PROGRAM STUDI INFORMATIKA
FAKULTAS TEKNIK DAN INFORMATIKA
UNIVERSITAS MULTIMEDIA NUSANTARA
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IF420 – ANALISIS NUMERIK

Pertemuan ke 10 – Numerical Differentiation

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Capaian Pembelajaran Mingguan Mata Kuliah (Sub-CPMK):

Sub-CPMK 10: Mahasiswa mampu memahami dan menerapkan teknik turunan numerik – C3

Reviews

- Root Finding Problem Statement
- Tolerance
- Bisection Method
- Newton-Raphson Method
- Root Finding in Python

Outlines

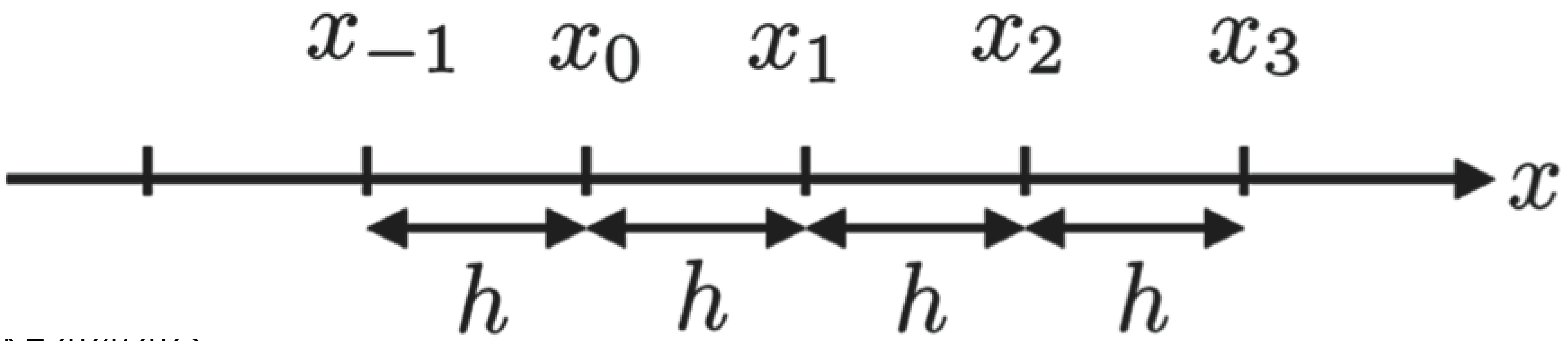
- Numerical Differentiation Problem Statement
- Finite Difference Approximating Derivatives
- Approximation of Higher Order Derivatives
- Numerical Differentiation with Noise

Motivation

- Many engineering and science systems **change** over **time**, **space**, and many other **dimensions** **of interest**.
- In Mathematics, function **derivatives** are often used to **model** these **changes**.
- However, in practice the function may **not** be explicitly **known**, or the function may be **implicitly represented** by a set of data points.
- In these cases and others, it may be desirable to **compute derivatives** **numerically** rather than **analytically**.

Numerical Differentiation Problem Statement

- A **numerical grid** is an **evenly spaced** set of points over the **domain** of a function (i.e., the independent variable), over some interval.
- The **spacing** or **step size** of a numerical grid is the **distance** between **adjacent points** on the grid.
- For the purpose of this text, if x is a **numerical grid**, then x_j is the j-th point in the numerical **grid** and h is the **spacing** between x_{j-1} and x_j.
- The following figure shows an example of a numerical grid.



Numerical Differentiation Problem Statement

- There are several **functions** in Python that can be used to generate **numerical grids**.
- For numerical grids in **one dimension**, it is sufficient to use the **linspace** function, which you have already used for creating regularly spaced arrays.
- In Python, a function $f(x)$ can be **represented** over an **interval** by **computing its value** on a grid.
- Although the function itself may be **continuous**, this **discrete** or **discretized** representation is useful for **numerical calculations** and **corresponds** to **data sets** that may be acquired in engineering and science practice.
- Specifically, the **function value** may only be known at **discrete points**.

Numerical Differentiation Problem Statement

- For example, a temperature sensor may deliver **temperature** versus **time** pairs at **regular time intervals**.
- Although temperature is a **smooth** and **continuous** function of time, the sensor only provides values at **discrete time intervals**, and in this particular case, the **underlying function** would **not** even be **known**.
- Whether f is an **analytic function** or a **discrete representation** of one, we would like to derive methods of **approximating** the **derivative** of f over a numerical **grid** and determine their **accuracy**.

Finite Difference Approximating Derivatives

- The **derivative** $f'(x)$ of a function $f(x)$ at the point $x = a$ is defined as:

$$f'(x) = \lim_{x \to a} \frac{f(x) - f(a)}{x - a}$$

- The **derivative** at $x = a$ is the **slope** at this **point**.
- In **finite difference approximations** of this **slope**, we can use values of the function in the neighborhood of the point $x = a$ to achieve the goal.
- There are **various finite difference formulas** used in different applications, and three of these, where the derivative is calculated using the **values** of **two points**, are presented next.

Forward & Backward Differences

- The **forward difference** is to estimate the **slope** of the function at x_j using the **line** that connects $\left(x_j, f\left(x_j\right)\right)$ and $\left(x_{j+1}, f\left(x_{j+1}\right)\right)$:

$$f'\left(x_j\right) = \frac{f\left(x_{j+1}\right) - f\left(x_j\right)}{x_{j+1} - x_j}$$

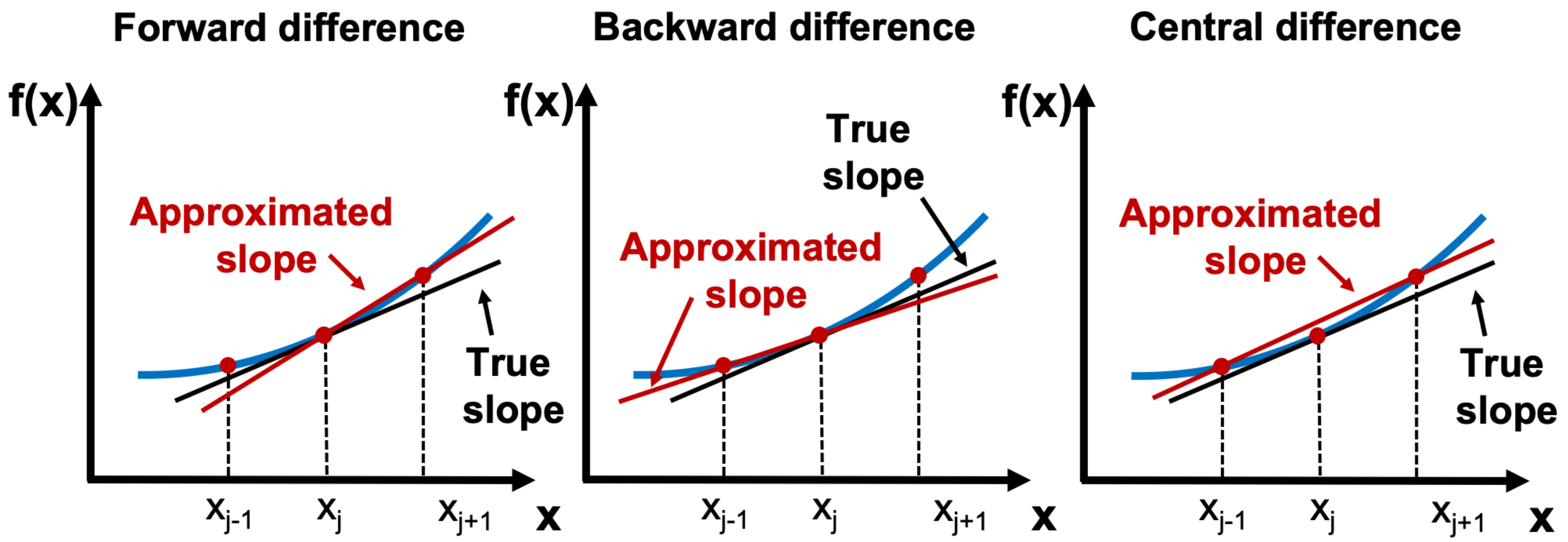
- The **backward difference** is to estimate the **slope** of the function at x_j using the **line** that connects $\left(x_{j-1}, f\left(x_{j-1}\right)\right)$ and $\left(x_j, f\left(x_j\right)\right)$:

$$f'\left(x_j\right) = \frac{f\left(x_j\right) - f\left(x_{j-1}\right)}{x_j - x_{j-1}}$$

Central Difference

- The **central difference** is to estimate the **slope** of the function at x_j using the **line** that connects $\left(x_{j-1}, f\left(x_{j-1}\right)\right)$ and $\left(x_{j+1}, f\left(x_{j+1}\right)\right)$:

$$f'\left(x_j\right) = \frac{f\left(x_{j+1}\right) - f\left(x_{j-1}\right)}{x_{j+1} - x_{j-1}}$$



Using Taylor Series

- To **derive** an **approximation** for the **derivative** of f, we return to **Taylor series**.
- For an **arbitrary function** $f(x)$ the **Taylor series** of f around $a = x_j$ is

$$f(x) = \frac{f(x_j)(x - x_j)^0}{0!} + \frac{f'(x_j)(x - x_j)^1}{1!} + \frac{f''(x_j)(x - x_j)^2}{2!} + \cdots$$

- If x is on a **grid** of points with **spacing** h, we can compute the **Taylor series** at $x = x_{j+1}$ to get

$$f(x_{j+1}) = \frac{f(x_j)(x_{j+1} - x_j)^0}{0!} + \frac{f'(x_j)(x_{j+1} - x_j)^1}{1!} + \frac{f''(x_j)(x_{j+1} - x_j)^2}{2!} + \cdots$$

- **Substituting** $h = x_{j+1} - x_j$ and solving for $f'(x_j)$ gives the equation

$$f'(x_j) = \frac{f(x_{j+1}) - f(x_j)}{h} + \left(-\frac{f''(x_j)h}{2!} - \frac{f'''(x_j)h^2}{3!} - \cdots\right)$$

- The terms that are in **parentheses**, $-\frac{f''(x_j)h}{2!} - \frac{f'''(x_j)h^2}{3!} - \cdots$, are called **higher order terms** of h.
- The **higher order terms** can be rewritten as

$$-\frac{f''(x_j)h}{2!} - \frac{f'''(x_j)h^2}{3!} - \cdots = h(\alpha + \epsilon(h))$$

where α is some **constant**, and $\epsilon(h)$ is a **function** of h that goes to **zero** as h goes to 0. You can verify with some algebra that this is true. We use the **abbreviation** "$O(h)$" for $h(\alpha + \epsilon(h))$, and in **general**, we use the abbreviation "$O(h^p)$" to denote $h^p(\alpha + \epsilon(h))$.

- Substituting $O(h)$ into the previous equation gives

$$f'(x_j) = \frac{f(x_{j+1}) - f(x_j)}{h} + O(h)$$

- This gives the **forward difference** formula for approximating derivatives as

$$f'(x_j) \approx \frac{f(x_{j+1}) - f(x_j)}{h}$$

and we say this formula is $O(h)$.

- Here, $O(h)$ describes the **accuracy** of the **forward difference** formula for approximating derivatives.
- For an approximation that is $O(h^p)$, we say that p is the **order** of the **accuracy** of the approximation.
- With few exceptions, **higher order accuracy** is **better** than **lower order**. To illustrate this point, assume $q < p$. Then as the spacing, $h > 0$, goes to 0, h^p goes to 0 **faster** than h^q. Therefore as h goes to 0, an approximation of a value that is $O(h^p)$ gets **closer** to the **true** value **faster** than one that is $O(h^q)$.

Using Taylor Series

- By computing the **Taylor series** around $a = x_j$ at $x = x_{j-1}$ and again solving for $f'(x_j)$, we get the **backward difference** formula

$$f'(x_j) \approx \frac{f(x_j) - f(x_{j-1})}{h}$$

which is also $O(h)$. You should try to verify this result on your own.

- Intuitively, the **forward** and **backward** **difference** formulas for the derivative at x_j are just the **slopes** between the point at x_j and the points x_{j+1} and x_{j-1}, respectively.

- We can construct an **improved approximation** of the derivative by clever manipulation of **Taylor series** terms taken at **different points**.
- To illustrate, we can compute the **Taylor series** around $a = x_j$ at both x_{j+1} and x_{j-1}.
- Written out, these equations are

$$f\left(x_{j+1}\right) = f\left(x_j\right) + f'\left(x_j\right)h + \frac{1}{2}f''\left(x_j\right)h^2 + \frac{1}{6}f'''\left(x_j\right)h^3 + \cdots$$

and

$$f\left(x_{j-1}\right) = f\left(x_j\right) - f'\left(x_j\right)h + \frac{1}{2}f''\left(x_j\right)h^2 - \frac{1}{6}f'''\left(x_j\right)h^3 + \cdots$$

- **Subtracting** the formulas above gives

$$f\left(x_{j+1}\right) - f\left(x_{j-1}\right) = 2f'\left(x_j\right)h + \frac{1}{3}f'''\left(x_j\right)h^3 + \cdots$$

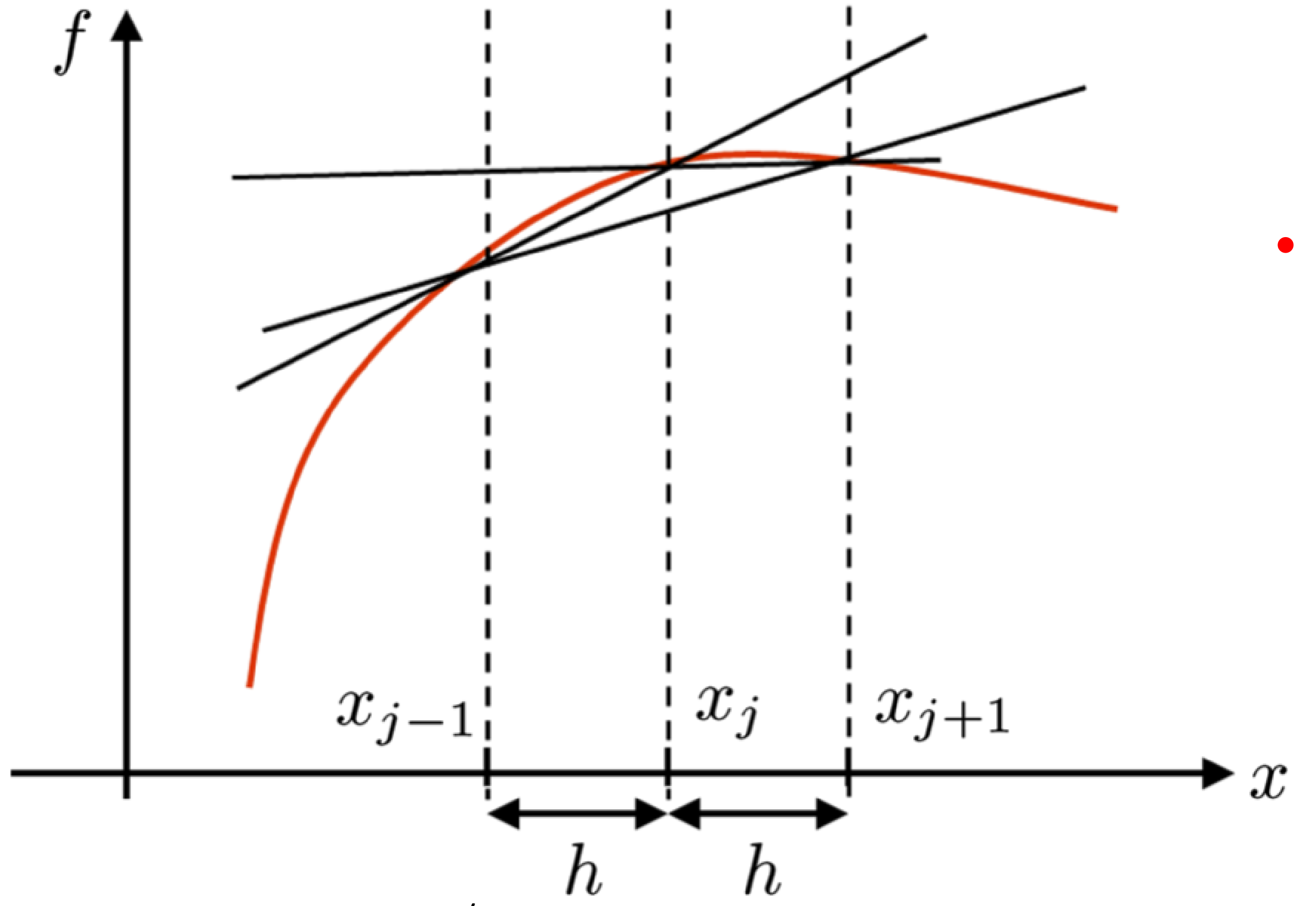
which when solved for $f'\left(x_j\right)$ gives the **central difference** formula

$$f'\left(x_j\right) \approx \frac{f\left(x_{j+1}\right) - f\left(x_{j-1}\right)}{2h}$$

Using Taylor Series

- Because of how we **subtracted** the two equations, the h terms **canceled out**; therefore, the **central difference formula** is $O(h^2)$, even though it requires the same amount of computational effort as the **forward** and **backward difference** formulas!
- Thus the **central difference** formula gets an **extra order** of **accuracy** for free.
- In general, formulas that utilize **symmetric** points around x_j, for example x_{j-1} and x_{j+1}, have **better accuracy** than **asymmetric** ones, such as the **forward** and **backward difference** formulas.

- The following figure shows the **forward difference** (line joining (x_j, y_j) and (x_{j+1}, y_{j+1})), **backward difference** (line joining (x_j, y_j) and (x_{j-1}, y_{j-1})), and **central difference** (line joining (x_{j-1}, y_{j-1}) and (x_{j+1}, y_{j+1})) approximation of the **derivative** of a function f.



- As can be seen, the **difference** in the value of the **slope** can be **significantly different** based on the size of the step h and the nature of the function.

Using Taylor Series

- **Example**: Take the Taylor series of f around $a = x_j$ and compute the series at $x = x_{j-2}, x_{j-1}, x_{j+1}, x_{j+2}$. Show that the resulting equations can be combined to form an approximation for $f'(x_j)$ that is $O(h^4)$.

- First, compute the **Taylor series** at the specified points.

$$f(x_{j-2}) = f(x_j) - 2hf'(x_j) + \frac{4h^2 f''(x_j)}{2} - \frac{8h^3 f'''(x_j)}{6} + \frac{16h^4 f''''(x_j)}{24} - \frac{32h^5 f'''''(x_j)}{120} + \cdots$$

$$f(x_{j-1}) = f(x_j) - hf'(x_j) + \frac{h^2 f''(x_j)}{2} - \frac{h^3 f'''(x_j)}{6} + \frac{h^4 f''''(x_j)}{24} - \frac{h^5 f'''''(x_j)}{120} + \cdots$$

$$f(x_{j+1}) = f(x_j) + hf'(x_j) + \frac{h^2 f''(x_j)}{2} + \frac{h^3 f'''(x_j)}{6} + \frac{h^4 f''''(x_j)}{24} + \frac{h^5 f'''''(x_j)}{120} + \cdots$$

$$f(x_{j+2}) = f(x_j) + 2hf'(x_j) + \frac{4h^2 f''(x_j)}{2} + \frac{8h^3 f'''(x_j)}{6} + \frac{16h^4 f''''(x_j)}{24} + \frac{32h^5 f'''''(x_j)}{120} + \cdots$$

- To get the h^2, h^3, and h^4 terms to **cancel out**, we can compute

$$f(x_{j-2}) - 8f(x_{j-1}) + 8f(x_{j+1}) - f(x_{j+2}) = 12hf'(x_j) - \frac{48h^5 f'''''(x_j)}{120}$$

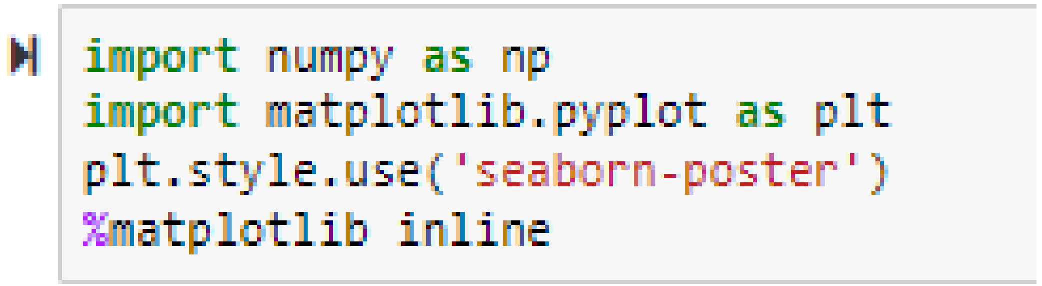
which can be rearranged to

$$f'(x_j) = \frac{f(x_{j-2}) - 8f(x_{j-1}) + 8f(x_{j+1}) - f(x_{j+2})}{12h} + O(h^4)$$

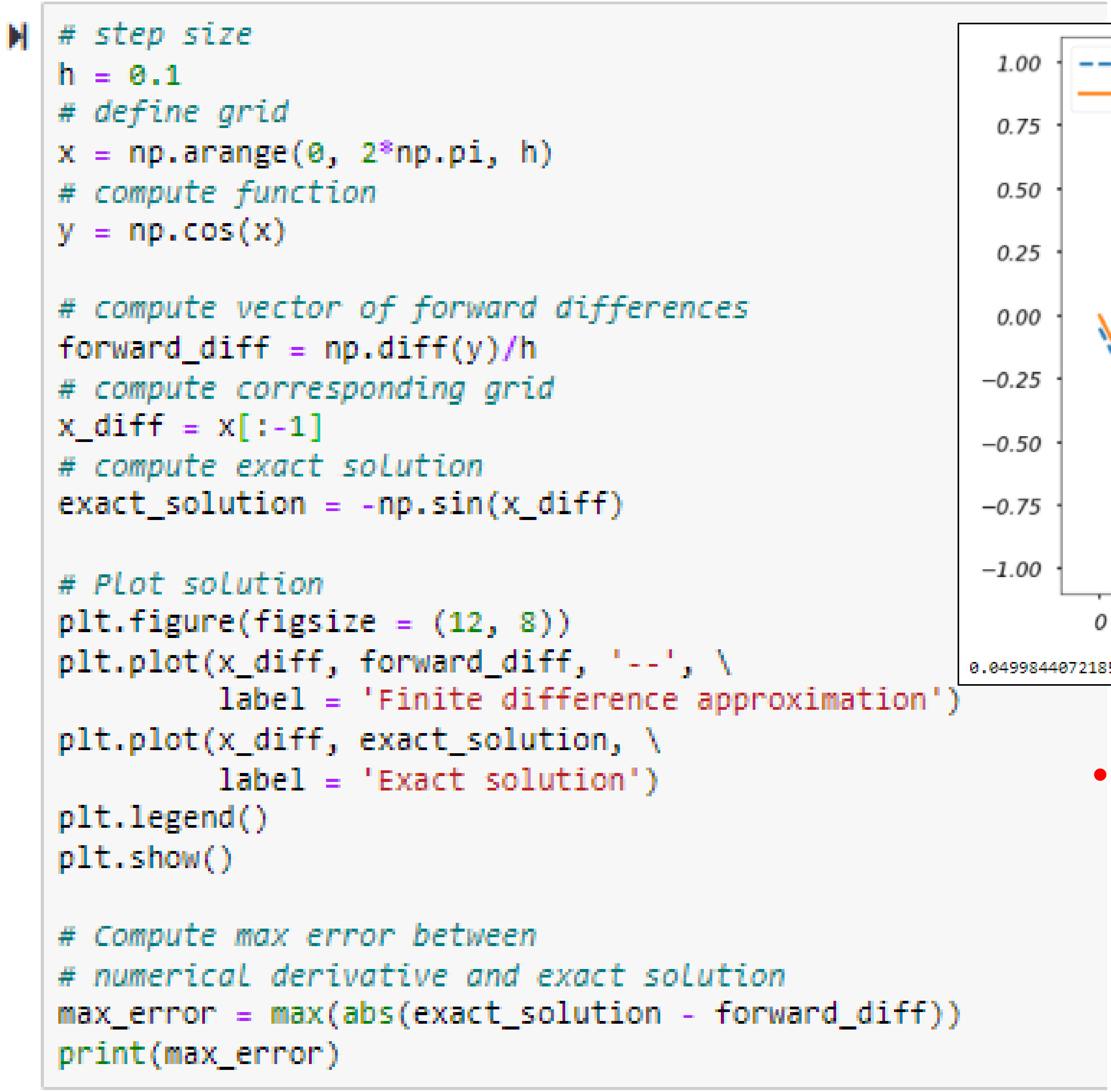
- This formula is a **better approximation** for the derivative at x_j than the **central difference** formula, but requires twice as many calculations.
- **TIPS**! Python has a command that can be used to compute **finite differences** directly: For a vector f, the command **d=np.diff(f)** produces an array d in which the entries are the differences of the adjacent elements in the initial array f.
- In other words $d(i) = f(i+1) - f(i)$.
- **WARNING**! When using the command **np.diff**, the size of the output is **one less** than the size of the input since it needs two arguments to produce a difference.

Using Taylor Series

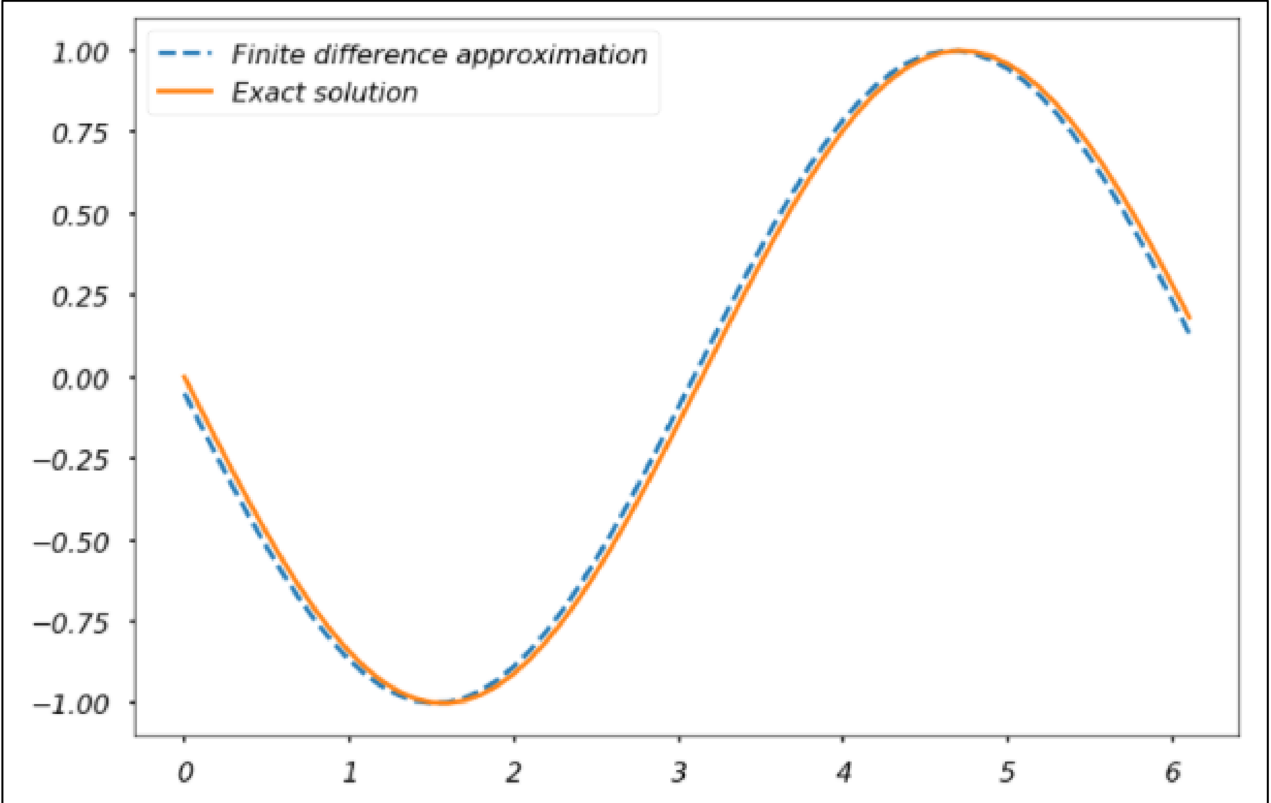
- **Example**: Consider the function $f(x) = \cos(x)$. We know the derivative of $\cos(x)$ is $-\sin(x)$. Although in practice we may not know the underlying function we are finding the derivative for, we use this simple example to illustrate the aforementioned **numerical differentiation** methods and their **accuracy**. The following code computes the derivatives numerically.



```
import numpy as np
import matplotlib.pyplot as plt
plt.style.use('seaborn-poster')
%matplotlib inline
```



```python
# step size
h = 0.1
# define grid
x = np.arange(0, 2*np.pi, h)
# compute function
y = np.cos(x)

# compute vector of forward differences
forward_diff = np.diff(y)/h
# compute corresponding grid
x_diff = x[:-1]
# compute exact solution
exact_solution = -np.sin(x_diff)

# Plot solution
plt.figure(figsize = (12, 8))
plt.plot(x_diff, forward_diff, '--', \
         label = 'Finite difference approximation')
plt.plot(x_diff, exact_solution, \
         label = 'Exact solution')
plt.legend()
plt.show()

# Compute max error between
# numerical derivative and exact solution
max_error = max(abs(exact_solution - forward_diff))
print(max_error)
```

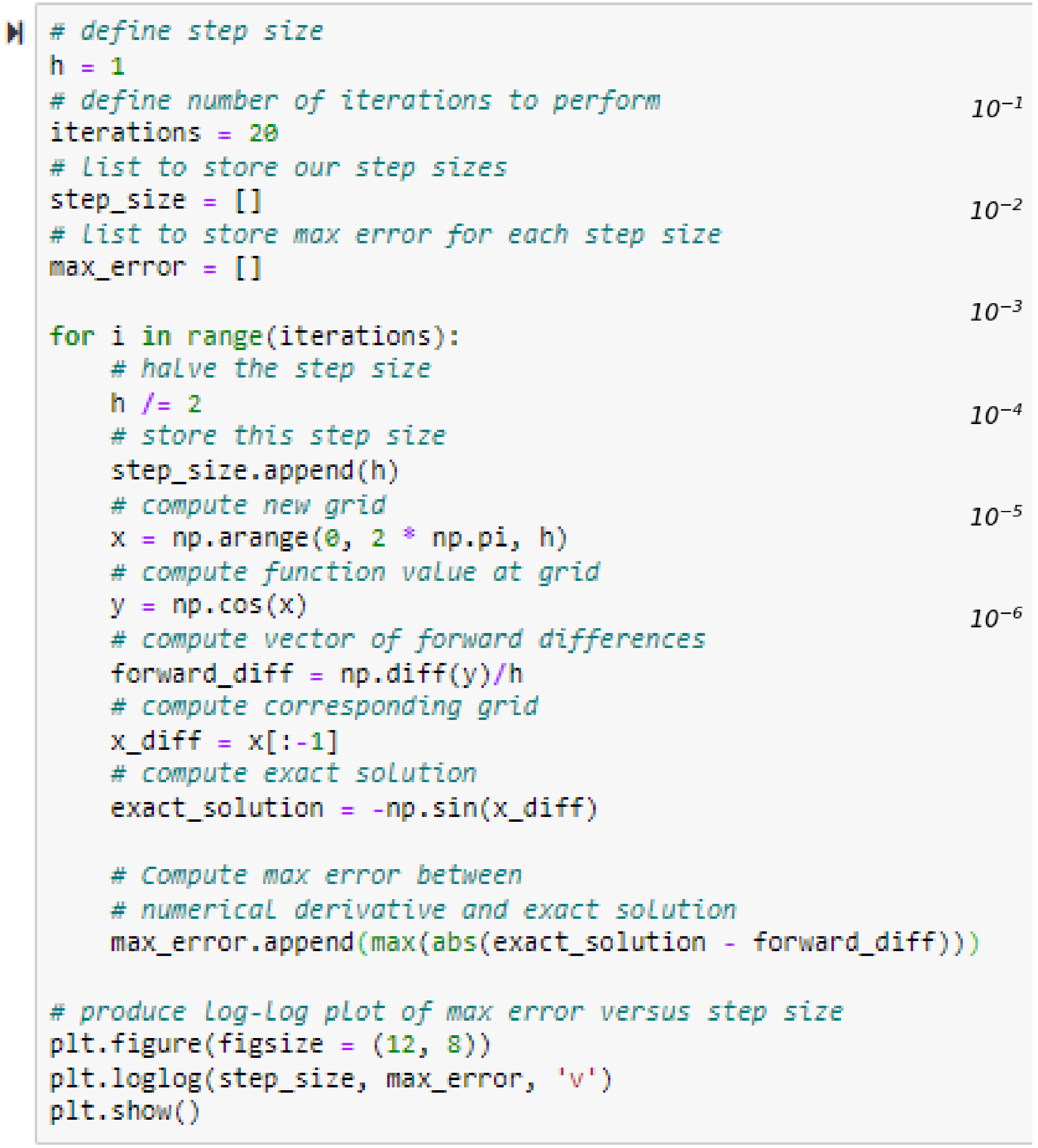


```
0.049984407218554114
```

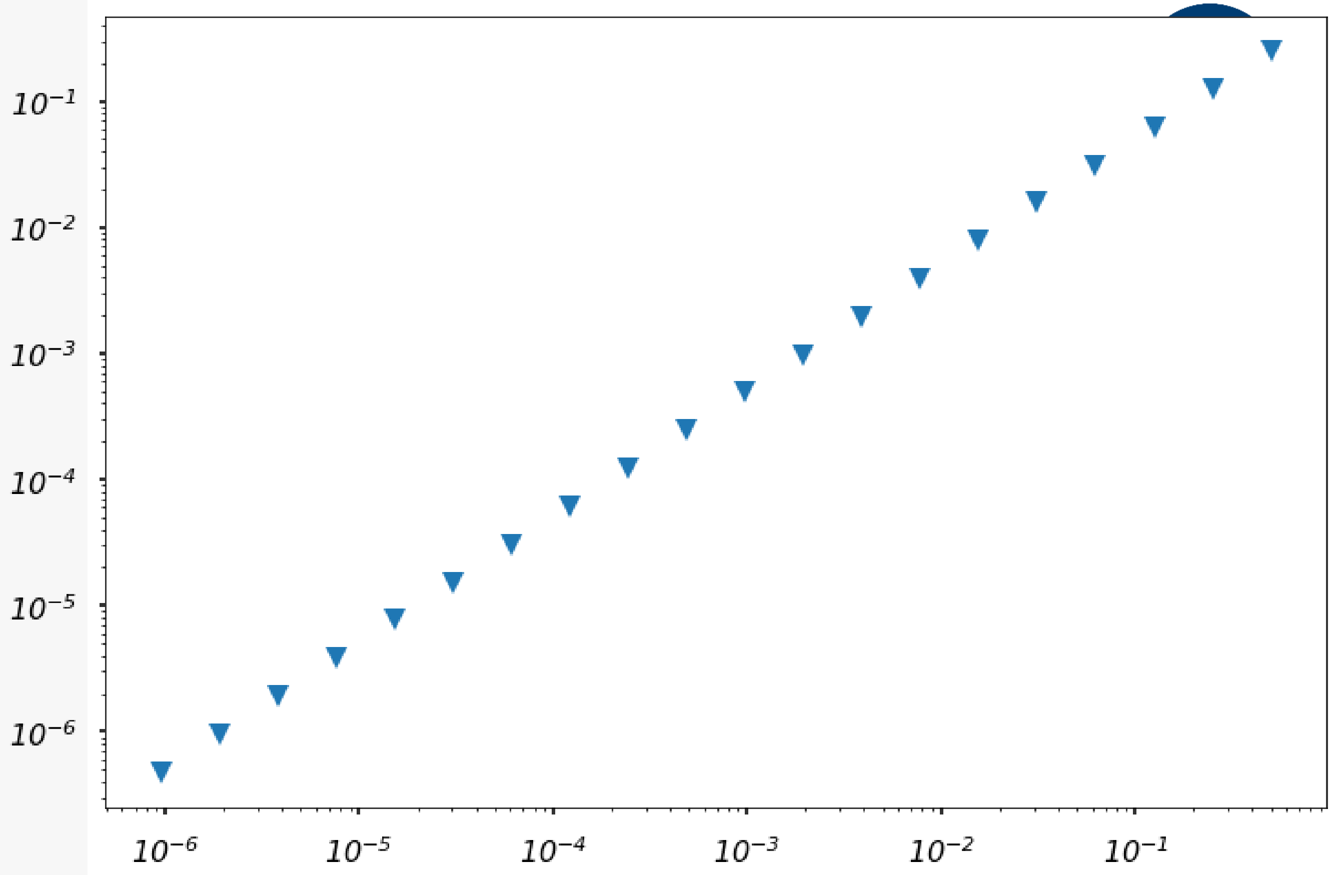
- As the above figure shows, there is a small **offset** between the **two curves**, which results from the **numerical error** in the evaluation of the **numerical derivatives**.

Using Taylor Series

- As illustrated in the previous example, the **finite difference scheme** contains a **numerical error** due to the approximation of the derivative.
- This difference **decreases** with the **size** of the **discretization step**, which is illustrated in the following example.
- **Example**: The following code computes the numerical derivative of $f(x) = \cos(x)$ using the **forward difference** formula with **decreasing** step sizes, h. It then plots the maximum error between the approximated derivative and the true derivative versus h as shown in the generated figure.



```python
# define step size
h = 1
# define number of iterations to perform
iterations = 20
# list to store our step sizes
step_size = []
# list to store max error for each step size
max_error = []

for i in range(iterations):
    # halve the step size
    h /= 2
    # store this step size
    step_size.append(h)
    # compute new grid
    x = np.arange(0, 2 * np.pi, h)
    # compute function value at grid
    y = np.cos(x)
    # compute vector of forward differences
    forward_diff = np.diff(y)/h
    # compute corresponding grid
    x_diff = x[:-1]
    # compute exact solution
    exact_solution = -np.sin(x_diff)

    # Compute max error between
    # numerical derivative and exact solution
    max_error.append(max(abs(exact_solution - forward_diff)))

# produce log-log plot of max error versus step size
plt.figure(figsize = (12, 8))
plt.loglog(step_size, max_error, 'v')
plt.show()
```



- The **slope** of the line in **log-log** space is 1; therefore, the error is **proportional** to h^1, which means that, as expected, the forward difference formula is $O(h)$.

Approximation of Higher Order Derivatives

- It is also possible to use **Taylor series** to approximate **higher order derivatives** (e.g., $f''(x_j), f'''(x_j)$, etc.). For example, taking the Taylor series around $a = x_j$ and then computing it at $x = x_{j-1}$ and x_{j+1} gives

$$f(x_{j-1}) = f(x_j) - hf'(x_j) + \frac{h^2 f''(x_j)}{2} - \frac{h^3 f'''(x_j)}{6} + \cdots$$

and

$$f(x_{j+1}) = f(x_j) + hf'(x_j) + \frac{h^2 f''(x_j)}{2} + \frac{h^3 f'''(x_j)}{6} + \cdots$$

- If we **add** these two equations together, we get

$$f(x_{j-1}) + f(x_{j+1}) = 2f(x_j) + h^2 f''(x_j) + \frac{2h^4 f''''(x_j)}{24} + \cdots$$

and with some rearrangement gives the approximation $f''(x_j) \approx \frac{f(x_{j+1}) - 2f(x_j) + f(x_{j-1})}{h^2}$ and $O(h^2)$.

Numerical Differentiation with Noise

- As stated earlier, sometimes f is given as a **vector,** where f is the corresponding function value for **independent data values** in another vector x, which is gridded.
- Sometimes data can be **contaminated** with **noise**, meaning its value is **off** by a small amount from what it would be if it were computed from a **pure** Mathematical function.
- This can often occur in engineering due to **inaccuracies** in **measurement devices** or the **data** itself can be slightly **modified** by perturbations outside the system of interest.
- For example, you may be trying to listen to your friend talk in a crowded room. The signal f might be the **intensity** and **tonal values** in your friend’s speech. However, because the room is crowded, **noise** from other conversations are heard along with your friend’s speech, and he becomes difficult to understand.

Numerical Differentiation with Noise

- To illustrate this point, we **numerically compute** the **derivative** of a simple **cosine** wave **corrupted** by a **small sin** wave.
- Consider the following **two functions**:

$$f(x) = \cos(x)$$

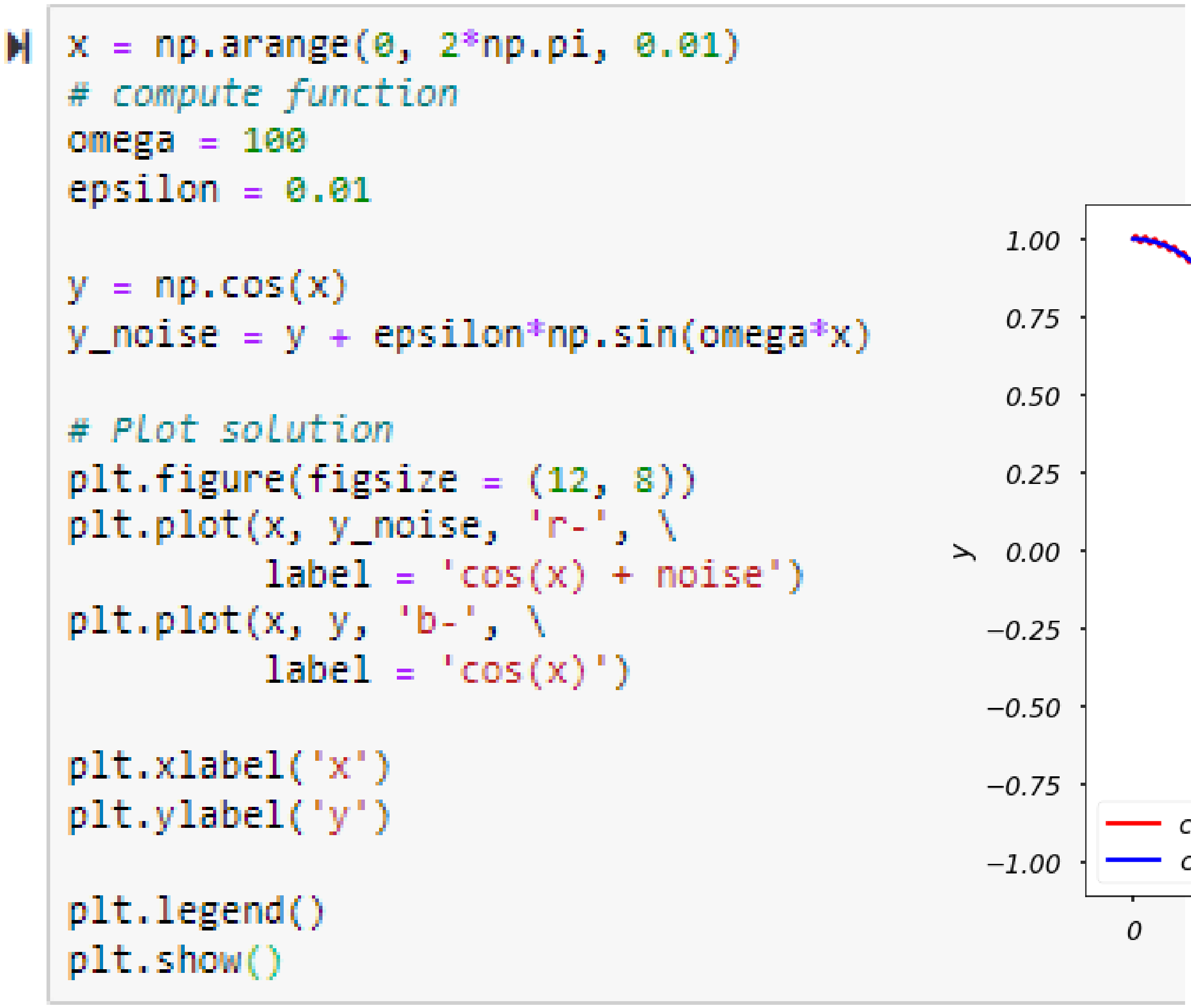
and

$$f_{\epsilon,\omega}(x) = \cos(x) + \epsilon \sin(\omega x)$$

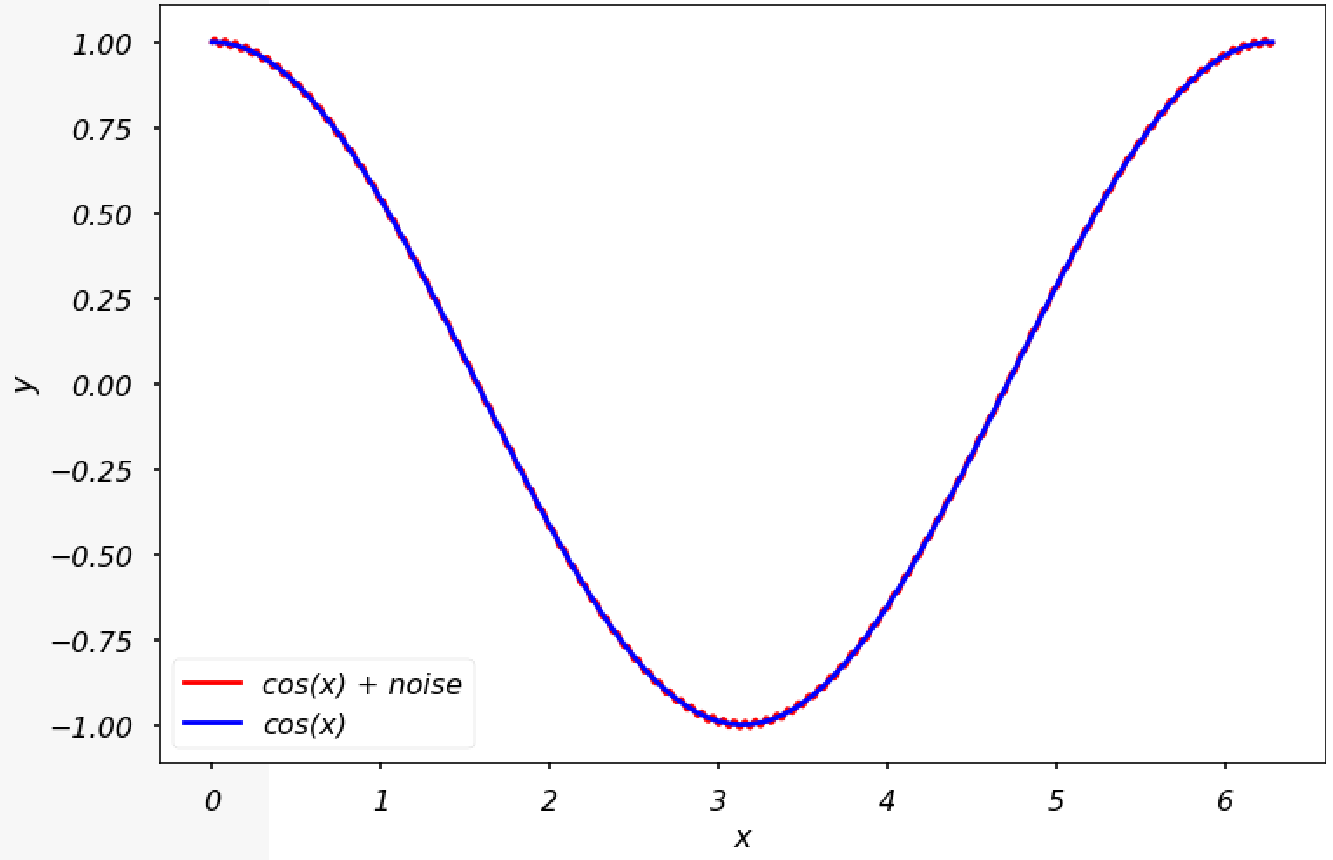
where $0 < \epsilon \ll 1$ is a very small number and ω is a large number.

- When ϵ is small, it is clear that $f \simeq f_{\epsilon,\omega}$.
- To illustrate this point, we plot $f_{\epsilon,\omega}(x)$ for $\epsilon = 0.01$ and $\omega = 100$, and we can see it is **very close** to $f(x)$, as shown in the following figure.

Numerical Differentiation with Noise



```
x = np.arange(0, 2*np.pi, 0.01)
# compute function
omega = 100
epsilon = 0.01

y = np.cos(x)
y_noise = y + epsilon*np.sin(omega*x)

# Plot solution
plt.figure(figsize = (12, 8))
plt.plot(x, y_noise, 'r-', \
         label = 'cos(x) + noise')
plt.plot(x, y, 'b-', \
         label = 'cos(x)')

plt.xlabel('x')
plt.ylabel('y')

plt.legend()
plt.show()
```



Numerical Differentiation with Noise

- The **derivatives** of our **two** test **functions** are

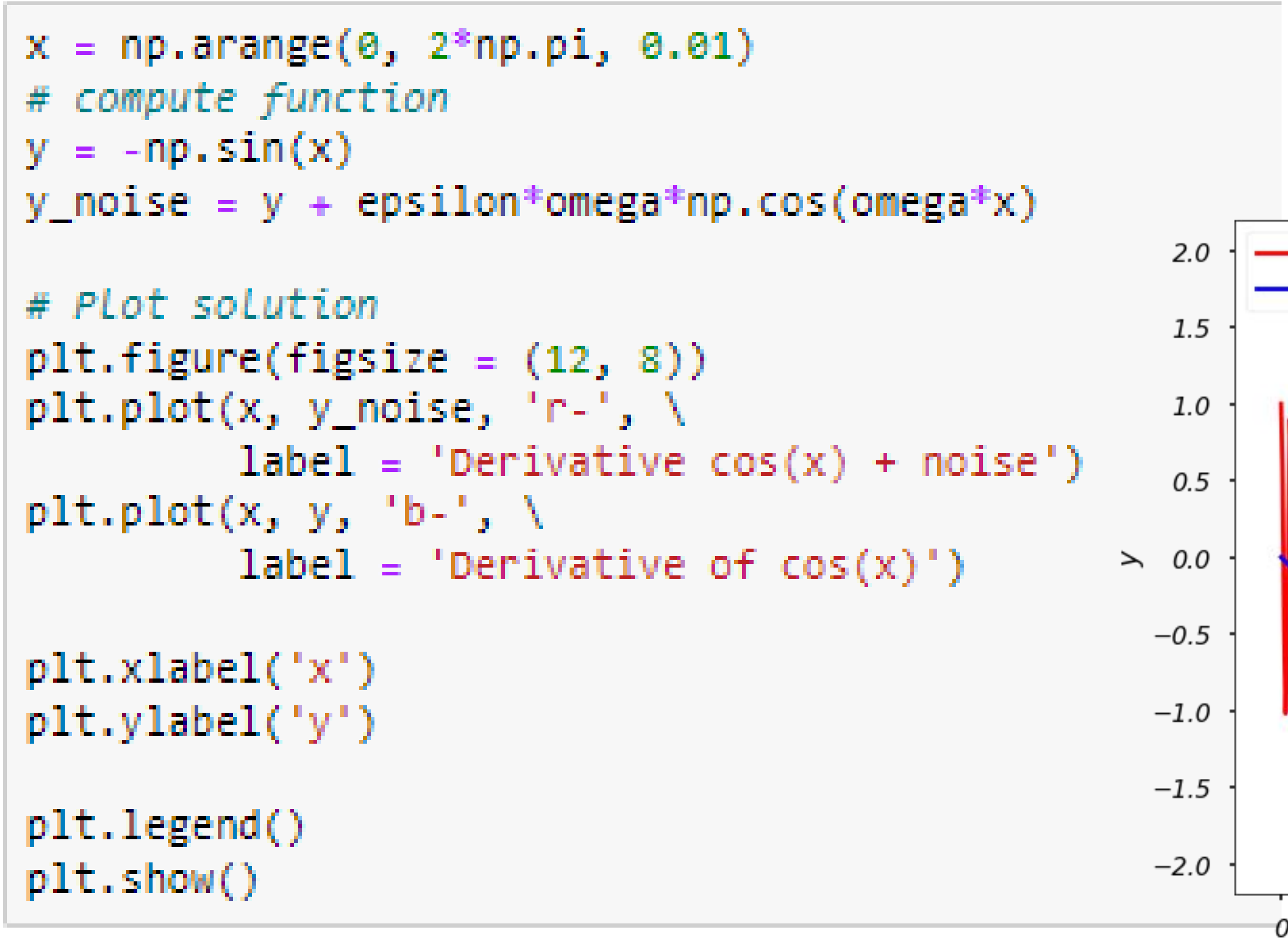
$$f'(x) = -\sin(x)$$

and

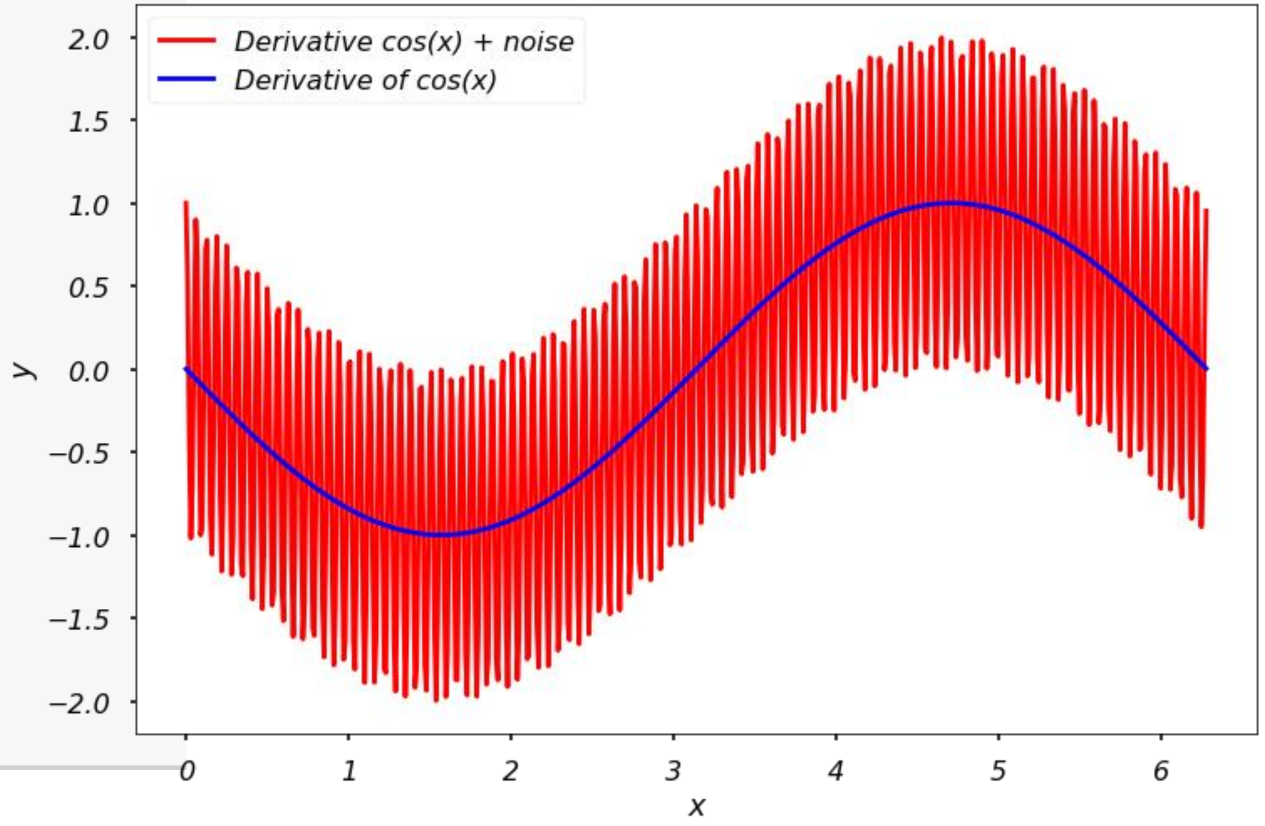
$$f'_{\epsilon,\omega}(x) = -\sin(x) + \epsilon\omega\cos(\omega x)$$

- Since $\epsilon\omega$ may not be small when ω is large, the **contribution** of the **noise** to the derivative **may not** be **small**.
- As a result, the **derivatives** (analytic and numerical) may **not** be **usable**.
- For instance, the following figure shows $f'(x)$ and $f'_{\epsilon,\omega}(x)$ for $\epsilon = 0.01$ and $\omega = 100$.

Numerical Differentiation with Noise

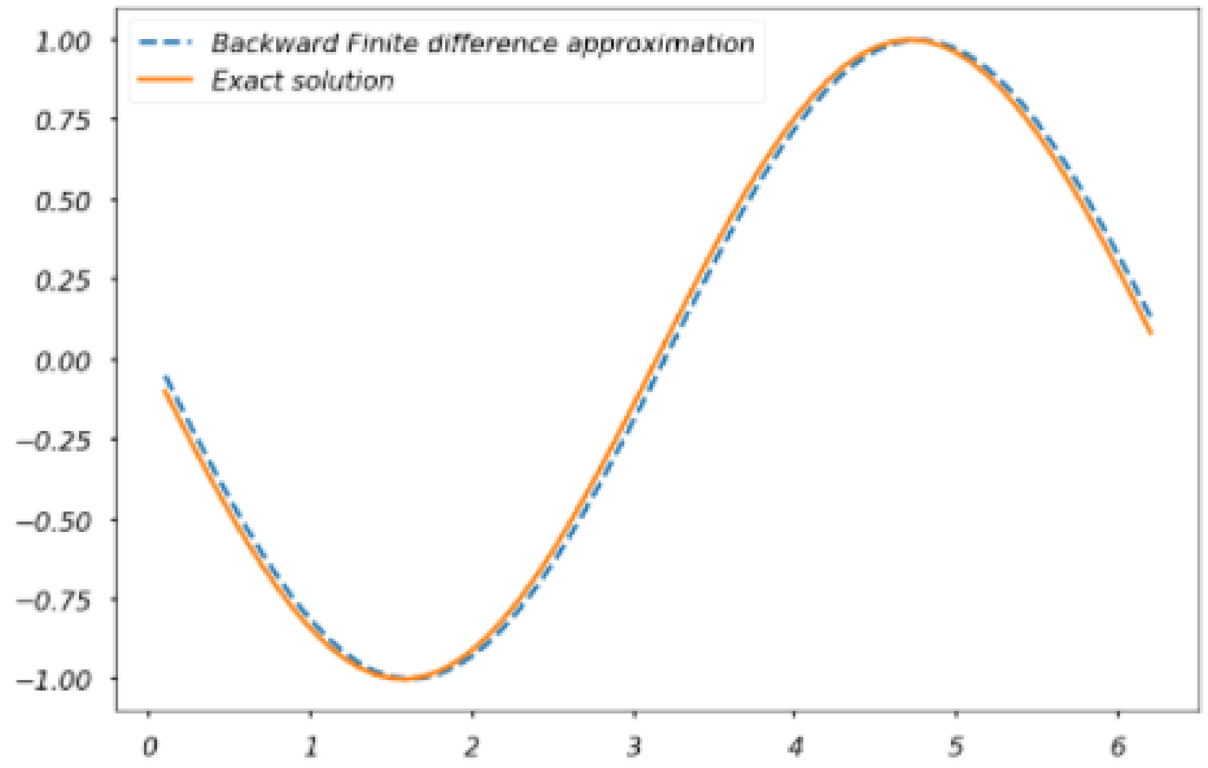


```
x = np.arange(0, 2*np.pi, 0.01)
# compute function
y = -np.sin(x)
y_noise = y + epsilon*omega*np.cos(omega*x)

# Plot solution
plt.figure(figsize = (12, 8))
plt.plot(x, y_noise, 'r-', \
         label = 'Derivative cos(x) + noise')
plt.plot(x, y, 'b-', \
         label = 'Derivative of cos(x)')

plt.xlabel('x')
plt.ylabel('y')

plt.legend()
plt.show()
```



Practice

1. **Modify** the code used to show the numerical differentiation of $f(x)$=cos(x) with forward difference method earlier. Modify it to show the result using '**backward difference**' method and compute the maximum error from this numerical approximation!



```
0.04997039864231646
```

Next Week's Outline

- Numerical Integration Problem Statement
- Riemann's Integral
- Trapezoid Rule
- Simpson's Rule
- Computing Integrals in Python

References

- Kong, Qingkai; Siauw, Timmy, and Bayen, Alexandre. 2020. Python Programming and Numerical Methods: A Guide for Engineers and Scientists. Academic Press. https://www.elsevier.com/books/python-programming-and-numerical-methods/kong/978-0-12-819549-9
- Other online and offline references

Visi

Menjadi Program Studi Strata Satu Informatika **unggulan** yang menghasilkan lulusan **berwawasan internasional** yang **kompeten** di bidang Ilmu Komputer (*Computer Science*), **berjiwa wirausaha** dan **berbudi pekerti luhur**.

INFORMATIKA
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Misi

1. Menyelenggarakan pembelajaran dengan teknologi dan kurikulum terbaik serta didukung tenaga pengajar profesional.
2. Melaksanakan kegiatan penelitian di bidang Informatika untuk memajukan ilmu dan teknologi Informatika.
3. Melaksanakan kegiatan pengabdian kepada masyarakat berbasis ilmu dan teknologi Informatika dalam rangka mengamalkan ilmu dan teknologi Informatika.