

Introduction to Computer Programming for the Physical Sciences

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- ☐ Open a new Jupyter notebook
- ☐ Name your notebook with your name and Homework 1
- ☐ Open a Markdown cell at the top and write your name and Homework 1
- ☐ Open a Markdown cell before each problem and write e.g. Problem 1, Problem 2(a), etc.
- ☐ Please abide by the [Policy and Guidelines on Using AI Tools](#)
- ☐ Once you finish the problems: 1) Restart the Python kernel and clear all cell outputs. 2) Rerun the notebook from start to finish so that all answers/outputs show up. 3) Save your notebook as a single .pdf file and upload it to Gradescope on Canvas by the deadline. **No late homeworks will be accepted except for illness accompanied by a doctor's note.**

Homework 3

Problem 1: Working with Python Data Containers

You are tasked with developing a program to manage information on business trips made by employees to various cities where your company has offices. Unfortunately, your company did not adopt a uniform method for recording this information, so you have to first develop a program that can convert the hybrid data into a homogenous format. Specifically, the business trip data is a python list containing a combination of dictionaries and tuples, where each dictionary or tuple represents information about a specific trip. The relevant data are the employee's name, destination city, round-trip mileage, and the date of the trip. The dictionaries contain the information in key-value pairs (i.e. name, destination, mileage, date), while the tuple contains the same information ordered sequentially (i.e. tuple_data = (name, destination, mileage, date)). The employee data is given in the code cell below:

```
In [ ]: import numpy as np
```

```
In [ ]: trips = [
    {'name': 'Alice', 'destination': 'New York', 'mileage': 200.0, 'date': '2022-01-01'},
    ('Bob', 'Chicago', 300, '2022-02-01'),
    {'name': 'Charlie', 'destination': 'Los Angeles', 'mileage': 400, 'date': '2022-03-01'},
    ('David', 'San Francisco', 500.0, '2022-04-01'),
    {'name': 'Eve', 'destination': 'Seattle', 'mileage': 620, 'date': '2022-05-01'},
    ('Frank', 'Boston', 705, '2022-06-01'),
    {'name': 'Grace', 'destination': 'Denver', 'mileage': 810, 'date': '2022-07-01'},
    ('Henry', 'Austin', 911, '2022-08-01'),
    {'name': 'Ivy', 'destination': 'Atlanta', 'mileage': 1000.0, 'date': '2022-09-01'},
    ('Jack', 'Miami', 1112.0, '2022-10-01'),
    {'name': 'Kate', 'destination': 'Dallas', 'mileage': 1200.0, 'date': '2022-11-01'},
    ('Liam', 'Houston', 134, '2022-12-01'),
    {'name': 'Mia', 'destination': 'Phoenix', 'mileage': 1400.0, 'date': '2023-01-01'},
    ('Noah', 'Las Vegas', 1526.0, '2023-02-01'),
    {'name': 'Olivia', 'destination': 'San Diego', 'mileage': 1600.0, 'date': '2023-03-01'},
    ('Peter', 'Portland', 1700, '2023-04-01'),
    ('Alice', 'Boston', 1322.0, '2023-01-01'),
    ('Bob', 'Los Angeles', 400, '2023-02-01'),
    {'name': 'Charlie', 'destination': 'Chicago', 'mileage': 500, 'date': '2023-03-01'},
    ('David', 'Miami', 600.0, '2023-04-01'),
    {'name': 'Eve', 'destination': 'Dallas', 'mileage': 700.0, 'date': '2023-05-01'},
    ('Frank', 'Houston', 800, '2023-06-01'),
    {'name': 'Grace', 'destination': 'Phoenix', 'mileage': 900.0, 'date': '2023-07-01'},
    ('Henry', 'Las Vegas', 1000, '2023-08-01'),
    {'name': 'Ivy', 'destination': 'San Diego', 'mileage': 1100.0, 'date': '2023-09-01'},
    ('Jack', 'Portland', 1200, '2023-10-01'),
    {'name': 'Kate', 'destination': 'New York', 'mileage': 1300.0, 'date': '2023-11-01'},
    ('Liam', 'Austin', 1400, '2023-12-01'),
    {'name': 'Mia', 'destination': 'Denver', 'mileage': 1500.0, 'date': '2024-01-01'},
    ('Noah', 'Atlanta', 1600, '2024-02-01'),
    {'name': 'Olivia', 'destination': 'Seattle', 'mileage': 1700.0, 'date': '2024-03-01'},
    ('Peter', 'San Francisco', 1800, '2024-04-01'),
    {'name': 'Alice', 'destination': 'Los Angeles', 'mileage': 210.0, 'date': '2024-05-01'},
    ('Alice', 'Boston', 3000.0, '2023-05-01'),
    ('Bob', 'San Francisco', 310, '2022-03-01'),
    {'name': 'Charlie', 'destination': 'Seattle', 'mileage': 410, 'date': '2022-04-01'},
    ('David', 'Boston', 510.0, '2022-05-01'),
    {'name': 'Eve', 'destination': 'Denver', 'mileage': 630, 'date': '2022-06-01'},
    ('Frank', 'Austin', 715, '2022-07-01'),
```

```
[
    {'name': 'Grace', 'destination': 'Atlanta', 'mileage': 820, 'date': '2022-08-01', 'driver': 'Henry', 'city': 'Miami', 'mileage': 921, 'date': '2022-09-01'},
    {'name': 'Ivy', 'destination': 'Dallas', 'mileage': 1010.0, 'date': '2022-10-01', 'driver': 'Jack', 'city': 'Houston', 'mileage': 1122.0, 'date': '2022-11-01'},
    {'name': 'Kate', 'destination': 'Phoenix', 'mileage': 1210.0, 'date': '2022-12-01', 'driver': 'Liam', 'city': 'Las Vegas', 'mileage': 144, 'date': '2023-01-01'},
    {'name': 'Mia', 'destination': 'San Diego', 'mileage': 1410.0, 'date': '2023-02-01', 'driver': 'Noah', 'city': 'Portland', 'mileage': 1536.0, 'date': '2023-03-01'},
    {'name': 'Olivia', 'destination': 'San Francisco', 'mileage': 1610.0, 'date': '2023-04-01', 'driver': 'Peter', 'city': 'New York', 'mileage': 1710, 'date': '2023-05-01'},
    {'name': 'Anne', 'destination': 'Seattle', 'mileage': 220.0, 'date': '2022-03-01', 'driver': 'Gerald', 'city': 'Boston', 'mileage': 320, 'date': '2022-04-01'},
    {'name': 'Charlie', 'destination': 'Denver', 'mileage': 420, 'date': '2022-05-01', 'driver': 'Dirk', 'city': 'Austin', 'mileage': 520.0, 'date': '2022-06-01'},
    {'name': 'Eve', 'destination': 'Atlanta', 'mileage': 640, 'date': '2022-07-01', 'driver': 'Joe', 'city': 'Miami', 'mileage': 725, 'date': '2022-08-01'},
    {'name': 'Grace', 'destination': 'Dallas', 'mileage': 830, 'date': '2022-09-01', 'driver': 'Dirk', 'city': 'Houston', 'mileage': 931, 'date': '2022-10-01'},
    {'name': 'Ivy', 'destination': 'Phoenix', 'mileage': 1020.0, 'date': '2022-11-01', 'driver': 'Henry', 'city': 'Las Vegas', 'mileage': 1132.0, 'date': '2022-12-01'},
    {'name': 'Kate', 'destination': 'San Diego', 'mileage': 1220.0, 'date': '2023-01-01', 'driver': 'Alison', 'city': 'Portland', 'mileage': 154, 'date': '2023-02-01'},
    {'name': 'Mia', 'destination': 'San Francisco', 'mileage': 1420.0, 'date': '2023-03-01', 'driver': 'Noah', 'city': 'New York', 'mileage': 1546.0, 'date': '2023-04-01'},
    {'name': 'Olivia', 'destination': 'Los Angeles', 'mileage': 1620.0, 'date': '2023-05-01', 'driver': 'Peter', 'city': 'Chicago', 'mileage': 1720, 'date': '2023-06-01'}
]
```

a) Write a function called `convert_trips` to convert the trip data into a homogenous format with behavior that follows the documentation string below:

```
def convert_trips(trips, append_new=None, filter_dict=None,
display=False):
    """
    Convert a list of trips containing dictionaries and tuples to a
    list of dictionaries.

    Parameters
    -----
    trips : list
        Trip database containing dictionaries and tuples, where each
        dictionary or tuple
        represents information about a specific trip.

    Returns
    -----
    output_list: list of dicts
        Trip database as a list of dictionaries.

    """
```

Test your function by performing a loop over each trip in the `output_list` and printing the trip data (i.e. the dictionary) to the screen.

```
In [ ]: # problem 1
# a)
def convert_trips(trips, append_new=None, filter_dict=None, display=False):
    """
```

Convert a list of trips containing dictionaries and tuples to a list of dict

Parameters

trips : list

Trip database containing dictionaries and tuples, where each dictionary represents information about a specific trip.

Returns

output_list: list of dicts

Trip database as a list of dictionaries.

"""

```
output_list = [0 for _ in range(len(trips))]
```

```
# set up a list with proper length for future operation
```

```
for i in range(len(trips)):
```

```
# going through each element of trips
```

```
if (type(trips[i]) == tuple):
```

```
# find out if the element is a tuple type, if it is, converted it in
```

```
output_list[i] = {'name':trips[i][0], 'destination': trips[i][1], 'mi
```

```
else:
```

```
# if the element is not tuple, which has to be dictionary, just copy
```

```
output_list[i] = trips[i]
```

```
return output_list
```

```
converted_trips = convert_trips(trips)
```

```
print(converted_trips)
```

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```
nix', 'mileage': 1020.0, 'date': '2022-11-01'}, {'name': 'Henry', 'destination':
'Las Vegas', 'mileage': 1132.0, 'date': '2022-12-01'}, {'name': 'Kate', 'destinat
ion': 'San Diego', 'mileage': 1220.0, 'date': '2023-01-01'}, {'name': 'Alison',
'destination': 'Portland', 'mileage': 154, 'date': '2023-02-01'}, {'name': 'Mia',
'destination': 'San Francisco', 'mileage': 1420.0, 'date': '2023-03-01'}, {'nam
e': 'Noah', 'destination': 'New York', 'mileage': 1546.0, 'date': '2023-04-01'},
{'name': 'Olivia', 'destination': 'Los Angeles', 'mileage': 1620.0, 'date': '2023
-05-01'}, {'name': 'Peter', 'destination': 'Chicago', 'mileage': 1720, 'date': '2
023-06-01'}]
```

b) Write a function called `query_trips` consistent with the behavior in the following documentation string.

```
def query_trips(trips, filter_dict):
    """
    Manage business trip data.

    Parameters
    -----
    trips : list
        Trip database containing a list of dictionaries with
    information about each trip.
    filter_dict : dict, optional
        If provided, return the list of trips that match the key-value
    pairs in
        this dictionary. The allowed keys in the dictionary are 'name',
        'destination', and 'date'. Multiple keys can be provided.

    Returns
    -----
    output_list: list of dicts
        List of trips that match the input parameters.

    Examples
    -----
    >>> filter_dict = {'name': 'Alice', 'destination': 'Boston'}
    >>> alice_trips = manage_trips(trips, filter_dict)
    Returns the list:

    alice_trips = [{'name': 'Alice', 'destination': 'Boston',
    'mileage': 1322.0, 'date': '2023-01-01'},
                    {'name': 'Alice', 'destination': 'Boston',
    'mileage': 3000.0, 'date': '2023-05-01'}]
```

Note: Make sure that if multiple trip parameters (name, destination, date) are provided in `filter_dict`, the output is a list of trips that match ALL of those parameters.

Test your code on the following example usage cases:

```
# Test filtering trips by destination, should print trips to New York
filter_dict = {'destination': 'New York'}
filtered_trips = query_trips(trips, filter_dict)

# Test filtering trips by name, should print trips by Noah
filter_dict = {'name': 'Noah'}
```

```
filtered_trips = query_trips(trips, filter_dict)
```

```
# Test filtering trips by date, should print trips on 2023-04-01
```

```
filter_dict = {'date': '2023-04-01'}
```

```
filtered_trips = query_trips(trips, filter_dict)
```

```
# Test filtering trips by name and destination, should print trips by Alice to New York
```

```
filter_dict = {'name': 'Alice', 'destination': 'New York'}
```

```
filtered_trips = query_trips(trips, filter_dict)
```

For each of these test, put the code in a separate code cell, and loop over each trip in `filtered_trips` and print the trip data (i.e. the dictionary) to the screen.

```
In [ ]: # b)
def query_trips(trips, filter_dict):
    """
    Manage business trip data.

    Parameters
    -----
    trips : list
        Trip database containing a list of dictionaries with information about e
    filter_dict : dict, optional
        If provided, return the list of trips that match the key-value pairs in
        this dictionary. The allowed keys in the dictionary are 'name',
        'destination', and 'date'. Multiple keys can be provided.

    Returns
    -----
    output_list: list of dicts
        List of trips that match the input parameters.

    Examples
    -----
    >>> filter_dict = {'name': 'Alice', 'destination': 'Boston'}
    >>> alice_trips = manage_trips(trips, filter_dict)
    Returns the list:

    alice_trips = [{'name': 'Alice', 'destination': 'Boston', 'mileage': 1322.0,
                    {'name': 'Alice', 'destination': 'Boston', 'mileage': 3000.0,
    """
    output_list = []
    # set up an empty list for operation
    for i in range(len(trips)):
        # going through all the elements in trips
        output_list.append(trips[i])
        # add this element of tips to the outputlist
        for j in filter_dict.keys():
            # gonging through the elements that we have to check
            if(trips[i][j] != filter_dict[j]):
                # find out if the element we want is in the element of trips
                output_list.remove(trips[i])
                # remove the element from output_list if it is not in the filter
                break
        # stop the cycle, since there is no need to check if other senar

    return output_list
```

```
filter_dict = {'name': 'Alice', 'destination': 'Boston'}
alice_trips = query_trips(converted_trips, filter_dict)
print(alice_trips)
```

```
[{'name': 'Alice', 'destination': 'Boston', 'mileage': 1322.0, 'date': '2023-01-01'}, {'name': 'Alice', 'destination': 'Boston', 'mileage': 3000.0, 'date': '2023-05-01'}]
```

```
In [ ]: # Test filtering trips by destination, should print trips to New York
filter_dict = {'destination': 'New York'}
filtered_trips = query_trips(converted_trips, filter_dict)
print(filtered_trips)
```

```
[{'name': 'Alice', 'destination': 'New York', 'mileage': 200.0, 'date': '2022-01-01'}, {'name': 'Kate', 'destination': 'New York', 'mileage': 1300.0, 'date': '2023-11-01'}, {'name': 'Peter', 'destination': 'New York', 'mileage': 1710, 'date': '2023-05-01'}, {'name': 'Noah', 'destination': 'New York', 'mileage': 1546.0, 'date': '2023-04-01'}]
```

```
In [ ]: # Test filtering trips by name, should print trips by Noah
filter_dict = {'name': 'Noah'}
filtered_trips = query_trips(converted_trips, filter_dict)
print(filtered_trips)
```

```
[{'name': 'Noah', 'destination': 'Las Vegas', 'mileage': 1526.0, 'date': '2023-02-01'}, {'name': 'Noah', 'destination': 'Atlanta', 'mileage': 1600, 'date': '2024-02-01'}, {'name': 'Noah', 'destination': 'Portland', 'mileage': 1536.0, 'date': '2023-03-01'}, {'name': 'Noah', 'destination': 'New York', 'mileage': 1546.0, 'date': '2023-04-01'}]
```

```
In [ ]: # Test filtering trips by date, should print trips on 2023-04-01
filter_dict = {'date': '2023-04-01'}
filtered_trips = query_trips(converted_trips, filter_dict)
print(filtered_trips)
```

```
[{'name': 'Peter', 'destination': 'Portland', 'mileage': 1700, 'date': '2023-04-01'}, {'name': 'David', 'destination': 'Miami', 'mileage': 600.0, 'date': '2023-04-01'}, {'name': 'Olivia', 'destination': 'San Francisco', 'mileage': 1610.0, 'date': '2023-04-01'}, {'name': 'Noah', 'destination': 'New York', 'mileage': 1546.0, 'date': '2023-04-01'}]
```

```
In [ ]: # Test filtering trips by name and destination, should print trips by Alice to New York
filter_dict = {'name': 'Alice', 'destination': 'New York'}
filtered_trips = query_trips(converted_trips, filter_dict)
print(filtered_trips)
```

```
[{'name': 'Alice', 'destination': 'New York', 'mileage': 200.0, 'date': '2022-01-01'}]
```

Problem 2: The Fibonacci Sequence

The Fibonacci sequence begins

0, 1, 1, 2, 3, 5, 8, 13, 21, 34, 55,

and is defined by the recursion relation

$$x_{n+1} = x_n + x_{n-1}$$

with $x_0 \equiv 0$ and $x_1 \equiv 1$. Write Python code to determine the largest Fibonacci number less than 10^6 ?

```
In [ ]: # problem 2
xn_small=0 # x0
xn=1 # x1
# set up initial value for the fibonacci number
xn_large = xn + xn_small # x2

while (xn_large < 10**6):
    # if the next number in Fibonacci number is less than 1e6, keep working on it
    xn_small = xn
    xn = xn_large
    # since we only need 2 numbers before the number we need to calculate in order
    # we are also saving a lot space by doing this.
    # in the while, xn_small represent x(n-1) in the formula and xn represent xn
    xn_large = xn + xn_small
    # xn_large is represent x(n+1) in the formula
    # we only need to add xn and x(n-1) to get x(n+1)

print(xn)
# since when the loop is break xn_large is the smallest number in Fibonacci which
# xn should be the largest number in Fibonacci which is smaller than 1e6
```

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Problem 3: Higher Order Derivatives

We can represent the n^{th} derivative of $f(x)$ as $f^{(n)}(x)$ where $f^0(x) \equiv f(x)$, $f^1(x) \equiv f'(x)$, $f^2(x) \equiv f''(x)$, etc.

Last week we learned how to compute numerical derivatives of a function $f(x)$, and found that the symmetric difference formula

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

performs significantly better than the forward difference formula.

As discussed at the end of the Week3 lecture notes, recursive functions are Python functions that call themselves.

a) Code up a **recursive** Python function to compute the n^{th} derivative of the function $f(x)$ using the symmetric difference formula and the recursion relation

$$f^{(n)}(x) \approx \frac{f^{(n-1)}(x+h) - f^{(n-1)}(x-h)}{2h}$$

Your function should be consistent with the following documentation string:

```
def deriv(f, x, n, h=1e-2):
    """
    Compute the nth derivative of a function f(x) using the symmetric
    difference formula.
```

```

Parameters
-----
f : function
    Function to take the derivative of.
x : float
    Point at which to evaluate the derivative.
n : int
    Order of the derivative.
h : float, optional
    Step size. The default is 1e-2.

Returns
-----
f^(n)(x): float
    The nth derivative of f(x) evaluated at x.

"""

```

b) Test your function by computing the derivatives of e^x at $x = 1$ for $n = 0, 1, 2, 3, 4, \dots, 10$ and compare to the analytic result. Print out your results to 16 decimal places. You can use the numpy function `np.exp()` to compute e^x .

c) Up to what order of the derivative n can you compute before you start getting numerical errors?

d) In your own words, what do you think is the source of these errors? Why do they set in at large values of n ?

```

In [ ]: # problem 3
# a)
def deriv(f, x, n, h=1e-2):
    """
    Compute the nth derivative of a function f(x) using the symmetric difference

    Parameters
    -----
    f : function
        Function to take the derivative of.
    x : float
        Point at which to evaluate the derivative.
    n : int
        Order of the derivative.
    h : float, optional
        Step size. The default is 1e-2.

    Returns
    -----
    f^(n)(x): float
        The nth derivative of f(x) evaluated at x.
    """
    if(n==0):
        return f(x)
    if(n==1):
        return (f(x+h)-f(x-h))/(2*h)
    return (deriv(f,x+h,n-1,h)-deriv(f,x-h,n-1,h))/(2*h)

# b)

```

```
for i in range(11):  
    print(deriv(np.exp,1.0,i,))
```

```
2.718281828459045  
2.718327133382714  
2.7183724390611452  
2.7184177454619984  
2.7184630602139492  
2.7185087514425277  
2.7184643425215427  
2.7144952952085077  
3.660266534311063  
44.23544863740858  
-9540.979117872439
```

b) continues:

the derivative of e^x should always be e^x no matter how many times of derivative are taken. Thus, all the results should be e. However, some of them shown on screen does not.

c)

starting from order 8 the result start to be far away from e, which is the analitical result.

d)

I think the source of the error may come from the limit of float numbers. Since h is 1e-2, when the order gets higher, the np.exp() may result in such a small number that float is no longer accurate enough. Than things will go wrong.