Computational Physics

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What is computational physics?

"Computational physics is the study and implementation of numerical analysis to solve problems in physics for which a quantitative theory already exists. Historically, computational physics was the first application of modern computers in science, and is now a subset of computational science. It is sometimes regarded as a subdiscipline (or offshoot) of theoretical physics, but others consider it an intermediate branch between theoretical and experimental physics - an area of study which supplements both theory and experiment". *from WIKIPEDIA*

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ONE

PYTHON BASICS

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The integrated development environments (IDEs)

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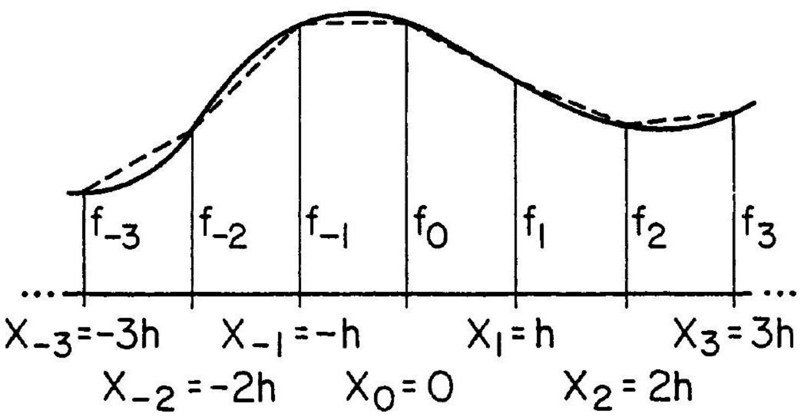
BASIC MATHEMATIC OPERATION

4.1 Discretization

$$f_n = f\left(x_n\right); x_n = nh(n = 0, \pm 1, \pm 2, \ldots),$$



4.2 Differentiation

We begin by using a Taylor series to expand f in the neighborhood of $x=0$:

$$f(x) = f_0 + xf' + \frac{x^2}{2!}f'' + \frac{x^3}{3!}f''' + \ldots$$

where all derivatives are evaluated at x=0. It is then simple to verify that

$$f_{\pm 1} \equiv f(x = \pm h) = f_0 \pm hf' + \frac{h^2}{2}f'' \pm \frac{h^3}{6}f''' + \mathcal{O}\left(h^4\right)$$
$$f_{\pm 2} \equiv f(x = \pm 2h) = f_0 \pm 2hf' + 2h^2 f'' \pm \frac{4h^3}{3}f''' + \mathcal{O}\left(h^4\right)$$

where $\mathcal{O}\left(h^4\right)$ means terms of order h^4 or higher.

To estimate the size of such terms, we can assume that and its derivatives are all of the same order of magnitude,
as is the case for many functions of physical relevance.

$$f' = \frac{f_1 - f_{-1}}{2h} - \frac{h^2}{6}f''' + \mathcal{O}\left(h^4\right)$$

$$f' \approx \frac{f_1 - f_{-1}}{2h}$$

Note: This "3-point" formula would be exact if were a second-degree polynomial in the 3-point interval *[-h,h]*, because the third- and all higherorder derivatives would then vanish.

It is more accurate (by one order in) than the forward or backward difference formulas:

$$\begin{aligned} f' &\approx \frac{f_1 - f_0}{h} + \mathcal{O}(h); \\ f' &\approx \frac{f_0 - f_{-1}}{h} + \mathcal{O}(h). \end{aligned}$$

extract thiese formula as a practice

$$f' \approx \frac{1}{12h}\left[f_{-2} - 8f_{-1} + 8f_1 - f_2\right] + \mathcal{O}\left(h^4\right)$$
$$f'' \approx \frac{f_1 - 2f_0 + f_{-1}}{h^2}.$$

4.2.1 Hands-On

```
import numpy as np
import matplotlib.pyplot as plt



##  we are looking for the derivative of the sin(x) from tw methods

steps=1000

x =np.linspace(-np.pi, np.pi,steps)
y =np.sin(x)

ydac = np.cos(x)

h = x[1]-x[0]

y1dif = np.diff(y)/h

yrol2=np.roll(y,2)[2:]
yt =y[2:]

y2dif = (yt-yrol2)/(2*h)

#plt.plot(x, ydac, '--', label="answer")
```

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```
plt.plot(x[:-1], y1dif-ydac[1:], lw=2, label='forward')
plt.plot(x[1:-1], y2dif-ydac[1:-1], lw=3, label='2points')

plt.legend()
```

Colab link

4.3 Numerical quadrature

4.4 Finding roots

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ERRORS

~To err is human, to forgive divine~

5.1 Types of Errors

5.2 Round-off Errors

5.3 Numerical Recursion

5.4 Error Assessment

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ORDINARY DIFFERENTIAL EQUATION

A linear differential equation:

$$a_0(x)y + a_1(x)y' + a_2(x)y'' + \cdots + a_n(x)y^{(n)} + b(x) = 0$$

A simple initial value problem

$$y' = f(x, y), \quad y(x_0) = y_0$$

We are interested in computing approximate values of the solution of above Equation in an interval $[x_0, b]$. Thus

$$x_i = x_0 + ih, \quad i = 0, 1, \ldots, n$$

$$h = \frac{b - x_0}{n}$$

10.1 Numerov Algorithm for Schrödinger ODE

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