Numerical-solver Assignment Report

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Chapter 1

Numerical methods

In real world problems, ODE systems are frequently used. However, these models cannot be solved analytically. Therefore, the solution has to be estimated by numerical methods. The most popular and simple method is the Euler's method.

Intuitively, the Euler's explicit method tries to estimate the value at the next step following the gradient of the solution at current point. If the step size is sufficiently small, the estimation will be accurate.

An initial value problem, has the general form of

$$y' = f(x, y) \tag{1.1}$$

$$y(x_0) = y_0 \tag{1.2}$$

for $x \in [x_0, X_M]$.

Notation: Throughout the report, we will use the following notation. y_n - numerical approximation of $y(x_n)$ $y(x_n)$ - analytical solution at mesh point x_n x_n - mesh points of defined range, where

$$x_n = x_0 + nh \tag{1.3}$$

$$h = \frac{(X_M - x_0)}{N} \tag{1.4}$$

for $n = 0, \ldots, N$

1.1 One-step methods

For the simple Euler's explicit method,

$$y_{n+1} = y_n + hf(x_n, y_n) \tag{1.5}$$

The implementation is as follows:

```python
y_n = [self.initial_value]
x_n = [self.x_min]

# Calculate approximated solution for each mesh point.
for n in range(1, self.mesh_points + 1):
    step = [self.mesh_size * f for f in self.func(x_n[-1], y_n
    [-1])]
    y_n.append([a + b for a, b in zip(y_n[-1], step)])
    x_n.append(self.x_min + n * self.mesh_size)

return x_n, y_n
```

The truncation error is defined to be the difference of exact solution with the numerical solution given the exact solution of previous mesh point is known. Therefore, we have that the truncation error for Euler's explicit method to be

$$T_n := \frac{y(x_{n+1}) - y(x_n)}{h} - f(x_n, y(x_n)) \tag{1.6}$$

According to Taylor's series expansion, we have

$$y(x_n + h) = y(x_n) + hy'(x_n) + \frac{1}{2}h^2 y''(\xi_n) \tag{1.7}$$

for $\xi_n \in (x_n, x_{n+1})$. Substitute this to the truncation error, noting that $f(x_n, y(x_n)) = y'(x_n)$ we get

$$T_n = \frac{1}{2}h^2 y''(\xi_n) \tag{1.8}$$

Therefore, the truncation error for Euler's explicit method varies linearly with the step size.

In this report, we will use an example model

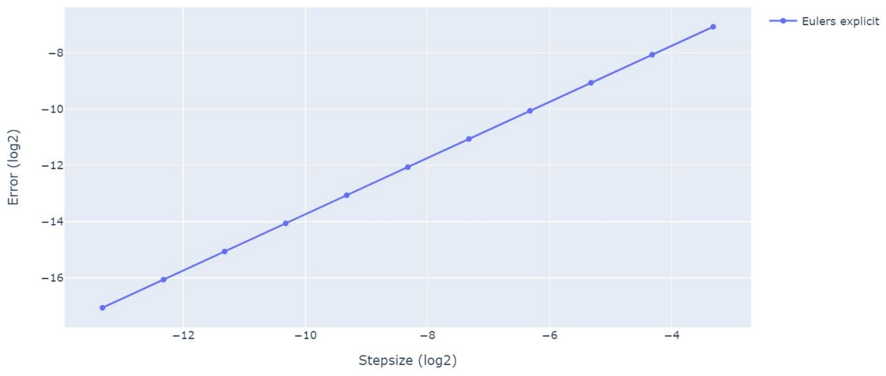
$$f(x, y) = -y \tag{1.9}$$

$$y(x_0) = 1 \tag{1.10}$$

for $x \in [0, 5]$ to show that the implementation follows the theory.

Some examples of the solution to the given model can be found here: Example model notebook

Result image extracted from the notebook above shows that the truncation error follows



Other than the Euler's explicit method, the other one-step methods implemented are the Euler's implicit method, trapezium rule method and four-stage explicit Runge-Kutta method.

The Euler's implicit method is defined to be

$$y_{n+1} = y_n + hf(x_{n+1}, y_{n+1}) \tag{1.11}$$

, while the trapezium rule method is

$$y_{n+1} = y_n + \frac{1}{2}h[f(x_n, y_n) + f(x_{n+1}, y_{n+1})] \tag{1.12}$$

. These methods, including Euler's explicit method, Euler's implicit method and trapezium rule method, can be generalised under the θ-method,

$$y_{n+1} = y_n + h[(1-\theta)f(x_n, y_n) + \theta f(x_{n+1}, y_{n+1})] \tag{1.13}$$

. For $\theta = 0$ and $\theta = 1$, the methods are Euler's explicit and Euler's implicit method respectively. Using the same definition for truncation error in 1.6, we can see that the truncation error are $T_n = -\frac{1}{2}hy''(\xi_n)$ for $\xi_n \in (x_n, x_{n+1})$ and $T_n = -\frac{1}{12}h^2y^{(3)}(\xi_n)$ for $\xi_n \in (x_n, x_{n+1})$ respectively.

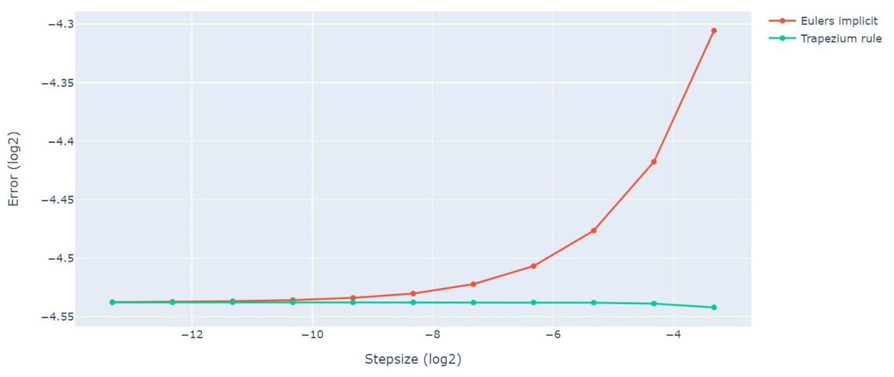
The Euler's implicit method implementation,

```python
y_n = [self.initial_value]
x_n = [self.x_min]

# Use value at previous mesh point as prediction for
# fixed point iteration if no prediction is given.
if prediction is None:
    prediction = y_n[-1]

# Calculate approximated solution for each mesh point.
# Use fixed point iteration to solve numerical equation.
for n in range(1, self.mesh_points + 1):

    def num_method(prediction):
        step = [self.mesh_size * f for f in self.func(
            x_n[-1] + self.mesh_size, prediction)]
        return [a + b for a, b in zip(y_n[-1], step)]

    est_y = self.fixed_pt_iteration(prediction, num_method)
    y_n.append(est_y)
    x_n.append(self.x_min + n * self.mesh_size)

return x_n, y_n
```

The trapezium rule method implementation,

```python
y_n = [self.initial_value]
x_n = [self.x_min]

# Use value at previous mesh point as prediction for
# fixed point iteration if no prediction is given.
if prediction is None:
    prediction = y_n[-1]

# Calculate approximated solution for each mesh point.
# Use fixed point iteration to solve numerical equation.
for n in range(1, self.mesh_points + 1):

    def num_method(prediction):
        previous_func = self.func(x_n[-1], y_n[-1])
        new_func = self.func(x_n[-1] + self.mesh_size,
    prediction)
        return [a + self.mesh_size / 2 * (b + c) for a, b, c in
     zip(
            y_n[-1], previous_func, new_func)]

    est_y = self.fixed_pt_iteration(prediction, num_method)
    y_n.append(est_y)
    x_n.append(self.x_min + n * self.mesh_size)

return x_n, y_n
```

When these methods are tested on the example model 1.9, the truncation error does not behave as expected. This is probably due to the use of fixed point iteration algorithm to estimate the solution of implicit functions. The error graph is shown below. Moreover, the error of the fixed point iteration algorithm is added to the error of the numerical method. Therefore, the difference of the numerical solution with the exact solution is larger for implicit methods as compared to Euler's explicit methods.



1.2 Predictor-corrector methods

For the implicit methods, numerical value at previous mesh point is chosen as the initial value for the fixed point iteration algorithm. The predictor-corrector method suggests a more carefully chosen initial guess for the implicit methods. An explicit numerical method is used as a predictor of the initial value of an implicit method. The initial value is then used as an initial guess for iterations to solve an implicit function. The implicit method that refines the solution is known as the corrector method.

The Euler-Trapezoidal method is a predictor-corrector that uses an Euler's explicit method as the predictor and trapezium rule method as the corrector. In this implementation, the trapezium rule method corrector is iterated until a set of conditions are satisfied. The conditions are defined to be the difference between current iteration and previous iteration is lesser than a given threshold value or the number of iterations exceeds a certain amount.

1.3 Adaptive method

In some types of problem or model, the solution to the problem exhibits a behaviour where step sizes have to be sufficiently small for a stable solution. In other words, as the mesh point varies, the solution have small changes. Such problems are called stiff problems. In order to obtain a stable solution, the computational cost is high. Moreover, such stable solution would have resolutions higher than required for practical purposes.

The adaptive method focus on the achieving desired accuracy with low computational cost. The main idea of an adaptive method is to control the precision at each mesh point. The truncation error at each mesh point is estimated. If the truncation error is larger than a threshold value, a smaller step size is chosen. These steps are repeated until the truncation error is smaller than the given threshold value.

The adaptive method implemented in this software is based on the BS23 (Bogacki and Shampine) and RK45 (Runge-Kutta-Fehlberg) method.

Absolute tolerance and relative tolerance were used in the implementation of the adaptive methods. Therefore two comparisons were made, one based on absolute tolerance and the other on relative tolerance. Similarly, the implemented adaptive method is used to solve the example model 1.9. The adaptive methods were tested for convergence. As shown in the graph below, the error of the method is smaller for smaller tolerance, regardless of absolute tolerance or relative tolerance.

Chapter 2

Code testing

In the progress of constructing the software, a unit testing infrastructure was put in place. The purpose of the unit testing is to create a robust and sustainable software. Written codes are tested to make sure it runs as intended and returns expected results. If code is tested while writing, it would be easier to fix bugs in the future as previously tested code would be correct and most probably free of bugs. Code coverage is used to define the percentage of codes covered in the unit testing process. It is usually aim to achieve a 100% code coverage. However, a 100% code coverage does not necessarily mean that the code is correct or free of errors. Nevertheless, it provides some confidence that the code is implemented correctly.

Every method in this numerical-solver software is tested. The numerical solution of each method is tested to give the same solution as a manually calculated solution. The methods are mostly tested against the example model 1.9.

The methods are classified into three classes: one-step methods, predictor-corrector methods and adaptive methods. The initialisations of each class are tested to ensure that variables are initialised correctly and input type satisfies the requirements. For example,

```python
def test__init__(self):

    def func(x, y):
        return [-y[0]]
    x_min = 0
    x_max = 1
    initial_value = [1]
    mesh_points = 10
```

```
 9
10      problem = solver.OneStepMethods(
11          func, x_min, x_max, initial_value, mesh_points)
12
13      # Test initialisation
14      self.assertEqual(problem.x_min, 0)
15      self.assertEqual(problem.mesh_points, 10)
16
17      # Test raised error for callable function
18      with self.assertRaises(TypeError):
19          solver.OneStepMethods(
20              x_min, x_min, x_max, initial_value, mesh_points)
21
22      # Test raised error if initial_value not list
23      with self.assertRaises(TypeError):
24          solver.OneStepMethods(
25              func, x_min, x_max, 1, mesh_points)
```

. A simple model with analytical solution is first initialised. Required inputs were check to make sure the problem is set up properly, in line 14 and 15 of the code snippet above. To ensure that the inputs to the function are of the desired data type, errors are raised whenever the user inputs a wrong data type. The unit testing also tests that these errors are raised appropriately (line 17 to 25) whenever the data type does not satisfy the requirements.

After checking that the problem is properly initialised, we then test that the numerical methods are working correctly. Take the adaptive method, BS23 algorithm, as an example,

```
def test_ode23(self):

def func(x, y):
    return [-y[0]]
x_min = 0
x_max = 1
initial_value = [1]

problem = solver.AdaptiveMethod(
    func, x_min, x_max, initial_value, initial_mesh=0.5)
mesh, soln = problem.ode23()

# Test end point of mesh
self.assertGreaterEqual(mesh[-1], 1.0)

# Test mesh point
self.assertAlmostEqual(mesh[1], 0.3483788976565)

# Test solution at first stepsize
self.assertAlmostEqual(soln[1][0], 0.7052580305097)
```

The method is first tested to execute the numerical computation up to the maximum mesh point indicated. Then the first adaptive mesh point and its solution, obtained from the software, matches the value computed manually.