DERIVATIVES

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Derivatives in Physics

- Pretty much all of physics involves differentials

$$\vec{v} = \frac{d\vec{x}}{dt}$$

$$\vec{a} = \frac{d\vec{v}}{dt}$$

- The definition of a differential is the limit of difference between dependent variable points over the difference between the independent variable, as that difference goes to zero

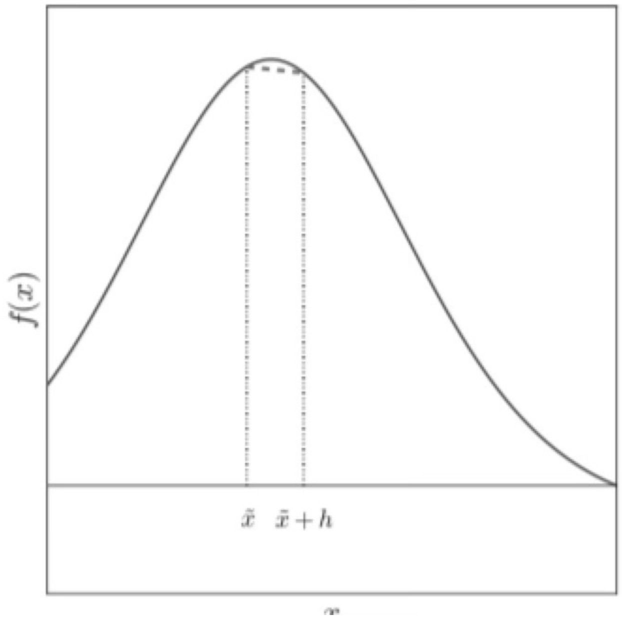
$$\frac{df(x)}{dx} \equiv \lim_{h\to 0} \frac{f(x+h) - f(x)}{h}$$

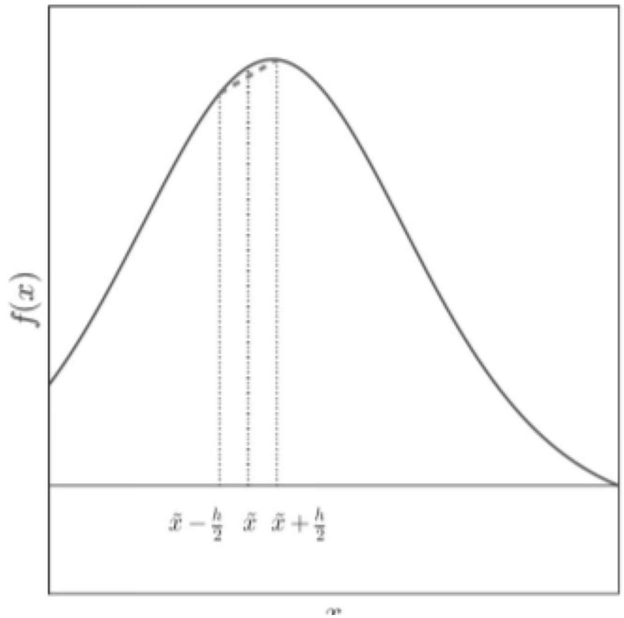
- And by now you know how to find the derivatives of arbitrarily complicated explicit functions using the chain rule.

$$\frac{d}{dx} e^{\sin(2x)} = \left(\frac{d}{dx} \sin(2x)\right) e^{\sin(2x)} = 2\cos(2x) e^{\sin(2x)}$$

Numerical Differentiation

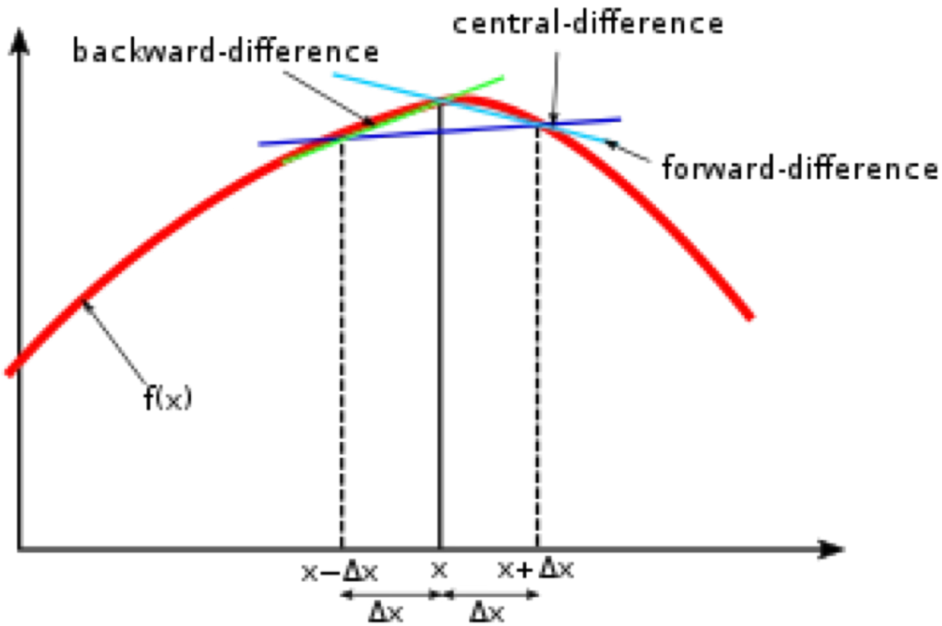
- Sometimes functions are not explicit
  - E.g. may be based on arbitrary distributions of real data.
- In this case, we need to numerically differentiate.





- We can't take h to zero, so we need to figure out how accurate we are if we don't.

Different Ways of Looking at the Derivative



Forward Difference:

$$\frac{df(x)}{dx} \equiv \lim_{h\to 0} \frac{f(x+h) - f(x)}{h}$$

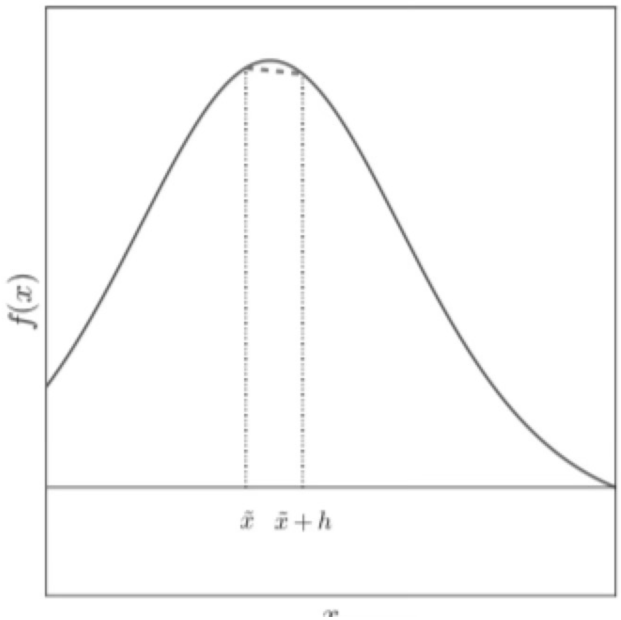
Backward Difference:

$$\frac{df(x)}{dx} \equiv \lim_{h\to 0} \frac{f(x) - f(x-h)}{h}$$

Central Difference:

$$\frac{df(x)}{dx} \equiv \lim_{h\to 0} \frac{f(x+\frac{h}{2}) - f(x-\frac{h}{2})}{h}$$

Consider the first



$$\frac{df(x)}{dx} \equiv \lim_{h\to 0} \frac{f(x+h)-f(x)}{h}$$

$$\to \left.\frac{df(x)}{dx}\right|_{x=\tilde{x}} = \lim_{h\to 0} \frac{f(\tilde{x}+h)-f(\tilde{x})}{h}$$

- Can't really go to zero, so we have to consider the errors
  - The smaller *h* is, the better our approximation is ε_{app}
  - BUT, the smaller *h* is, the bigger our round-off error is. ε_{ro}
- Need to optimize!

Approximation Error

- Taylor expand

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(x) + \cdots$$

$$\begin{aligned}\frac{f(\tilde{x}+h) - f(\tilde{x})}{h} &= f'(\tilde{x}) + \boxed{\frac{h}{2}f''(\tilde{x}) + \frac{h^2}{6}f'''(\tilde{x})} \\ &= f'(\tilde{x}) + \mathcal{O}(h)\end{aligned}$$

- As *h* gets small, the first term will dominate, so the error of our approximation is approximately

$$\varepsilon_{app} \approx \frac{h}{2}|f''(x)|$$

Looking backward?

$$\frac{f(\tilde{x}) - f(\tilde{x} - h)}{h} = f'(\tilde{x}) - \frac{h}{2} f''(\tilde{x}) + \frac{h^2}{6} f'''(\tilde{x}) + \ldots$$
$$= f'(\tilde{x}) - \mathcal{O}(h)$$

$$\frac{f(\tilde{x}) - f(\tilde{x} - h)}{h} = f'(\tilde{x}) - \frac{h}{2} f''(\tilde{x}) + \frac{h^2}{6} f'''(\tilde{x})$$
$$= f'(\tilde{x}) - \mathcal{O}(h)$$

Again

$$\varepsilon_{app} \approx \frac{h}{2} |f''(x)|$$

Round-off Error

- The round off error comes into play when *f(x)* and *f(x+h)* are very close.

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

$$\varepsilon_{ro} \approx \frac{1}{h}\Delta(f(x+h) - f(x)) \approx \frac{2|f(x)|\epsilon_m}{h}$$

- So the total error is roughly

$$\epsilon_m \approx 2.22 \times 10^{-16}$$

$$\varepsilon = \varepsilon_{app} + \varepsilon_{ro}$$

Gets bigger with *h*

$$\approx \frac{h}{2}|f''(x)| + \frac{2|f(x)|}{h}\epsilon_m$$

Gets smaller with *h*

Errors

- We can't take our *h* to zero, so we need to choose and optimum value
- There are two types of errors associated with our calculation
  - The error associated with the Taylor approximation, which will get smaller as *h* gets smaller. ε_{app}
  - The round-off error when taking the difference, which will get larger as *h* gets smaller. ε_{ro}

$$\varepsilon_{app} \approx \frac{h}{2}|f''(x)|$$

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

$$\varepsilon_{ro} \approx \frac{1}{h}\Delta(f(x+h) - f(x)) \approx \frac{2|f(x)|\epsilon_m}{h}$$

$$\rightarrow \varepsilon = \varepsilon_{app} + \varepsilon_{ro}$$

$$\approx \frac{h}{2}|f''(x)| + \frac{2|f(x)|}{h}\epsilon_m$$

Find the Minimum

- Take the derivative wrt h

$$\frac{d\varepsilon}{dh} = \frac{1}{2}|f''(x)| - \frac{2|f(x)|}{h^2}\epsilon_m$$

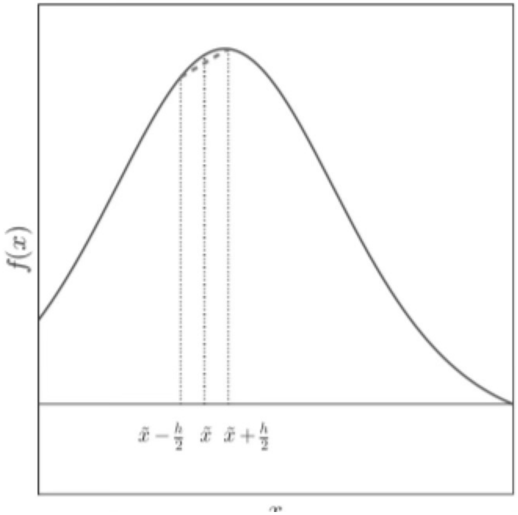
$$\rightarrow h_{opt} = \sqrt{4\epsilon_m \left|\frac{f(x)}{f''(x)}\right|}$$

$$\boxed{= (3 \times 10^{-8})\sqrt{\left|\frac{f(x)}{f''(x)}\right|}}$$

$$\varepsilon_{opt} = \sqrt{4\epsilon_m |f(x)f''(x)|}$$

$$\boxed{= (3 \times 10^{-8})\sqrt{|f(x)f''(x)|}}$$

Central Difference Derivative



$$\frac{df(x)}{dx} \equiv \lim_{h\to 0} \frac{f(x+\frac{h}{2}) - f(x-\frac{h}{2})}{h}$$

$$f(x+\frac{h}{2}) \approx f(x) + \left(\frac{h}{2}\right) f'(x) + \left(\frac{h}{2}\right)^2 \frac{1}{2} f''(x) + \left(\frac{h}{2}\right)^3 \frac{1}{6} f'''(x) + \ldots$$

$$= \cancel{f(x)} + \frac{h}{2} f'(x) + \cancel{\frac{h^2}{8} f''(x)} + \frac{h^3}{48} f'''(x) + \ldots$$

$$f(x-\frac{h}{2}) \approx \cancel{f(x)} - \frac{h}{2} f'(x) + \cancel{\frac{h^2}{8} f''(x)} - \frac{h^3}{48} f'''(x) + \ldots$$

$$\mathcal{O}(h^2)$$

$$\to \frac{f(x+\frac{h}{2}) - f(x-\frac{h}{2})}{h} \approx f'(x) + \frac{h^2}{24} f'''(x) + \ldots$$

Minimizing the Error…

- In this case

$$\varepsilon = \varepsilon_{app} + \varepsilon_{ro} = \frac{h^2}{24}|f'''(x)| + \frac{2|f(x)|}{h}\epsilon_m$$

$$\frac{d\varepsilon}{dh} = \frac{h}{12}|f'''(x)| - \frac{2|f(x)|}{h^2}\epsilon_m$$

$$\to h_{opt} =$$

Bigger step

$$\boxed{= (1 \times 10^{-5}) \left(\left| \frac{f(x)}{f'''(x)} \right| \right)^{1/3}}$$

Compare to forward or backward only

$$(3 \times 10^{-8}) \sqrt{\left| \frac{f(x)}{f''(x)} \right|}$$

$$\varepsilon_{opt} = \left(\frac{9}{8}\epsilon_m^2 |f(x)|^2 |f'''(x)| \right)^{1/3}$$

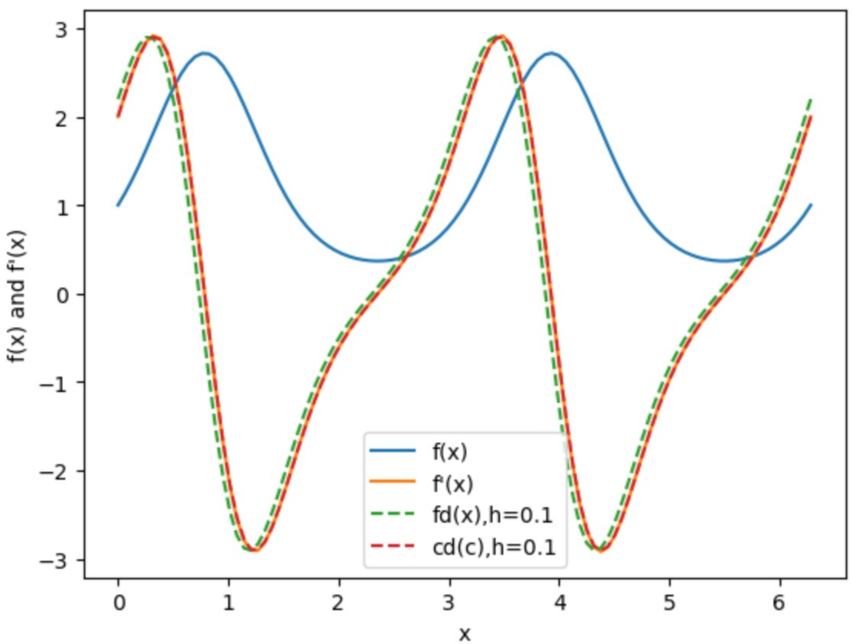
$$\boxed{= (4 \times 10^{-11}) \left(|f(x)|^2 |f'''(x)| \right)^{1/3}}$$

$$(3 \times 10^{-8}) \sqrt{|f(x) f''(x)|}$$

Smaller error

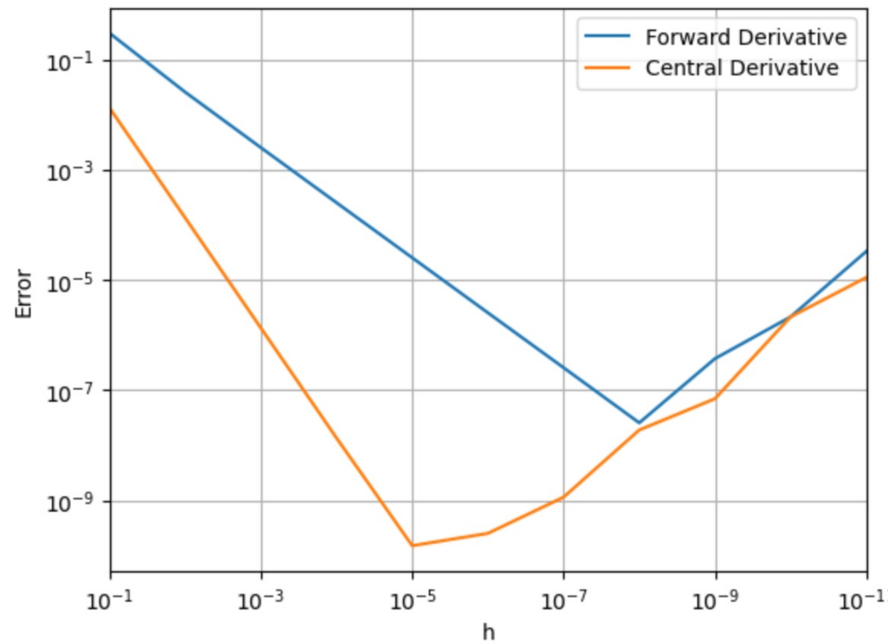
Test*

Plot:
- f(x)
- f'(x)
- Forward derivative (fd)
- Central derivative (cd)



$$f(x) = e^{\sin 2x}$$

Compare errors for forward and central derivatives



Central Derivative
- Optimum step size 1000 time larger
- Minimum error 100 times smaller

*see 'Lecture 7 – Derivatives.ipynb'

Second Derivatives

- We can derive second derivatives from first derivatives in the same way.

$$\frac{d^2 f(x)}{dx^2} = \frac{f'\left(x+\frac{h}{2}\right) - f'\left(x-\frac{h}{2}\right)}{h}$$

$$= \frac{\left(\frac{f(x+h)-f(x)}{h}\right) - \left(\frac{f(x)-f(x-h)}{h}\right)}{h}$$

$$\boxed{= \frac{f(x+h) + f(x-h) - 2f(x)}{h^2}}$$

Digression: Laplace Equation

- Many things, including:
  - Static electric fields in the absence of charges
  - Static magnetic fields in the absence of currents
  - Temperature gradients

  obey the Laplace equation, which is essentially a conservation of flux
- In three dimensions

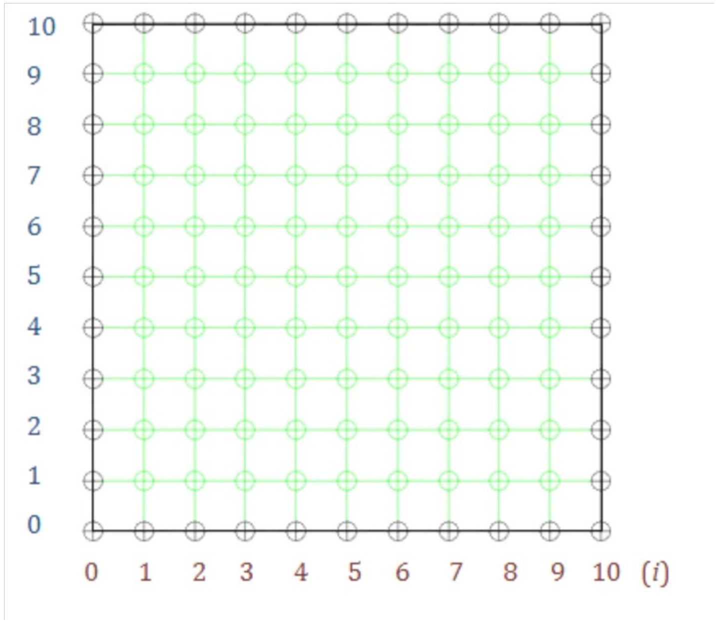
$$\nabla^2\phi = \frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} + \frac{\partial^2\phi}{\partial z^2} = 0$$

- In two dimensions

$$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} = 0$$

Example: 2-Dimensional Temperature Gradient

- Temperatures on a uniformly conducting plane will obey the 2D Laplace equation.



$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

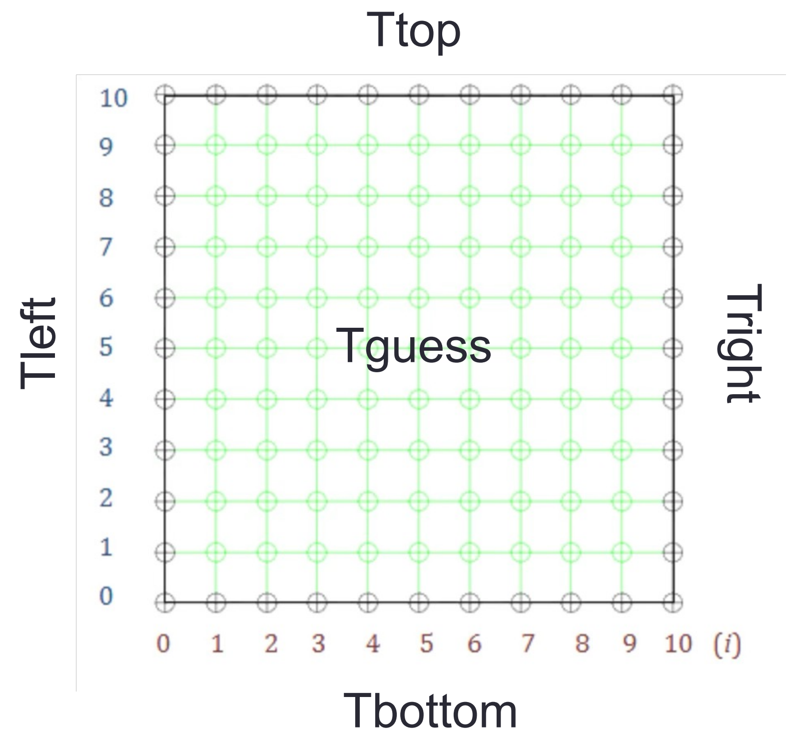
$$0 = \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{(\Delta x)^2} + \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{(\Delta y)^2}$$

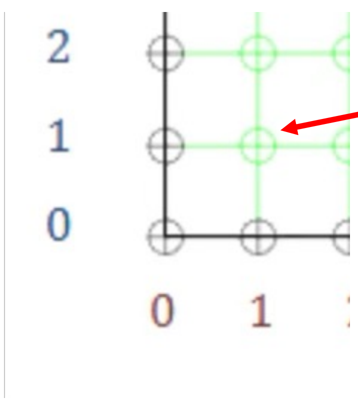
$$\Delta x = \Delta y = h \qquad \text{(grid spacing)}$$

$$\to T_{i,j} = \frac{1}{4}\left(T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1}\right)$$

Solving this in practice…

- Set the boundary conditions on the edges of the array
- Make a guess about the temperatures in the middle
- Keep applying our interpolation algorithm to the points in the plane until they converge on a stable equilibrium solution
  - Example: first guess for lower right corner





$$T_{1,1} = \frac{1}{4}\left(T_{2,1} + T_{0,1} + T_{1,2} + T_{1,0}\right)$$
$$= \frac{1}{4}\left(T_{guess} + T_{left} + T_{guess} + T_{bottom}\right)$$

A Word About Plotting Arrays…

- Python arrays are "row priority". Example

```
arr = np.array([[1.,2.,3.],[4.,5.,6]])  # 2 row x 3 columns
print(arr)
```

```
[[1. 2. 3.]
 [4. 5. 6.]]
```

- When we plot an array, it will plot as
- In other words, the first index corresponds to *y* and the second index corresponds to *x*
  - Which is a bit counterintuitive