

AMSC 460 Homework Set 3

Due: 21.05.04

Note:

- Due: 2pm, May 4, 2021. Late submission is subject to automatic 20% reduction.
- When submitting, make sure you upload your matlab or python codes, in addition to your answer sheets to analytical questions.

Topic: Differentiation

Consider numerical differentiation schemes using

- $-f(x_0-2h) + 4f(x_0-h) - 3f(x_0)$
- $f(x_0-h) - 2f(x_0) + f(x_0+h)$
- $f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)$
- $-f(x_0-2h) + 16f(x_0-h) - 30f(x_0) + 16f(x_0+h) - f(x_0+2h)$

These are the same as Quiz no.7

For each scheme,

1. [5pts] identify the order of derivative
2. [5pts] Identify the order of truncation error
3. [10pts] Write a matlab or python code that gives the corresponding derivative at arbitrary x_0 any h
4. [20pts] For $f(x)=\exp(2x)$,
 - a. obtain analytical form of corresponding derivative at arbitrary point x
 - b. At $x_0=0$, obtain expected numerical value of the corresponding derivative
 - c. Generate a figure equivalent to Fig.14.2 in the text book
 - d. Comment on the figure.

Bonus Points: Quiz 6. Data Fitting Using Normal Equation

Indicate your choice:

- A. Redo Quiz 6, and submit a new one
- ☒ B. Keep original submission/points of Quiz.

Four points correspond to 2% towards final grade either way.

1,2 a) ^(backward difference) One-sided three point formula, ^(derivative of order 1) 2nd order method w/ truncation error $O(h^2)$
b) Centered three point formula for derivative of order 2, 2nd order method w/ trunc error $O(h^2)$
c) Centered 5-point formula for derivative of order 4, 4th order method w/ trunc error $O(h^4)$
d) Centered 5-point formula for derivative of order 2, 4th order method w/ trunc error $O(h^4)$.

4u, b)

for Scheme a and c

$$\frac{de^{2x}}{dx} = 2e^{2x}, \quad \left. \frac{de^{2x}}{dx} \right|_{x=0} = 2$$

for Scheme b and d,

$$\frac{d^2 e^{2x}}{dx^2} = 4e^{2x}, \quad \left. \frac{d^2 e^{2x}}{dx^2} \right|_{x=0} = 4$$

```
In [1]: import numpy as np
import matplotlib.pyplot as plt
from decimal import *
```

Resources: <https://stackoverflow.com/questions/316238/python-float-to-decimal-conversion> This was used to determine an accurate way to represent IEEE standard for floating point numbers so that ideal measurements could be taken. The repr() function returns the shortest representation of the floating point number that has the same standard as IEEE-754 double precision. Was going to implement code from these papers but did not finish it in enough time: (Read through all these resources. It was a fun learning experience.)

<https://www.maths.manchester.ac.uk/~higham/narep/narep440.pdf>

<https://people.maths.ox.ac.uk/trefethen/barycentric.pdf>

<http://terpconnect.umd.edu/~petersd/666/BarycentricLagrange1.pdf>

<https://math.stackexchange.com/questions/200924/why-is-lagrange-interpolation-numerically-unstable>

<https://math.stackexchange.com/questions/1509340/newton-form-vs-lagrange-form-for-interpolating-polynomials>

http://www.math.niu.edu/~dattab/MATH435.2013/NUMERICAL_DIFFERENTIATIONandINTEGRATION.pdf

```
In [2]: def func_for_a(func, h: np.float_, x_0: np.float_) -> np.float_:
        return -np.divide(np.float_(-3.0) * func(x_0) + np.float_(4.0) * func(x_0 - h) - fu
            np.float_(2) * h)

def func_for_b(func, h: np.float_, x_0: np.float_) -> np.float_:
        return np.divide(func(x_0 - h) + np.float_(-2.0) * func(x_0) + func(x_0 + h), np.fl

def func_for_c(func, h: np.float_, x_0: np.float_) -> np.float_:
        return np.divide(func(x_0 + np.float_(-2.0) * h) + np.float_(8.0) * (func(x_0 + h)
            func(x_0 + np.float_(2.0) * h), np.float_(12.0) * h)

def func_for_d(func, h: np.float_, x_0: np.float_) -> np.float_:
        return np.divide(np.float_(-1) * func(x_0 + np.float_(-2.0) * h) + np.float_(16.0)
            - func(x_0 + np.float_(2.0) * h) + np.float_(-30.0) * func(x_0),
            np.float_(12.0) * np.float_power(h,2))
```

```
In [3]: func = lambda x: np.exp((np.float_(2.0) * x))
x_0 = np.float_(0.0)
h = np.float_(0.00001)

func_for_a(func, h, x_0)
```

Out[3]: 1.9999999997355464

```
In [4]: start = np.float_power(np.float_(10), np.float_(-8))
stop = np.float_(0.1)
h = np.arange(start, stop, np.divide(stop - start, np.float_(10**7)))
fill_value = Decimal('2.2')/Decimal(repr(np.float_power(np.float_(10), np.float_(16))))
nu = np.full_like(h, dtype=Decimal, fill_value=fill_value)
```

```
In [5]: second_deriv_at_zero = list(np.full_like(h, dtype=Decimal, fill_value=Decimal('4')))
first_deriv_at_zero = list(np.full_like(h, dtype=Decimal, fill_value=Decimal('2')))
```

In []:

```
In [6]: x_zeros = (np.full_like(h, dtype=np.float_, fill_value=np.float_(0.0)))

## The Numerical Derivative is calculated using floating point representations of the n
## the IEEE standard. (Unlike Python float which is not using true division since it at
## regular floating point arithmetic.
## Source:

numerical_derivative = list(map(lambda x: Decimal(repr(x)), list(func_for_a(func, h, x_z
zip_object = zip(first_deriv_at_zero, numerical_derivative)
a_measured_error = []
for list1_i, list2_i in zip_object:
    a_measured_error.append((list1_i-list2_i).copy_abs())

numerical_derivative = list(map(lambda x: Decimal(repr(x)), list(func_for_b(func, h, x_z
zip_object = zip(second_deriv_at_zero, numerical_derivative)
b_measured_error = []
for list1_i, list2_i in zip_object:
    b_measured_error.append((list1_i-list2_i).copy_abs())

numerical_derivative = list(map(lambda x: Decimal(repr(x)), list(func_for_c(func, h, x_z
zip_object = zip(first_deriv_at_zero, numerical_derivative)
c_measured_error = []
for list1_i, list2_i in zip_object:
    c_measured_error.append((list1_i-list2_i).copy_abs())

numerical_derivative = list(map(lambda x: Decimal(repr(x)), list(func_for_d(func, h, x_z
zip_object = zip(second_deriv_at_zero, numerical_derivative)
d_measured_error = []
for list1_i, list2_i in zip_object:
    d_measured_error.append((list1_i-list2_i).copy_abs())
```

```
In [7]: h = list(map(lambda x: Decimal(repr(x)), list(h)))
```

```
In [8]: ## using the midpoint and endpoints of the interval on which the truncation error is de

a_ideal_trunc_error = []
a_max_ideal_trunc_error = []
a_min_ideal_trunc_error = []
for h_value in h:
    exponent = Decimal('-2')*h_value
    a_ideal_trunc_error.append(((h_value*h_value*exponent.exp()*Decimal('8'))/Decimal('
a_max_ideal_trunc_error.append(((h_value*h_value*Decimal('8'))/Decimal('3')).copy_a
    exponent = Decimal('-4')*h_value
    a_min_ideal_trunc_error.append(((h_value*h_value*exponent.exp()*Decimal('8'))/Decim

b_ideal_trunc_error = []
b_max_ideal_trunc_error = []
b_min_ideal_trunc_error = []
for h_value in h:
    b_ideal_trunc_error.append(((h_value*h_value*Decimal('-1')*Decimal('16'))/(Decimal(
    exponent = Decimal('2')*h_value
    b_max_ideal_trunc_error.append(((h_value*h_value*Decimal('-1')*exponent.exp()*Decim
    exponent = Decimal('-2')*h_value
    b_min_ideal_trunc_error.append(((h_value*h_value*Decimal('-1')*exponent.exp()*Decim

c_ideal_trunc_error = []
c_max_ideal_trunc_error = []
c_min_ideal_trunc_error = []
```

```

for h_value in h:
    c_ideal_trunc_error.append(((h_value*h_value*h_value*h_value*Decimal('32'))/(Decimal(
exponent = Decimal('-4')*h_value
c_min_ideal_trunc_error.append(((h_value*h_value*h_value*h_value*exponent.exp()*Dec
exponent = Decimal('4')*h_value
c_max_ideal_trunc_error.append(((h_value*h_value*h_value*h_value*exponent.exp()*Dec

d_ideal_trunc_error = []
d_max_ideal_trunc_error = []
d_min_ideal_trunc_error = []
for h_value in h:
    d_ideal_trunc_error.append(((h_value*h_value*h_value*h_value*Decimal('16'))/(Decimal(
exponent = Decimal('-4')*h_value
d_min_ideal_trunc_error.append(((h_value*h_value*h_value*h_value*exponent.exp()*Dec
exponent = Decimal('4')*h_value
d_max_ideal_trunc_error.append(((h_value*h_value*h_value*h_value*exponent.exp()*Dec

# a_ideal_trunc_error = abs(np.divide(np.float_power(h, 2) * np.exp(np.float_(-2) * h)
# b_ideal_trunc_error = abs(np.divide(np.float_power(h, 2) * np.float_(-1) * np.float_(
# c_ideal_trunc_error = abs(np.divide(np.float_power(h, 4) * np.float_(1) * np.float_(3
# d_ideal_trunc_error = abs(np.divide(np.float_power(h, 4) * np.float_(1) * np.float_(1

```

```

In [9]: ideal_label = 'Ideal Roundoff Error'
trunc_label = 'Ideal Truncation Error'
measure_label = 'Measured Error'

```

```

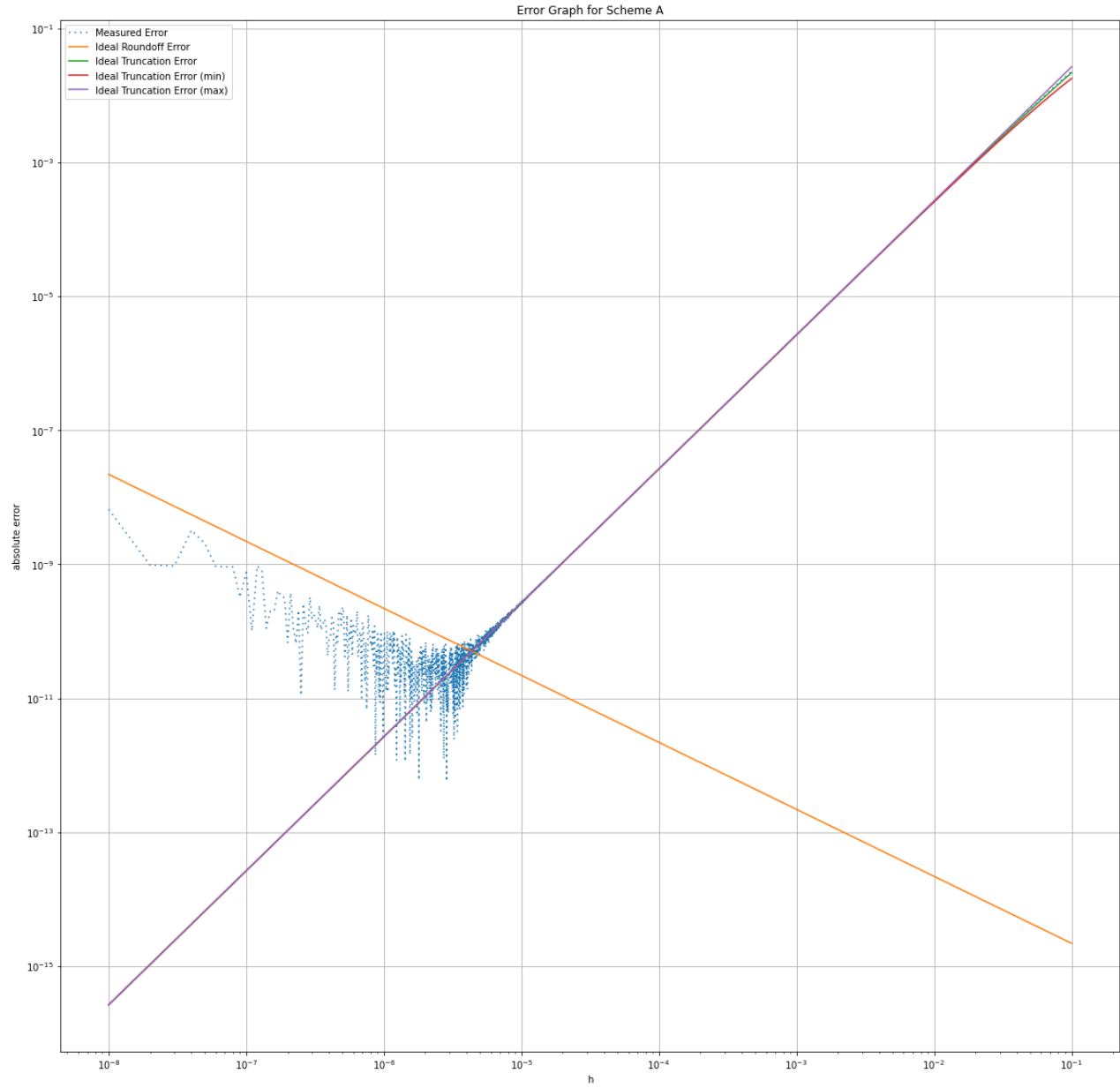
In [ ]: ideal_roundoff_error = []
zip_object = zip(h, nu)
for hs, nus in zip_object:
    ideal_roundoff_error.append(nus/hs)
#ideal_roundoff_error = np.divide(nu, h)
schemes = ['A', 'B', 'C', 'D']
measured_error = [a_measured_error, b_measured_error, c_measured_error, d_measured_error]
trunc_error = [a_ideal_trunc_error, b_ideal_trunc_error, c_ideal_trunc_error, d_ideal_trunc_error]
min_trunc_error = [a_min_ideal_trunc_error, b_min_ideal_trunc_error, c_min_ideal_trunc_error, d_min_ideal_trunc_error]
max_trunc_error = [a_max_ideal_trunc_error, b_max_ideal_trunc_error, c_max_ideal_trunc_error, d_max_ideal_trunc_error]

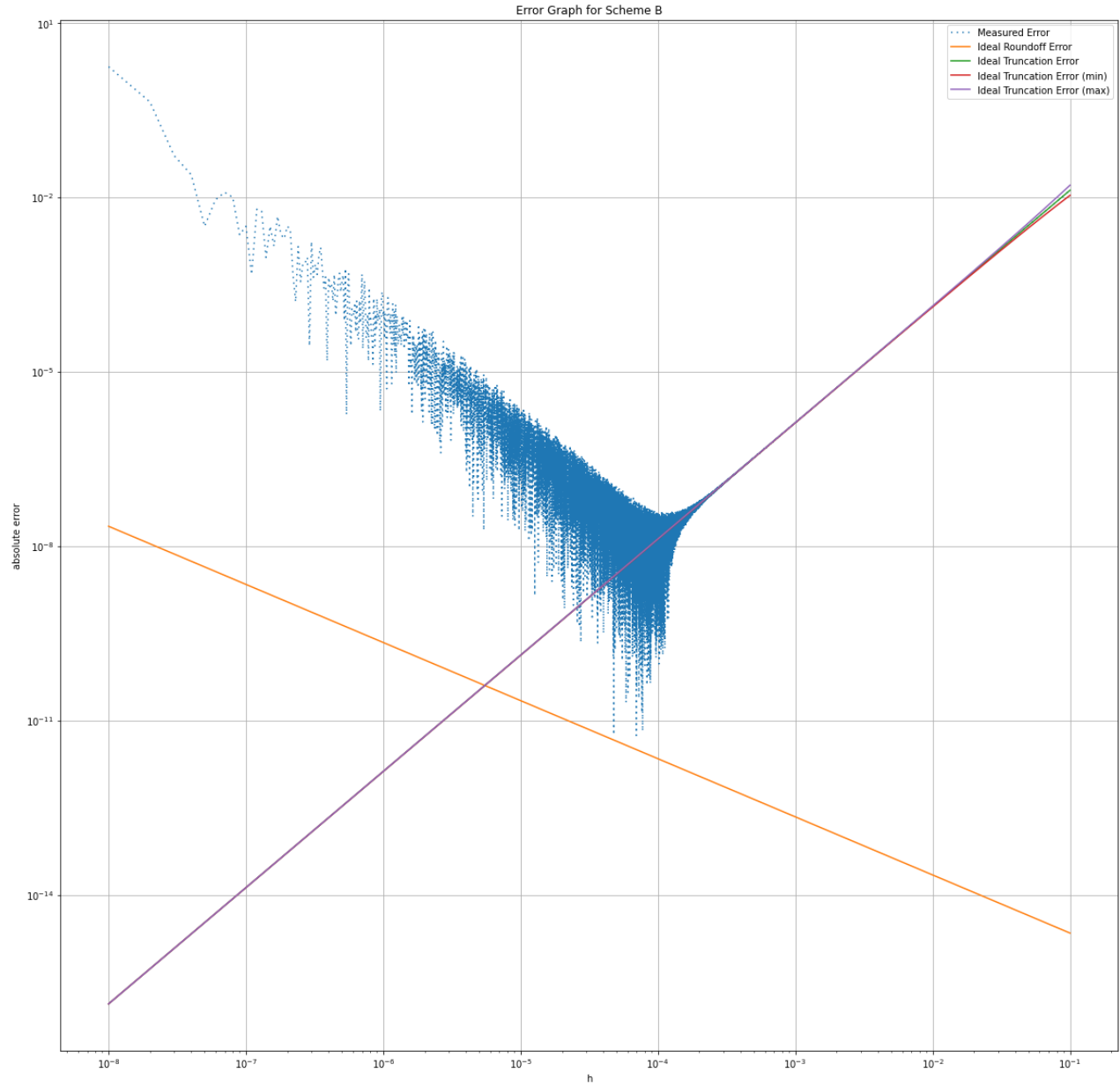
```

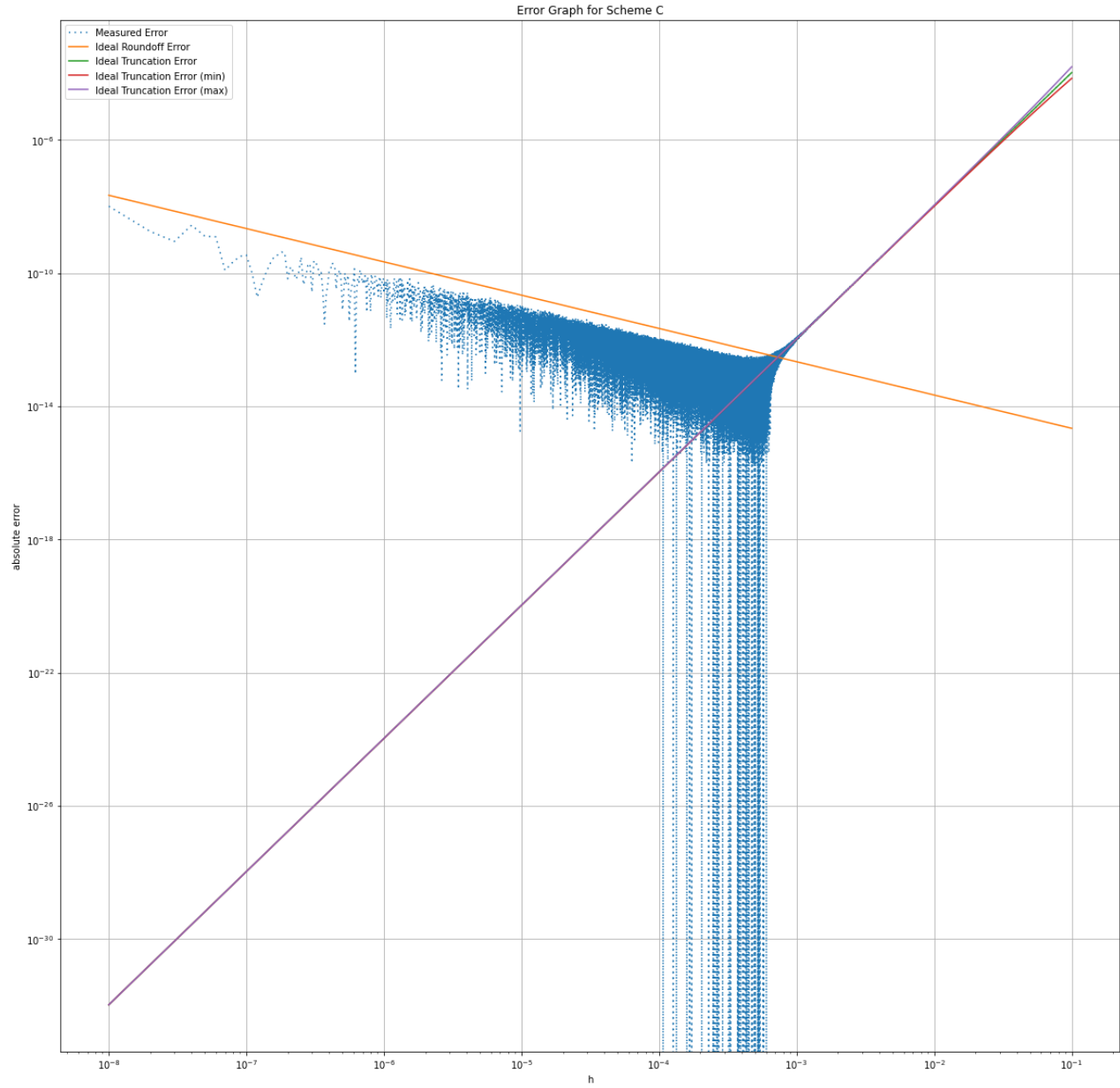
```

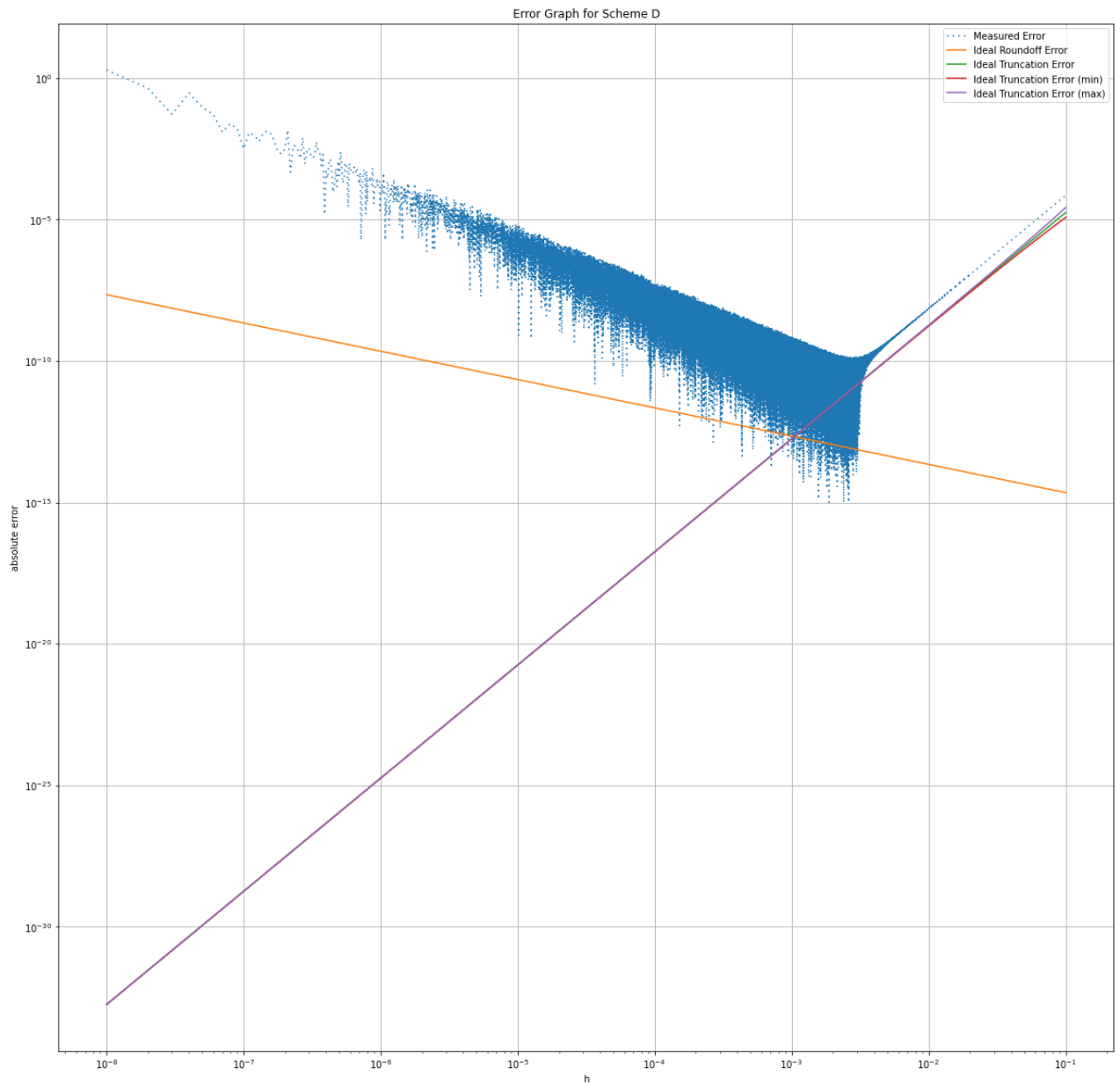
In [15]: for idx, scheme in enumerate(schemes):
plt.figure(figsize=(20,20))
title = 'Error Graph for Scheme ' + scheme
plt.title(title)
plt.ylabel('absolute error')
plt.xlabel('h')
plt.loglog(h, measured_error[idx], linestyle=(0,(1,3)), label=measure_label)
plt.loglog(h, ideal_roundoff_error, label=ideal_label)
plt.loglog(h, trunc_error[idx], label=trunc_label)
plt.loglog(h, min_trunc_error[idx], label=trunc_label + ' (min)')
plt.loglog(h, max_trunc_error[idx], label=trunc_label + ' (max)')
plt.grid()
plt.legend()
plt.show()

```









Scheme A Graph Comments

We see here that the minimizing h value does not correspond to the intersection of the ideal roundoff error or the ideal truncation error. Even with the use of the decimal class to try and get a truer approximation of the floating point round off error it is most likely the result of roundoff error in floating point calculations that prevents the measured error min to match up with the ideal roundoff and ideal truncation errors. A fix for this issue would be to change the precision to be less than the IEEE double precision numbers to be able to see this result more clearly that indeed the measured error and ideal error lines correspond to the intersection. It could also be beneficial to compute by hand an analytic solution for the ideal errors lines and plot those instead. This would remove any errors that are cropping up because of the roundoff error present in every calculation.

Scheme B Graph Comments

The second derivative has a division by h^2 which results in different ideal roundoff error. The ideal roundoff error must also be computed with h^2 in order to see that the plots of measured error and ideal errors will align. See the

graphs below where the ideal round off was computed with again with the h^2 denominator to quickly verify this result.

Scheme C Graph Comments

The results of this graph and its discussion aligns with the discussion of Scheme A, roundoff errors present in every calculation prevent us from seeing the optimal h value that minimizes measured error line up with the intersection of the ideal roundoff errors and truncation error.

Scheme D Graph Comments

The results of this graph and its discussion aligns with the discussion of Scheme B. See the discussion of the graphs with h^2 for more information. It is however puzzling why the measured error does not converge with the truncation error as h becomes much smaller. This is also seen in the graphs with the modified ideal roundoff error. This may be the result of the truncation error for the second derivative having h^4 present. It also could be because this truncation error was taken from the section using richardson extropolation instead of being calculated by hand.

Schemes with five-point formulas and 2nd derivatives (C, D)

There is more noise in the measured error for choices of h smaller than the optimal h value for 5 points methods. This likely because when using more points there is more error introduced per point chosen leading to a noiser graph. Similarly for the second derivative three point method, the error is compounded by the addition of dividing by h twice.

Schemes A,B,C Graph Comments

Note we see that the measured error converges with the midpoint of the truncation errors which is what we expect from fig 14.2 as roundoff no longer dominates the calculations.

All graphs comment

The measured error is noisy. This is to be expected. Floating point calculations are not necessarily going to be the same since their representations in binary are at times better or worse computationally than what we may expect for math done analytically (i.e. by hand). Even tho $h_1=0.00000250$ and $h=0.00000251$ are close in decimal form, in binary operations with floatining point representations they may be causing wildly different amounts of error. It was noticed that when using smaller h vectors that had more space between each h , the plots for ideal error would not even cross. This was the first warning that these ideal lines may not be as accurate as we like and suffer the effects of roundoff error even with the pragmatic approach of the decimal class attempting to remove round off errors. We do see, as expected however, that for larger values of h (after the optimal h) that these differences in computations begin to converge. This is because we move further away from the limit of floating point representations and have less variations in the amount of round off errors we might expect. This is stated on page 422 right above Fig 14.2

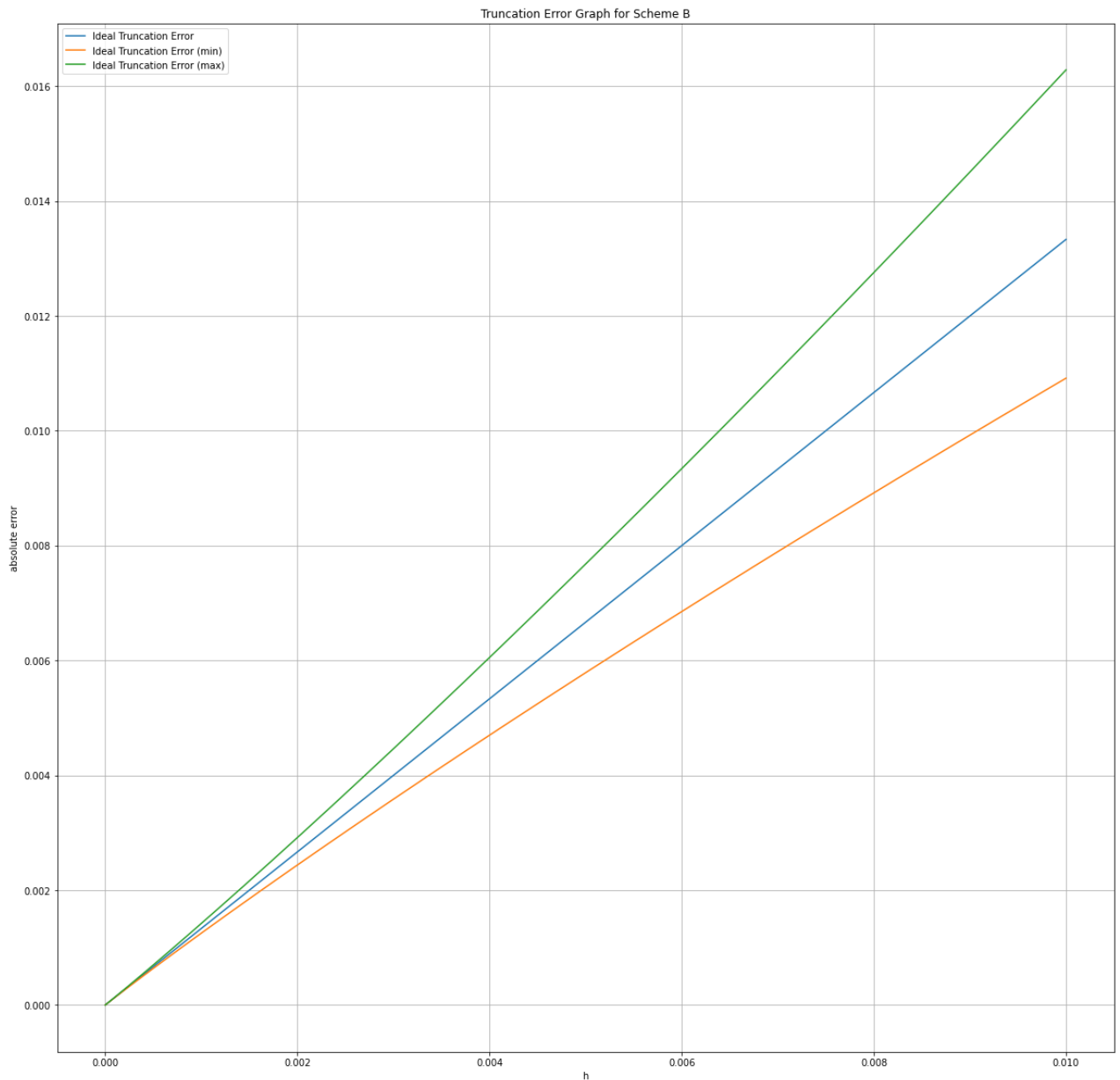
The roundoff error present in the calculation of the ideal error lines appears to over estimate the optimal h .

In the higher order methods (C,D) we see that they achieve a much lower error with far fewer steps (i.e. larger h). This is expected since they are more accurate. In log-log axis they also have a much steeper slope for their truncation error since the 2nd order methods since their truncation term is $O(h^4)$. In theory, if the optimal h is produced at the intersection of ideal round off error and truncation error, this steeper slope graphically suggests they are indeed more accurate with larger step sizes since it will intersect with the roundoff error at a larger value of h .

The truncation errors for the midpoint and endpoints of the range on which they are defined appear to diverge for large values of h . The graph below confirms this idea. We know this to be the result of under or overestimating by our choice of a forward or backward method, and when viewing a graph for scheme B, a centered method, we see that very clearly. The farther we move from the point we wish to approximate (with larger values of h) the more we over estimate errors. Similarly, the further behind we move away the more we underestimate errors.

```
In [14]: plt.figure(figsize=(20,20))
         title = 'Truncation Error Graph for Scheme B'
         plt.title(title)
         plt.ylabel('absolute error')
         plt.xlabel('h')
         plt.plot(h, b_ideal_trunc_error, label=trunc_label)
         plt.plot(h, b_min_ideal_trunc_error, label=trunc_label + ' (min)')
         plt.plot(h, b_max_ideal_trunc_error, label=trunc_label + ' (max)')
         plt.grid()
         plt.legend()
```

```
Out[14]: <matplotlib.legend.Legend at 0x1d1ce7236a0>
```

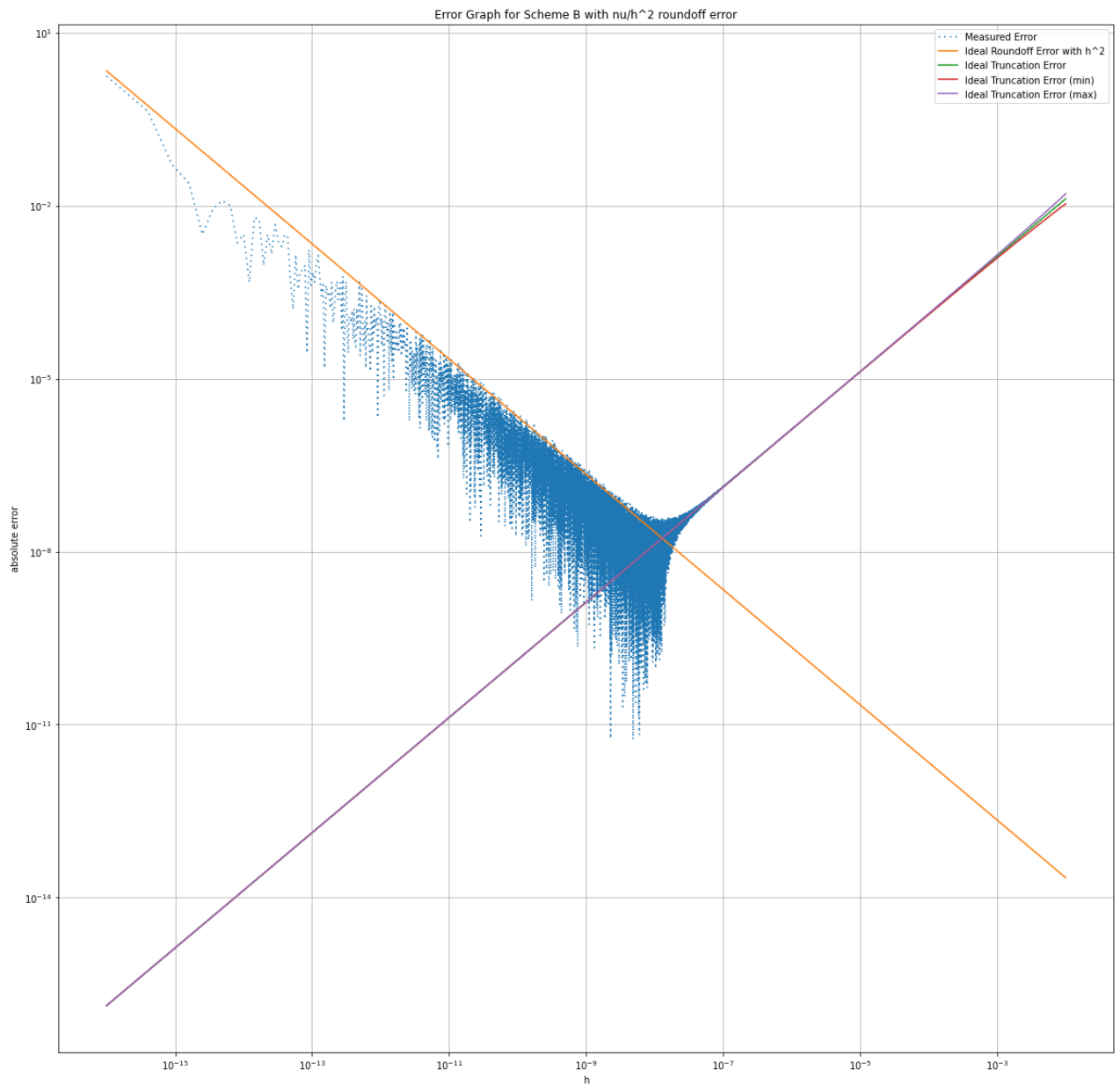


```
In [10]: h = np.float_power(np.arange(start, stop, np.divide(stop - start, np.float_(10**7))), 2)
h = list(map(lambda x: Decimal(repr(x)), list(h)))
#ideal_roundoff_error = np.divide(nu, h)
zip_object = zip(h, nu)
ideal_roundoff_error = []
for hs, nus in zip_object:
    ideal_roundoff_error.append(nus/hs)
```

```
In [13]: plt.figure(figsize=(20,20))
title = 'Error Graph for Scheme B with nu/h^2 roundoff error'
plt.title(title)
plt.ylabel('absolute error')
plt.xlabel('h')
plt.loglog(h, b_measured_error, linestyle=(0,(1,3)), label=measure_label)
plt.loglog(h, ideal_roundoff_error, label='Ideal Roundoff Error with h^2')
plt.loglog(h, b_ideal_trunc_error, label=trunc_label)
plt.loglog(h, b_min_ideal_trunc_error, label=trunc_label + ' (min)')
plt.loglog(h, b_max_ideal_trunc_error, label=trunc_label + ' (max)')
```

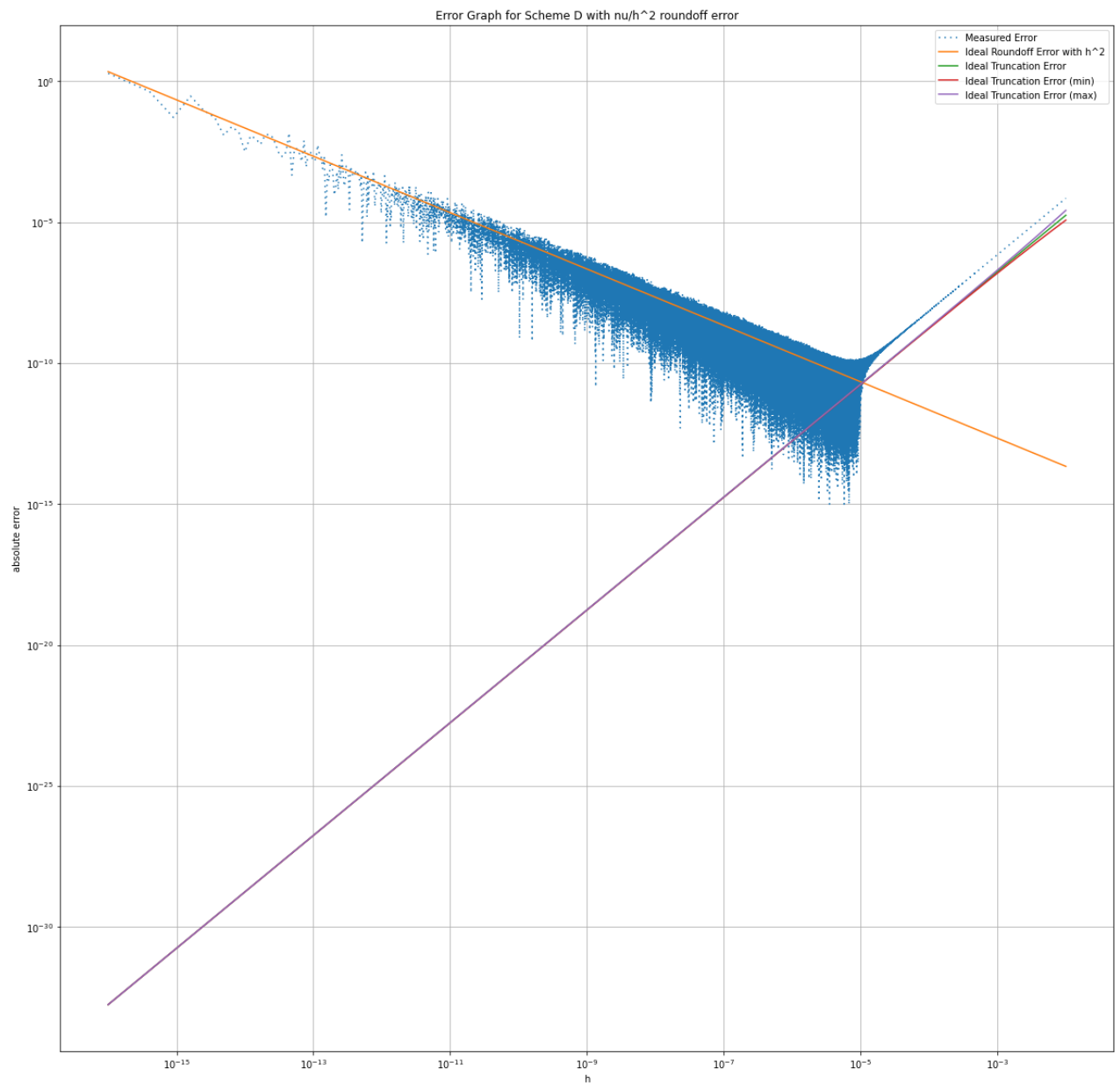
```
plt.grid()
plt.legend()
```

Out[13]: <matplotlib.legend.Legend at 0x1d1cea528b0>



```
In [12]: plt.figure(figsize=(20,20))
title = 'Error Graph for Scheme D with nu/h^2 roundoff error'
plt.title(title)
plt.ylabel('absolute error')
plt.xlabel('h')
plt.loglog(h, d_measured_error, linestyle=(0,(1,3)), label=measure_label)
plt.loglog(h, ideal_roundoff_error, label='Ideal Roundoff Error with h^2')
plt.loglog(h, d_ideal_trunc_error, label='Ideal Truncation Error')
plt.loglog(h, d_min_ideal_trunc_error, label=trunc_label + ' (min)')
plt.loglog(h, d_max_ideal_trunc_error, label=trunc_label + ' (max)')
plt.grid()
plt.legend()
```

Out[12]: <matplotlib.legend.Legend at 0x1d1ceab4c70>



Comments for 2nd derivative methods

Immediately we notice that the measured error does not seem to follow the same pattern as what was stated in the book for the graph of Fig 14.2, which is plotting a first derivative. This is most likely found in the math if we were to compute the analytic solution. Also, without an explanation, I do note that the 2nd order method (graph B) appears to reach its optimal h at the intersection of our ideal error lines. This might be because of the roundoff error lining up just right since scheme B uses fewer points and also has an h^2 in it. Trying to say that... the round off error in the numerator and the denominator of scheme B match and thus maybe are cancelling out leading to a result that aligns with our ideal error lines roundoff error as well.

In []: