SEMT30002: Scientific Computing and Optimisation

Week 1 Demos: Finite differences and Euler's method

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Finite differences

In the first demo, we look at how to numerically approximate the derivative of the function $f(x) = e^{2x}$ using the forwards differencing formula given by

$$f'(a) = \frac{f(a + \Delta x) - f(a)}{\Delta x} + O(\Delta x).$$

We start by importing some functions and packages:

In [1]:

```python
from math import exp
import numpy as np
import matplotlib.pyplot as plt
```

Now we define a Python function that implements the first-order accurate forwards difference approximation

In [2]:

```python
def forward(f, a, dx):
    """
    Implements the first-order forwards difference formula
    """
    return (f(a+dx) - f(a)) / dx
```

We also define a Python function for the mathematical function $f(x) = e^{2x}$.

In [3]:

```python
def f(x):
    """
    Implements the exponential function given by
    f(x) = exp(2 * x) using NumPy functions
    """
    return np.exp(2 * x)
```

Now we use the forwards difference formula to approximate $f'(1)$ using 20 different values of Δx that are logarithmically spaced between 10^{-4} and 10^{-1}.

In [4]:

```
# The point where we want to evaluate the derivative
a = 1

# A NumPy array with values of \Delta x
dx = np.logspace(-4, -1, 20)

# Approximate the derivative using forwards differencing
dfdx_f = forward(f, a, dx)
```

- Now we calculate the exact value of the derivative, which is given by $f'(1) = 2e$.
- Using the exact value of the derivative, we can calculate the truncation error to convince ourselves that our code is working as expected

In [5]:

```
# Compute the exact value of the derivative
dfdx_exact = 2 * exp(2 * a)

# Compute the (absolute value) of the truncation error
TE_f = np.abs(dfdx_exact - dfdx_f)
```

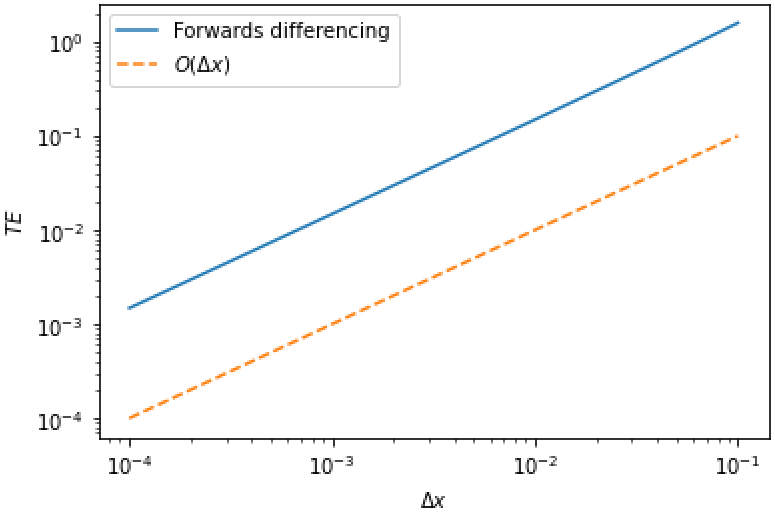
- We now create a log-log plot of the truncation error as a function of Δx.
- The use of logarithmic axes will make it easier to determine the rate at which the truncation error decreases with Δx, since the slope of the curve will indicate the power of Δx that the truncation error depends on.

- To see this, suppose that $TE = K(\Delta x)^p$ for some constant K and exponent p.
- Then $\log(TE) = p\log(\Delta x) + \log K$.
- Thus, $\log(TE)$ is linear in $\log(\Delta x)$ and has slope p.

- Theory tells us that the truncation error of the forwards difference formula should linearly decrease with Δx.
- Therefore, we also plot the curve $TE = \Delta x$.
- When plotted using log axes, the slopes of the two curves should be the same since the power of Δx is the same

In [6]:

```
plt.loglog(dx, TE_f, label = 'Forwards differencing')
plt.loglog(dx, dx, '--', label = '$O(\\Delta x)$')
plt.xlabel('$\\Delta x$')
plt.ylabel('$TE$')
plt.legend()
plt.show()
```



Forwards vs central differencing

We will now re-calculate the derivatives using the central difference approximation to showcase the increase in accuracy.

We start by defining a Python function that implements the central difference formula

In [7]:
```
def central(f, a, dx):
    """
    Implements the second-order central difference formula
    """
    return (f(a+dx) - f(a-dx)) / 2 / dx
```

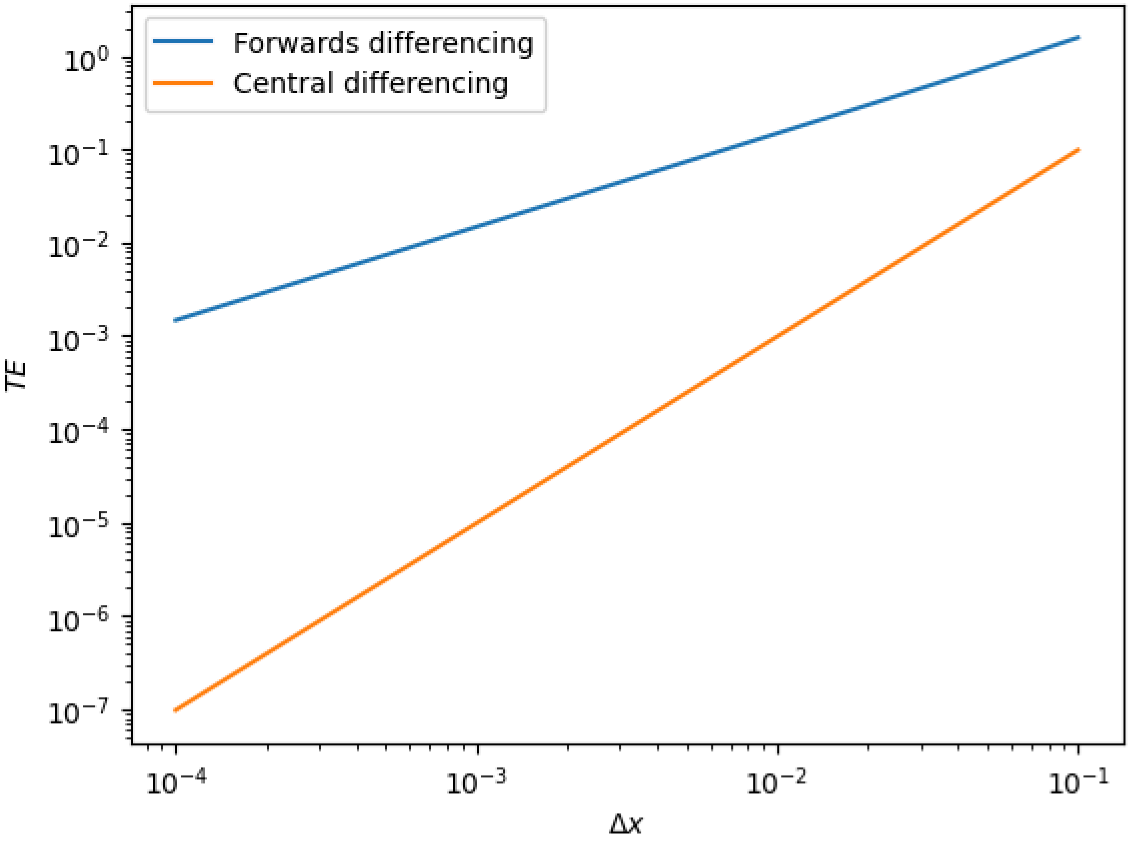
Now we approximate the derivative and calculate the truncation error

In [8]:
```
# Approximate the derivative using forwards differencing
dfdx_c = central(f, a, dx)

# Calculate the truncation error
TE_c = np.abs(dfdx_exact - dfdx_c)
```

Finally, we plot the truncation errors obtained using the forwards and central difference formulae.

In [9]:
```
plt.loglog(dx, TE_f, label = 'Forwards differencing')
plt.loglog(dx, TE_c, label = 'Central differencing')
plt.xlabel('$\\Delta x$')
plt.ylabel('$TE$')
plt.legend()
plt.show()
```



- The truncation error is much smaller when central differencing is used, indicating this is a much more accurate method.
- It is easy to see that the slope of the orange curve is two, indicating that the truncation error of the central difference formula is $O((\Delta x)^2)$, as expected from theory.

Is my differentiation formula correct?

In this demo, we deliberately introduce an error into the forwards difference formula for the first derivative. We then see how this manifests in the truncation error.

We start by defining an incorrect Python function for the forwards difference formula:

In [10]:
```
def forward_error(f, a, dx):
    """
    Implements a buggy version of the forwards difference formula
    for the first-order derivative
    """
    return (f(a+dx) - f(a)) / 2 / dx
```

As before, we calculate the derivative and the truncation error. The results are then plotted

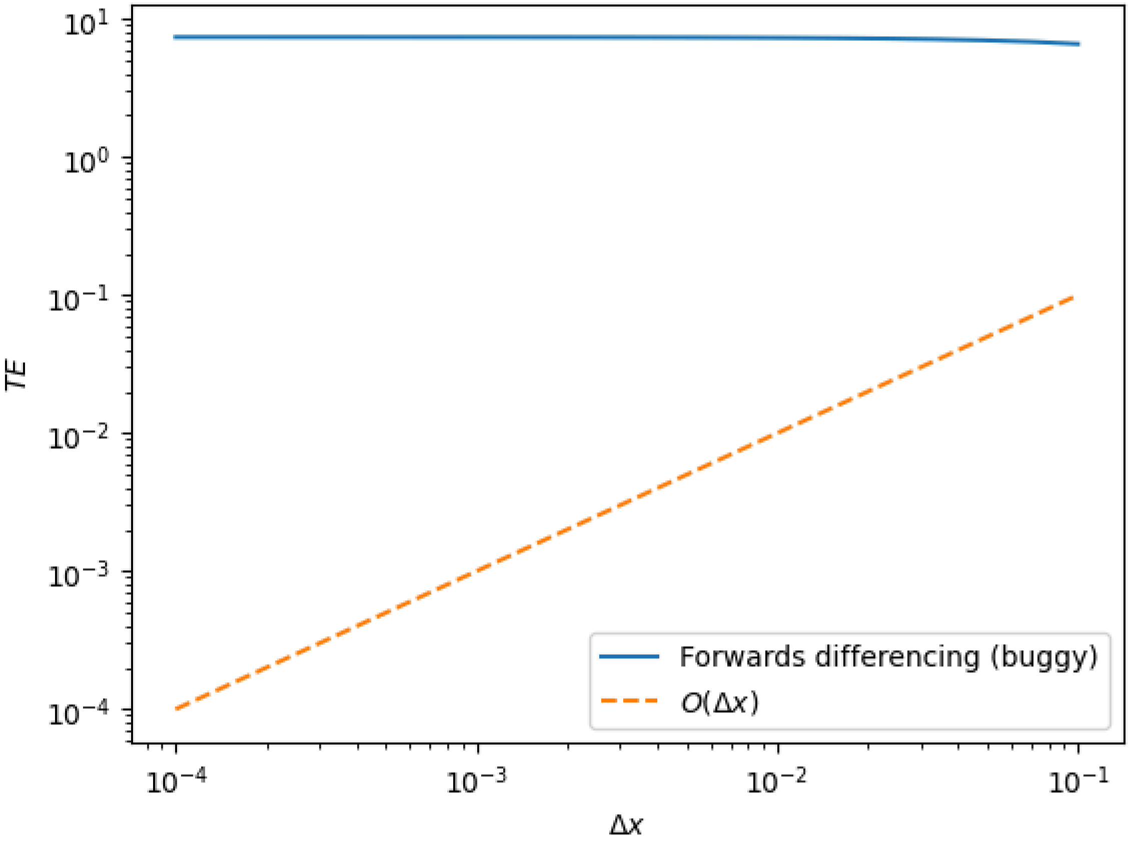
In [11]:

```
# calc the derivative
dfdx_num = forward_error(f, a, dx)

# calc the truncation error
TE = np.abs(dfdx_exact - dfdx_num)
```

In [12]:

```
# plot
plt.loglog(dx, TE, label = 'Forwards differencing (buggy)')
plt.loglog(dx, dx, '--', label = '$O(\\Delta x)$')
plt.xlabel('$\\Delta x$')
plt.ylabel('$TE$')
plt.legend()
plt.show()
```



We clearly see that the truncation error is not decreasing with Δx, so there must be a bug in the code!

Euler's method and vectorisation

This demo will showcase the benefits of vectorisation through Euler's method.

Consider the system of M linear ODEs given by

$$\frac{d\boldsymbol{u}}{dt} = -\mathbf{A}\boldsymbol{u}$$

where $\boldsymbol{u} = (u_1, u_2, \ldots, u_M)^T$ and $\mathbf{A}$ is an $M \times M$ random matrix with entries between 0 and 10^{-2}. The initial condition is $\boldsymbol{u}(0) = (1, 1, \ldots, 1)^T$.

We will use two versions of Euler's method to solve this problem over the time range $0 \leq t \leq 1$ using $N_t = 100$ time steps. We'll assume the system has $M = 200$ ODEs.

Let's define some Python variables for this problem

In [13]:

```
# Max time
t_max = 1

# Number of time steps
Nt = 100

# Calculation of time step size \Delta t
dt = t_max / Nt

# Calculation of time points (including t = 0)
t = dt * np.arange(Nt + 1)

"""
Parameters for the ODE system
"""
# Size of the ODE system
M = 200

# Generate the random matrix
A = 1e-2 * np.random.random((M, M))
```

- We will also pre-allocate an array to store the solution at each time step to improve the performance of the solver.
- This array will have size $M \times (N_t + 1)$, where the $N_t + 1$ arises from storing the initial condition and the solution computed at N_t Euler steps.
- This shaping of the array implies that columns of the array will correspond to different time points and rows will correspond to different solution components.

We initially set the values in the array to zero. The correct values will be placed in the array as they are computed.

In [14]:

```
"""
Pre-allocation
"""
u = np.zeros((M, Nt+1))
```

Slow implementation without vectorisation

- We now write the right-hand side of the ODE system using native Python operations that do not use vectorised operations.

- That is, we use nested for loops to compute the matrix-vector product $-\boldsymbol{A}\boldsymbol{u}$.

In [15]:

```
def f(u, t, A):
    """
    Computes the RHS of the ODE system; in this case,
    f(u, t) = -A * u
    """

    # Get dimension of ODE system
    M = len(u)

    # Pre-allocate an array to store the RHS of the ODE
    rhs = np.zeros(M)

    # Compute matrix-vector product and store in the RHS array
    for i in range(M):
        for j in range(M):
            rhs[i] -= A[i,j] * u[j]

    # Return the RHS array
    return rhs
```

Now we set the initial condition. We do this by overwriting the first column of the solution array `u` that was pre-allocated

In [16]:

```
"""
Setting the initial condition
"""
for i in range(M):
    u[i,0] = 1
```

- Having defined all this, we can now define a Python function that implements Euler's method.
- Recall, that Euler's method is defined through the iteration formula as

$$\boldsymbol{u}^{n+1} = \boldsymbol{u}^n + \Delta t \boldsymbol{f}(\boldsymbol{u}^n, t^n)$$

In [17]:

```
def euler():
    """
    Slow implementation of Euler's method.  The lack of arguments
    to this function means global variables are used, which is
    not good programming practice, but it keeps the demo simple
    """

    # Loop over time steps
    for n in range(Nt):

        # Compute the RHS using the solution at the current time step
        f_array = f(u[:, n], t[n], A)

        # Loop over solution components.  Notice here the values
        # in the pre-allocated array are being overwritten
        for i in range(M):
            u[i, n+1] = u[i, n] + dt * f_array[i]
```

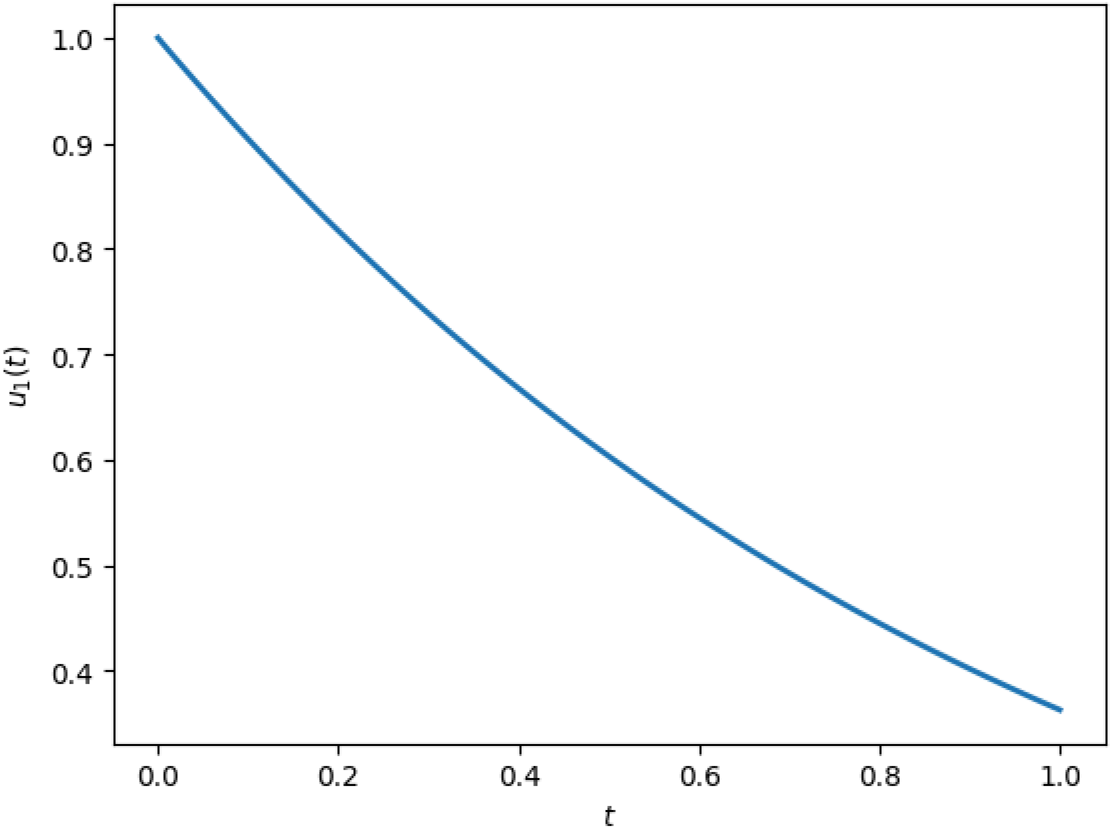
We now run the code three times and time each run:

In [18]:
```
%timeit -r 3 -n 1 euler()
```

```
726 ms ± 3.94 ms per loop (mean ± std. dev. of 3 runs, 1 loop each)
```

And we can plot the first component of the solution

In [19]:
```
plt.plot(t, u[0,:], lw = 2)
plt.xlabel('$t$')
plt.ylabel('$u_1(t)$')
plt.show()
```



Fast (vectorised) implementation

We can speed-up Euler's method using vectorised operations.

One place this can be done is in the function that evaluates the right-hand side of the ODE.

Rather than using nested for loops to compute the matrix-vector product, vectorised NumPy operations can be used:

In [20]:

```
def f_vectorised(u, t, A):
    """
    Computes the RHS of the ODE system; in this case,
    f(u, t) = -A * u using vectorised operations.
    Recall that matrix-vector multiplication in NumPy
    is done using @ and not *
    """

    return -A @ u
```

We first reset the solution and assign the initial condition:

In [21]:

```
# set solution array to zero
u = np.zeros((M, Nt+1))

# overwrite the first column of the array and set to ones
u[:, 0] = 1
```

We now define a vectorised version of Euler's method that uses NumPy arrays:

In [22]:

```
def euler_vectorised():
    """
    Fast implementation of Euler's method.  The lack of arguments
    to this function means global variables are used, which is
    not good programming practice, but it keeps the demo simple
    """

    # Loop over time steps
    for n in range(Nt):

        # Compute the RHS of the eqn at time step n
        f = f_vectorised(u[:, n], t[n], A)

        # Euler update
        u[:, n+1] = u[:, n] + dt * f

    return u
```

Now the IVP is solved using Euler's method and timed:

In [23]:

```
%timeit -r 5 -n 5 euler_vectorised()
```

```
1.39 ms ± 185 µs per loop (mean ± std. dev. of 5 runs, 5 loops each)
```

We see the vectorised code is much faster (about 200 times faster).