Lecture 3:

Vector Calculus

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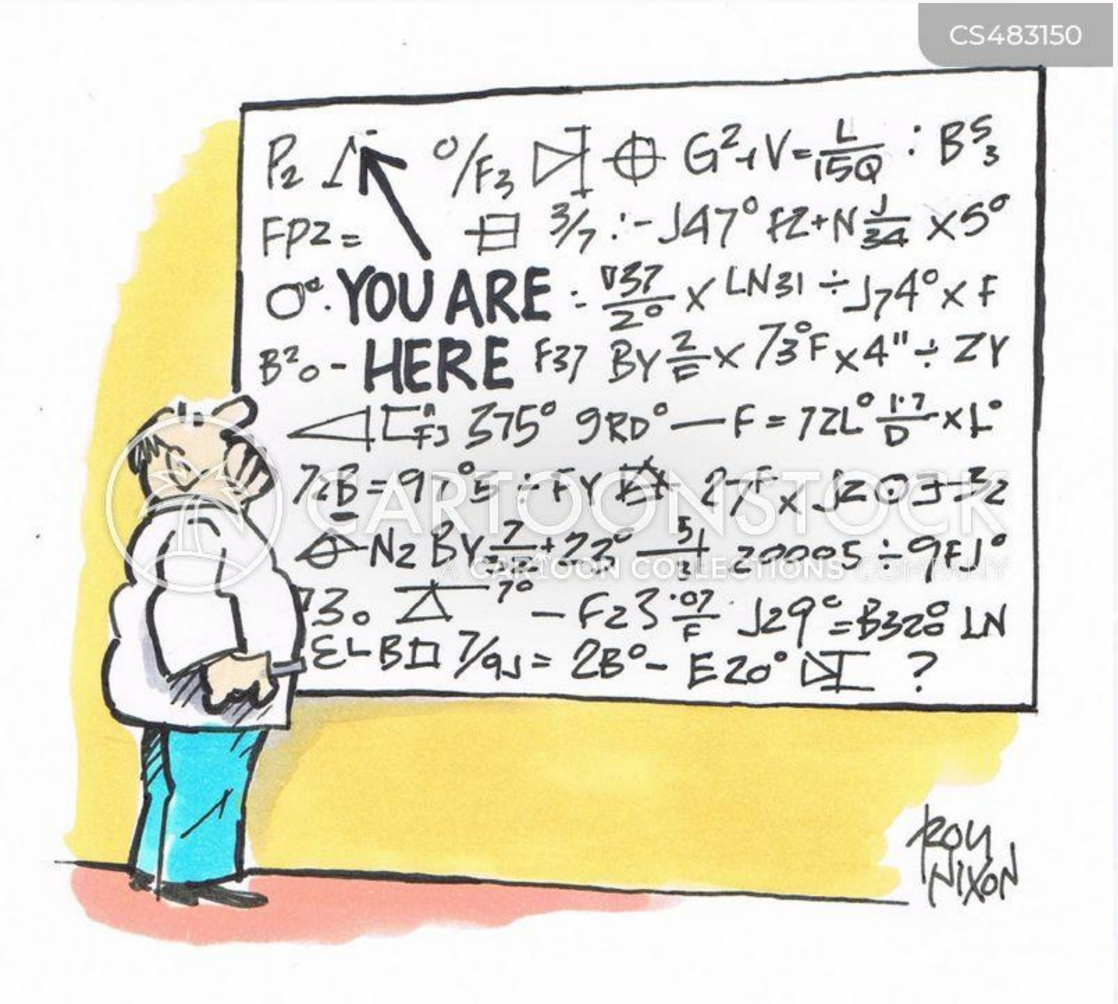
Numerical Methods for Computational Science

MSSE 273, 3 Units

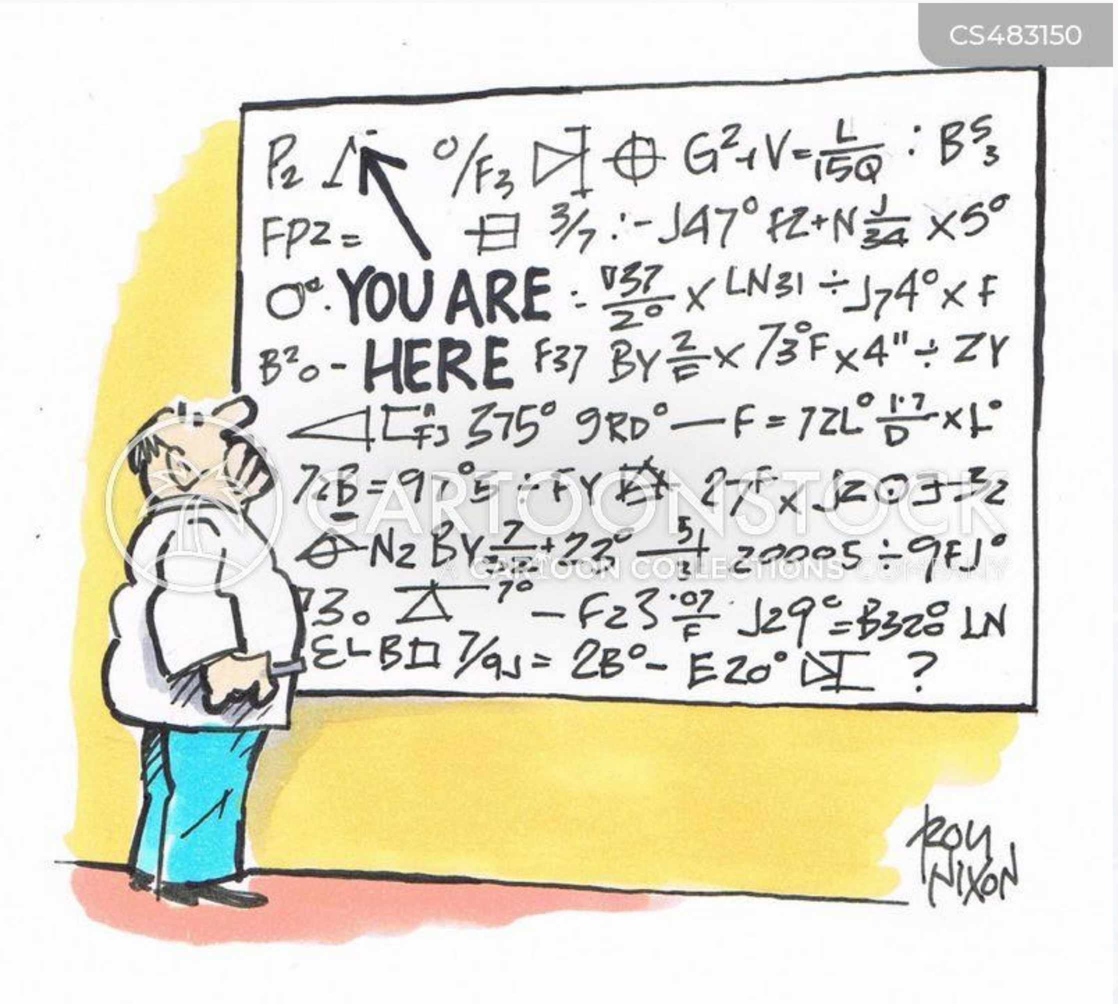
Course Map

Week 1:	Introduction to Scientific Computing and Python Libraries
Week 2:	Linear Algebra Fundamentals
Week 3:	**Vector Calculus**
Week 4:	Numerical Differentiation and Integration
Week 5:	Solving Nonlinear Equations
Week 6:	Probability Theory Basics
Week 7:	Random Variables and Distributions
Week 8:	Statistics for Data Science
Week 9:	Eigenvalues and Eigenvectors
Week 10:	Simulation and Monte Carlo Method
Week 11:	Data Fitting and Regression
Week 12:	Optimization Techniques
Week 13:	Machine Learning Fundamentals



Outline

- Recap: Calculus
- Gradient
- Line Integrals
- Divergence
- Curl



Outline

- **Recap: Calculus**
- Gradient
- Line Integrals
- Divergence
- Curl

derivatives

motivation:

- optimization algorithms (gradient descent and related)
- ANNs learn via **backpropagation** → chain rule
- approximation methods (Taylor series)
- maximum entropy distributions (data analysis, data modelling)
- error estimation and error propagation
- and more…

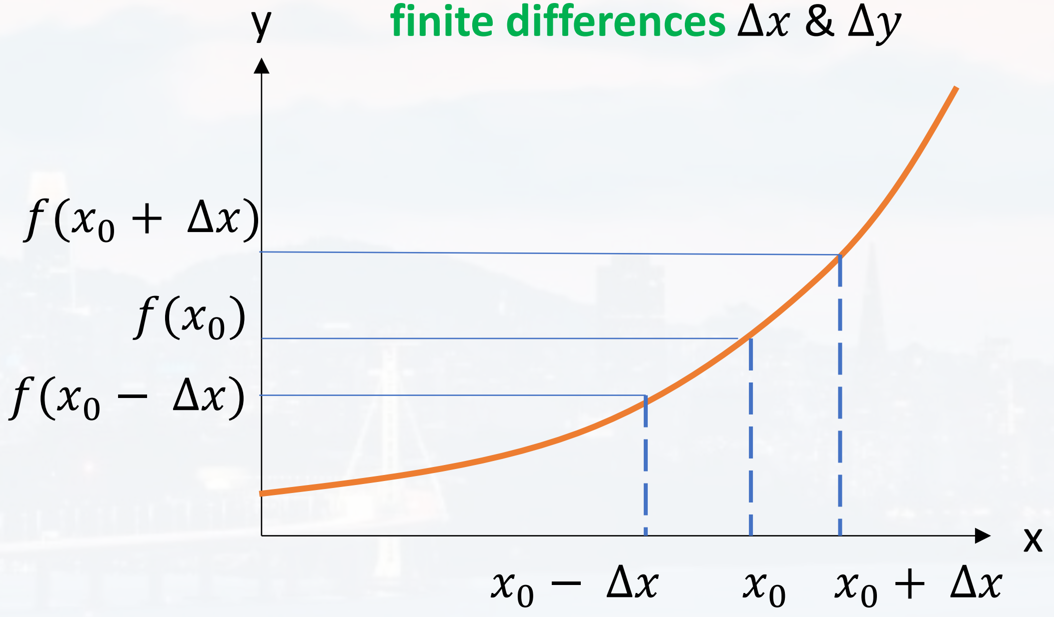
derivatives

slope of a function at $x = x_0$

$$\left.\frac{df^+}{dx}\right|_{x=x_0} = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x}$$

$$\left.\frac{df^-}{dx}\right|_{x=x_0} = \lim_{\Delta x \to 0} \frac{f(x_0) - f(x_0 - \Delta x)}{\Delta x}$$

finite differences Δx & Δy



$$\boxed{\left.\frac{df}{dx}\right|_{x=x_0} = \frac{1}{2}\left(\left.\frac{df^+}{dx}\right|_{x=x_0} + \left.\frac{df^-}{dx}\right|_{x=x_0}\right) = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - f(x_0 - \Delta x)}{2\Delta x}}$$

1st derivative at $x = x_0$

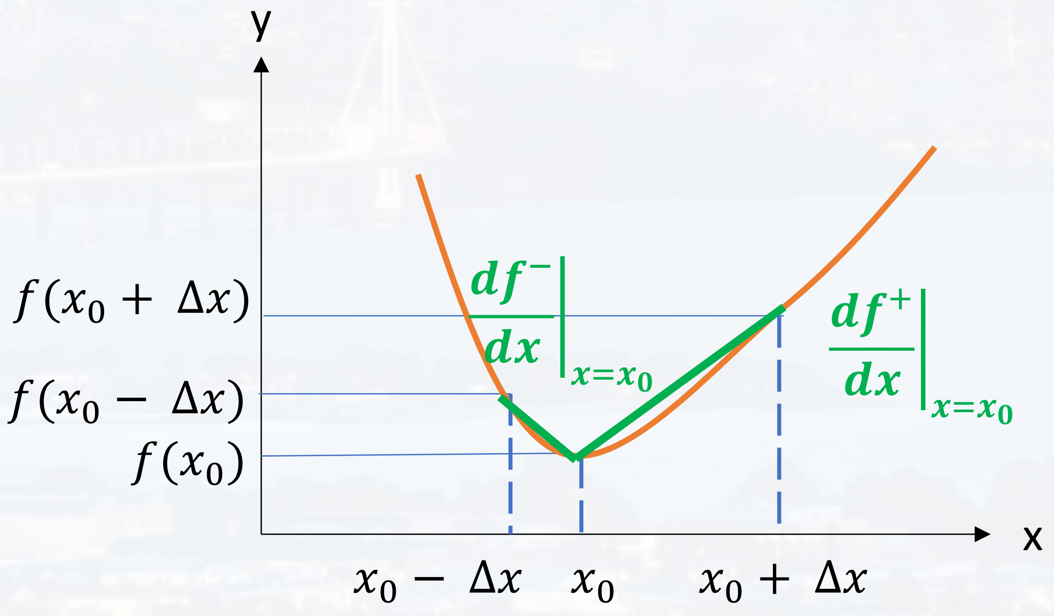
derivatives

$$\boxed{\left.\frac{df}{dx}\right|_{x=x_0} = \frac{1}{2}\left(\left.\frac{df^+}{dx}\right|_{x=x_0} + \left.\frac{df^-}{dx}\right|_{x=x_0}\right) = \lim_{\Delta x\to 0}\frac{f(x_0+\Delta x)-f(x_0-\Delta x)}{2\Delta x}}$$

1st derivative at $x = x_0$

change of the slope of a function at $x = x_0$, aka *curvature*

$$\left.\frac{d^2f}{dx^2}\right|_{x=x_0} = \lim_{\Delta x\to 0}\frac{1}{\Delta x}\left(\left.\frac{df^+}{dx}\right|_{x=x_0} - \left.\frac{df^-}{dx}\right|_{x=x_0}\right)$$



derivatives

$$\boxed{\left.\frac{df}{dx}\right|_{x=x_0} = \frac{1}{2}\left(\left.\frac{df^+}{dx}\right|_{x=x_0} + \left.\frac{df^-}{dx}\right|_{x=x_0}\right) = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - f(x_0 - \Delta x)}{2\Delta x}}$$

1st derivative at $x = x_0$

change of the slope of a function at $x = x_0$, aka *curvature*

$$\left.\frac{d^2 f}{dx^2}\right|_{x=x_0} = \lim_{\Delta x \to 0} \frac{1}{\Delta x}\left(\left.\frac{df^+}{dx}\right|_{x=x_0} - \left.\frac{df^-}{dx}\right|_{x=x_0}\right) = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - 2f(x_0) + f(x_0 - \Delta x)}{\Delta x^2}$$

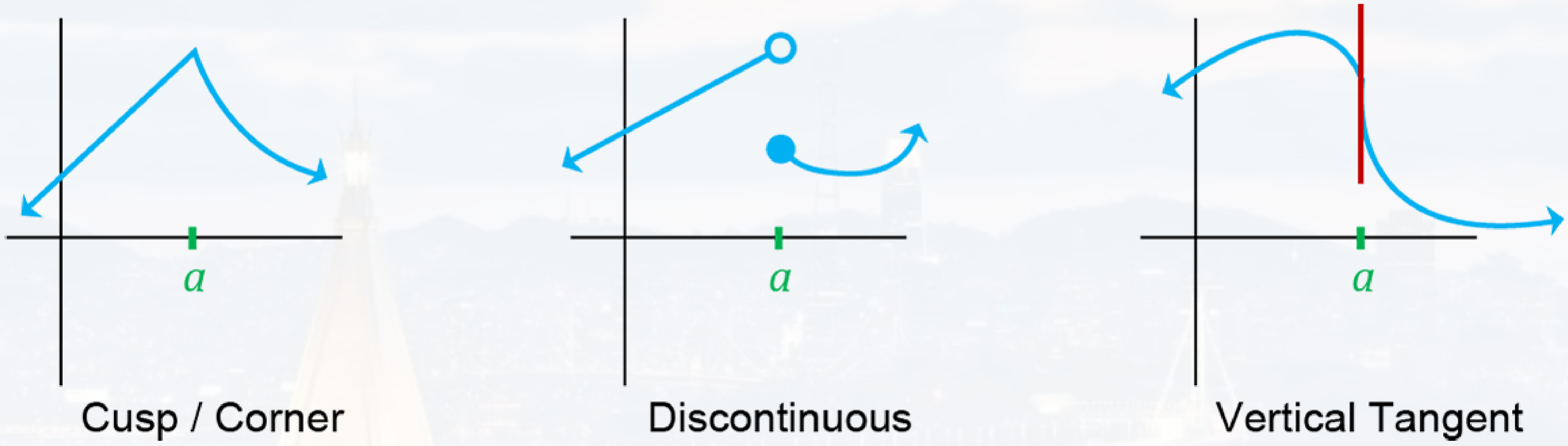
$$\boxed{\left.\frac{d^2 f}{dx^2}\right|_{x=x_0} = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - 2f(x_0) + f(x_0 - \Delta x)}{\Delta x^2}}$$

2nd derivative at $x = x_0$

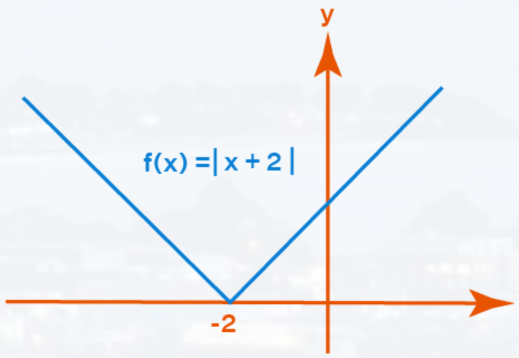
…and so on

derivatives

derivatives are not always defined:

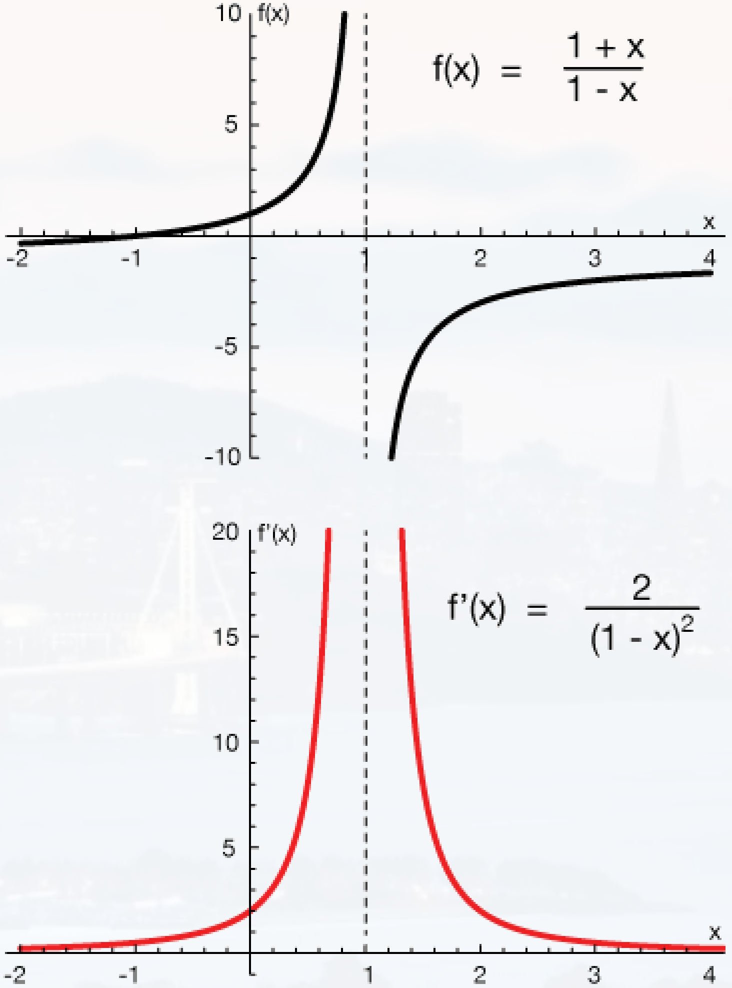


function needs to be **continuous *and* differentiable**



derivatives

derivatives are not always defined:



function needs to be **continuous *and* differentiable**

derivatives

example: $f(x) = \sqrt{x}$

$$\left.\frac{df}{dx}\right|_{x=x_0} = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - f(x_0 - \Delta x)}{2\Delta x}$$

$$= \lim_{\Delta x \to 0} \frac{\sqrt{x_0 + \Delta x} - \sqrt{x_0 - \Delta x}}{2\Delta x}$$

$$= \lim_{\Delta x \to 0} \frac{\left(\sqrt{x_0 + \Delta x} - \sqrt{x_0 - \Delta x}\right)\left(\sqrt{x_0 + \Delta x} + \sqrt{x_0 - \Delta x}\right)}{2\,\Delta x\left(\sqrt{x_0 + \Delta x} + \sqrt{x_0 - \Delta x}\right)}$$

$$= \lim_{\Delta x \to 0} \frac{x_0 + \Delta x - x_0 + \Delta x}{2\,\Delta x\left(\sqrt{x_0 + \Delta x} + \sqrt{x_0 - \Delta x}\right)}$$

$$= \lim_{\Delta x \to 0} \frac{2\Delta x}{2\,\Delta x\left(\sqrt{x_0 + \Delta x} + \sqrt{x_0 - \Delta x}\right)} = \frac{1}{2\sqrt{x_0}}$$

derivatives

$a \in \mathbb{C}$

$n \in \mathbb{R}$

rules:

$$\frac{d}{dx}\, ax^n = \; a\, nx^{n-1}$$

$$\frac{d}{dx}[f(x) + g(x)] = \frac{d}{dx}f(x) + \frac{d}{dx}g(x)$$

sum rule: derivatives are linear

$$\frac{d}{dx}[f(x)g(x)] = g(x)\frac{d}{dx}f(x) + f(x)\frac{d}{dx}g(x)$$

product rule

$$\frac{d}{dx}\boldsymbol{f}[\boldsymbol{g}(\boldsymbol{x})] = \underbrace{\frac{df(x)}{dg(x)}}_{\text{outer derivative}}\;\underbrace{\frac{d}{dx}g(x)}_{\text{inner derivative}}$$

chain rule

derivatives

$a \in \mathbb{C}$
$n \in \mathbb{R}$

special derivatives

$$\frac{d}{dx}\, e^x = e^x$$

the actual definition of e

$$\frac{d}{dx}\, b^x = \ln(b)\, b^x$$

$b > 0$

$$\frac{d}{dx}\, log_b(x) = \frac{1}{x\ln(b)}$$

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

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

derivatives

$a \in \mathbb{C}$
$n \in \mathbb{R}$

$$\frac{d}{dx}\, ax^n = \ a\, nx^{n-1}$$

$$\frac{d}{dx}\, 3x^5 = 15x^4$$

$$\frac{d}{dx}[f(x)+g(x)] = \frac{d}{dx}f(x) + \frac{d}{dx}g(x)$$

$$\frac{d}{dx}\,[3x^5 - 2x] = 15x^4 - 2$$

$$\frac{d}{dx}[f(x)g(x)] = g(x)\frac{d}{dx}f(x) + f(x)\frac{d}{dx}g(x)$$

$$\frac{d}{dx}\,[3x^5\sin(x)] = 15x^4\sin(x) + 3x^5\cos(x)$$

$$\frac{d}{dx}\boldsymbol{f}[\boldsymbol{g}(\boldsymbol{x})] = \frac{df(x)}{dg(x)}\,\frac{d}{dx}g(x)$$

outer derivative inner derivative

$$\frac{d}{dx}\,\mathbf{sin}(\mathbf{3x^5}) = \cos(3x^5)\ 15x^4$$

outer derivative inner derivative

derivatives

Taylor Series

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left.\frac{d^n f}{dx^n}\right|_{x=x_0} (x - x_0)^n$$

n = 0: $f(x) \approx f(x_0)$

n = 1: $f(x) \approx f(x_0) + \left.\frac{df}{dx}\right|_{x=x_0} (x - x_0)$ tangent on f at $x = x_0$

$$\frac{f(x) - f(x_0)}{x - x_0} \approx \left.\frac{df}{dx}\right|_{x=x_0}$$

$$\left.\frac{df^+}{dx}\right|_{x=x_0} = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x}$$

definition of the 1st derivative!

derivatives

Taylor Series

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n f}{dx^n}\bigg|_{x=x_0} (x - x_0)^n$$

n = 0: $f(x) \approx f(x_0)$

n = 1: $f(x) \approx f(x_0) + \frac{df}{dx}\bigg|_{x=x_0} (x - x_0)$ tangent of f at $x = x_0$

n = 2: $f(x) \approx f(x_0) + \frac{df}{dx}\bigg|_{x=x_0} (x - x_0) + \frac{1}{2} \frac{d^2 f}{dx^2}\bigg|_{x=x_0} (x - x_0)^2$

derivatives

Taylor Series

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left.\frac{d^n f}{dx^n}\right|_{x=x_0} (x - x_0)^n$$

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n = 2: $f(x) \approx f(x_0) + \left.\frac{df}{dx}\right|_{x=x_0} (x - x_0) + \frac{1}{2} \left.\frac{d^2 f}{dx^2}\right|_{x=x_0} (x - x_0)^2$

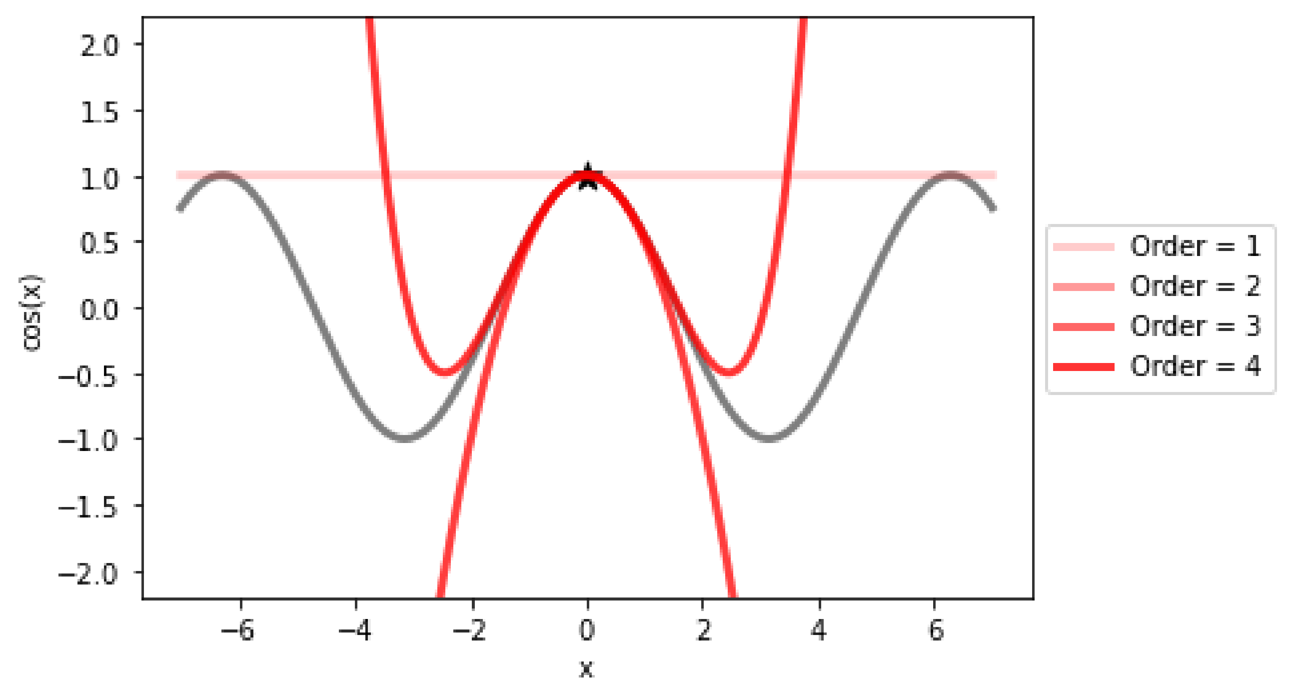
exercise:
- write down the Taylor Series of *sin(x)*, *cos(x)* and e^x at $x_0 = 0$
- express all three series as an infinite sum
- try to combine all three equations by introducing a new mathematical object $\boldsymbol{i}$ which only property is $\boldsymbol{i^2 = -1}$

derivatives

Taylor Series

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left. \frac{d^n f}{dx^n} \right|_{x=x_0} (x - x_0)^n$$

run the function `PlotTaylorSeries.py`



derivatives

Taylor Series

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n f}{dx^n}\bigg|_{x=x_0} (x - x_0)^n$$

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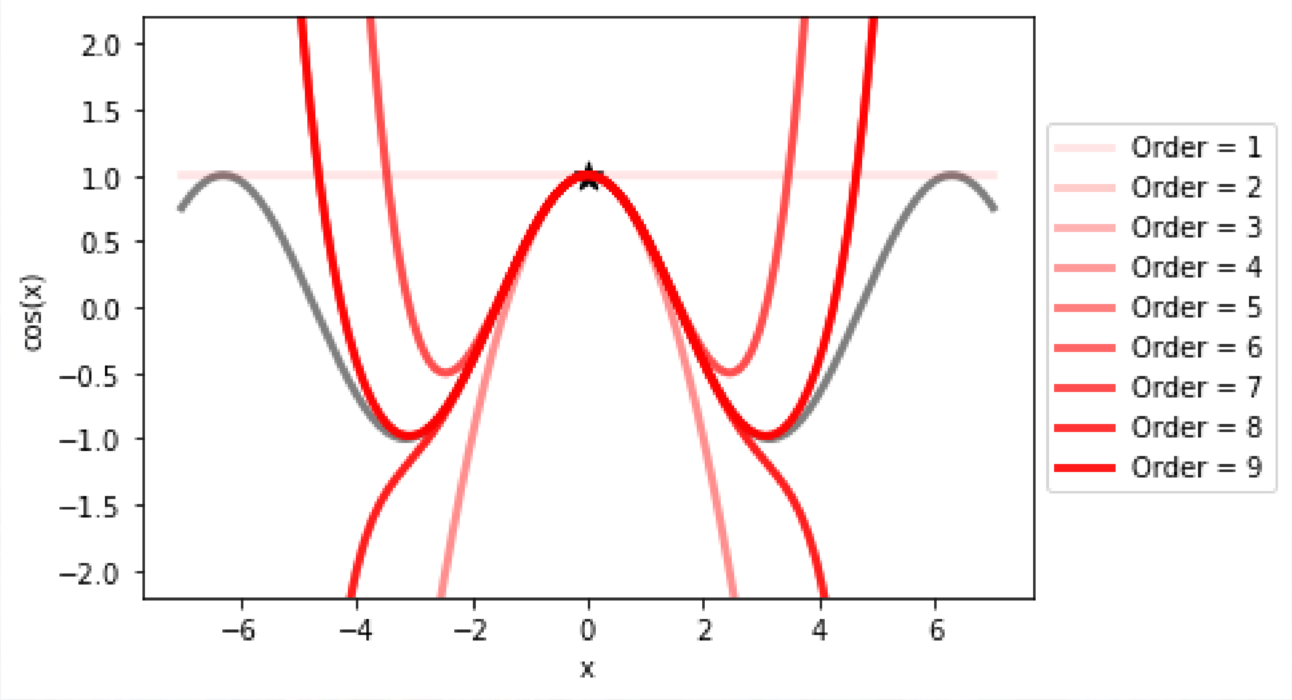

derivatives

Taylor Series

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n f}{dx^n}\bigg|_{x=x_0} (x - x_0)^n$$

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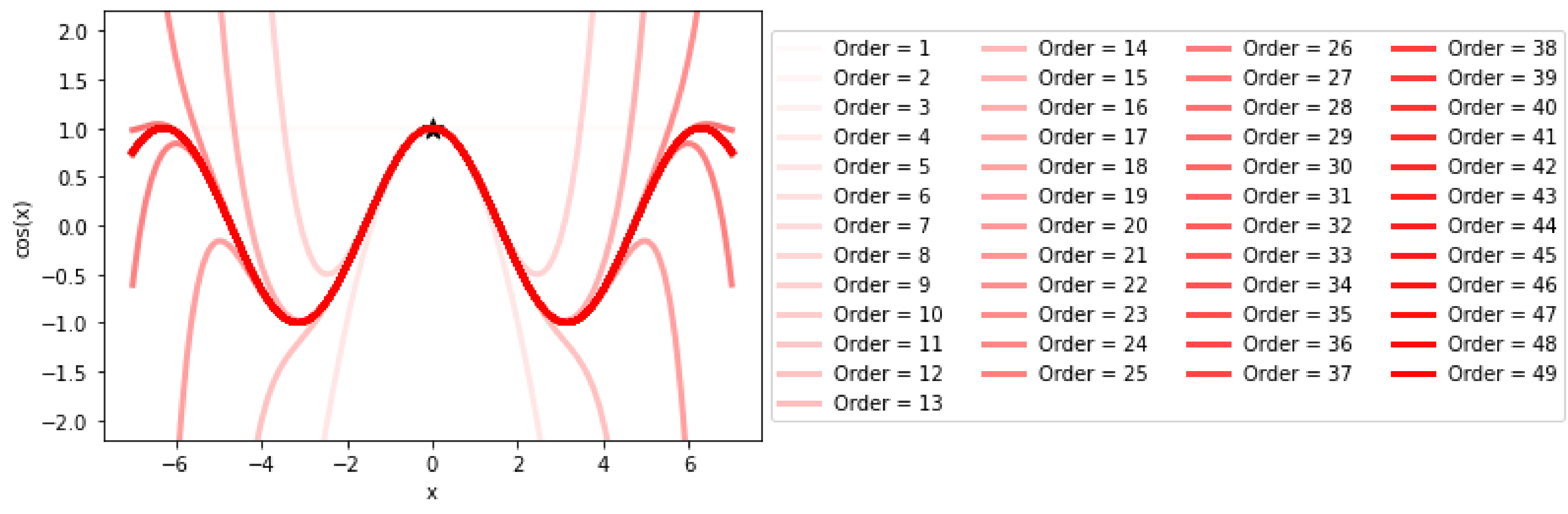


integrals

motivation:

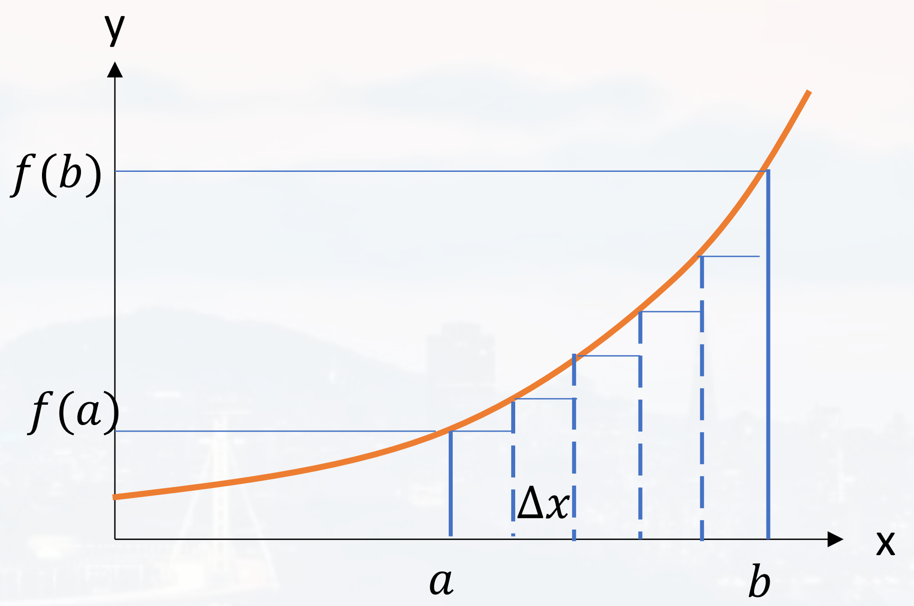
- deriving probabilities from likelihood functions
- normalization tools
- calculating volumes, areas, flow, energy, etc….
- sums → integral

integrals area under a curve (1D)

$$\int_a^b f(x)\,dx = \lim_{\Delta x \to 0} \boxed{\sum_{i=0}^{N-1} f(a + i\,\Delta x)\,\Delta x}$$

$$N = \frac{b - a}{\Delta x}$$

$$\boxed{A_{tot} \approx}$$



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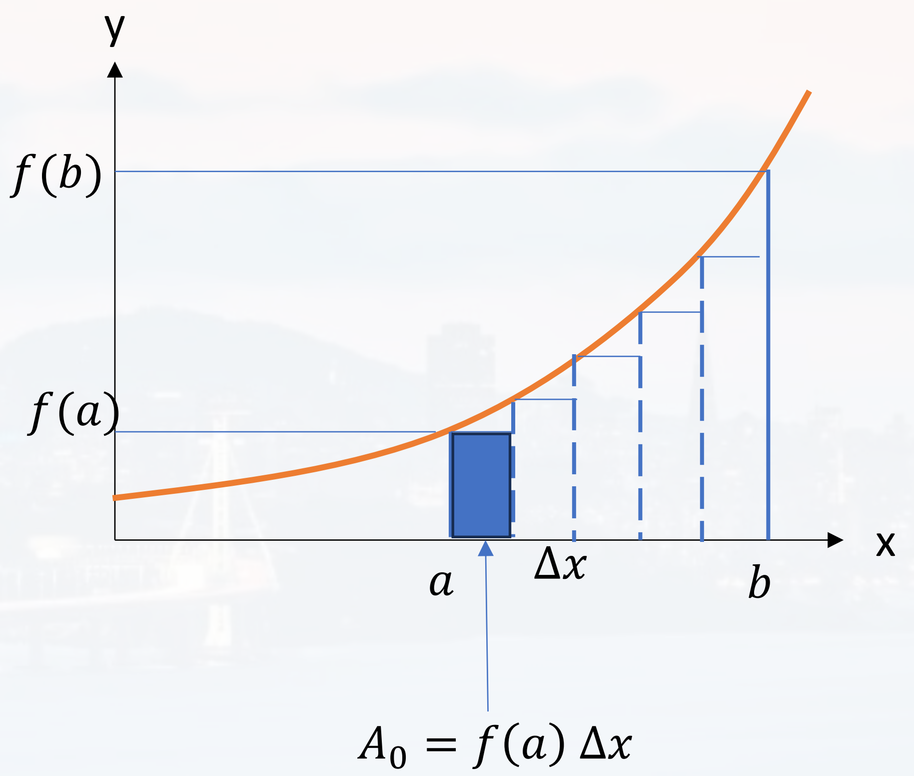
$$\int_a^b f(x)\,dx = \lim_{\Delta x \to 0} \boxed{\sum_{i=0}^{N-1} f(a + i\,\Delta x)\,\Delta x}$$

$$N = \frac{b-a}{\Delta x}$$

$$\boxed{A_{tot} \approx}\ f(a)\,\Delta x$$

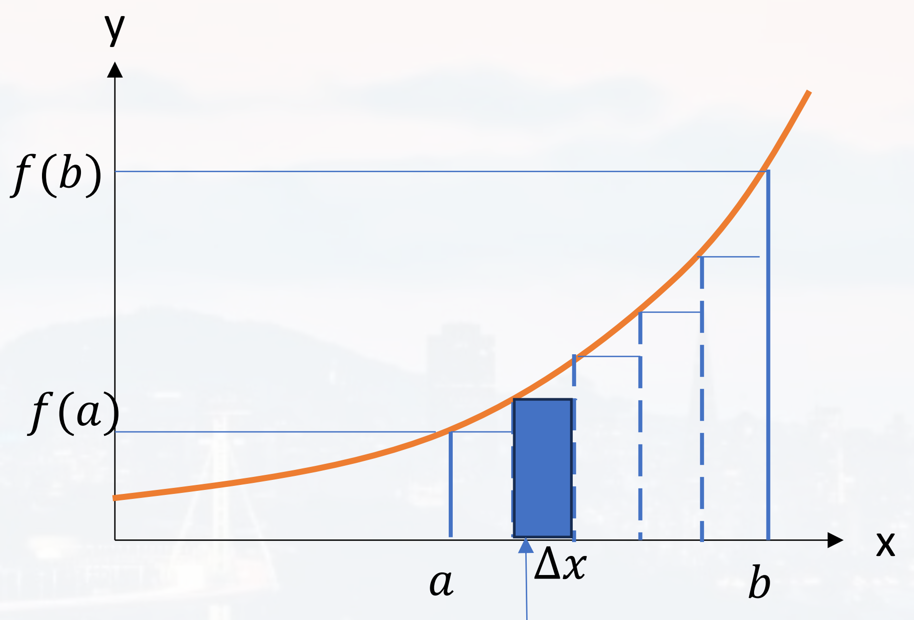


integrals area under a curve (1D)

$$\int_a^b f(x)\,dx = \lim_{\Delta x \to 0} \boxed{\sum_{i=0}^{N-1} f(a + i\,\Delta x)\,\Delta x}$$

$$N = \frac{b - a}{\Delta x}$$

$$\boxed{A_{tot} \approx} \; f(a)\,\Delta x + f(a + \Delta x)\,\Delta x$$



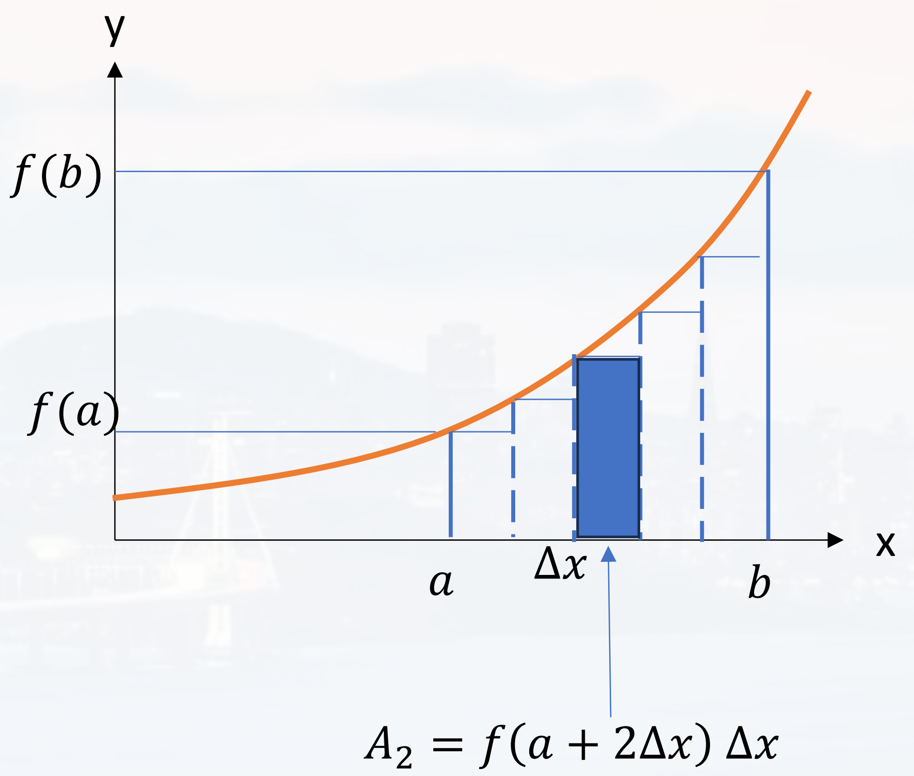
$$A_1 = f(a + \Delta x)\,\Delta x$$

integrals area under a curve (1D)

$$\int_a^b f(x)\,dx = \lim_{\Delta x \to 0} \boxed{\sum_{i=0}^{N-1} f(a + i\,\Delta x)\,\Delta x}$$

$$N = \frac{b-a}{\Delta x}$$

$$\boxed{A_{tot} \approx} \; f(a)\,\Delta x + f(a+\Delta x)\,\Delta x + f(a+2\Delta x)\,\Delta x$$

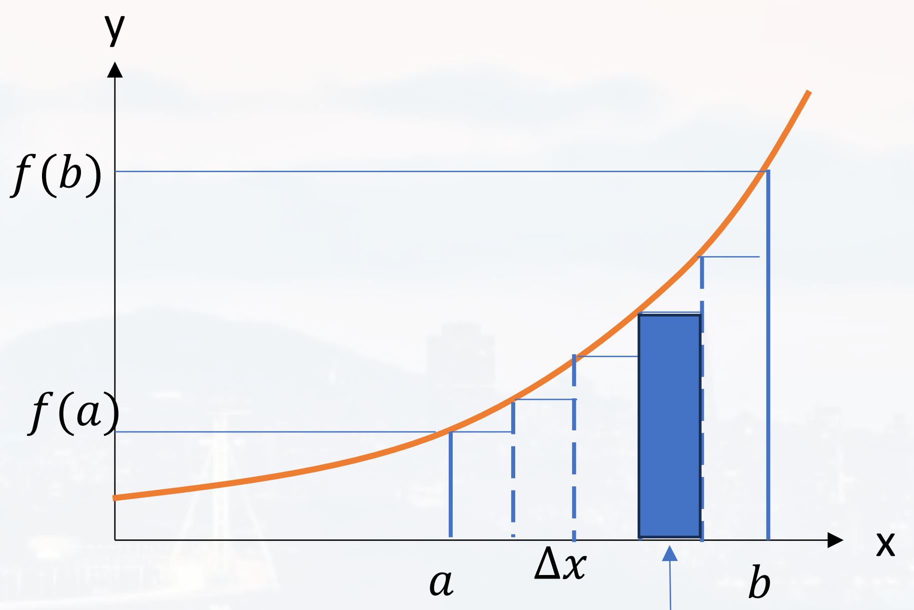


integrals area under a curve (1D)

$$\int_a^b f(x)\,dx = \lim_{\Delta x \to 0} \boxed{\sum_{i=0}^{N-1} f(a + i\,\Delta x)\,\Delta x}$$

$$N = \frac{b-a}{\Delta x}$$

$$\boxed{A_{tot} \approx} \; f(a)\,\Delta x + f(a+\Delta x)\,\Delta x + f(a+2\Delta x)\,\Delta x + f(a+3\Delta x)\,\Delta x$$



$$A_3 = f(a+3\Delta x)\,\Delta x$$

integrals

area under a curve (1D)

$$\int_a^b f(x)\,dx = \lim_{\Delta x \to 0} \boxed{\sum_{i=0}^{N-1} f(a + i\,\Delta x)\,\Delta x}$$

$$N = \frac{b - a}{\Delta x}$$

$$\boxed{A_{tot} \approx} \; f(a + \mathbf{0}\Delta x)\,\Delta x$$

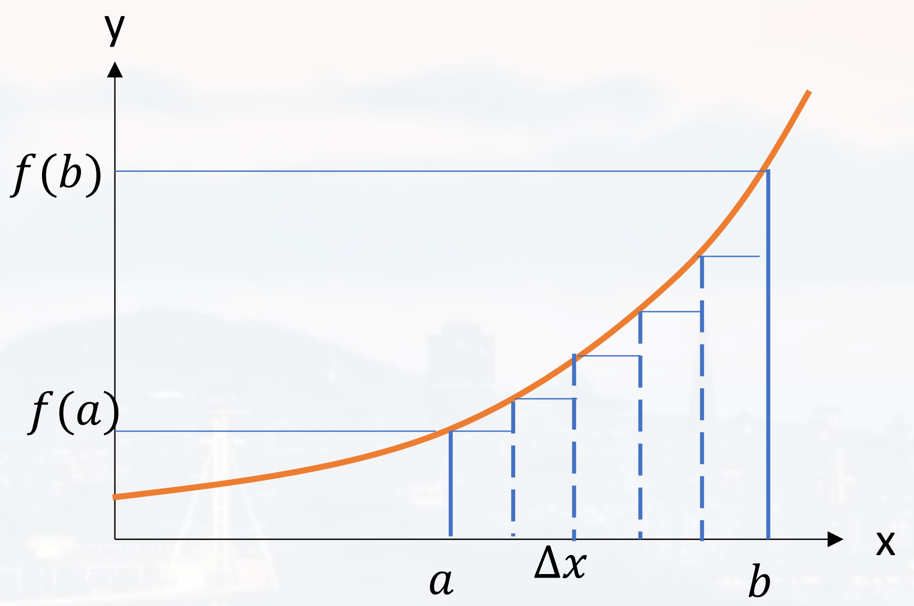
$$+ f(a + \mathbf{1}\Delta x)\,\Delta x$$

$$+ f(a + \mathbf{2}\Delta x)\,\Delta x$$

$$+ f(a + \mathbf{3}\Delta x)\,\Delta x$$

$$+ f(a + \mathbf{4}\Delta x)\,\Delta x$$

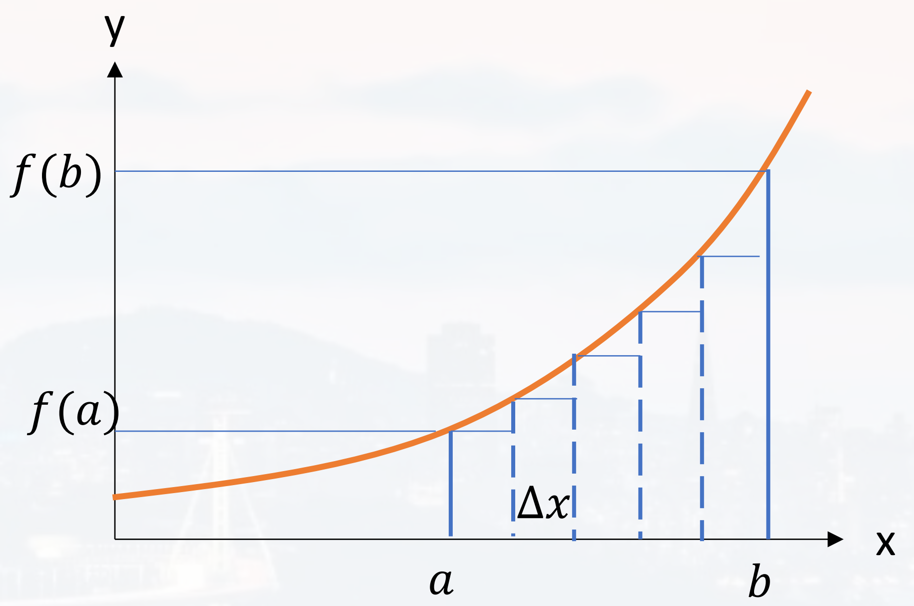
$$+ \cdots \qquad = \sum_{i=0}^{N-1} f(a + i\,\Delta x)\,\Delta x$$



integrals area under a curve (1D)

$$\int_a^b f(x)\,dx = \lim_{\Delta x \to 0} \sum_{i=0}^{N-1} f(a + i\,\Delta x)\,\Delta x$$

$$N = \frac{b-a}{\Delta x}$$



more accurate:

$$\int_a^b f(x)\,dx = \lim_{\Delta x \to 0} \sum_{i=0}^{N-1} [f(a + i\,\Delta x) + f(a + (i+1)\,\Delta x)]\,\frac{\Delta x}{2}$$

trapezoidal rule

error (for large N):

$$\varepsilon = -\frac{(b-a)^2}{12\,N^2}\,[f'(b) - f'(a)] + O(N^{-3})$$

integrals

$$\int_a^b f(x)\,dx = \lim_{\Delta x\to 0}\sum_{i=0}^{N-1}[f(a+i\,\Delta x)+f(a+(i+1)\,\Delta x)]\,\frac{\Delta x}{2} \qquad N=\frac{b-a}{\Delta x}$$

example: $f(x) = x^2$

$$\int_a^b x^2\,dx = \lim_{\Delta x\to 0}\sum_{i=0}^{N-1}[(a+i\,\Delta x)^2+(a+(i+1)\,\Delta x)^2]\,\frac{\Delta x}{2}$$

$$= \lim_{\Delta x\to 0}\sum_{i=0}^{N-1}[2a^2+i^2\Delta x^2+2ai\Delta x+a^2+(i+1)^2\Delta x^2+2a(i+1)\Delta x]\,\frac{\Delta x}{2}$$

$$= \lim_{\Delta x\to 0}\sum_{i=0}^{N-1}[2a^2+i^2\Delta x^2+2ai\Delta x+i^2\Delta x^2+\Delta x^2+2i\Delta x^2+2ai\Delta x+2a\Delta x]\,\frac{\Delta x}{2}$$

integrals

example: $f(x) = x^2$

$$N = \frac{b - a}{\Delta x}$$

$$= \lim_{\Delta x \to 0} \sum_{i=0}^{N-1} [2a^2 + i^2\Delta x^2 + 2ai\Delta x + i^2\Delta x^2 + \Delta x^2 + 2i\Delta x^2 + 2ai\Delta x + 2a\Delta x] \frac{\Delta x}{2}$$

$$= \lim_{\Delta x \to 0} \left[\Delta x a^2 N + \Delta x^3 \sum_{i=0}^{N-1} i^2 + 2a\Delta x^2 \sum_{i=0}^{N-1} i + \frac{\Delta x^3}{2} N + \Delta x^3 \sum_{i=0}^{N-1} i + a\Delta x^2 N\right]$$

$$= \lim_{\Delta x \to 0} \left[\Delta x a^2 N + \Delta x^3 \sum_{i=0}^{N-1} i^2 + 2a\Delta x^2 \sum_{i=0}^{N-1} i + \Delta x^3 \sum_{i=0}^{N-1} i\right]$$

integrals

$$N = \frac{b - a}{\Delta x}$$

example: $f(x) = x^2$

$$= \lim_{\Delta x \to 0} \left[\Delta x a^2 N + \Delta x^3 \sum_{i=0}^{N-1} i^2 + 2a\Delta x^2 \sum_{i=0}^{N-1} i + \Delta x^3 \sum_{i=0}^{N-1} i \right]$$

$$= \lim_{\Delta x \to 0} \left[\Delta x a^2 N + \Delta x^3 \frac{N(N+1)(2N+1)}{6} + a\Delta x^2 N(N+1) + \Delta x^3 \frac{N(N+1)}{2} \right]$$

$$= \lim_{\Delta x \to 0} \left[\Delta x a^2 N + \Delta x^3 \frac{N(N+1)(2N+1)}{6} + a\Delta x^2 N(N+1) \right]$$

$$= \lim_{\Delta x \to 0} \left[\Delta x a^2 N + \Delta x^3 \frac{(N^2+N)(2N+1)}{6} + a\Delta x^2 N^2 + a\Delta x^2 N \right]$$

integrals

$$N = \frac{b - a}{\Delta x}$$

example: $f(x) = x^2$

$$= \lim_{\Delta x \to 0} \left[\Delta x a^2 N + \Delta x^3 \frac{(N^2 + N)(2N + 1)}{6} + a\Delta x^2 N^2 + a\Delta x^2 N\right]$$

$$= \lim_{\Delta x \to 0} \left[\Delta x a^2 N + \Delta x^3 \frac{2N^3 + 3N^2 + N}{6} + a\Delta x^2 N^2\right]$$

$$= \lim_{\Delta x \to 0} \left[\Delta x a^2 \frac{b - a}{\Delta x} + \Delta x^3 \frac{2\left(\frac{b - a}{\Delta x}\right)^3 + 3\left(\frac{b - a}{\Delta x}\right)^2 + \frac{b - a}{\Delta x}}{6} + a\Delta x^2 \left(\frac{b - a}{\Delta x}\right)^2\right]$$

$$= a^2(b - a) + \frac{(b - a)^3}{3} + a(b - a)^2 = \frac{(b - a)^3}{3}$$

$$\int_a^b x^2\, dx = \frac{(b - a)^3}{3}$$

integrals

$a, c \in \mathbb{C}$

$n \in \mathbb{R}$

rules:

$$\int \frac{d}{dx} f(x)\, dx = \int df(x) = f(x) + c$$

therefore: an integral is an **anti derivative!**

$$\int a x^n \, dx = a \frac{1}{n+1} x^{n+1} + c \quad n \neq -1$$

$$\int f(x) + g(x)\, dx = \int f(x)\, dx + \int g(x)\, dx + c$$

sum rule: integrals are linear

$$\int f(x) \frac{d}{dx} g(x) \; dx = f(x) g(x) + \int \frac{d}{dx} f(x) \cdot \; g(x) dx + c$$

product rule

integrals

$a, c \in \mathbb{C}$
$n \in \mathbb{R}$

special integrals

$$\int e^x \, dx = e^x + c$$

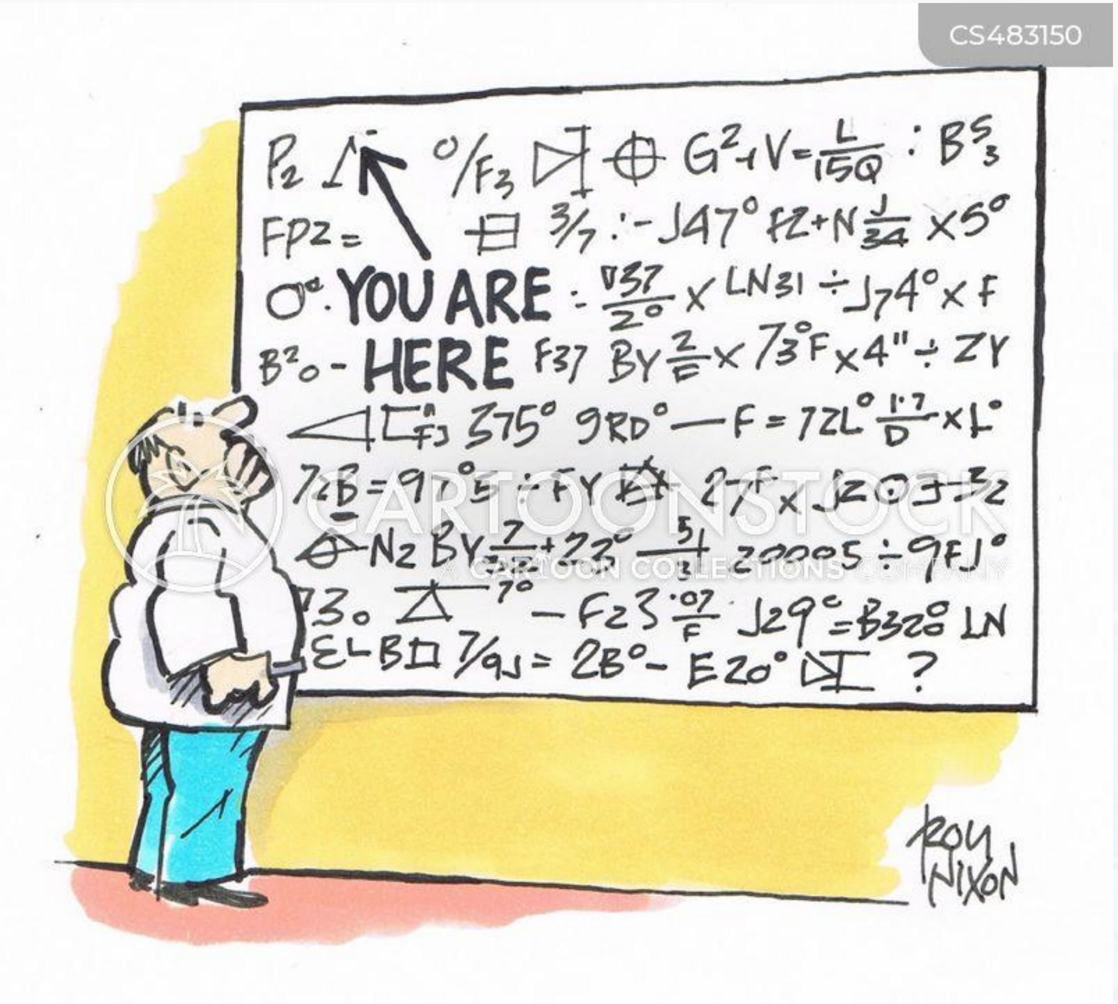
$$\int a^x \, dx = \frac{a^x}{\ln(a)} + c$$

$$\int \frac{1}{x} dx = \ln(|x|) + c$$

$$\int log_b(x) \, dx = x log_b(x) - \frac{x}{\ln(b)} + c$$

$$\int cos(x) \, dx = \sin(x) + c$$

$$\int sin(x) \, dx = -\cos(x) + c$$



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- **Gradient**
- Line Integrals
- Divergence
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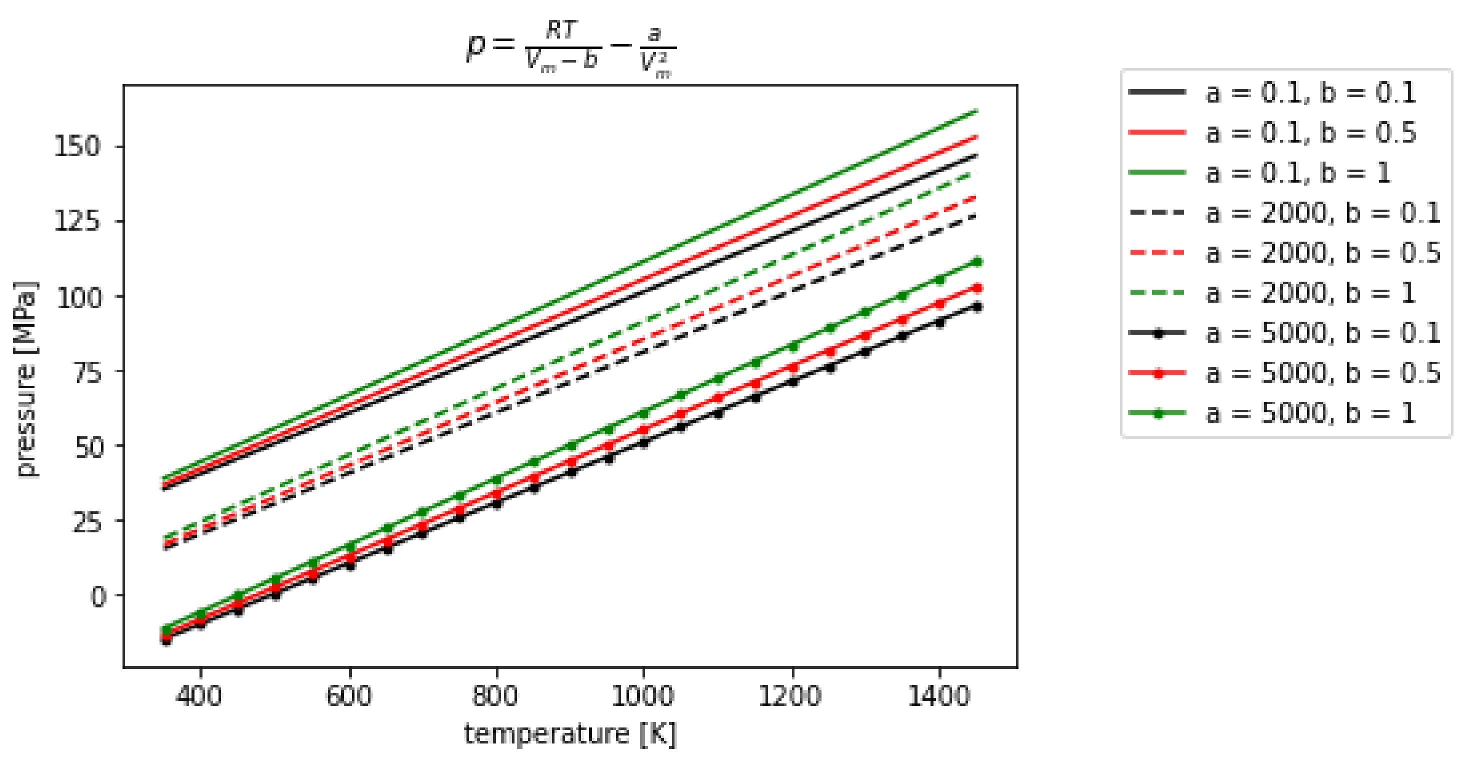
the problem: often we need to find the minimum of a geometrical complex function

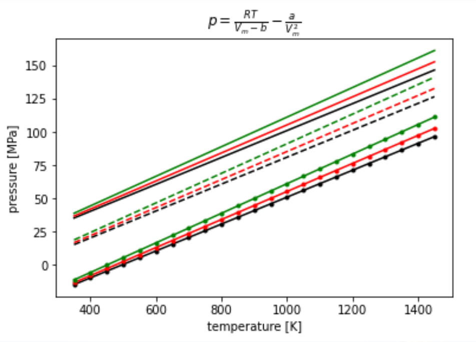


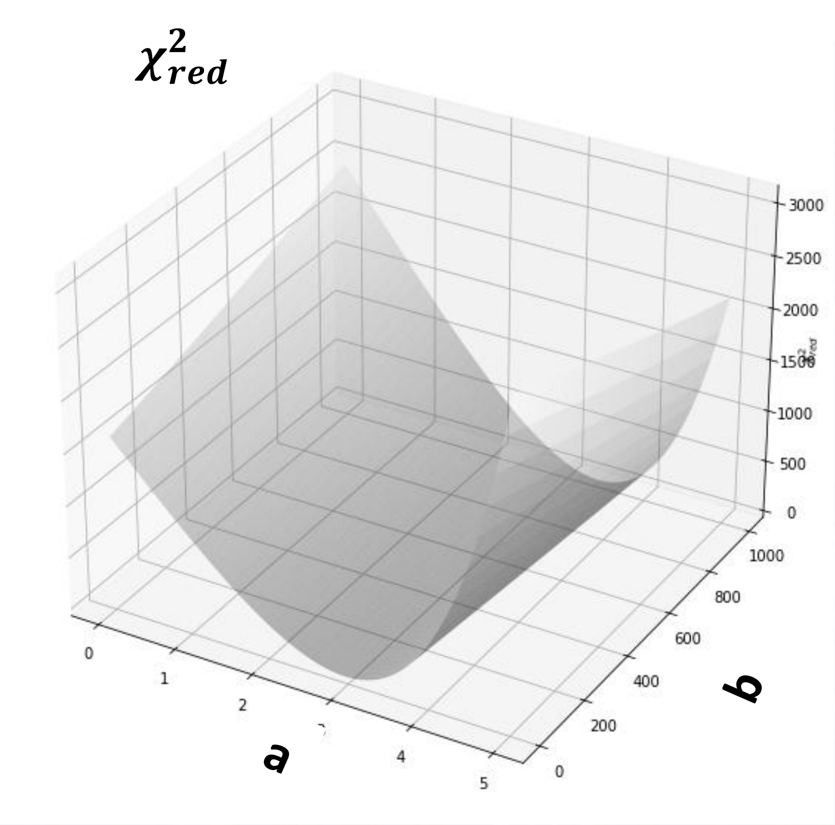
finding ***a*** and ***b*** of a van-der-Waals gas

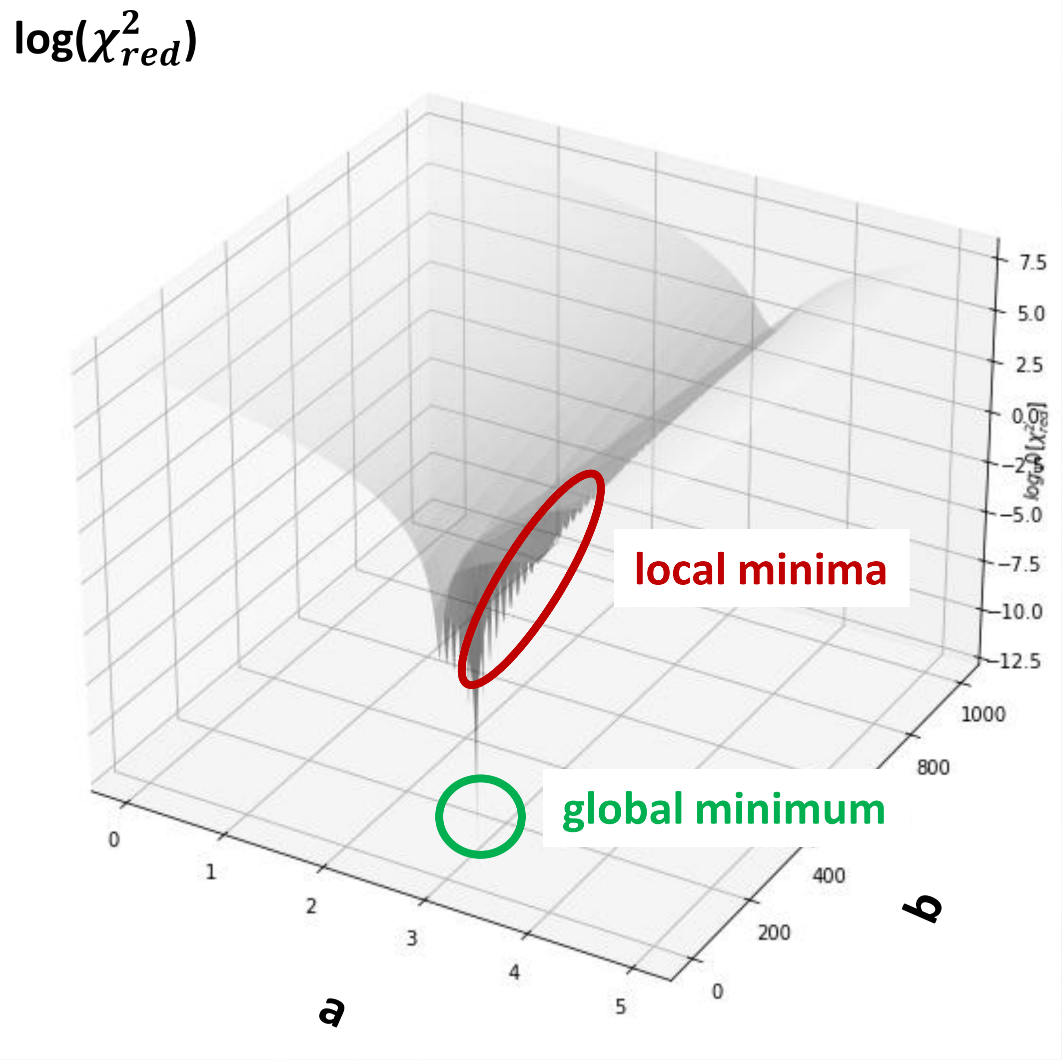
if critical points are not accessible
→ fitting curve, finding ***a*** and ***b***

the problem:

often we need to find the minimum of a geometrical complex function

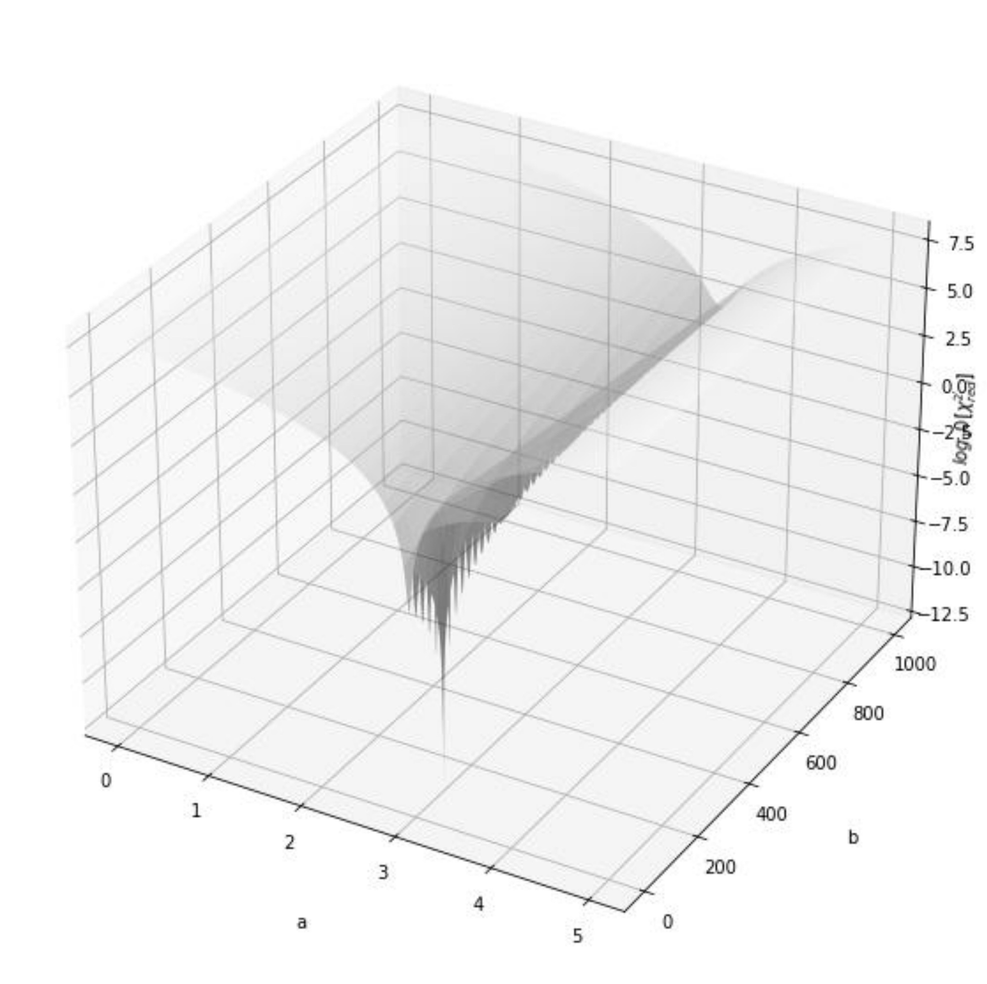




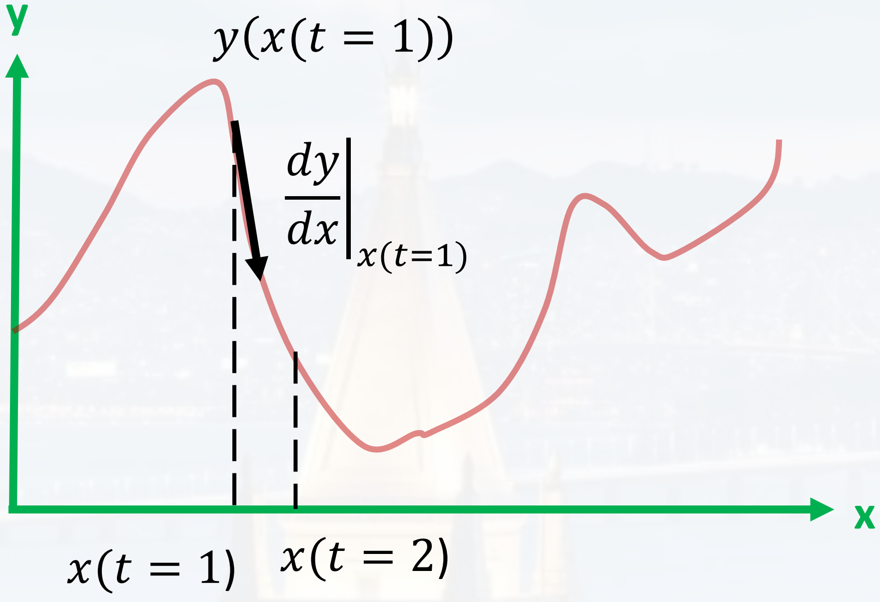


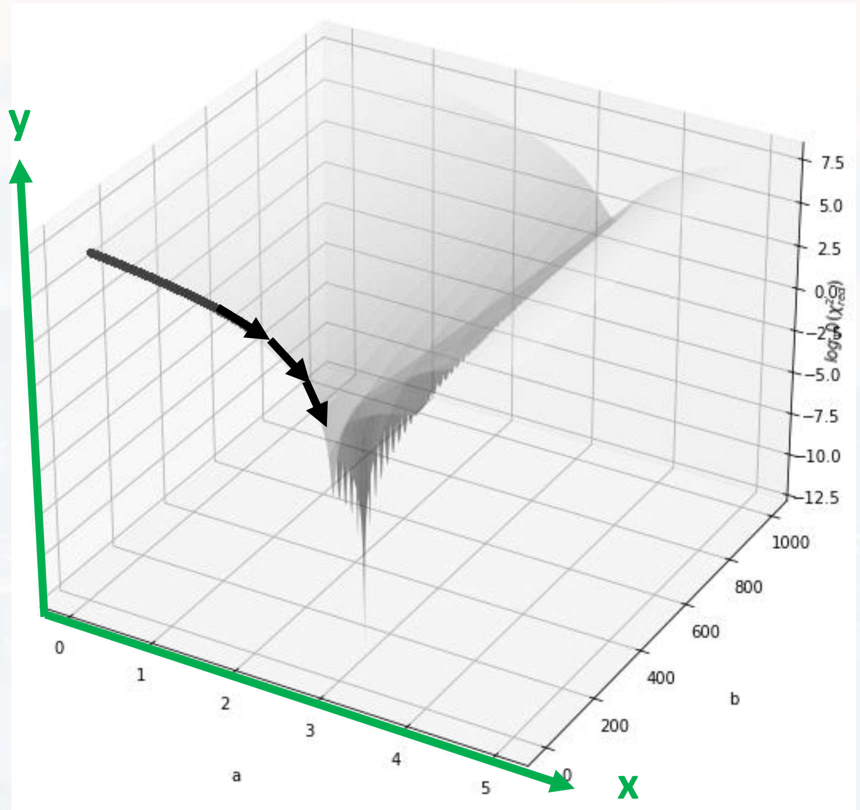
the problem: often we need to find the minimum of a geometrical complex function

These functions are very complicated, not analytical at all



$$\left.\frac{dy}{dx}\right|_{x_0} \approx \frac{y(x_0+\Delta x) - y(x_0-\Delta x)}{2\Delta x}$$





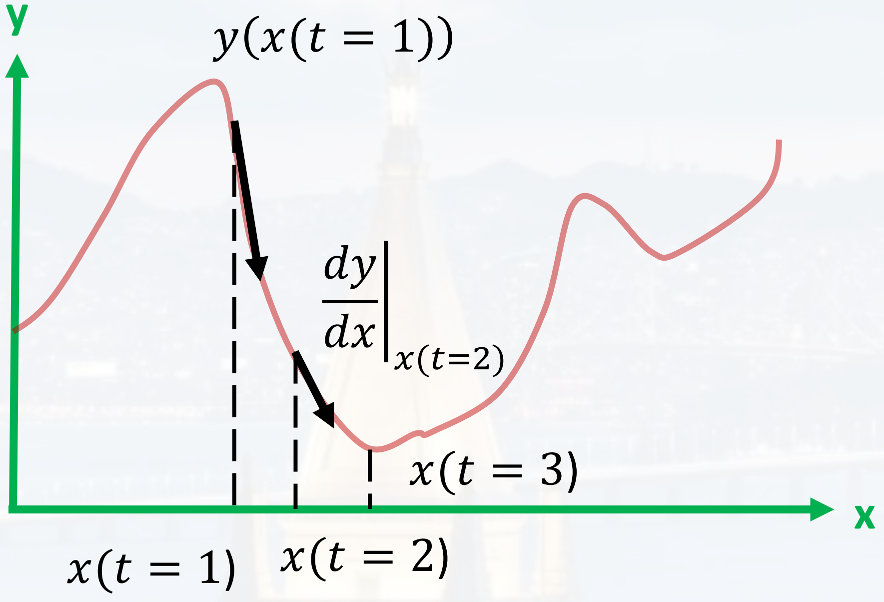
$$x(t=2) = x(t=1) - \varepsilon \left.\frac{dy}{dx}\right|_{x(t=1)}$$

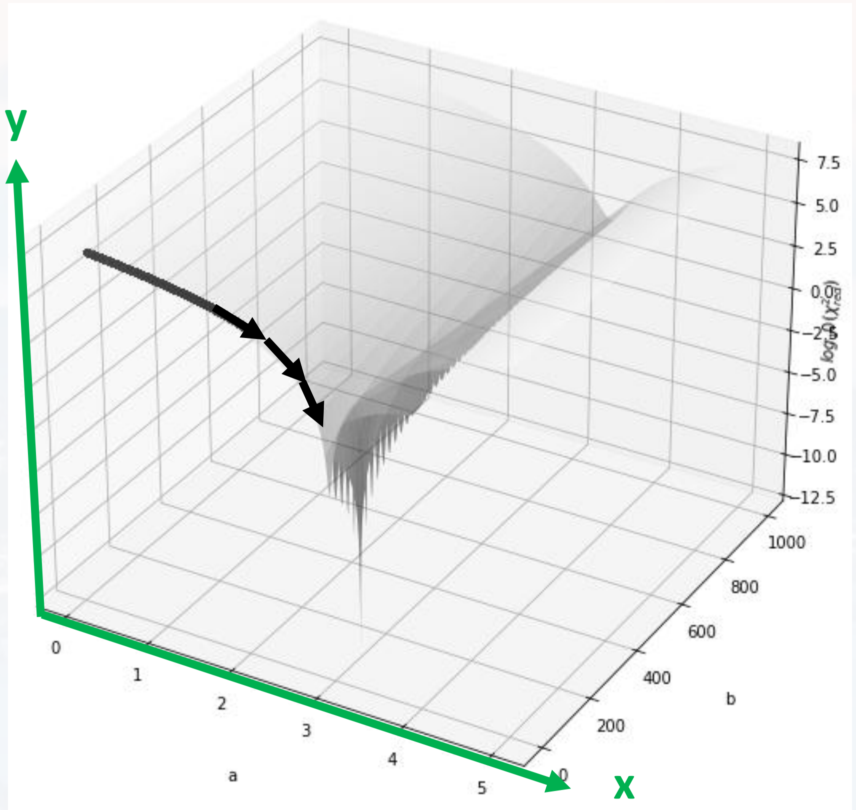
$\varepsilon > 0$

Vector Calculus

Gradient

$$\left.\frac{dy}{dx}\right|_{x_0} \approx \frac{y(x_0+\Delta x) - y(x_0-\Delta x)}{2\Delta x}$$

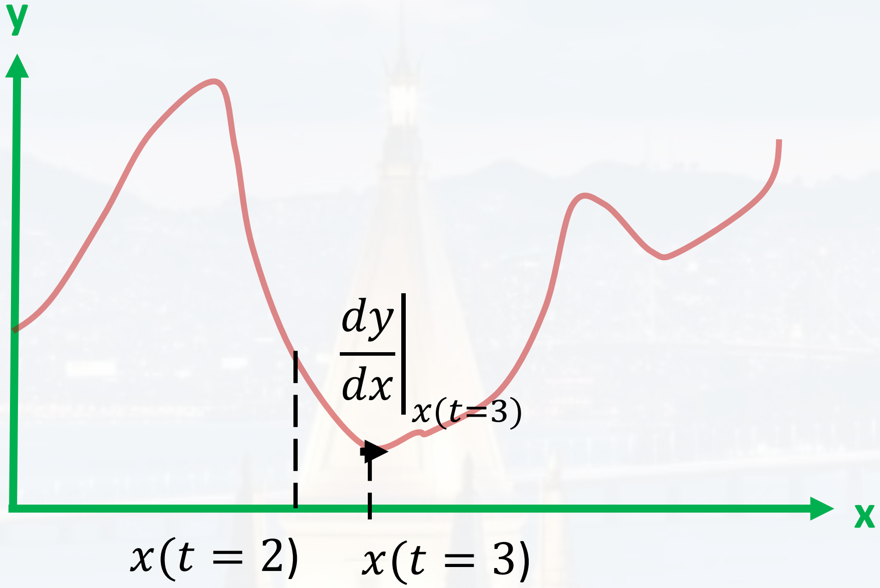


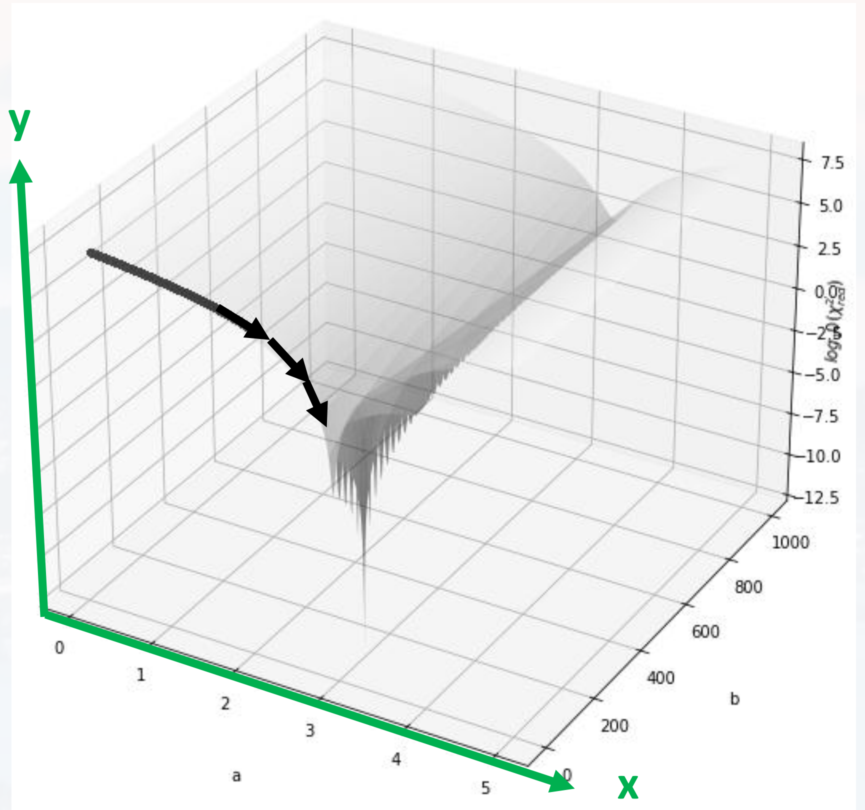


$$x(t=3) = x(t=2) - \varepsilon \left.\frac{dy}{dx}\right|_{x(t=2)}$$

$\varepsilon > 0$

$$\left.\frac{dy}{dx}\right|_{x_0} \approx \frac{y(x_0+\Delta x) - y(x_0-\Delta x)}{2\Delta x}$$





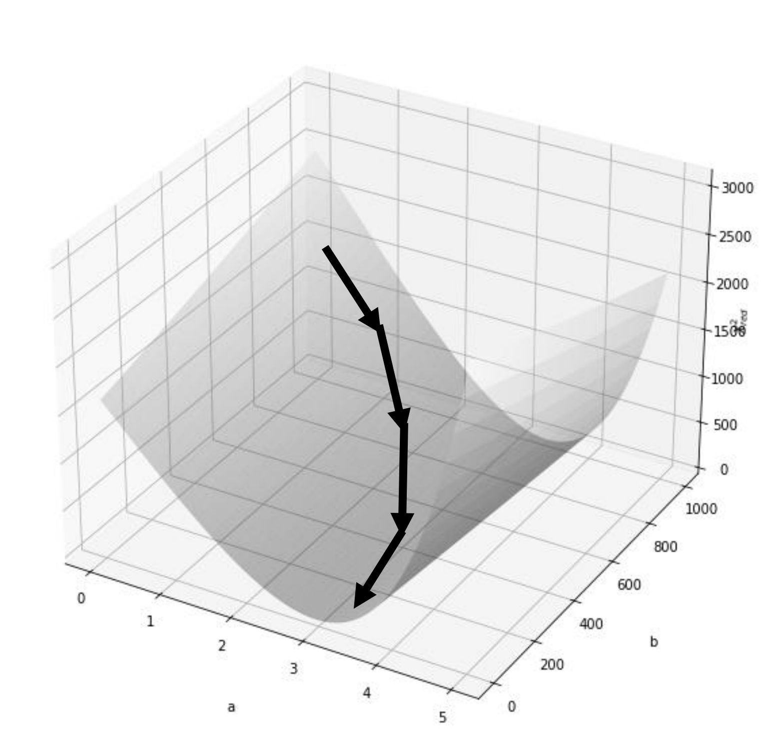
$$x(t=4) = x(t=3) - \varepsilon\left.\frac{dy}{dx}\right|_{x(t=3)}$$

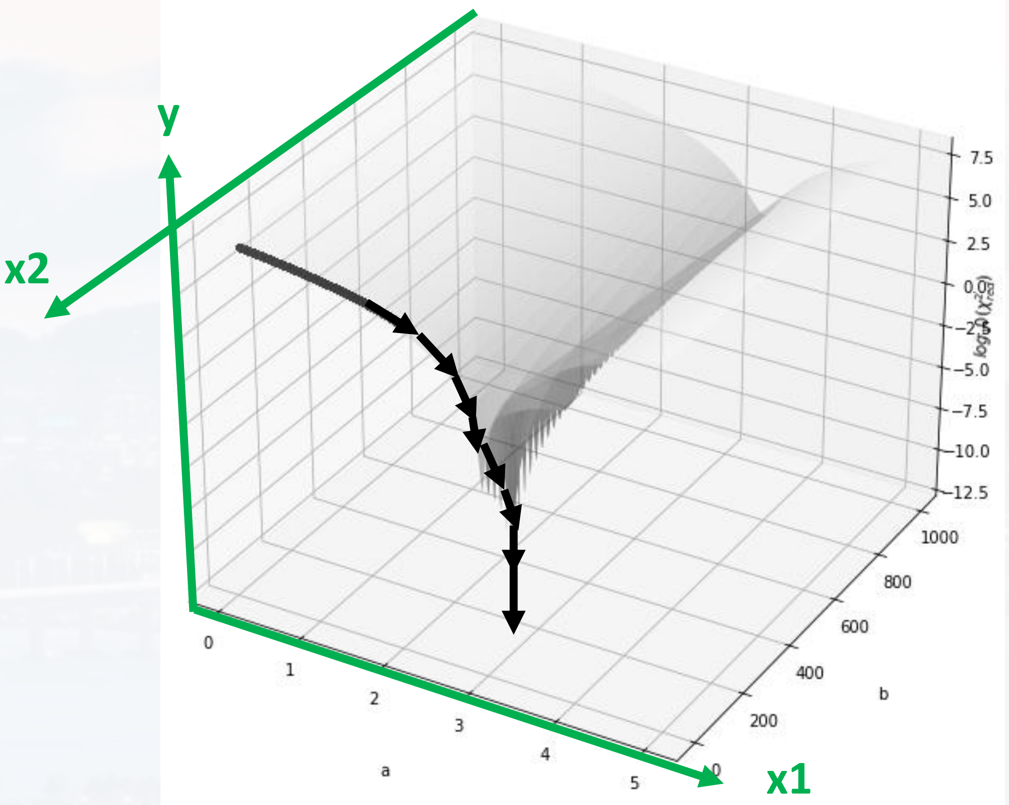
$\varepsilon > 0$

Vector Calculus

$$\left.\frac{\partial y}{\partial x_1}\right|_{x_1^*;\,x_2^*} \approx \frac{y(x_1^* + \Delta x_1,\ x_2^*) - y(x_1^* - \Delta x_1,\ x_2^*)}{2\Delta x_1}$$

$$\left.\frac{\partial y}{\partial x_2}\right|_{x_1^*;\,x_2^*} \approx \frac{y(x_1^*,\ x_2^* + \Delta x_2)\ - y(x_1^*,\ x_2^* - \Delta x_2)}{2\Delta x_2}$$





$$\left.\frac{\partial y}{\partial x_1}\right|_{x_1^*;\, x_2^*; \ldots;\, x_N^*} \approx \frac{y(x_1^* + \Delta x_1,\ x_2^*, \ldots, x_N^*) - y(x_1^* - \Delta x_1,\ x_2^*, \ldots, x_N^*)}{2\Delta x_1}$$

$$\left.\frac{\partial y}{\partial x_2}\right|_{x_1^*;\, x_2^*; \ldots;\, x_N^*} \approx \frac{y(x_1^*, x_2^* + \Delta x_2, \ldots, x_N^*) - y(x_1^*, x_2^* - \Delta x_2, \ldots, x_N^*)}{2\Delta x_2}$$

$$\vdots$$

$$\left.\frac{\partial y}{\partial x_i}\right|_{x_1^*;\, x_2^*; \ldots;\, x_N^*} \approx \frac{y(\ldots, x_i^* + \Delta x_i, \ldots, x_N^*) - y(\ldots, x_i^* - \Delta x_i, \ldots, x_N^*)}{2\Delta x_i}$$

$$\vdots$$

$$\left.\frac{\partial y}{\partial x_N}\right|_{x_1^*;\, x_2^*; \ldots;\, x_N^*} \approx \frac{y(x_1^*, x_2^*, \ldots, x_N^* + \Delta x_N) - y(x_1^*, x_2^*, \ldots, x_N^* - \Delta x_N)}{2\Delta x_N}$$

$$\begin{pmatrix} \left.\frac{\partial y}{\partial x_1}\right|_{x_1^*;\, x_2^*; \ldots;\, x_N^*)} \\ \ldots \\ \left.\frac{\partial y}{\partial x_i}\right|_{x_1^*;\, x_2^*; \ldots;\, x_N^*} \\ \ldots \\ \left.\frac{\partial y}{\partial x_N}\right|_{x_1^*;\, x_2^*; \ldots;\, x_N^*} \end{pmatrix} = grad(y)_x$$

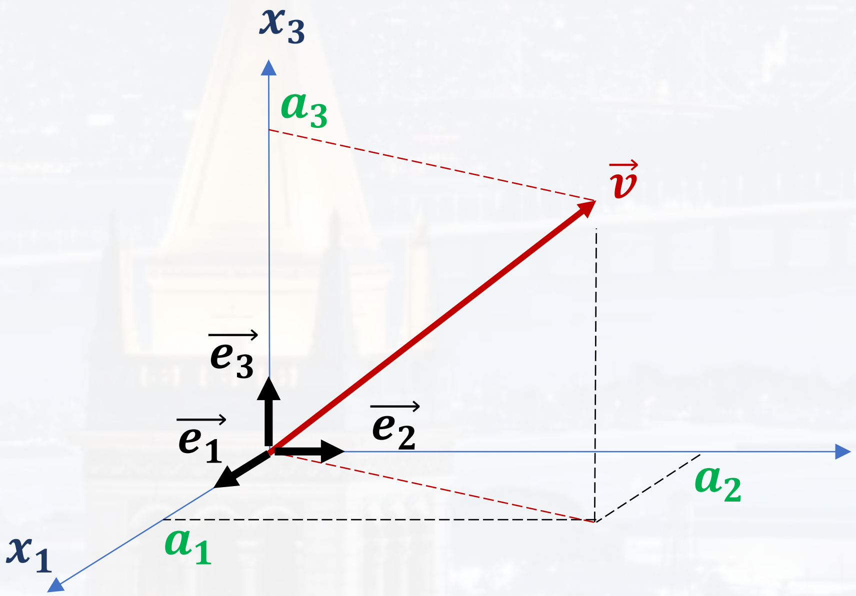
gradient of y wrt x

$$\begin{pmatrix} \left.\frac{\partial y}{\partial x_1}\right|_{x_1^*;\, x_2^*;\ldots;\, x_N^*)} \\ \ldots \\ \left.\frac{\partial y}{\partial x_i}\right|_{x_1^*;\, x_2^*;\ldots;\, x_N^*} \\ \ldots \\ \left.\frac{\partial y}{\partial x_N}\right|_{x_1^*;\, x_2^*;\ldots;\, x_N^*} \end{pmatrix} = grad(y)_x \equiv \vec{\nabla} y$$

The gradient of a function f is **a vector**, because the derivatives have a direction!

unit vectors $\vec{e_1}$, $\vec{e_2}$ and $\vec{e_3}$

$$\vec{e_1} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad \vec{e_2} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad \vec{e_3} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$



length 1 (normalized)
mutually orthogonal

ortho normal

$$\vec{v} = a_1\vec{e_1} + a_2\vec{e_2} + a_3\vec{e_3}$$

$$\vec{v} = a_1\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + a_2\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + a_3\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

$$\begin{pmatrix} \left.\frac{\partial y}{\partial x_1}\right|_{x_1^*;\, x_2^*;\ldots;\, x_N^*)} \\ \ldots \\ \left.\frac{\partial y}{\partial x_i}\right|_{x_1^*;\, x_2^*;\ldots;\, x_N^*} \\ \ldots \\ \left.\frac{\partial y}{\partial x_N}\right|_{x_1^*;\, x_2^*;\ldots;\, x_N^*} \end{pmatrix} = grad(y)_x \equiv \vec{\nabla} y$$

The gradient of a function f is **a vector**, because the derivatives have a direction!

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$$\vec{v} = a_1\overrightarrow{e_1} + a_2\overrightarrow{e_2} + a_3\overrightarrow{e_3}$$

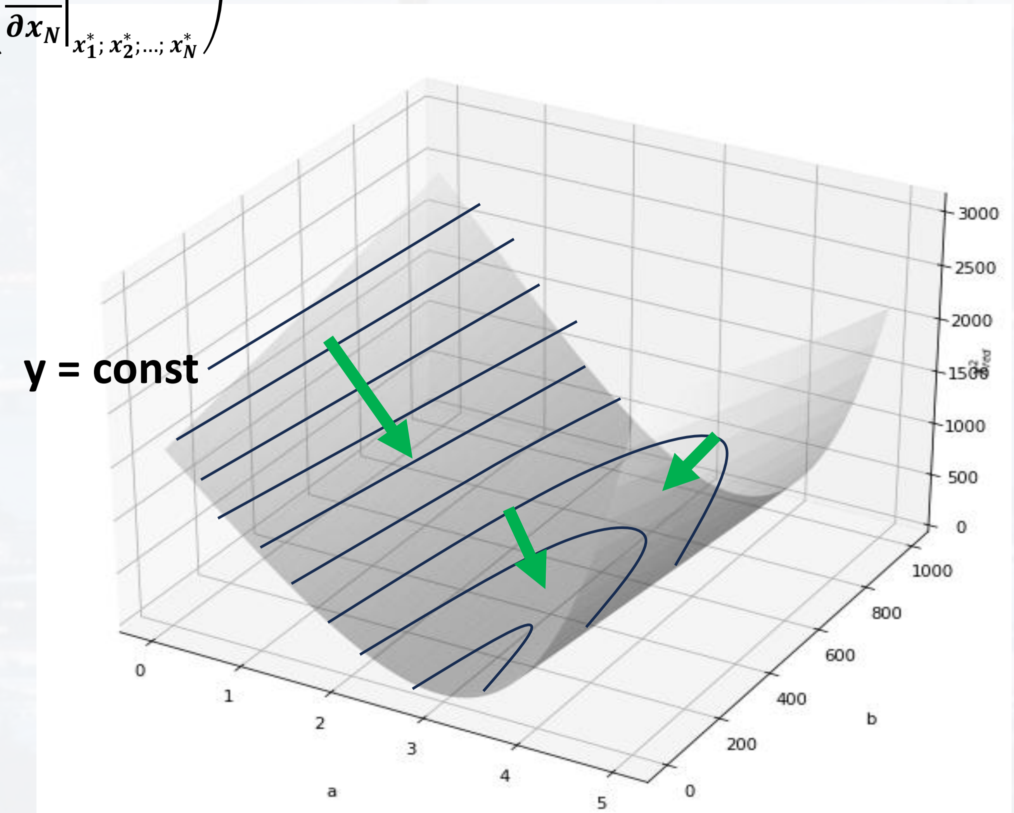
$$\vec{\nabla} y = \frac{\partial y}{\partial x_1}\overrightarrow{e_1} + \frac{\partial y}{\partial x_2}\overrightarrow{e_2} + \ldots \frac{\partial y}{\partial x_i}\overrightarrow{e_i}\ldots + \frac{\partial y}{\partial x_N}\overrightarrow{e_N} = \left(\frac{\partial}{\partial x_1}\overrightarrow{e_1} + \frac{\partial}{\partial x_2}\overrightarrow{e_2} + \ldots \frac{\partial}{\partial x_i}\overrightarrow{e_i}\ldots + \frac{\partial}{\partial x_N}\overrightarrow{e_N}\right) y$$

Gradient

$$\begin{pmatrix} \left.\frac{\partial y}{\partial x_1}\right|_{x_1^*;\, x_2^*;\dots;\, x_N^*)} \\ \dots \\ \left.\frac{\partial y}{\partial x_i}\right|_{x_1^*;\, x_2^*;\dots;\, x_N^*} \\ \dots \\ \left.\frac{\partial y}{\partial x_N}\right|_{x_1^*;\, x_2^*;\dots;\, x_N^*} \end{pmatrix} = grad(y)_x \equiv \vec{\nabla} y$$

$$\vec{\nabla} y = \frac{\partial y}{\partial x_1}\vec{e_1} + \frac{\partial y}{\partial x_2}\vec{e_2} + \dots \frac{\partial y}{\partial x_i}\vec{e_i}\dots + \frac{\partial y}{\partial x_N}\vec{e_N}$$

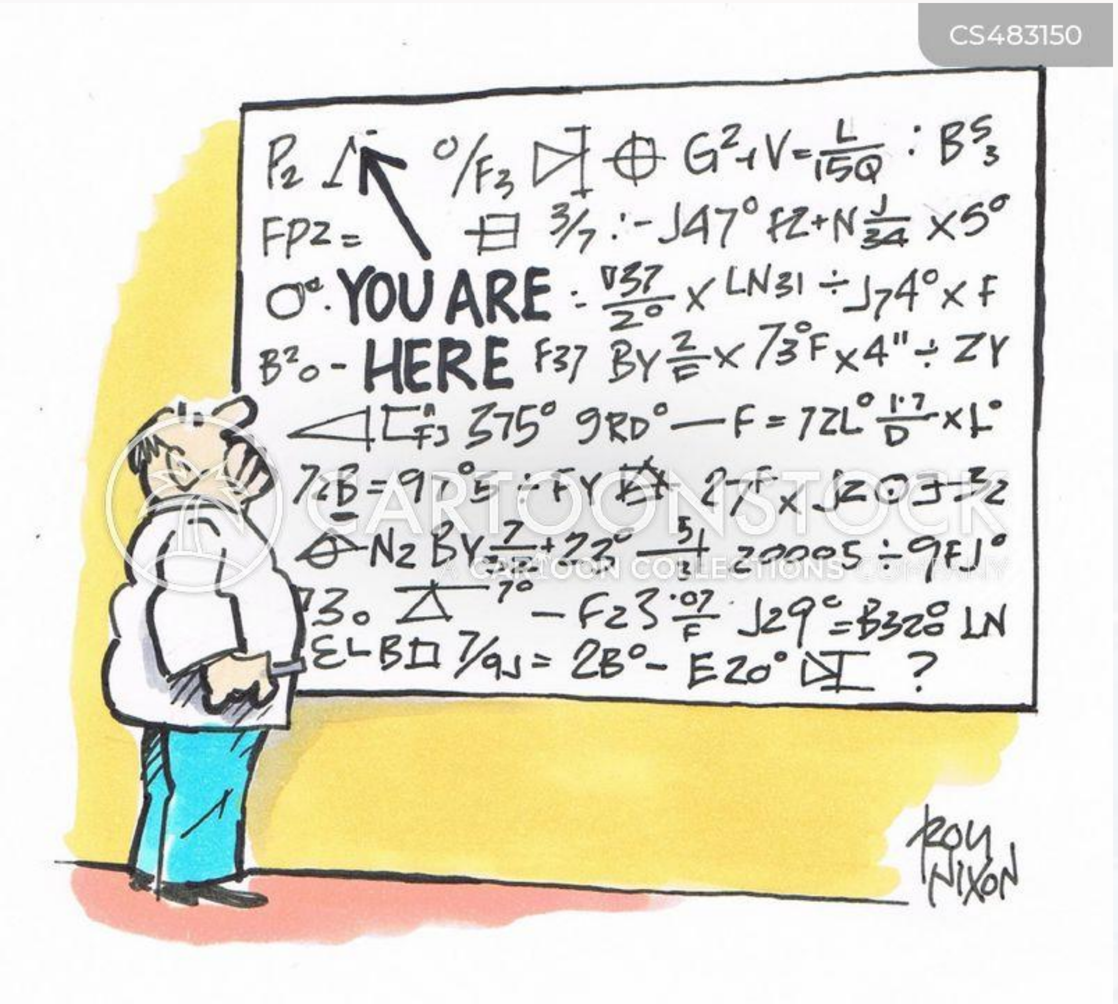
$$= \left(\frac{\partial}{\partial x_1}\vec{e_1} + \frac{\partial}{\partial x_2}\vec{e_2} + \dots \frac{\partial}{\partial x_i}\vec{e_i}\dots + \frac{\partial}{\partial x_N}\vec{e_N}\right) y$$



<u>gradient:</u> vector containing all the partial derivatives at point $P = P(\boldsymbol{x_1^*};\ \boldsymbol{x_2^*};\dots;\ \boldsymbol{x_N^*})$

$grad(y)_x$ is perpendicular to y = const

$\frac{\partial y}{\partial x_i} = 0$ for y = const, hence $\vec{\nabla} y = 0$



<u>Outline</u>

- Recap: Calculus
- Gradient
- **Line Integrals**
- Divergence
- Curl

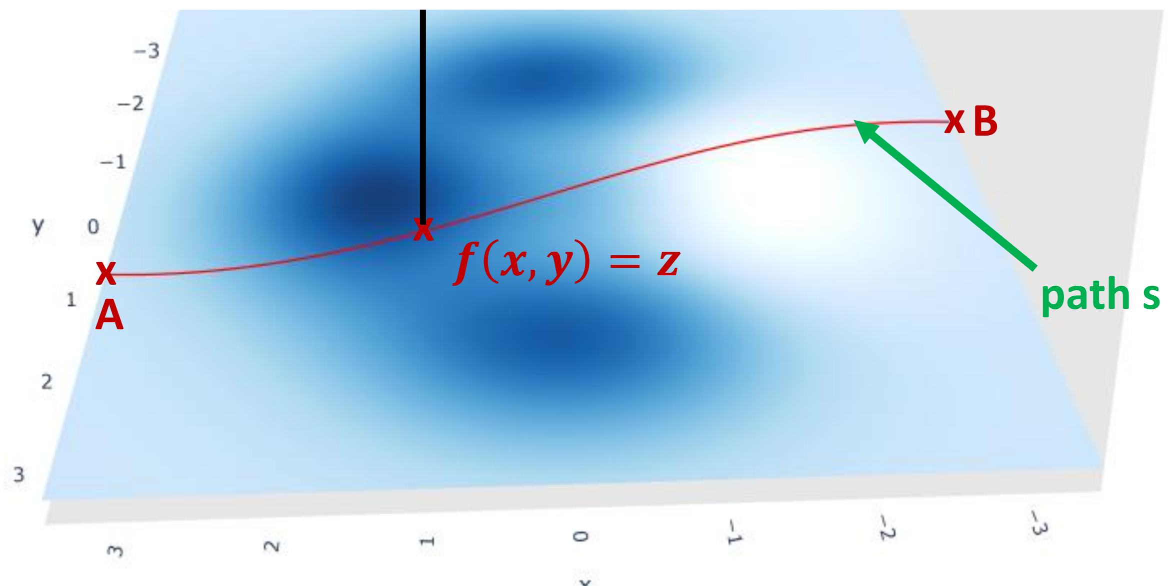
We will be integrating over a path:
line integral

If the path is **closed**
(start and endpoint
are identical): $\oint_C$

We can integrate over a
scalar function/field or over a
vector field (see previous slides)

integrating the scalar function
$f(x, y)$ over the path s

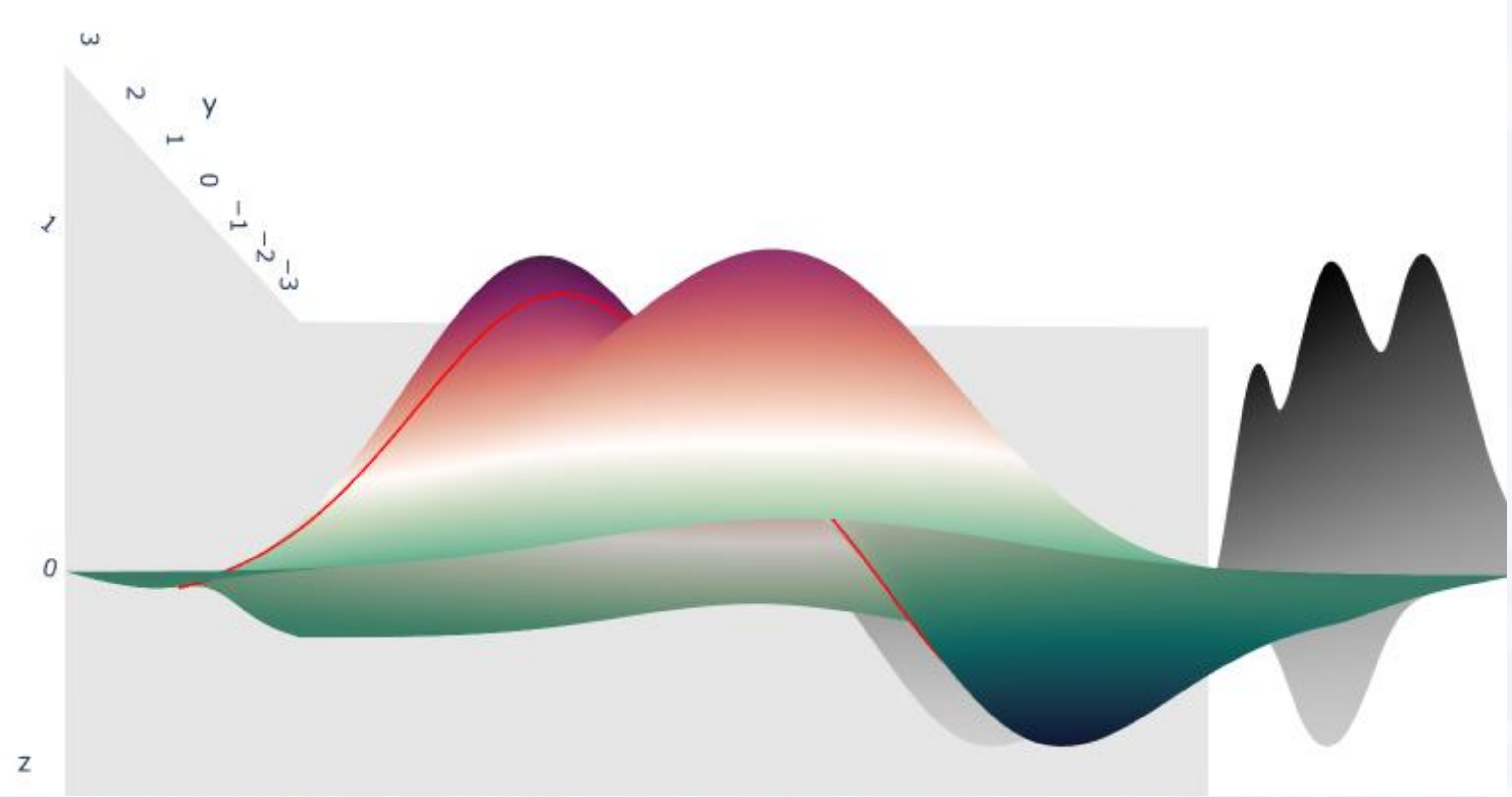
$$\int_A^B f(x, y)\, ds$$



see `PlotLineIntegral.ipynb`

integrating the scalar function $f(x, y)$ over the path s: $\int_A^B f(x, y)\, ds$

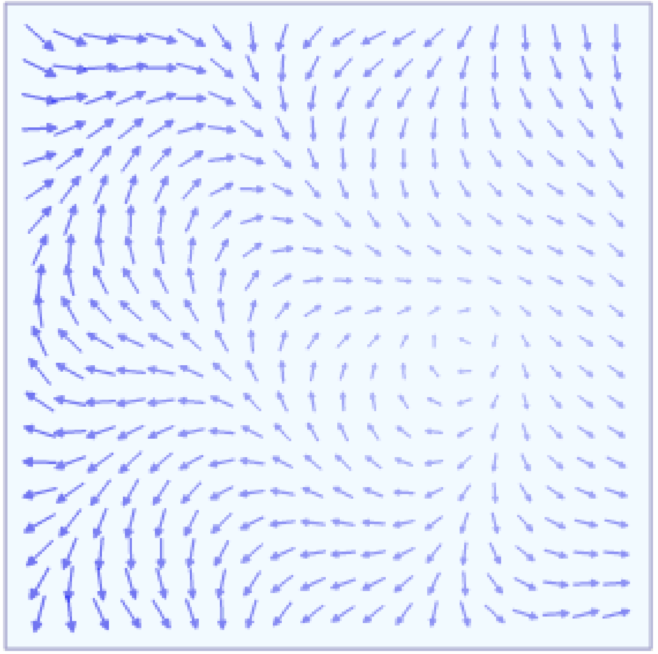
A line integral over a **scalar field** can be interpreted as the area under the curve s along the surface $z = f(x, y)$



see `PlotLineIntegral.ipynb`

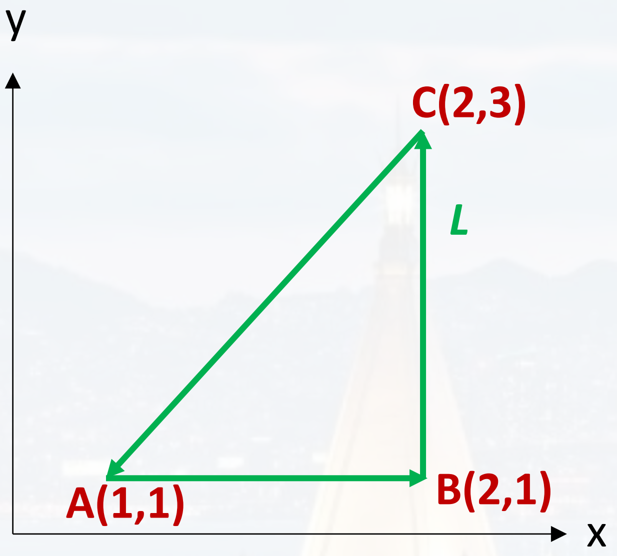
integrating the **vector field** $\vec{\boldsymbol{v}}(x, y)$ over the path s: $$\int_A^B \vec{\boldsymbol{v}}(x, y) \cdot \boldsymbol{d}\vec{\boldsymbol{r}}$$

A line integral over a **vector field** can be interpreted as multiplying the vector $\vec{\boldsymbol{v}}(x, y)$ with the **tangent vector** $\boldsymbol{d}\vec{\boldsymbol{r}}$ (= current direction) of the path/curve and adding this product up along the curve.



credit: Wikipedia

example 1: scalar field $f(x,y) = 2xy^2 + 3$



$$\oint_L f(x,y)\,ds = \int_A^B f(x,y)\,ds + \int_B^C f(x,y)\,ds + \int_C^A f(x,y)\,ds$$

$$ds^2 = dx^2 + dy^2$$

A → B $\quad y = const = 1 \quad ds^2 = dx^2 + 0$

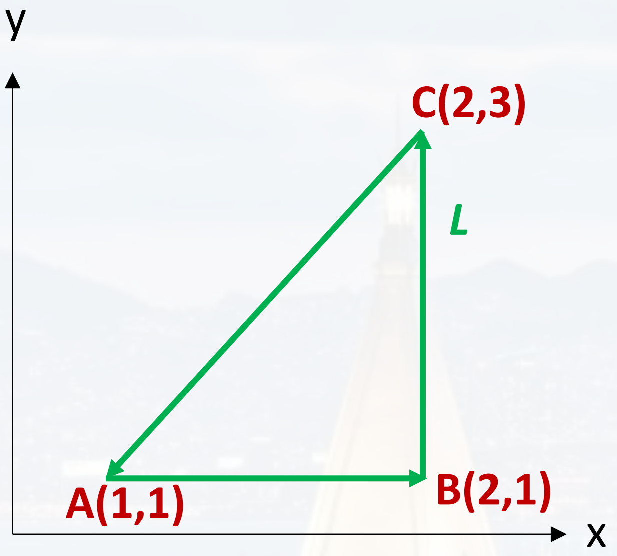
$$\int_A^B f(x,y)\,ds = \int_{(1,1)}^{(2,1)} 2xy^2 + 3\,ds$$

$$= \int_{(1)}^{(2)} 2x\,dx + \int_{(1)}^{(2)} 3\,dx$$

$$= x^2\Big|_1^2 + 3x\Big|_1^2$$

$$= 4 - 1 + 6 - 3 = 6$$

example 1: scalar field $f(x,y) = 2xy^2 + 3$



$$\oint_L f(x,y)\,ds = \int_A^B f(x,y)\,ds + \int_B^C f(x,y)\,ds + \int_C^A f(x,y)\,ds$$

$$ds^2 = dx^2 + dy^2$$

B → C $\quad x = const = 2 \qquad ds^2 = 0 + dy^2$

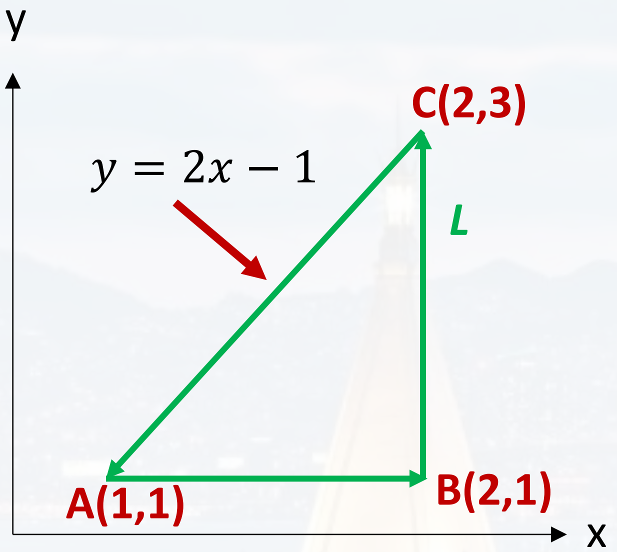
$$\int_B^C f(x,y)\,ds = \int_{(2,1)}^{(2,3)} 2xy^2 + 3\,ds$$

$$= 4\int_{(1)}^{(3)} y^2\,dy + \int_{(1)}^{(3)} 3\,dy$$

$$= \frac{4}{3}y^3\Big|_1^3 + 3y\Big|_1^3$$

$$= 36 - \frac{4}{3} + 9 - 3 = \frac{122}{3}$$

example 1: scalar field $f(x,y) = 2xy^2 + 3$



$$\oint_L f(x,y)\,ds = \int_A^B f(x,y)\,ds + \int_B^C f(x,y)\,ds + \int_C^A f(x,y)\,ds$$

C → A $\quad y = 2x - 1$

$$dy = 2dx \qquad \boxed{ds = \sqrt{dx^2 + dy^2} = \sqrt{5}dx}$$

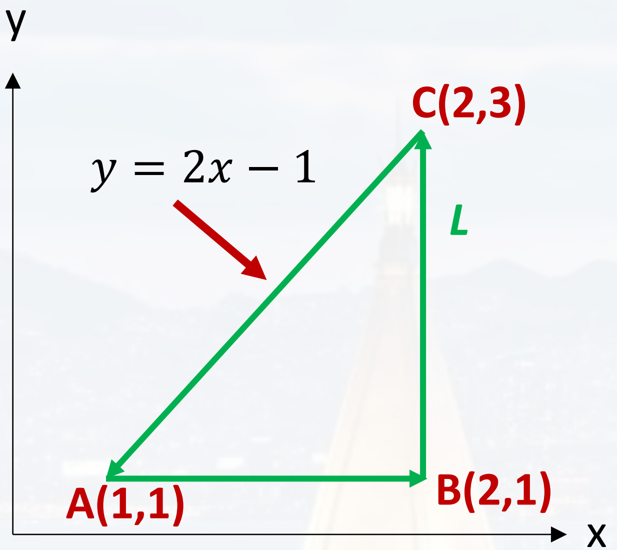
$$\int_C^A f(x,y)\,ds = -\int_A^C f(x,y)\,ds$$

$$= -\int_{(1)}^{(2)} [2x(2x-1)^2 + 3]\sqrt{5}dx = -\int_{(1)}^{(2)} [2x(4x^2 - 4x + 1) + 3]\sqrt{5}dx$$

$$= -\sqrt{5}\int_{(1)}^{(2)} 8x^3 - 8x^2 + 2x + 3\,dx = \sqrt{5}\left[-2x^4\Big|_1^2 + \frac{8}{3}x^3\Big|_1^2 - x^2\Big|_1^2 - 3x\Big|_1^2\right] = -38.76$$

example 1: scalar field $f(x,y) = 2xy^2 + 3$

We could have also substituted x!



$$\oint_L f(x,y)\,ds = \int_A^B f(x,y)\,ds + \int_B^C f(x,y)\,ds + \int_C^A f(x,y)\,ds$$

C → A $\quad y = 2x - 1$

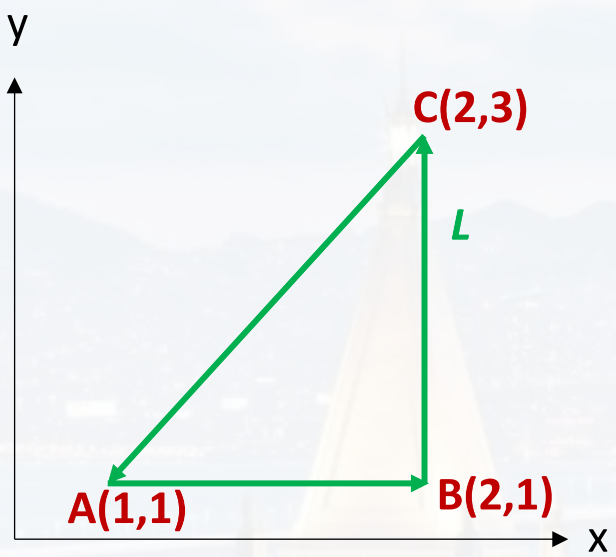
$$\frac{dy}{2} = dx$$

$$\boxed{ds = \sqrt{dx^2 + dy^2} = \frac{\sqrt{5}}{2}dy}$$

$$-\int_A^C f(x,y)\,ds = -\int_{(1)}^{(3)} \left[2\left(\frac{y}{2} + \frac{1}{2}\right)y^2 + 3\right]\frac{\sqrt{5}}{2}dy$$

$$= -\frac{\sqrt{5}}{2}\int_{(1)}^{(3)} y^3 + y^2 + 3\,dy = -\frac{\sqrt{5}}{2}\left[\frac{y^4}{4}\bigg|_1^3 + \frac{1}{3}y^3\bigg|_1^3 + 3y\bigg|_1^3\right] = -38.76$$

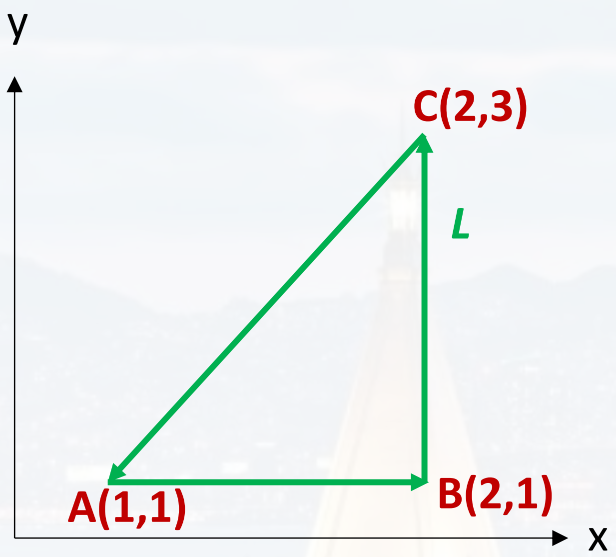
example 1: scalar field $f(x, y) = 2xy^2 + 3$



$$\oint_L f(x,y)\,ds = \int_A^B f(x,y)\,ds + \int_B^C f(x,y)\,ds + \int_C^A f(x,y)\,ds$$

$$= 6 + \frac{122}{3} - 38.76$$

example 2: vector field $\vec{v} = \begin{pmatrix} 2xy^2 \\ 3 \end{pmatrix}$



$$\oint_L \vec{v}\, d\vec{r} = \int_A^B \vec{v}\, d\vec{r} + \int_B^C \vec{v}\, d\vec{r} + \int_C^A \vec{v} d\vec{r}$$

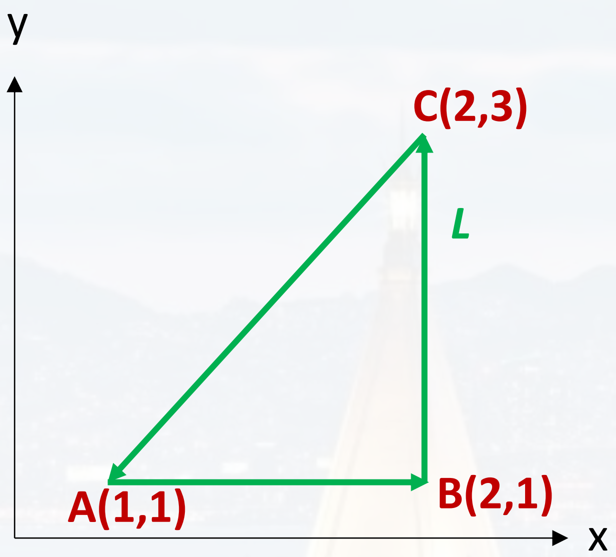
A → B $\quad y = const = 1$

$$\int_A^B \begin{pmatrix} 2xy^2 \\ 3 \end{pmatrix} \begin{pmatrix} dx \\ 0 \end{pmatrix} = \int_1^2 2x\, dx = x^2 \Big|_1^2 = 3$$

B → C $\quad x = const = 2$

$$\int_B^C \begin{pmatrix} 2xy^2 \\ 3 \end{pmatrix} \begin{pmatrix} 0 \\ dy \end{pmatrix} = \int_1^3 3\, dy = 3y|_1^3 = 6$$

example 2: vector field $\vec{v} = \begin{pmatrix} 2xy^2 \\ 3 \end{pmatrix}$



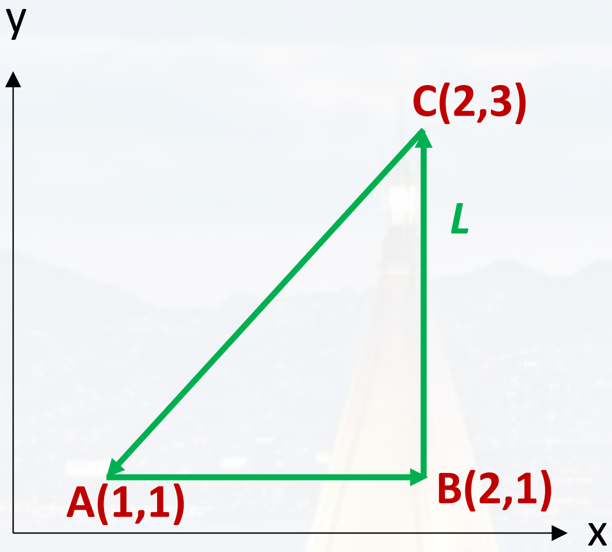
$$\oint_L \vec{v}\, d\vec{r} = \int_A^B \vec{v}\, d\vec{r} + \int_B^C \vec{v}\, d\vec{r} + \int_C^A \vec{v} d\vec{r}$$

C → A $\quad y = 2x - 1 \qquad dy = 2dx$

$$-\int_A^C \begin{pmatrix} 8x^3 - 8x^2 + 2x \\ 3 \end{pmatrix} \begin{pmatrix} dx \\ 2dx \end{pmatrix} = -\int_1^2 8x^3 - 8x^2 + 2x + 6\, dx$$

$$= -2x^4\Big|_1^2 + \frac{8}{3}x^3\Big|_1^2 - x^2\Big|_1^2 - 6x\Big|_1^2 \quad = -39 + \frac{56}{3} = -20.33$$

example 2: vector field $\vec{v} = \begin{pmatrix} 2xy^2 \\ 3 \end{pmatrix}$



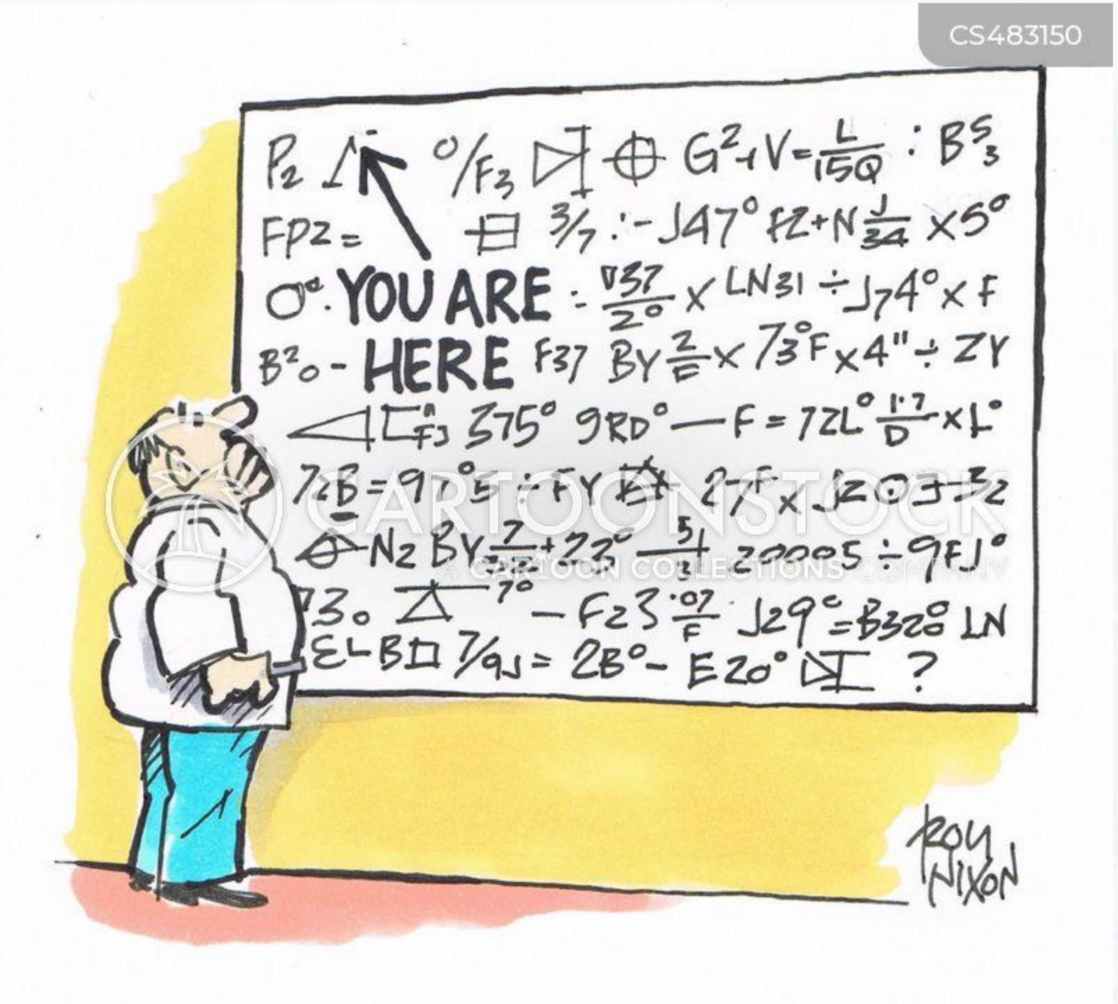
$$\oint_L \vec{v}\,d\vec{r} = \int_A^B \vec{v}\,d\vec{r} + \int_B^C \vec{v}\,d\vec{r} + \int_C^A \vec{v}d\vec{r}$$

C → A $\quad y = 2x - 1 \qquad dy = 2dx$

$$-\int_A^C \begin{pmatrix} (y+1)y^2 \\ 3 \end{pmatrix} \begin{pmatrix} 0.5\,dy \\ dy \end{pmatrix} = -\frac{1}{2}\int_1^3 y^3 + y^2 + 6\,dy$$

$$= -\frac{1}{8}y^4\Big|_1^3 - \frac{1}{6}y^3\Big|_1^3 - 3y\Big|_1^3 \quad = -20.33$$

total: 3 + 6 – 20.33 = - 11.33



Outline

- Recap: Calculus

- Gradient

- Line Integrals

- Divergence

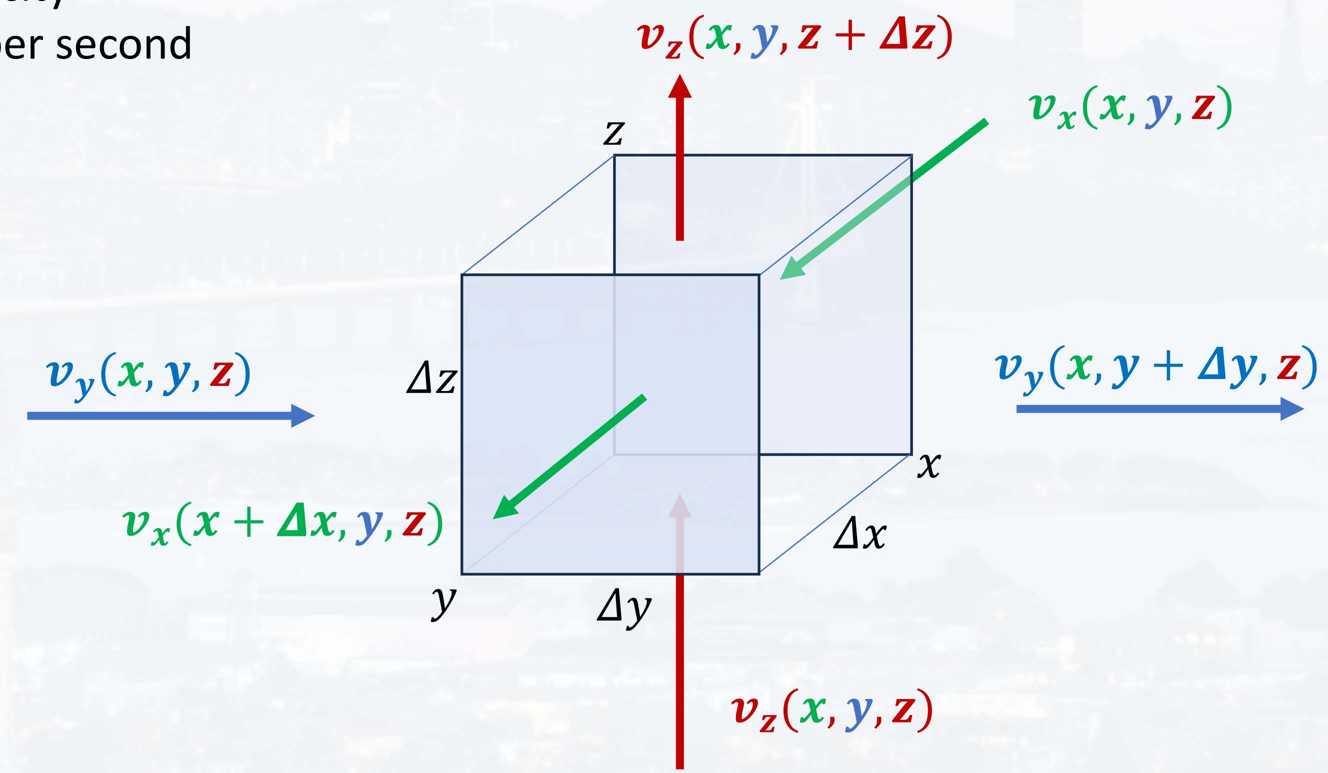
- Curl

calculating volume flux density

flux: $\Psi = something/time$ → number/s, mass/s, energy/s etc

flux density: $\varphi = \frac{something}{time * area}$ → number/s/m^2, mass/s/m^2, energy/s/m^2 etc

vector field $\vec{v}$, e. g. wind velocity
→ flux would be molecules per second



calculating volume flux density

vector field $\vec{v}$, e. g. wind velocity
→ flux would be molecules per second

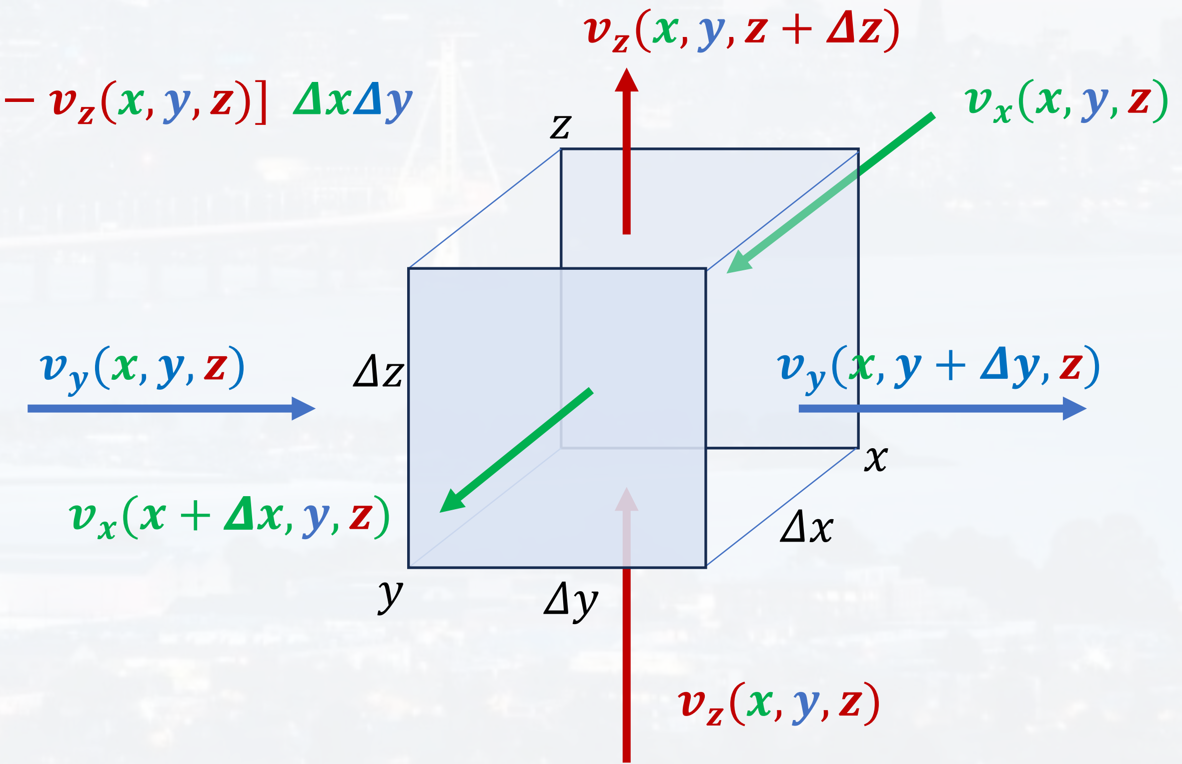
flux: $\Psi = something/time$

flux density: $\varphi = \frac{something}{time * area}$

net flux in **x** direction: $[v_x(x+\Delta x, y, z) - v_x(x, y, z)]\ \Delta y \Delta z$

net flux in **y** direction: $[v_y(x, y+\Delta y, z) - v_y(x, y, z)]\ \Delta x \Delta z$

net flux in **z** direction: $[v_z(x, y, z+\Delta z) - v_z(x, y, z)]\ \Delta x \Delta y$



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net flux in **x** direction: $[v_x(x+\Delta x, y, z) - v_x(x, y, z)]\ \Delta y \Delta z$

net flux in **y** direction: $[v_y(x, y+\Delta y, z) - v_y(x, y, z)]\ \Delta x \Delta z$

net flux in **z** direction: $[v_z(x, y, z+\Delta z) - v_z(x, y, z)]\ \Delta x \Delta y$

total net flux:

$$[v_x(x+\Delta x, y, z) - v_x(x, y, z)]\ \Delta y \Delta z + \\ [v_y(x, y+\Delta y, z) - v_y(x, y, z)]\ \Delta x \Delta z + \\ [v_z(x, y, z+\Delta z) - v_z(x, y, z)]\ \Delta x \Delta y$$

total net flux **per volume**:

$$\frac{[v_x(x+\Delta x,y,z)-v_x(x,y,z)]\ \Delta y\Delta z + [v_y(x,y+\Delta y,z)-v_y(x,y,z)]\ \Delta x\Delta z + [v_z(x,y,z+\Delta z)-v_z(x,y,z)]\Delta x\Delta y}{\Delta x\Delta y\Delta z}$$

calculating volume flux density

total net flux **per volume**:

$$\frac{[v_x(x+\Delta x,y,z)-v_x(x,y,z)]\,\Delta y\Delta z+[v_y(x,y+\Delta y,z)-v_y(x,y,z)]\,\Delta x\Delta z+[v_z(x,y,z+\Delta z)-v_z(x,y,z)]\Delta x\Delta y}{\Delta x\Delta y\Delta z}$$

total net flux **per volume**: $\boxed{\frac{v_x(x+\Delta x,y,z)-v_x(x,y,z)}{\Delta x}+\frac{v_y(x,y+\Delta y,z)-v_y(x,y,z)}{\Delta y}+\frac{v_z(x,y,z+\Delta z)-v_z(x,y,z)}{\Delta z}}$

first derivatives for Δx, Δy, $\Delta z \rightarrow 0$

$$\frac{\partial v_x}{\partial x}+\frac{\partial v_y}{\partial y}+\frac{\partial v_z}{\partial z} = \begin{pmatrix}\frac{\partial}{\partial x}\\ \frac{\partial}{\partial y}\\ \frac{\partial}{\partial z}\end{pmatrix}\cdot\begin{pmatrix}v_x\\ v_y\\ v_z\end{pmatrix} \equiv \vec{\nabla}\cdot\vec{v}$$

divergence of $\vec{v}$

calculating volume flux density

divergence

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} \cdot \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} \equiv \vec{\boldsymbol{\nabla}} \cdot \vec{\boldsymbol{v}} \equiv \mathbf{div}\, \vec{\boldsymbol{v}}$$

dot product with a **vector** ($\vec{\boldsymbol{v}}$), returns a **scalar**

gradient

$$\left(\frac{\partial}{\partial x}\vec{\boldsymbol{e}_x} + \frac{\partial}{\partial y}\vec{\boldsymbol{e}_y} + \frac{\partial}{\partial z}\vec{\boldsymbol{e}_z}\right) f = \begin{pmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \\ \frac{\partial f}{\partial z} \end{pmatrix} = grad(f) \equiv \vec{\nabla} f$$

turns a **scalar** (***f***) into a **vector** grad(*f*),

$\vec{\nabla} \cdot \vec{v} \equiv \mathbf{div}\,\vec{v}$

divergence: net flux at a given point, if >0 → source term
if <0 → sink term

$$\frac{[v_x(x+\Delta x,y,z)-v_x(x,y,z)]\,\Delta y\Delta z+[v_y(x,y+\Delta y,z)-v_y(x,y,z)]\,\Delta x\Delta z+[v_z(x,y,z+\Delta z)-v_z(x,y,z)]\Delta x\Delta y}{\Delta x\Delta y\Delta z}$$

We derived the divergence, by

1) multiplying the vector $\vec{v}$ with the surface element $\Delta x_i \Delta x_j$
2) summing this product over all surface elements
3) dividing by the volume
4) let $\Delta x, \Delta y, \Delta z$ → 0 , i. e. $\partial x, \partial y, \partial z$

$$\mathbf{div}\,\vec{v} \equiv \lim_{V\to 0}\frac{1}{V}\int_{(V)}\vec{v}\cdot d\vec{f}$$

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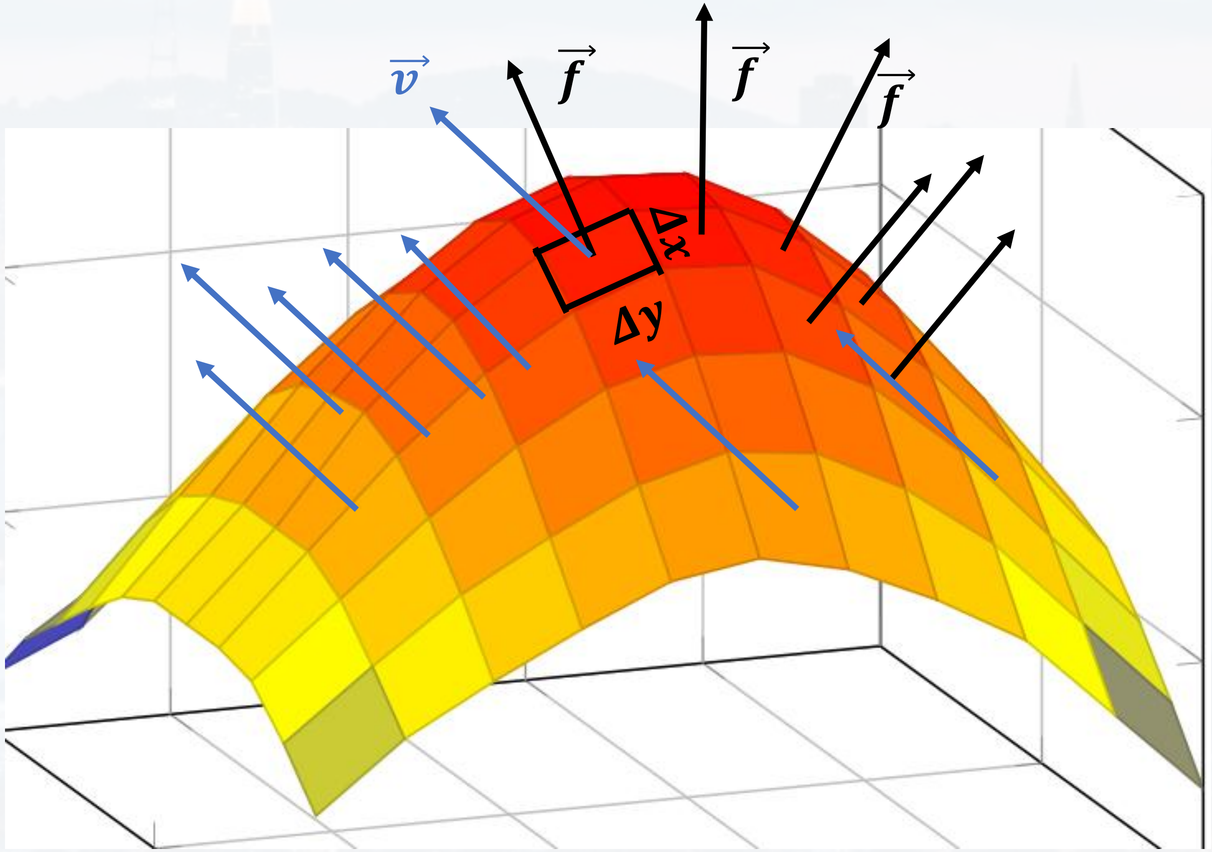
4) let $\boldsymbol{\Delta x}, \boldsymbol{\Delta y}, \boldsymbol{\Delta z} \rightarrow 0$, i. e. $\boldsymbol{\partial x}, \boldsymbol{\partial y}, \boldsymbol{\partial z}$

$$\mathbf{div}\,\vec{\boldsymbol{v}} \equiv \lim_{V\to 0} \frac{1}{V} \int_{(V)} \vec{\boldsymbol{v}} \cdot d\vec{\boldsymbol{f}}$$

$\vec{\boldsymbol{f}}$ is **perpendicular** to the surface element

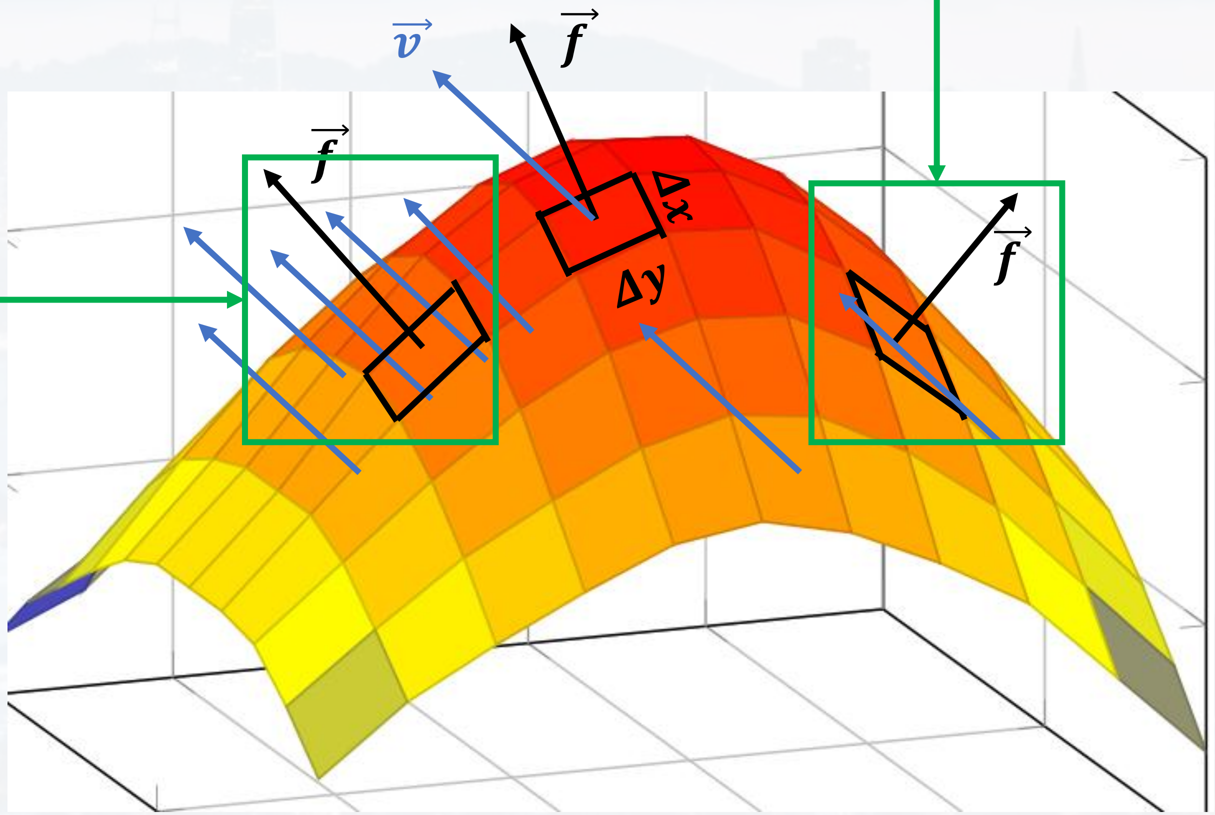


$$\mathbf{div}\,\vec{\boldsymbol{v}} \equiv \lim_{V\to 0}\frac{1}{V}\int_{(V)} \vec{\boldsymbol{v}}\cdot d\vec{\boldsymbol{f}}$$

dot product of $\vec{\boldsymbol{f}}$ and $\vec{\boldsymbol{v}}$

no flux in or out:
$\vec{\boldsymbol{v}}\cdot d\vec{\boldsymbol{f}} = \mathbf{0}$

max flux out:
$\vec{\boldsymbol{v}}\cdot d\vec{\boldsymbol{f}} = |\vec{\boldsymbol{v}}|$



$$\mathbf{div}\,\vec{\boldsymbol{v}} \equiv \lim_{V\to 0}\frac{1}{V}\int_{(V)} \vec{\boldsymbol{v}} \cdot d\vec{\boldsymbol{f}}$$

divergence = net flux at a given **point**

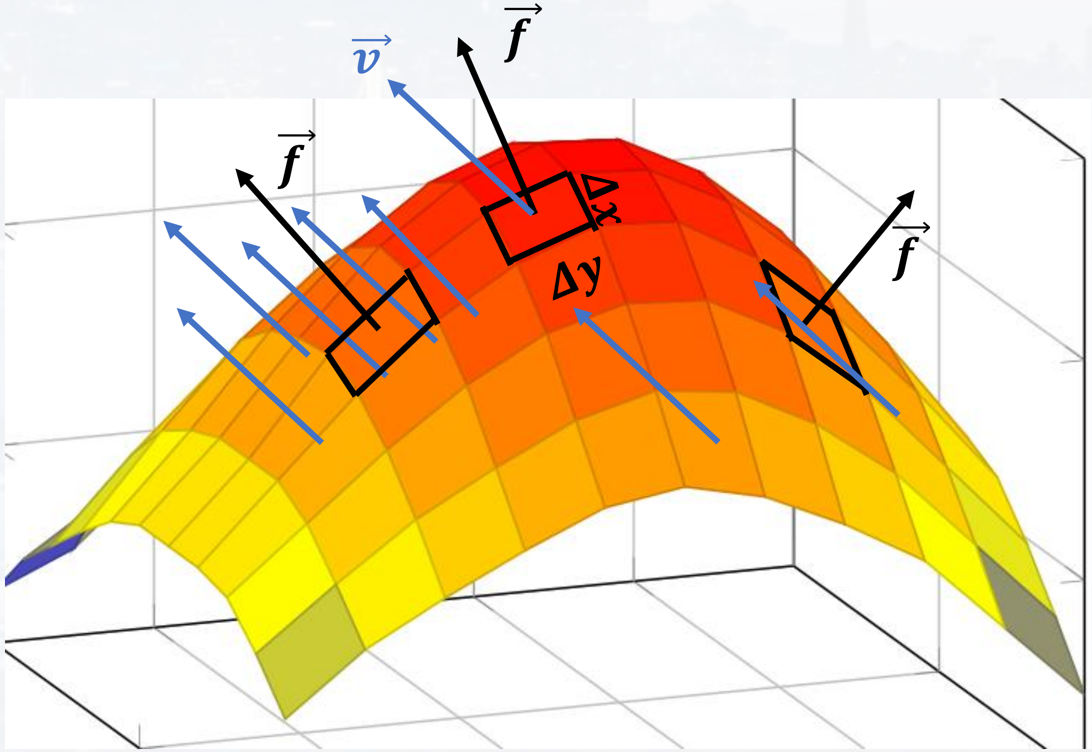
summing over the entire volume:

$$\int_V \mathbf{div}\,\vec{\boldsymbol{v}} \cdot dV = \int_V \lim_{V\to 0}\frac{1}{V}\int_{(V)} \vec{\boldsymbol{v}} \cdot d\vec{\boldsymbol{f}} \cdot dV$$

$$= \int_{(V)} \vec{\boldsymbol{v}} \cdot d\vec{\boldsymbol{f}}$$

$$\boxed{\int_V \mathbf{div}\,\vec{\boldsymbol{v}} \cdot dV = \int_{(V)} \vec{\boldsymbol{v}} \cdot d\vec{\boldsymbol{f}}}$$

Gauss' Theorem



$$\mathbf{div}\,\vec{\boldsymbol{v}} \equiv \lim_{V\to 0}\frac{1}{V}\int_{(V)}\vec{\boldsymbol{v}}\cdot d\vec{\boldsymbol{f}}$$

divergence = net flux at a given point

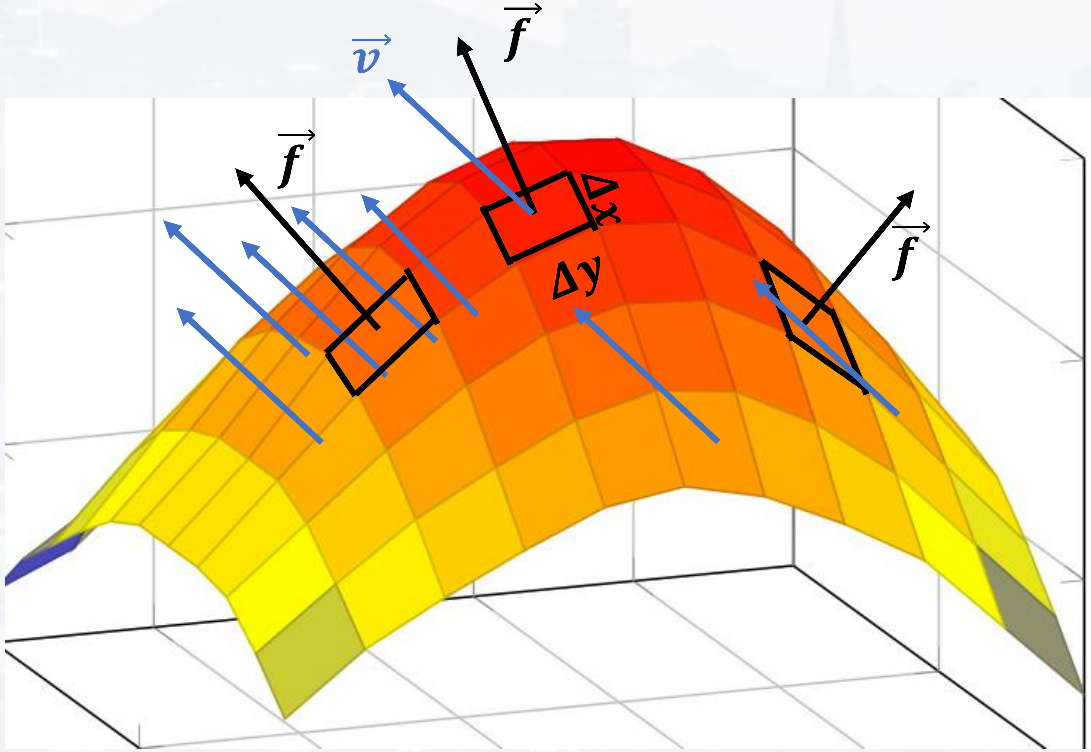
$$\boxed{\int_{V}\mathbf{div}\,\vec{\boldsymbol{v}}\cdot dV = \int_{(V)}\vec{\boldsymbol{v}}\cdot d\vec{\boldsymbol{f}}}$$

Gauss' Theorem

Interpretation:

(right-hand side of the equation)
Summing up the flux that goes through all the surface elements around a given volume,

(left-hand side)
tells us how strong the source/sink within that volume is.



$$\mathbf{div}\,\vec{\boldsymbol{v}} \equiv \lim_{V\to 0}\frac{1}{V}\int_{(V)} \vec{\boldsymbol{v}} \cdot d\vec{\boldsymbol{f}}$$

divergence = net flux at a given point

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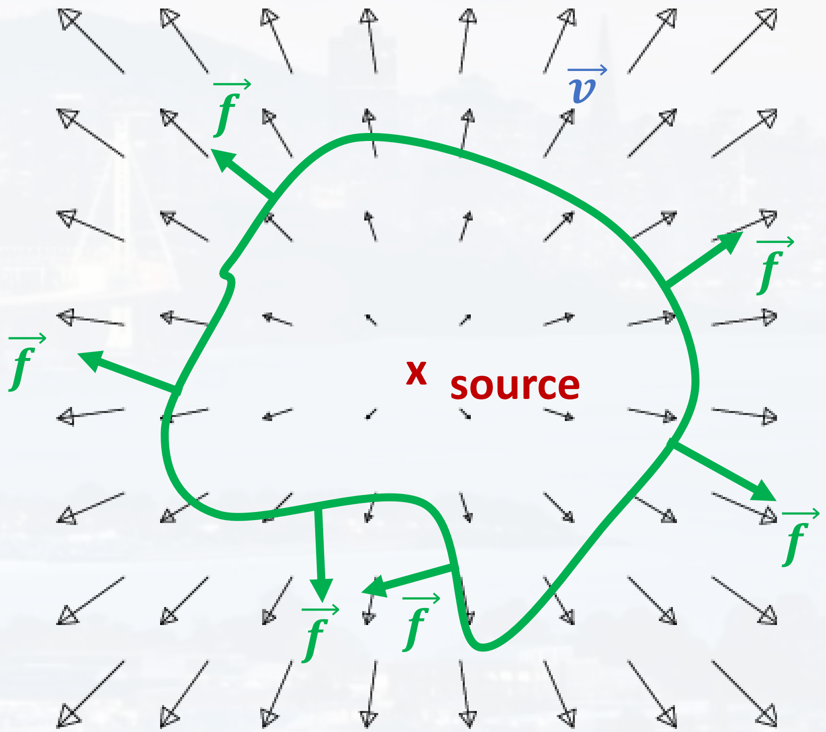
Gauss' Theorem



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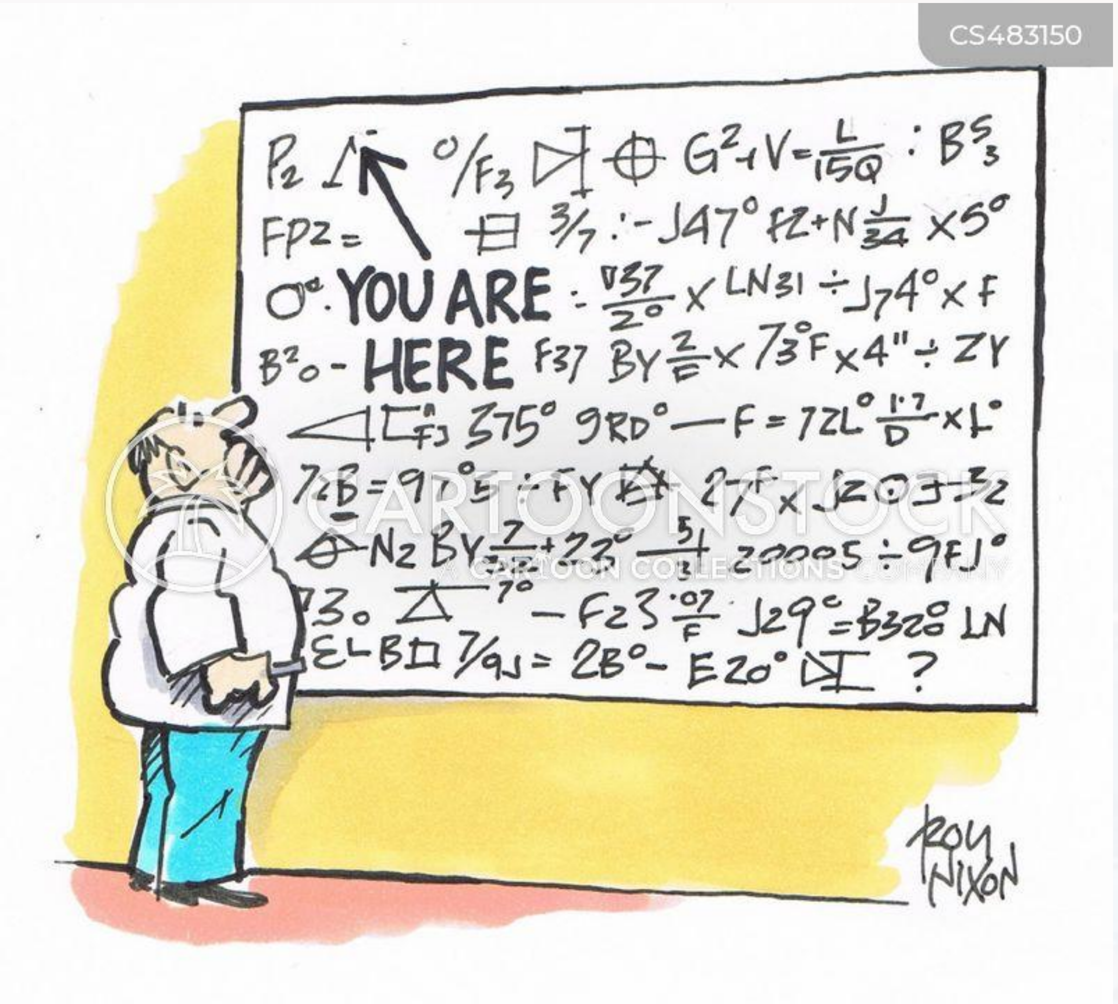
Credit:
Corinne A. Manogue,
Tevian Dray



Outline

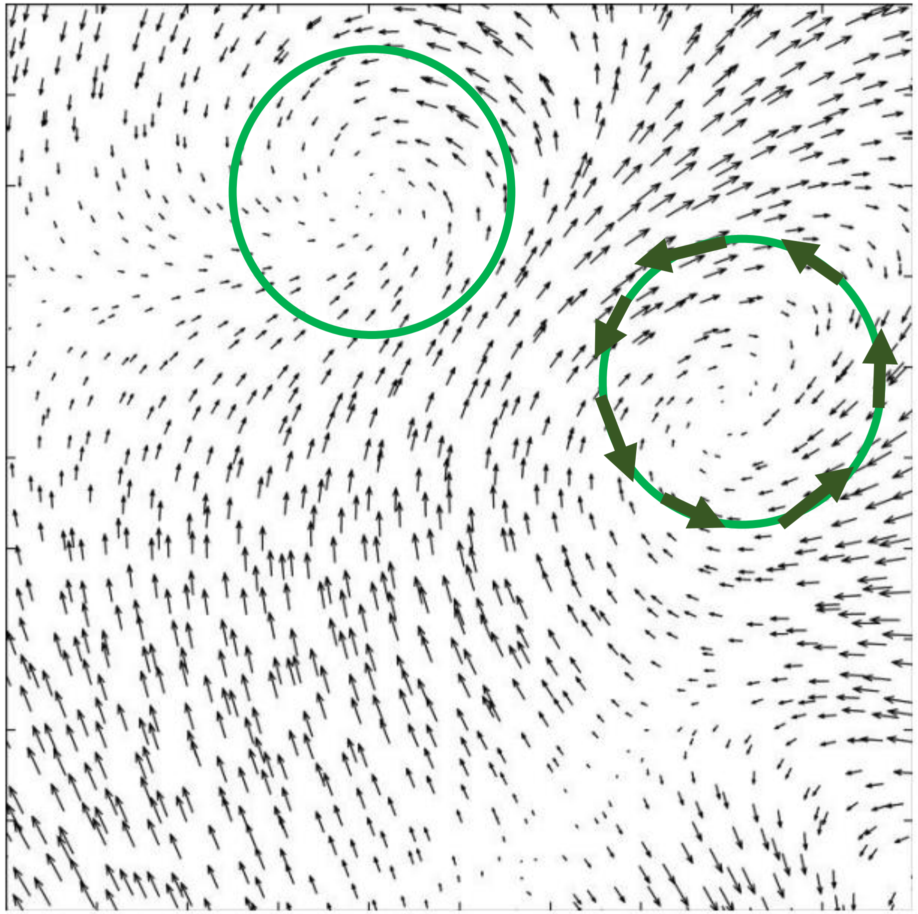
- Recap: Calculus
- Gradient
- Line Integrals
- Divergence
- **Curl**

$$\mathbf{div}\,\vec{\boldsymbol{v}} \equiv \lim_{V\to 0}\frac{1}{V}\int_{(V)} \vec{\boldsymbol{v}} \cdot d\vec{\boldsymbol{f}}$$

divergence = net flux at a given **point** → tells if source/sink

$\vec{\boldsymbol{v}}$ can also have **curls**

curls



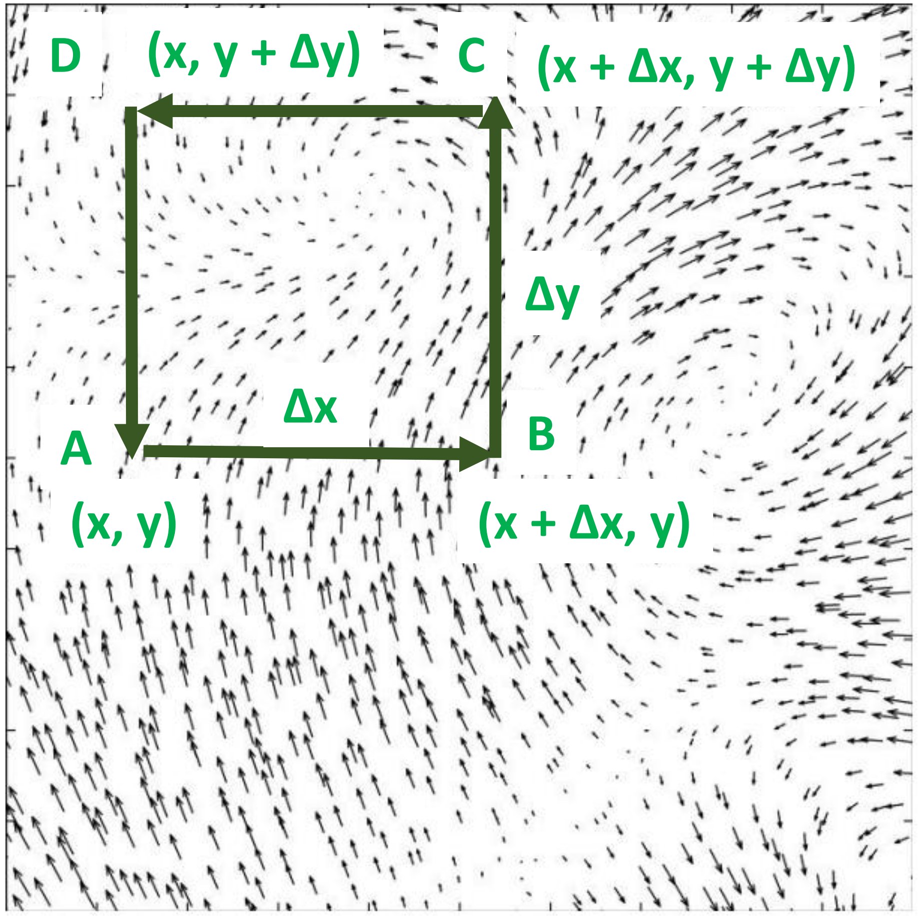
credit:
Daniel Vieira

divergence: in order to get the flux in/out, we had to multiply $d\vec{\boldsymbol{f}}$ with $\vec{\boldsymbol{v}}$

curl: in order to get the curl/rotation we need to multiply $\vec{\boldsymbol{v}}$ with the **direction $\mathbf{d}\vec{\boldsymbol{r}}$ of the path we move along**

curl: in order to get the curl/rotation we need to multiply $\vec{v}$ with the **direction $\mathbf{d}\vec{r}$ of the path we move along**

curls



at A) $\Delta\vec{r} = \begin{pmatrix} \Delta x \\ 0 \end{pmatrix}$ $\vec{v} = \begin{pmatrix} v_x(x, y) \\ v_y(x, y) \end{pmatrix}$

at B) $\Delta\vec{r} = \begin{pmatrix} 0 \\ \Delta y \end{pmatrix}$ $\vec{v} = \begin{pmatrix} v_x(x + \Delta x, y) \\ v_y(x + \Delta x, y) \end{pmatrix}$

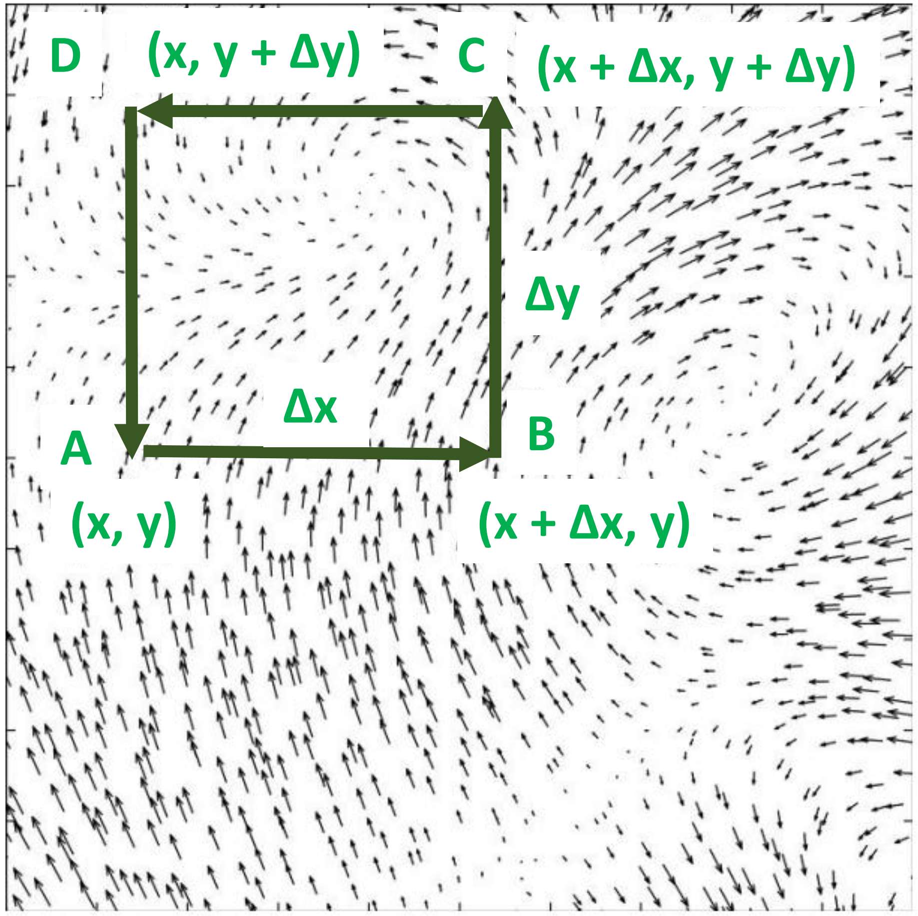
at C) $\Delta\vec{r} = \begin{pmatrix} -\Delta x \\ 0 \end{pmatrix}$ $\vec{v} = \begin{pmatrix} v_x(x + \Delta x, y + \Delta y) \\ v_y(x + \Delta x, y + \Delta y) \end{pmatrix}$

at D) $\Delta\vec{r} = \begin{pmatrix} 0 \\ -\Delta y \end{pmatrix}$ $\vec{v} = \begin{pmatrix} v_x(x, y + \Delta y) \\ v_y(x, y + \Delta y) \end{pmatrix}$

credit:
Daniel Vieira

curl: in order to get the curl/rotation we need to multiply $\vec{v}$ with the **direction $\mathrm{d}\vec{r}$ of the path we move along**

curls



at A) $\Delta\vec{r}\cdot\vec{v} = v_x(x,y)\Delta x$

at B) $\Delta\vec{r}\cdot\vec{v} = v_y(x+\Delta x, y)\Delta y$

at C) $\Delta\vec{r}\cdot\vec{v} = -v_x(x+\Delta x, y+\Delta y)\Delta \mathrm{x}$
$= -v_x(x, y+\Delta y)\Delta \mathrm{x}$

at D) $\Delta\vec{r}\cdot\vec{v} = -v_y(x, y+\Delta y)\Delta y$
$= -v_y(x,y)\Delta y$

credit:
Daniel Vieira

curl: in order to get the curl/rotation we need to multiply $\vec{v}$ with the **direction $\mathrm{d}\vec{r}$ of the path we move along**

summing all up and approximating terms like:

$$v_y(x+\Delta x, y) \approx v_y(x,y) + \frac{\partial v_y(x,y)}{\partial x}\Delta x$$

(Taylor series)

$$C = \underbrace{v_x(x,y)\Delta x}_{\text{A) to B)}} + \underbrace{\left[v_y(x,y) + \frac{\partial v_y(x,y)}{\partial x}\Delta x\right]\Delta y}_{\text{B) to C)}} \underbrace{- \left[v_x(x,y) + \frac{\partial v_x(x,y)}{\partial y}\Delta y\right]\Delta x}_{\text{C) to D)}} \underbrace{- v_y(x,y)\Delta y}_{\text{D) to A)}}$$

$$C = \frac{\partial v_y(x,y)}{\partial x}\Delta x\Delta y - \frac{\partial v_x(x,y)}{\partial y}\Delta y\Delta x = \underbrace{\left[\frac{\partial v_y(x,y)}{\partial x} - \frac{\partial v_x(x,y)}{\partial y}\right]}_{\text{curl of } \vec{v}}\Delta y\Delta x$$

curl: in order to get the curl/rotation we need to multiply $\vec{v}$ with the **direction $\mathbf{d}\vec{r}$ of the path we move along**

$$C = \frac{\partial v_y(x,y)}{\partial x}\Delta x \Delta y - \frac{\partial v_x(x,y)}{\partial y}\Delta y \Delta x = \underbrace{\left[\frac{\partial v_y(x,y)}{\partial x} - \frac{\partial v_x(x,y)}{\partial y}\right]}_{\text{curl of } \vec{v}} \Delta y \Delta x$$

<u>that was 2D, but in 3D:</u>

"**curl** of $\vec{v}$" $\equiv \boldsymbol{rot}\,\vec{v} \equiv \vec{\nabla} \times \vec{v}$

cross product $\vec{a} \times \vec{b}$

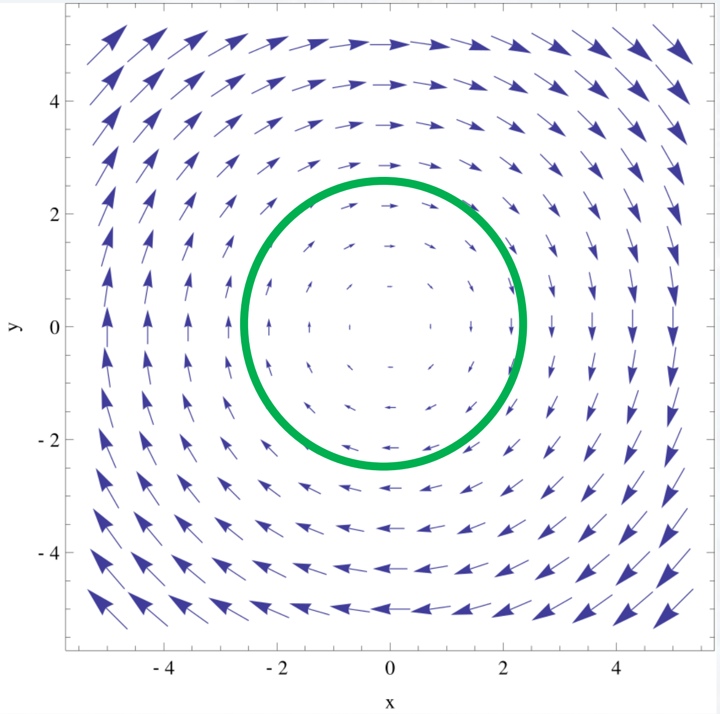
trick for 2D and 3D

$$\vec{a} \times \vec{b} = \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} \begin{pmatrix} b_x \\ b_y \\ b_z \end{pmatrix} \atop \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} \begin{pmatrix} b_x \\ b_y \\ b_z \end{pmatrix} = \begin{pmatrix} a_y b_z - a_z b_y \\ a_z b_x - a_x b_z \\ a_x b_y - a_y b_x \end{pmatrix}$$

curl: in order to get the curl/rotation we need to multiply $\vec{v}$ with the **direction $\mathrm{d}\vec{r}$ of the path we move along**

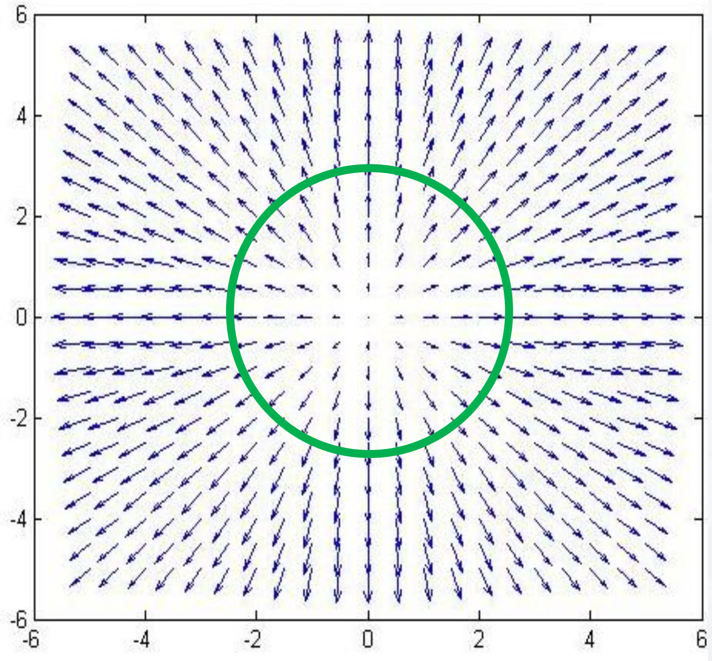
$$\text{“curl of } \vec{v}\text{"} \equiv rot\,\vec{v} \equiv \vec{\nabla}\times\vec{v} = \vec{e_x}\left(\frac{\partial v_z}{\partial y}-\frac{\partial v_y}{\partial z}\right)+\vec{e_y}\left(\frac{\partial v_x}{\partial z}-\frac{\partial v_z}{\partial x}\right)+\vec{e_z}\left(\frac{\partial v_y}{\partial x}-\frac{\partial v_x}{\partial y}\right)$$

$rot\,\vec{v} \neq 0$
$div\,\vec{v} = 0$



credit: Wikipedia

$rot\,\vec{v} = 0$
$div\,\vec{v} \neq 0$



credit: Stackoverflow

Vector Calculus

curl

$$\vec{e}_x\left(\frac{\partial v_z}{\partial y}-\frac{\partial v_y}{\partial z}\right)+\vec{e}_y\left(\frac{\partial v_x}{\partial z}-\frac{\partial v_z}{\partial x}\right)+\vec{e}_z\left(\frac{\partial v_y}{\partial x}-\frac{\partial v_x}{\partial y}\right)=\mathbf{rot}\,\vec{v}\equiv\vec{\nabla}\times\vec{v}$$

cross product of two **vectors** ($\vec{\nabla}$ and $\vec{v}$), returns a **vector**

divergence

$$\frac{\partial v_x}{\partial x}+\frac{\partial v_y}{\partial y}+\frac{\partial v_z}{\partial z}=\begin{pmatrix}\frac{\partial}{\partial x}\\ \frac{\partial}{\partial y}\\ \frac{\partial}{\partial z}\end{pmatrix}\cdot\begin{pmatrix}v_x\\ v_y\\ v_z\end{pmatrix}\equiv\vec{\nabla}\cdot\vec{v}\equiv\mathbf{div}\,\vec{v}$$

dot product with a **vector** ($\vec{v}$), returns a **scalar**

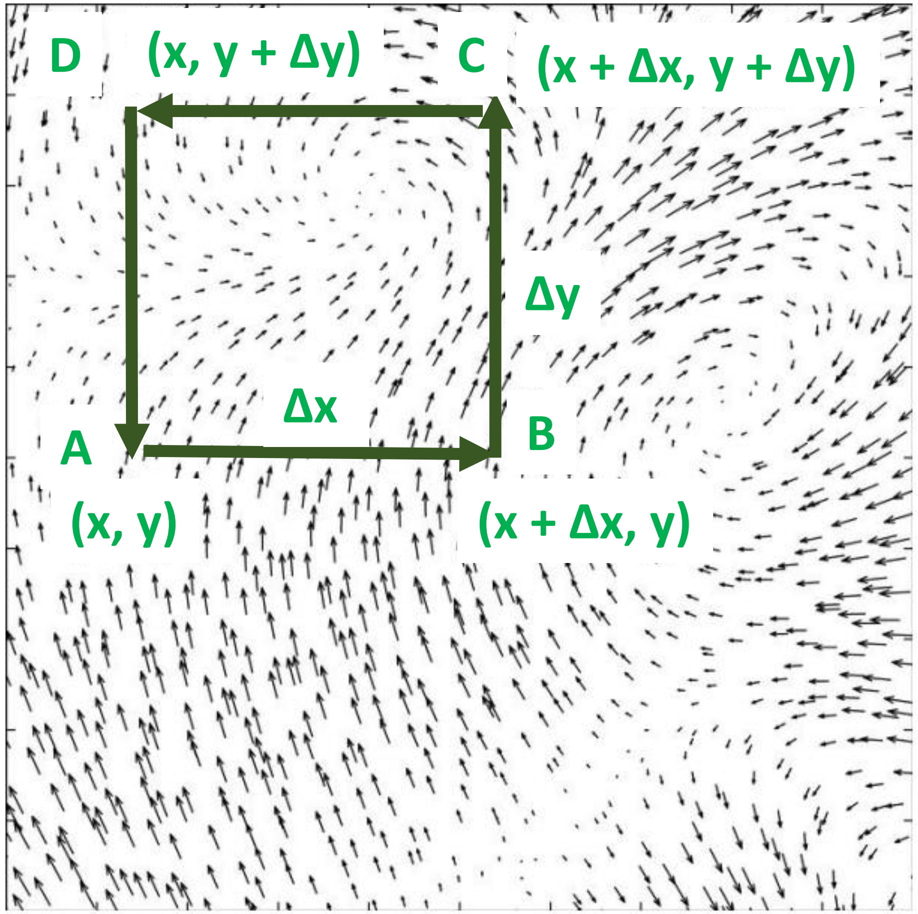
gradient

$$\left(\frac{\partial}{\partial x}\vec{e}_x+\frac{\partial}{\partial y}\vec{e}_y+\frac{\partial}{\partial z}\vec{e}_z\right)f=\begin{pmatrix}\frac{\partial f}{\partial x}\\ \frac{\partial f}{\partial y}\\ \frac{\partial f}{\partial z}\end{pmatrix}=grad(f)\equiv\vec{\nabla}f$$

turns a **scalar** (***f***) into a **vector** grad(*f*), multiply $\vec{v}$ with the **direction $\mathbf{d}\vec{r}$** of the **closed path *C* we move along** and **adding it all up**

$$v_x(x,y)\Delta x + \left[v_y(x,y) + \frac{\partial v_y(x,y)}{\partial x}\Delta x\right]\Delta y - \left[v_x(x,y) + \frac{\partial v_x(x,y)}{\partial y}\Delta y\right]\Delta x - v_y(x,y)\Delta y =$$

A) to B) | B) to C) | C) to D) | D) to A)



equals the **difference** of the **mixed partial derivatives**, **times the area *A* defined by *C***

$$= \left[\frac{\partial v_y(x,y)}{\partial x} - \frac{\partial v_x(x,y)}{\partial y}\right]\Delta y \Delta x$$

$$\oint_C \vec{v}\cdot \mathbf{d}\vec{r} = \iint \left[\frac{\partial v_y}{\partial x} - \frac{\partial v_x}{\partial y}\right] dA$$

Green's Theorem

(Stoke's Theorem in 2D)

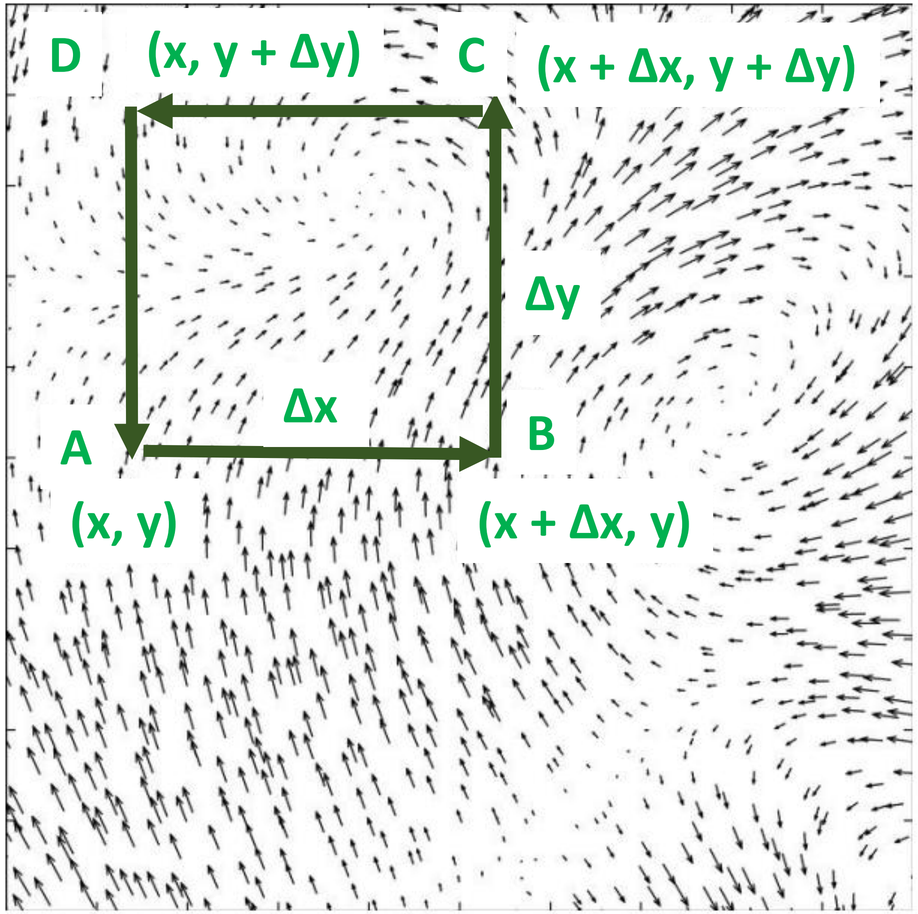
$$\oint_C \vec{v}\cdot \mathbf{d}\vec{r} = \int_A \left(\vec{\nabla}\times\vec{v}\right)\cdot d\vec{f}$$

Stoke's Theorem

credit:
Daniel Vieira

multiply $\vec{v}$ with the **direction $\mathbf{d}\vec{r}$** of the closed path C we move along and adding it all up

$$v_x(x,y)\Delta x + \left[v_y(x,y) + \frac{\partial v_y(x,y)}{\partial x}\Delta x\right]\Delta y - \left[v_x(x,y) + \frac{\partial v_x(x,y)}{\partial y}\Delta y\right]\Delta x - v_y(x,y)\Delta y =$$



equals the difference of the mixed partial derivatives, times the area A defined by C

$$= \left[\frac{\partial v_y(x,y)}{\partial x} - \frac{\partial v_x(x,y)}{\partial y}\right]\Delta y \Delta x$$

$$\oint_C \vec{v}\cdot \mathbf{d}\vec{r} = \iint \left[\frac{\partial v_y}{\partial x} - \frac{\partial v_x}{\partial y}\right] dA$$

Green's Theorem

(Stoke's Theorem in 2D)

$$\oint_C \vec{v}\cdot \mathbf{d}\vec{r} = \int_A (\vec{\nabla}\times\vec{v})\cdot d\vec{f}$$

Stoke's Theorem

credit: Daniel Vieira

Thank you very much for your attention!