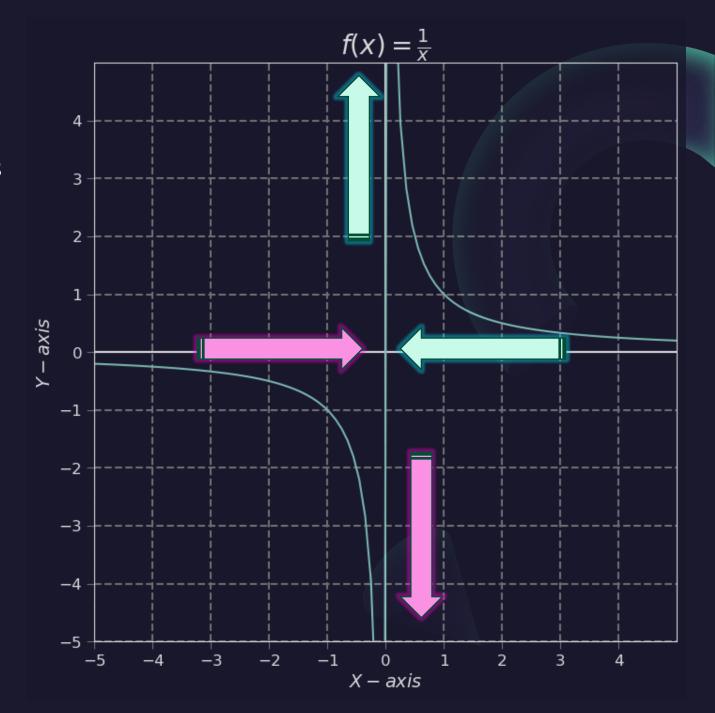
• You won't always end with a finite number as a limit, for some functions you the limit may be infinity ∞ , for example $\lim_{x\to 0^+}(\frac{1}{x})=\infty$, try inputting (0.1, 0.01, 0.001,...).

| 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.

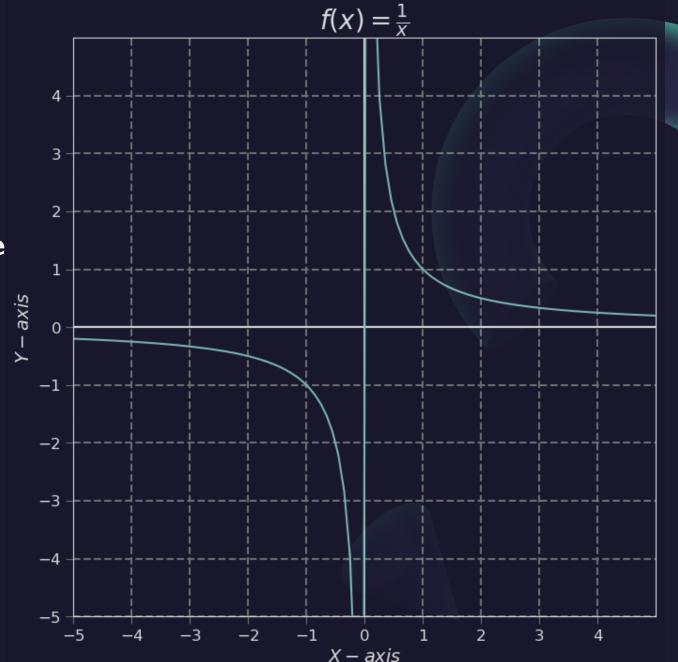


- Till now we treated this function from the positive side only, but it has two parts.
- When we inputted numbers that are close to zero in positive side it goes to infinity.
- Let's input number that are closer to zero but for the negative part of the function.
- For the negative part of this function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





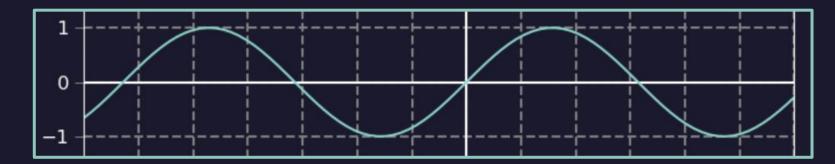
- $\lim_{x\to 0^+} (\frac{1}{x}) = \infty$ for the positive side
- $\lim_{x\to 0^-} (\frac{1}{x}) = -\infty$ for the negative side
- What is the limit $\lim_{x\to 0} (\frac{1}{x}) = ?$
- This <u>limit doesn't exist</u> for this function as the two parts of the functions are not approaching the same value.





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))



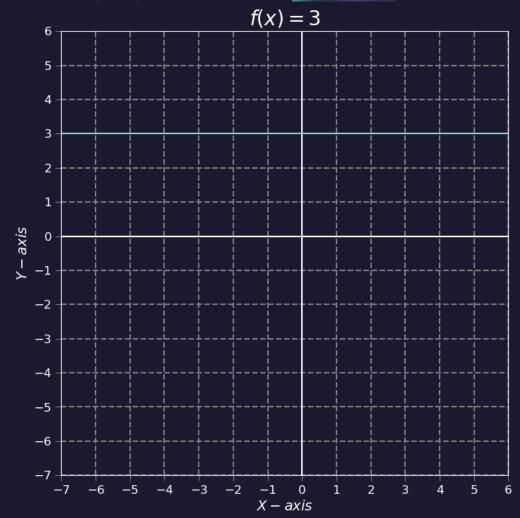
Limits and continuity

- 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.

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





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

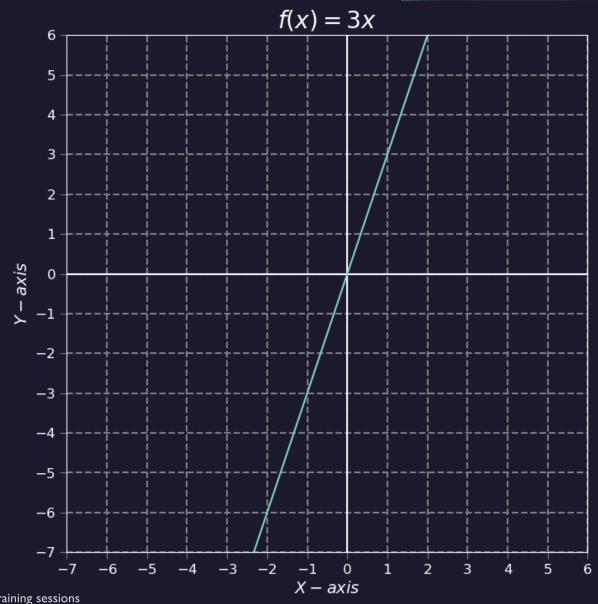
• function f(x) = 3x constant function.

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

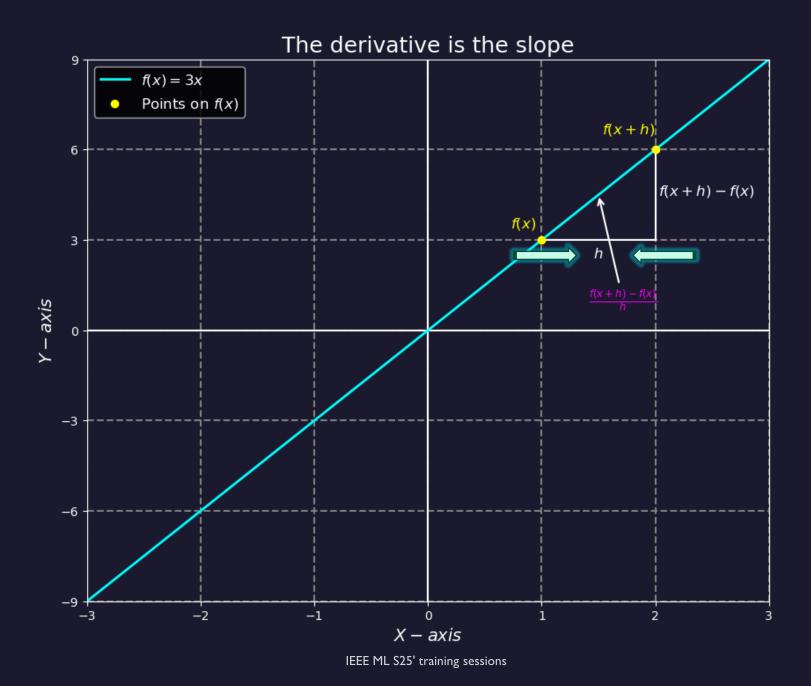
$$= \lim_{h\to 0} \frac{3x + 3h - 3x}{h}$$

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

• 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.



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

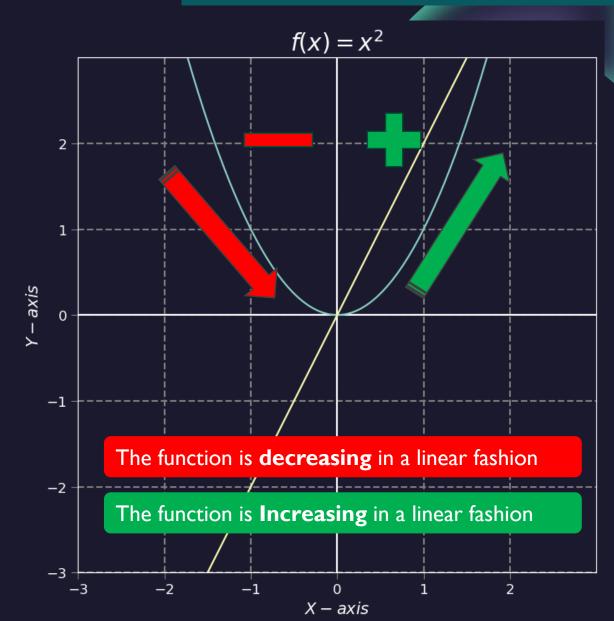
• function $f(x) = x^2$ quadratic equation.

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

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

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

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

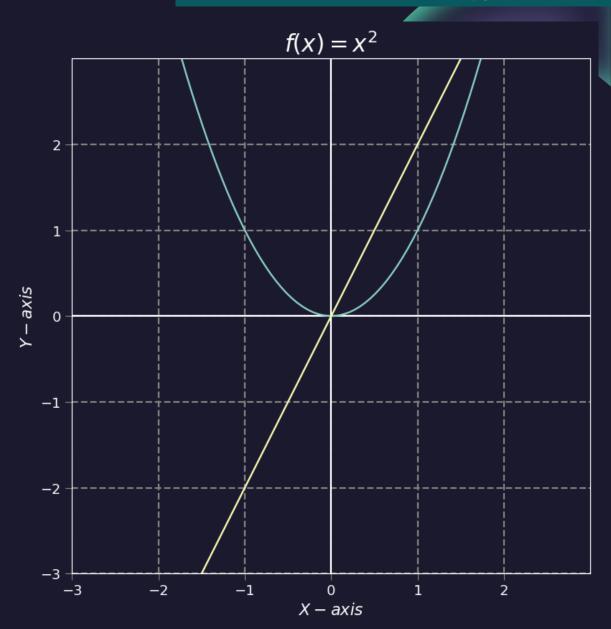




$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$

• 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.

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 $f'(x) = \frac{1}{x ln(a)}$
 - If $f(x) = log_a(2x^2 + 4x)$, then $f'(x) = \frac{4x+4}{(2x^2+4x)ln(a)}$

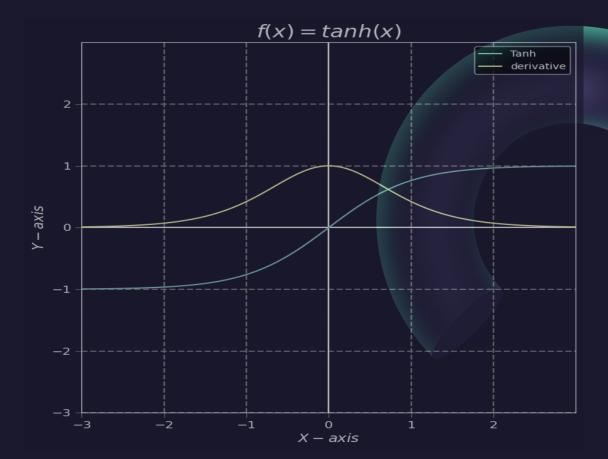


Differentiation Rules

•
$$\frac{d}{dx}(\sin(x)) = \cos(x)$$

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

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



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

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



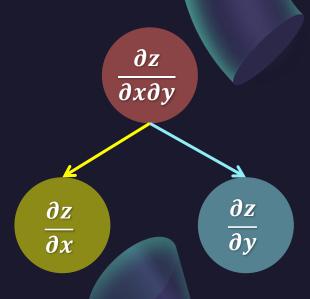
- Partial derivative of a function of several variables is its derivative with respect to one of those variables, with the other held constant.
 - Notation $\frac{\partial f}{\partial x}$

•
$$z = f(x, y) = x^2 + y^2$$

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

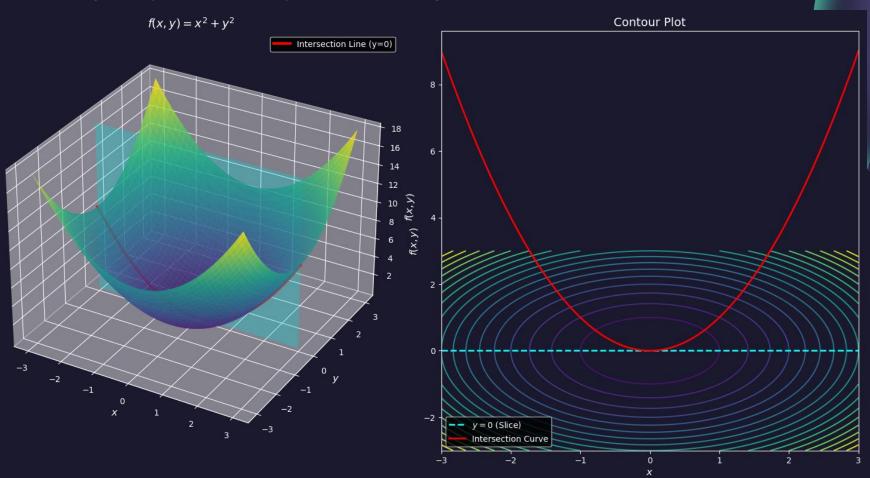
•
$$\frac{\partial z}{\partial y} = \frac{\partial}{\partial y}(x^2) + 2y = 0 + 2y = 2y$$

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





• 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 $f(x,y)=x^2+y^2=x^2, \rightarrow f(x,0)=x^2$

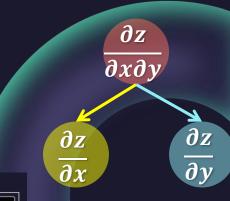


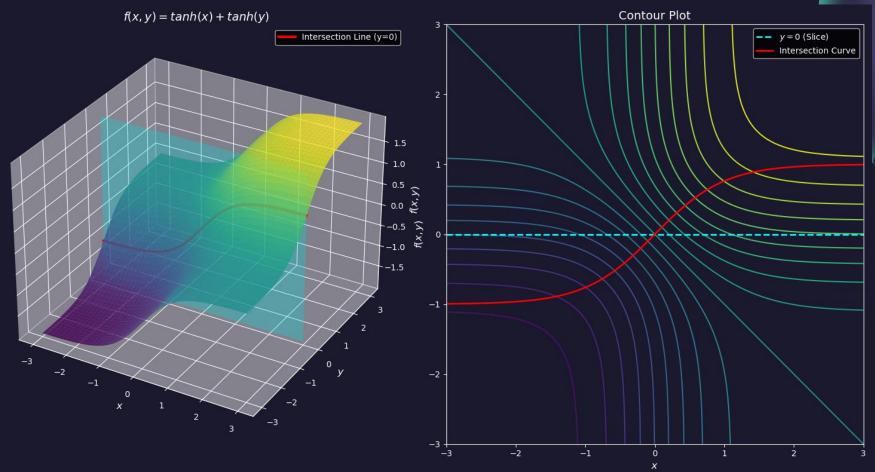
 $\partial x \partial y$

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



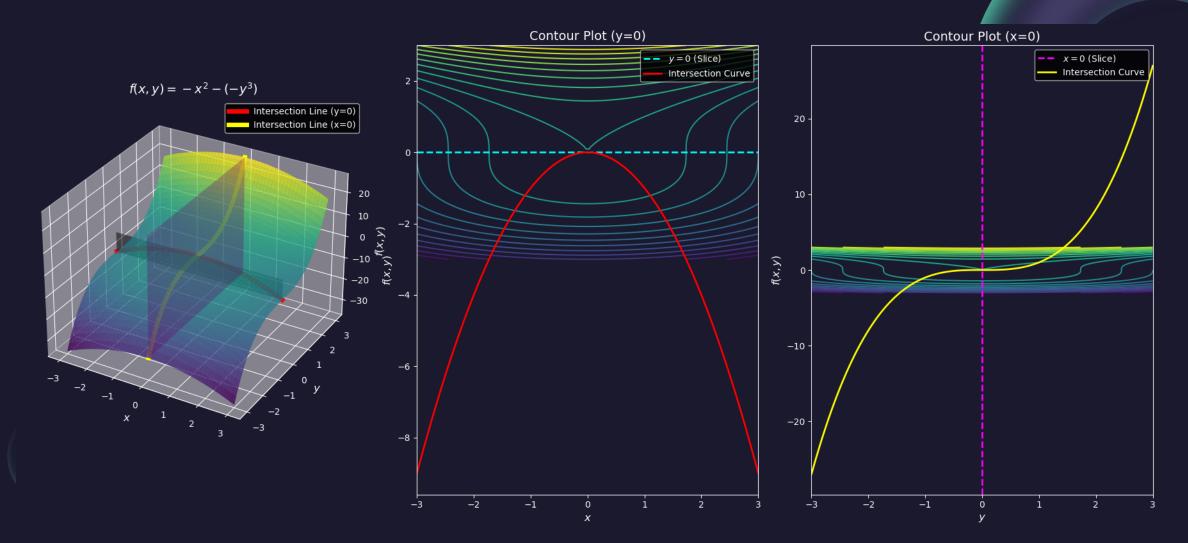
• Another example on the function f(x, y) = tanh(x) + tanh(y)





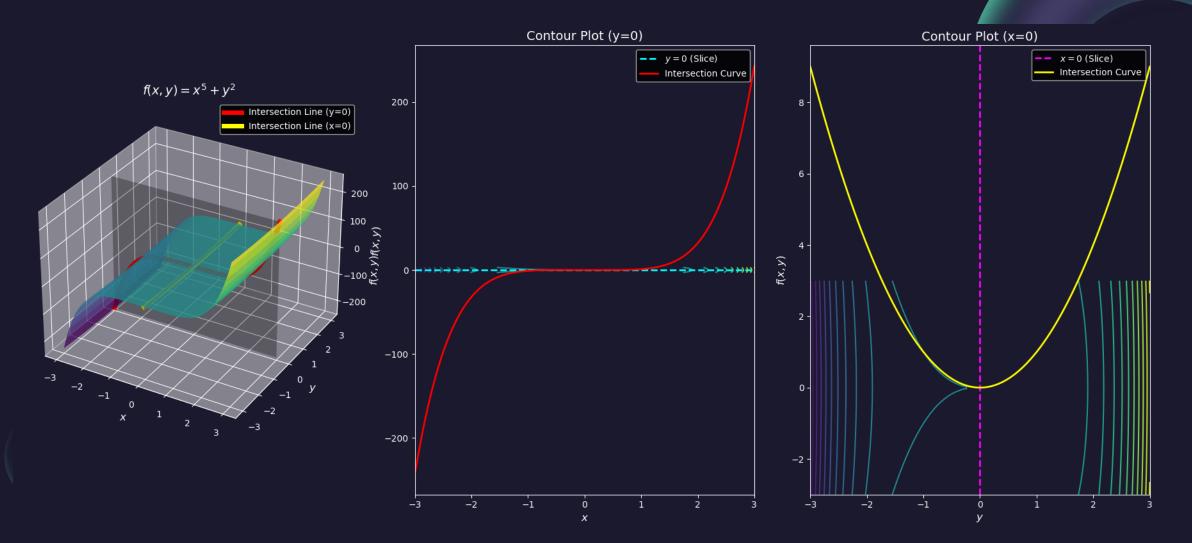


• Another example on the function $f(x, y) = -x^2 - (-y^3)$





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

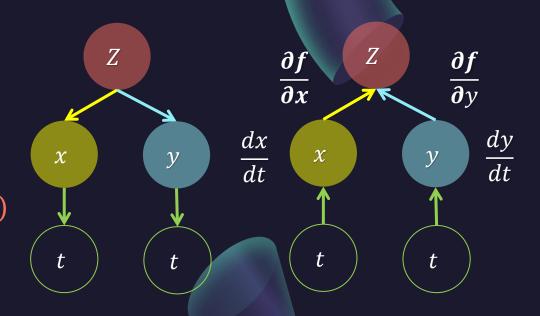


Chain Rule

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

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

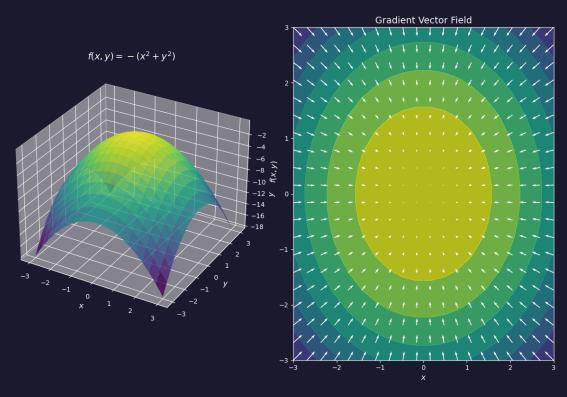
$$\frac{dz}{dt} = (2x - 3y)(6\cos 2t) + (-3x + 4y)(-8\sin 2t)$$
$$= -64\sin 4t - 72\cos t 4t$$

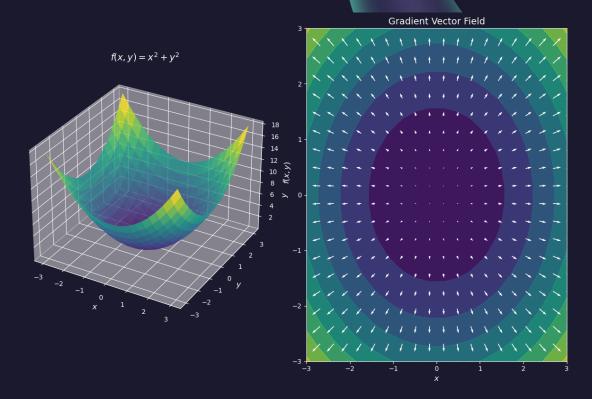




• The gradient of a scaler function f(x, y) is a vector field that points in the <u>direction of</u> the greatest rate of change of f, for a function f(x, y) the gradient is defined as:

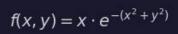
• $\nabla f(x, y) = (\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y})$ vector of partial derivatives.

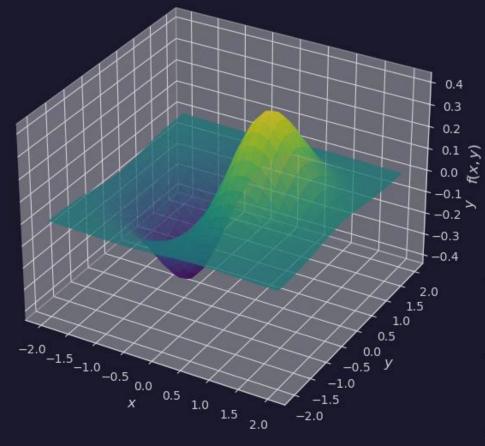


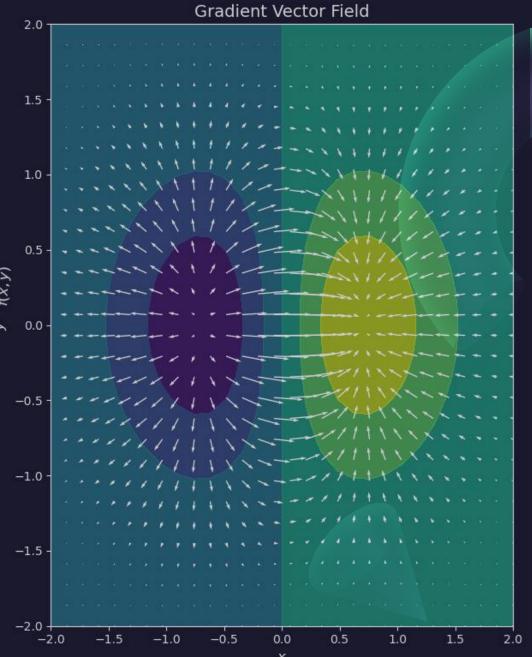


IEEE ML S25' training sessions











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

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

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

- 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.

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

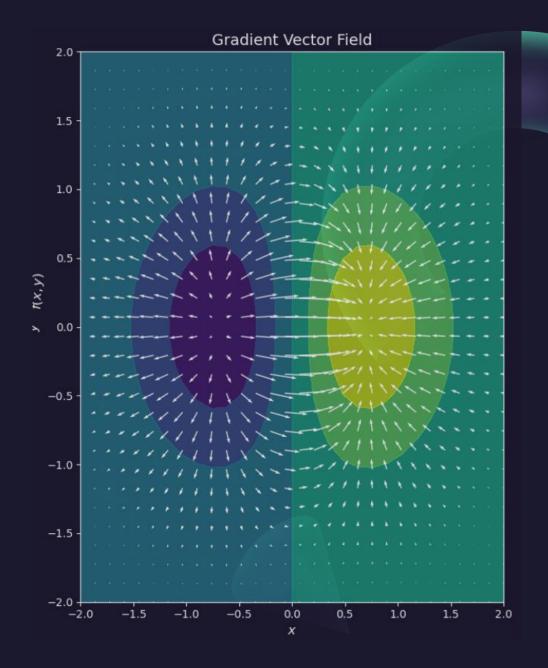
- Since the gradient is a vector, it has a direction and a magnitude represented by the arrows we plotted in the vector field.
- These vectors represent the steepest ascent, and the magnitude tell us how fast the function increase in that direction.



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

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

• 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:

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

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

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



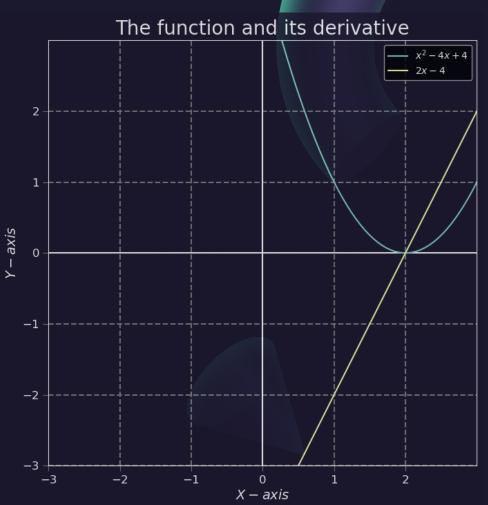
Optimization

- 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

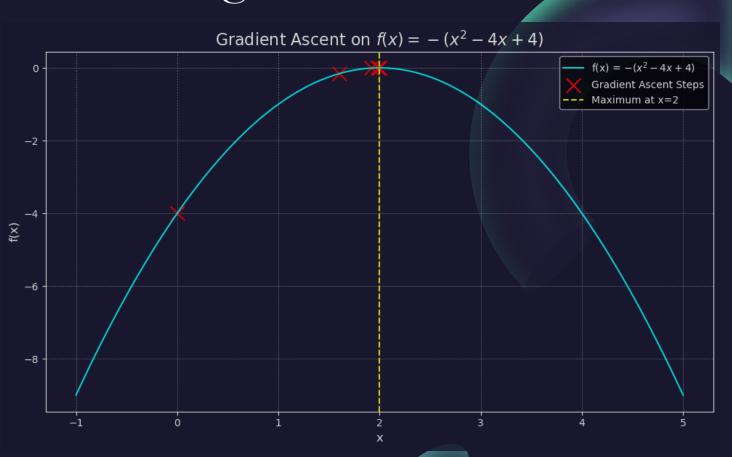
•
$$x_{new} = 1.92 + 0.4 (-(2(1.92) - 4))$$

•
$$x_{new} = 1.984$$

• 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.

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

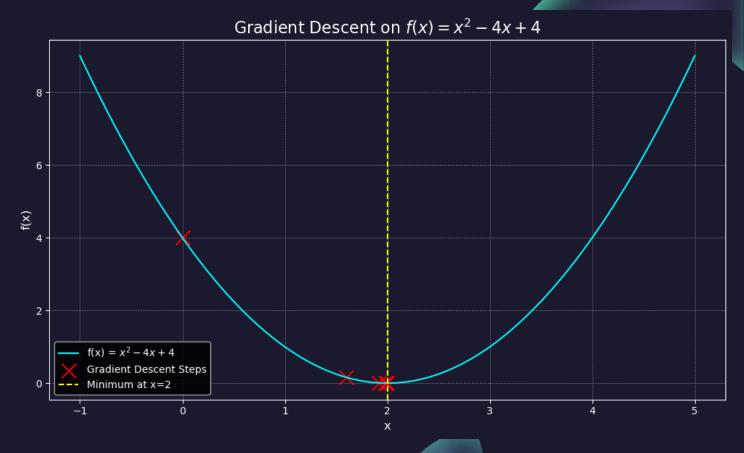
Gradient Descent for minimizing

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



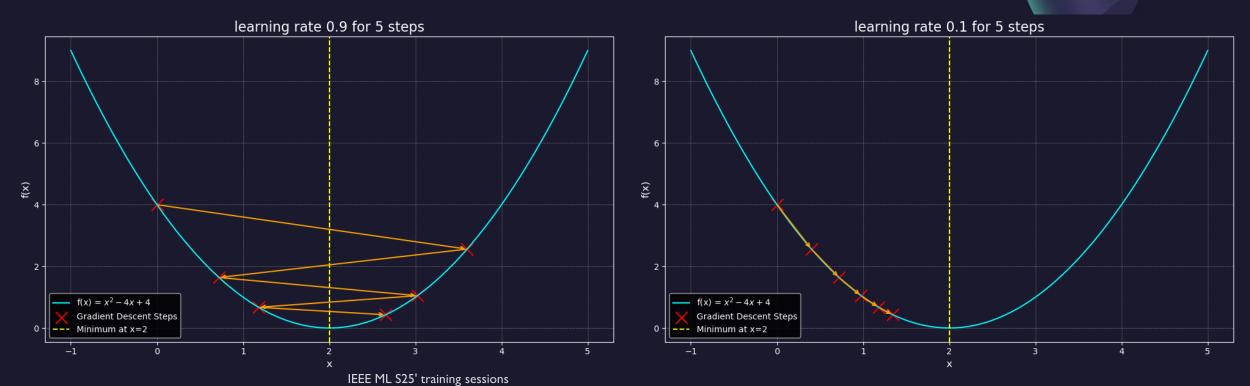
Gradient Ascent 🚺 vs Gradient Descent 🖳

| 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