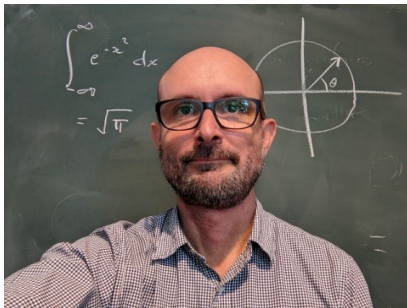


# **35006 Numerical Methods**

Your Subject Coordinator/Lecturer this semester:



Chris Poulton (“Dr Chris, Dr Poulton”, “Chris”, etc etc, just please not “Christopher”)

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Emails answered by Monday, Wednesday mornings.

## What do we mean by Numerical Methods?

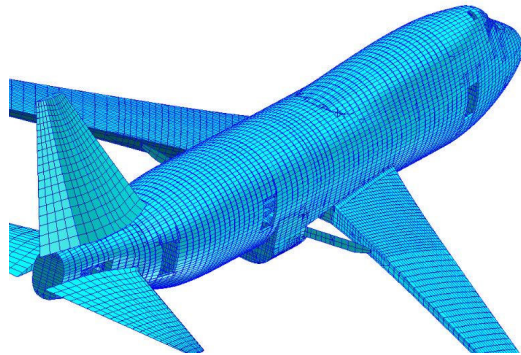
*Procedure*: what the computer does

**Definition**: A numerical method is a *procedure* run by a computer to give an approximate answer to some mathematical problem.

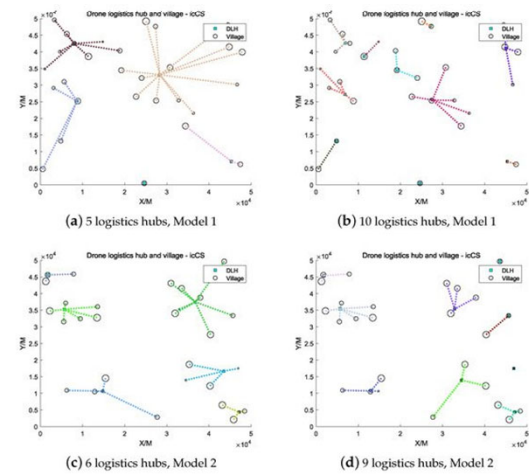
*approximate*: because while sometimes you can get an *exact* solution, almost always you can't.

By *mathematical* we mean any problem that can be stated mathematically, not limited to pure mathematics, but often arising in (say) physics and engineering.

Important applications:



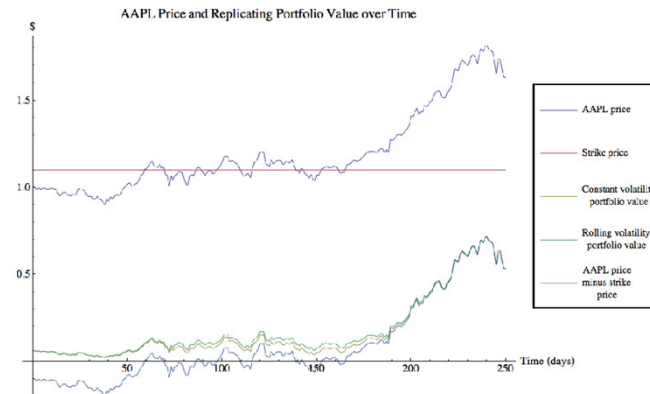
Structural engineering



Supply chain optimisation



Physics engines

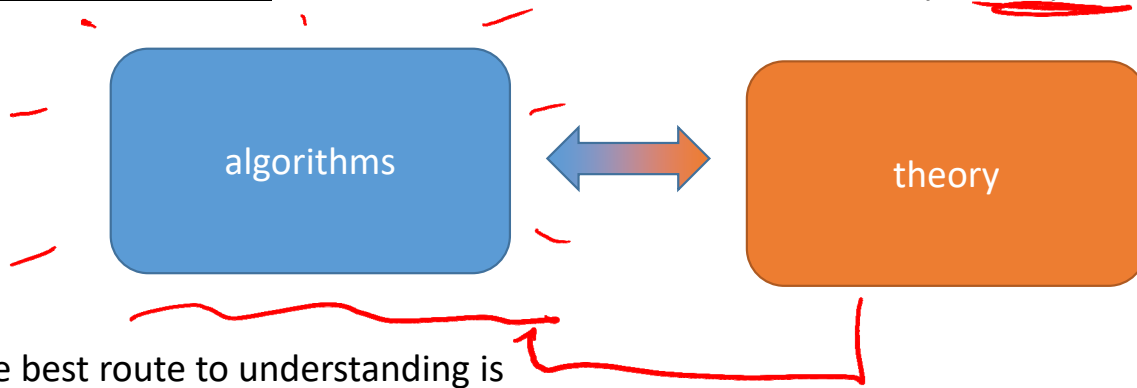


Mathematical finance

It is sometimes useful to distinguish between *Numerical Methods* and *Numerical Analysis*:

Numerical Methods: what works

Numerical Analysis: why things work



The best route to understanding is

- 1) To use a mixture of *what* and *why*
- 2) To “get your hands dirty” fiddling around with things

This subject will mix the *what* and the *why*, but will concentrate mostly on practical implementation.

## Why are numerical methods necessary?

Nowadays can't we just "vibe code" everything?

1. Even if you rely on AI tools, it's good to know what the bots are doing
2. Efficiency – if you know how things work you can make them better
3. Knowledge of the methods means that you know where things *don't* work
4. In the end knowing how code works is a valuable (and highly employable) skill.

Main aims of this subject:

1. Introduce the main numerical methods currently in use in scientific and engineering computing
2. Get an appreciation for *how* these methods work, and more importantly when they don't
3. Give you practice in implementing each of these methods



## Subject structure by week\*:

1. Programming basics. Intro to Python: control structures, data types, style and technique. Numerical precision. Graphing functions. Numerical differentiation
2. Root finding and Numerical solution to nonlinear equations. Newton's method. Bisection, the secant method, etc.
- 3. Minimisation and maximisation in 1D
- 4. Numerical optimisation in higher dimensions – gradient descent, simplex methods
- 5. Interpolation and extrapolation – splines etc
- 6. Integration in 1D: quadrature etc.
- 7. Integration in multiple dimensions: Monte Carlo methods
- 8. Solution of linear systems
9. Methods for sparse linear systems
- 10. Solution to ODEs – Euler, Runge Kutta, Predictor-Corrector
- 11. Numerical solution of ODEs and PDEs by finite differences
- 12. The Fast Fourier Transform (time permitting)

\*Note that this is the first time that this subject has been run, so this is (I hope) only a *good approximation* of what will be covered.

Classes and materials:

Workshop (Wrk1): Weekly workshop held online

Computer Labs (Cmp1): 3 hours per week

Assessment

The assessment has the following components:

3 Assignments:	Due weeks <u>4,7,10</u>	<u>30%</u>
<u>Final Project:</u>	Due end of Week 12	<u>40%</u>
<u>Live coding exercise:</u>	Held in the Lab class in Week 12	<u>30%</u>

---

Each week:

- Week 1: Intro to Python; Error, precision and numerical differentiation
  - Workshop Class
    - Blank slides.pdf ←
    - Annotated Slides ←
  - Computer Lab this week
    - Computer Lab 1.pdf ←
    - Lab 1 solutions and scripts |||
  - Preparation for next week
    - Preparation Tasks ||
  - Other Resources
    - Link to Numerical Recipes Textbook ]
    - Additional Reading ]

Assumed Knowledge and skills:

1. Thorough algebra
2. Calculus from Maths 2 / IMAM / MM2
3. Some previous coding experience  
(if not, then please let me know) ]

# Programming Basics

Why Python?

Overall structure of non-parallel code

The important control structures

Stopping conditions

Data types

Style and Technique



## Why are we using Python?

### **Disadvantages:**

- it's relatively slow
- it is not very "elegant" as a language
- the module libraries are a bit of a mess
- not great for memory-intensive tasks

### **Advantages**

- it's free
- it's easy to learn
- it's easy to read
- it is now the Industry Standard in computing

## Overall structure (of non-parallel code):

```
1  # -*- coding: utf-8 -*-|
2  """
3  sum_integers.py
4
5  Created on Wed Jul 20 17:31:57 2022
6  @author: Chris Poulton
7
8  Script to add the first N integers together
9  """
10
11
12 import numpy as np
13 import matplotlib.pyplot as plt
14 import math as math
15
16
17 Function definitions
18 -----
19 """
20 def foo(n):
21     foo = n*(n+1)/2
22     return foo
23
24 """
25 Main script starts
26 -----
27 """
28 print("Please enter the maximum value:")
29 nmaxstr = input()
30 nmax = int(nmaxstr) #convert the input to an integer type
31
32 print("Summing all integers from 1 up to",nmax)
33
34 nsum = 0
35 for i in range(1,int(nmax)+1): #note that range(1,N) creates a list from 1 to n-1
36     print(i,"+")
37     nsum = nsum + i
38
39 print("=",nsum)
40
41 print("Analytic formula: sum =",foo(nmax))
```

Header

Modules

Function definitions

Main script starts

← starts running here

←

A good “beginners cheat sheet” for python is given in canvas  
 (from [https://nbisweden.github.io/workshop-python/img/cheat\\_sheet.pdf](https://nbisweden.github.io/workshop-python/img/cheat_sheet.pdf))

## Python for Beginners – Cheat Sheet

### Data types and Collections

integer	10
float	3.14
boolean	True/False
string	'abcde'
list	[1, 2, 3, 4, 5]
tuple	(1, 2, 'a', 'b')
set	{'a', 'b', 'c'}
dictionary	{'a':1, 'b':2}

### Numerical Operators

+	addition
-	subtraction
*	multiplication
/	division
**	exponent
%	modulus
//	floor division

### Comparison Operators

<	less
<=	less or equal
>	greater
>=	greater or equal
==	equal
!=	not equal

### List Methods

L.append(x)	append x to end of list
L.insert(i, x)	insert x at position i
L.remove(x)	remove first occurrence of x
L.reverse()	reverse list in place

### Dictionary Methods

d.keys()	returns a list of keys
d.values()	returns a list of values
d.items()	returns a list of (key, value)

### String Methods

s.strip()	remove trailing whitespace
s.split(x)	return list, delimiter x
s.join(l)	return string, delimiter s
s.startswith(x)	return True if s starts with x
s.endswith(x)	return True if s ends with x
s.upper()	return copy, uppercase only
s.lower()	return copy, lowercase only

### Logical Operators

and	logical AND
or	logical OR
not	logical NOT

### Membership Operators

in	value in object
not in	value not in object

### Conditional Statements

```

if condition:
    <code>
elif condition:
    <code>
else:
    <code>
            
```

### Import from Module

```

from module import func    import func
from module import func as f  import func as f
            
```

### Operations

Index starts at 0

**Strings:**

s[i]            i:th item of s  
s[-1]            last item of s

**Lists:**

l = []            define empty list  
l[i:j]            slice in range i to j  
l[i] = x            replace i with x  
l[i:j:k]            slice range i to j, step k

**Dictionaries:**

d = {}            create empty dictionary  
d[i]            retrieve item with key i  
d[i] = x            store x to key i  
i in d            is key i in dictionary

## Python for Beginners – Cheat Sheet

### Built-in Functions

<code>float(x)</code>	convert x to float
<code>int(x)</code>	convert x to integer
<code>str(x)</code>	convert x to string
<code>set(x)</code>	convert x to set
<code>type(x)</code>	returns type of x
<code>len(x)</code>	returns length of x
<code>max(x)</code>	returns maximum of x
<code>min(x)</code>	returns minimum of x
<code>sum(x)</code>	returns sum of values in x
<code>sorted(x)</code>	returns sorted list
<code>round(x, d)</code>	returns x rounded to d
<code>print(x)</code>	print object x

### Loops

`while` condition:  
    <code>

`for` var in list:  
    <code>

#### Control statements:

<code>break</code>	terminate loop
<code>continue</code>	jump to next iteration
<code>pass</code>	does nothing

### String Formatting

"Put {} into a {}".format("values", "string")  
'Put values into a string'

"Put whitespace after: {:<10}, or before: {:>10}".format("a", "b")  
'Put whitespace after: a           , or before:            b'

"Put whitespace around: {:^10}".format("c")  
'Put whitespace around:        c        .'

### Regular Expressions

```
import re
p = re.compile(pattern)  compile search query
p.search(text)           search for all matches
p.sub(sub, text)         substitute match with sub
```

<code>.</code>	any one character
<code>*</code>	repeat previous 0 or more times
<code>+</code>	repeat previous 1 or more times
<code>?</code>	repeat previous 0 or 1 times
<code>\d</code>	any digit
<code>\s</code>	any whitespace
<code>[abc]</code>	any character in this set {a, b, c}
<code>[^abc]</code>	any character *not* in this set
<code>[a-z]</code>	any letter between a and z
<code>a b</code>	a or b

### Reading and Writing Files

```
fh = open(<path>, 'r')
for line in fh:
    <code>
fh.close()
```

```
out = open(<path>, 'w')
out.write(<str>)
out.close()
```

### Functions

```
def Name(param1, param2 = val):
    <code>
    #param2 optional, default: val
    return <data>
```

### sys.argv

<code>import sys</code>	import module
<code>sys.argv[0]</code>	name of script
<code>sys.argv[1]</code>	first cmd line arg

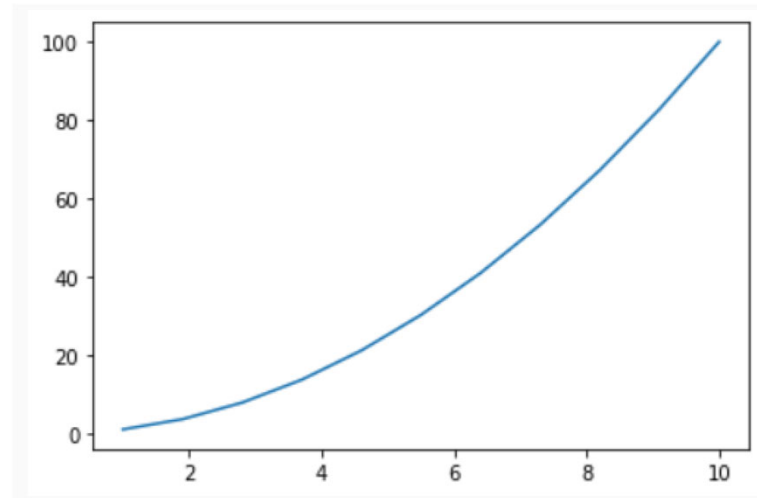
## The important control structures

### 1. Sequential statements

Tells computer to run commands in a fixed order

*line number*

```
8 import numpy as np
9 import matplotlib.pyplot as plt
10 import math as math
11
12 x = np.linspace(1,10,11)
13 b = 2
14
15 c = x**b
16
17 plt.plot(x,c)
```



See: <https://www.educative.io/answers/what-are-control-flow-statements-in-python>

## 2. Conditional statements

Creates two (or more) paths for the computer to follow

Instructions: if, else, elif

*else if.*

```
8 a = 5
9 b = 10
10 c = 15
11 if a > b:
12     if a > c:
13         print("a value is big")
14     else:
15         print("c value is big")
16 elif b > c:
17     print("b value is big")
18 else:
19     print("c is big")
```

*test if true*  
*colon (don't forget!)*

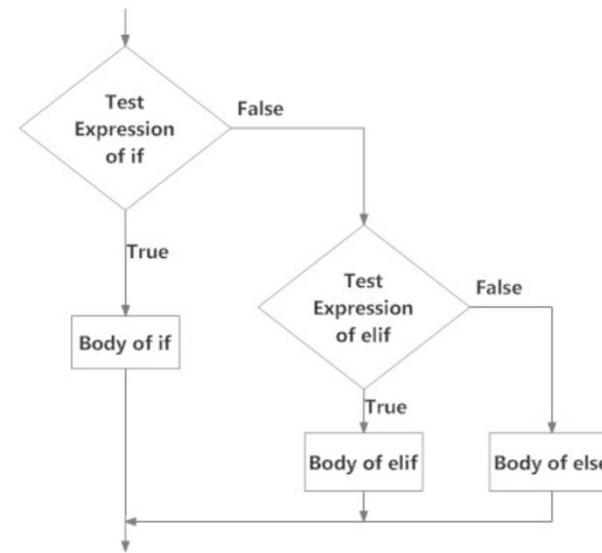


Fig: Operation of if...elif...else statement

```
In [1]: run selection.py
c is big
```

```
In [2]:
```

### 3. Iteration (loops)

Performs a loop a number of times (**for**) or while a specified condition is true (**while**)

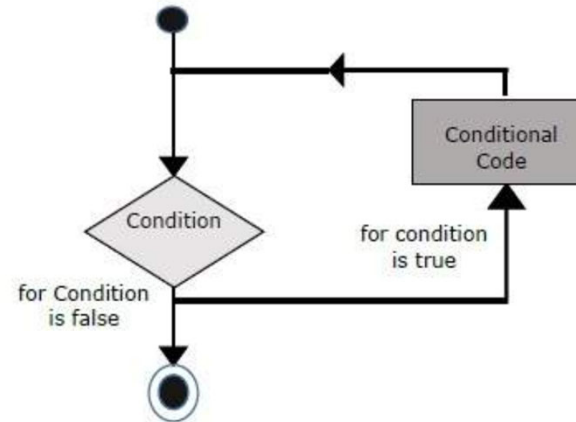
```
8 import numpy as np
9 import matplotlib.pyplot as plt
10 import math as math
11
12
13 for j in range(0,10):
14     print(j, end = " ")
15
16
17
```

*[0, 1, 2, 3, 4 ... 10]*

In [5]: run iteration1 ↵  
0 1 2 3 4 5 6 7 8 9

In [6]:

FOR loop:



## Aside: The range() instruction in python

The instruction range(N) returns a list of integers, starting at zero and ending at N-1. It is good for creating lists of integers.

```
 /
▲ 8 import numpy as np
▲ 9 import matplotlib.pyplot as plt
▲ 10 import math as math
11
12
13 for j in range(0,10): (
14     print(j, end = " ")
15
16
17
```

You can change the starting value from zero to anything you like:

```

13 for j in range(4,10):
14     print(j, end = " ")
15
16
17
```

↙ [4, 5, 6, 7, 8, 9, 10].

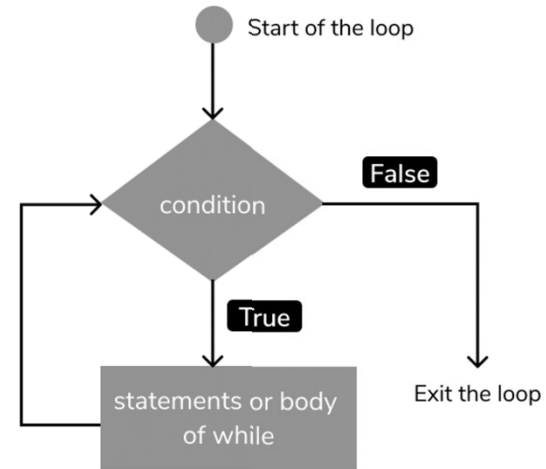
```
8 m = 5
9 i = 0
10 while i < m:
11     print(i, end = " ")
12     i = i + 1
13 print("End")
14
15
```

In [5]: run iteration1  
0 1 2 3 4 5 6 7 8 9

In [6]: run iteration2  
0 1 2 3 4 End

In [7]:

## WHILE loop:



### Dangers of a while loop:

The code can run forever!

e.g. what happens here?

```
8 m = -1
9 i = 0
10 while i > m:
11     print(i, end = " ")
12     i = i + 1
13 print("End")
14
```

## Stopping conditions

It is very important to have a built-in “fail-safe” that tells your code where to stop (otherwise you have to stop it manually).

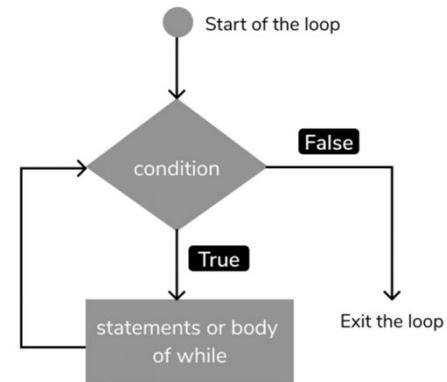
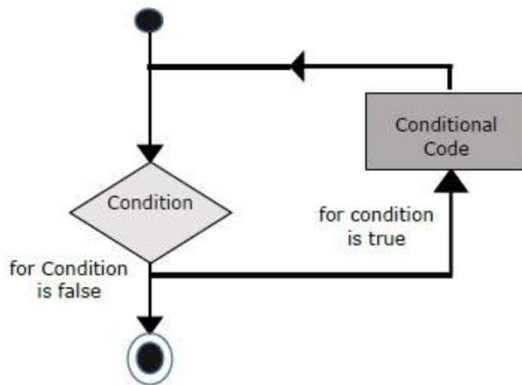
- **break**: terminate the loop and go to the end
- **continue**: jump over the remaining code inside the loop and go to the next iteration
- **pass**: do nothing

```
Loops

while condition:
    <code>

for var in list:
    <code>

Control statements:
break        terminate loop
continue     jump to next iteration
pass        does nothing
```



## Data types in python

Data types and Collections	
integer	10
float	3.14
boolean	True/False
string	'abcde'
list	[1, 2, 3, 4, 5]
tuple	(1, 2, 'a', 'b')
set	{'a', 'b', 'c'}
dictionary	{'a':1, 'b':2}

Mostly we will be using *integers, floats, Booleans, and Lists.*

## Lists

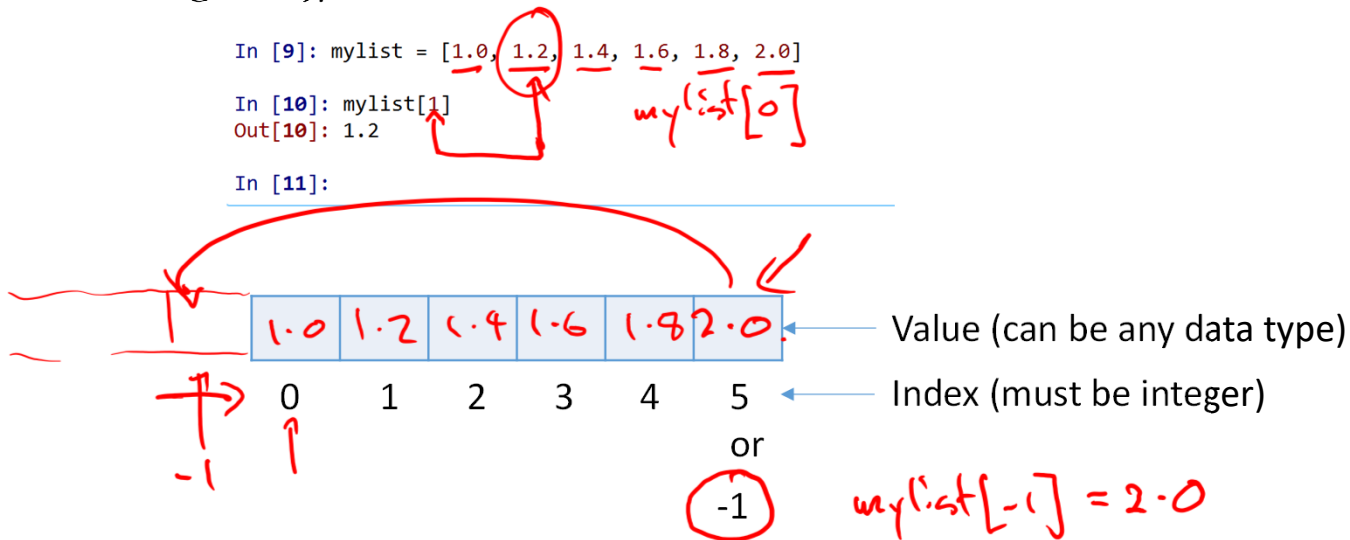
It will become important to gather numbers together in *Lists*.  
Think of a list as a set of boxes into which we put numbers of a given type.

```
In [9]: mylist = [1.0, 1.2, 1.4, 1.6, 1.8, 2.0]
```

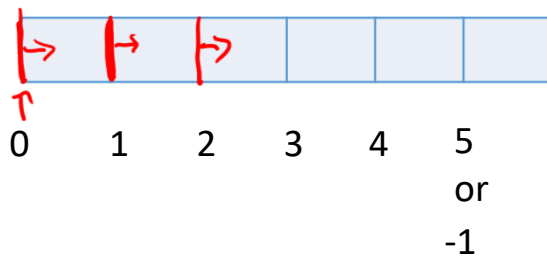
```
In [10]: mylist[1]
```

```
Out[10]: 1.2
```

```
In [11]:
```



It is sometimes useful to think of the index as labelling the *boundary* between two boxes



Lists can be created in the following ways

### 1. Manually:

```
In [9]: mylist = [1.0, 1.2, 1.4, 1.6, 1.8, 2.0]
```

```
In [10]: mylist[1]  
Out[10]: 1.2
```

```
In [11]:
```

---

### 2. Using range():

```
In [1]: xrange = range(4,10)
```

```
In [2]: xrange[2]  
Out[2]: 6
```

```
In [3]: |
```

Or if you're careful, in a contracted form using range:

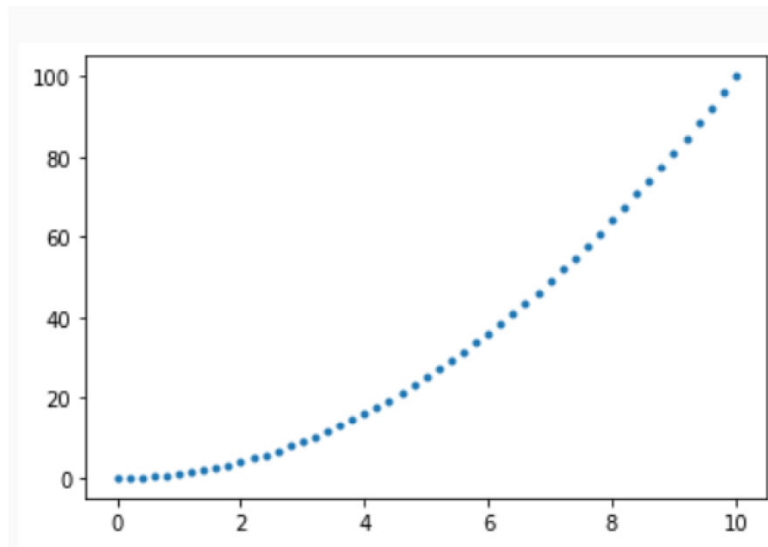
```
In [1]: pow2 = [x**2 for x in range(0,10)]
```

```
In [2]: print(*pow2)  
0 1 4 9 16 25 36 49 64 81
```

```
In [3]:
```

### 3. Using np.linspace (very important for this subject)

```
8 import numpy as np
9 import matplotlib.pyplot as plt
10 import math as math
11
12
13 x = np.linspace(0,10,51)
14 y = x**2
15
16 plt.plot(x,y, '.')
17
18
```



## Style

Developing good programming *style* is key to well-running code (and getting good marks in this subject!)

Three general rules:

1. Always comment your code!
2. Be clear, not clever
3. Divide work into bite-size chunks (functions) and *only give each chunk what it needs to know (i.e. use information hiding)*

1. Always comment your code!  
(You will thank yourself later)

```
1
2 import numpy as np
3 def three(n):
4     x3 = n**3
5     return x3
6 x1 = 10
7 x2 = 0
8 for i in range(0,x1+1):
9     x2 = x2 + three(i)
10 x2 = x2/(x1+1)
11 print(x2)
12
13
```

```
1 # -*- coding: utf-8 -*-
2 """
3 Created on Thu Jul 21 13:17:16 2022
4
5 @author: Chris
6
7 Code to compute the average of the first N cubes
8 starting from 0
9
10 """
11
12 import numpy as np
13 import matplotlib.pyplot as plt
14 import math as math
15
16 """
17 Function definitions
18 -----
19 """
20 def powfn(n):
21     # takes n and raises it to the power of 3
22     powfn = n**3
23     return powfn
24
25 """
26 Main script starts
27 -----
28 """
29
30 N = 10 # input maximum number
31
32 # sum over the first N
33 rsum = 0
34 for i in range(0,N+1):
35     rsum = rsum + powfn(i)
36
37 # compute average by dividing by the number of terms:
38 av = rsum/len(range(0,N+1))
39
40 print("average:",av)
41
```

## 2. Be clear, not clever

```
22 # confusing
23 x = float(input())
24 print("no") if x > 42 else print("yes") if x == 42 else print("maybe")
25
```

```
26 #better
27 x = float(input())
28 if x>42:
29     print('no')
30 elif x==42:
31     print('yes')
32 else:
33     print('maybe')
34
```

### 3. Divide work into bite-size chunks (functions) and *only give each chunk what it needs to know (i.e. use information hiding)*

```
15 """
16 Main script starts
17 -----
18 """
19
20 pi = math.pi
21
22 xrange = np.linspace(0,2*pi,100)
23 dx = xrange[2]-xrange[1]
24
25 sin_int = 0
26 for x in xrange:
27     # print and plot the values
28     print(x, (math.sin(x))**2)
29     plt.plot(x,(math.sin(x))**2, '.')
30
31     sin_int = sin_int+(math.sin(x))**2*dx
32
33 av_sin = sin_int/(2*pi)
34
35 # show the plot with all the points and display result:
36 plt.show()
37 print("Average:",av_sin)
38
39
40 """
41 Now do the same for cos**2(x):
42 """
43
44 cos_int = 0
45 for x in xrange:
46     # print and plot the values
47     print(x, (math.cos(x))**2)
48     plt.plot(x,(math.cos(x))**2, '.')
49
50     cos_int = cos_int+(math.cos(x))**2*dx
51
52 av_cos = cos_int/(2*pi)
53
54 # show the plot with all the points and display result:
55 plt.show()
56 print("Average:",av_cos)
```

```

16 """
17 Function definitions
18 -----
19 """
20 def mysquav(input_fun,xrange):
21     # returns the average of the square of an input function
22     # over the range given by xr, using Riemann integration.
23     # input_fun: a single-variabed function
24     # a range of evenly-spaced real numbers to integrate over
25
26     dx = xrange[2]-xrange[1] # width of each interval
27     L = xrange[-1]-xrange[0] # total length of interval
28
29     fun_int = 0
30     for x in xrange:
31         # print and plot the values
32         #print(x, (input_fun(x))**2)
33         plt.plot(x,(input_fun(x))**2,'.')
34
35         fun_int = fun_int+input_fun(x)**2*dx
36
37     mysquav = fun_int/L
38
39     return mysquav
40
41 """
42 Main script starts
43 -----
44 """
45
46 pi = math.pi
47 xrange = np.linspace(0,2*pi,100)
48
49 av_sin = mysquav(math.sin,xrange)
50 plt.show()
51 print("Average sin**2(x):",av_sin)
52
53 av_cos = mysquav(math.cos,xrange)
54 plt.show()
55 print("Average cos**2(x):",av_cos)

```

The golden rule: never write the same code segment twice!

# Precision and numerical differentiation

How computers store real numbers

Machine precision

Types of errors

Finding numerical derivatives



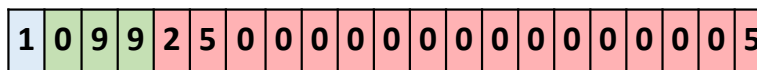




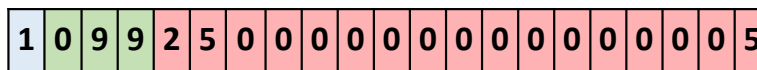
An error due to machine precision is a *fractional* or *relative* error – it tells us how much a number can be “off” as a fraction of the number itself.

To see this, consider the example from earlier: The machine cannot distinguish

2.500000000000000052

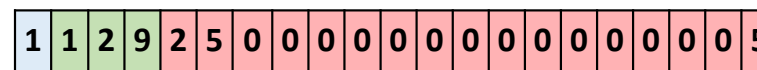


2.500000000000000057

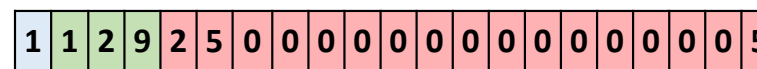


But it has equal trouble distinguishing

$2.500000000000000052 \times 10^{30}$



$2.500000000000000057 \times 10^{30}$



Two types of errors:

**Round-off error** occurs when errors in the storing of numbers accumulate.

This error depends on the machine, and on how the machine stores numbers.

There is generally not much that can be done about this\*.

**Truncation error** occurs when there is a difference between what you compute and the true answer. It occurs even when the round-off error is zero.

This error depends on your algorithm.

Reducing truncation error is practically the entire goal of all numerical methods.

\*there are actually a few things that you can do to minimise round-off error but we'll get to them later

## Numerical accuracy and convergence

For anything that a computer does you have to know *how good it is at solving the problem*.

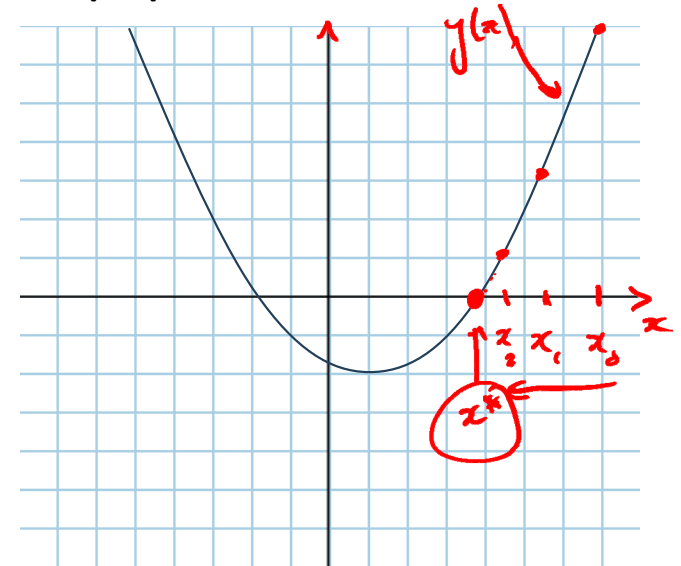
*There are two main quantities:*

1. Accuracy: how close is your numerical answer to the "true" solution?
2. Speed: how fast does it converge to its solution?

In a practical situation we often put it this way:

How accurate do you want your answer? Can we get to within this accuracy in a reasonable time?

**Example problem: find the zeros of a function**



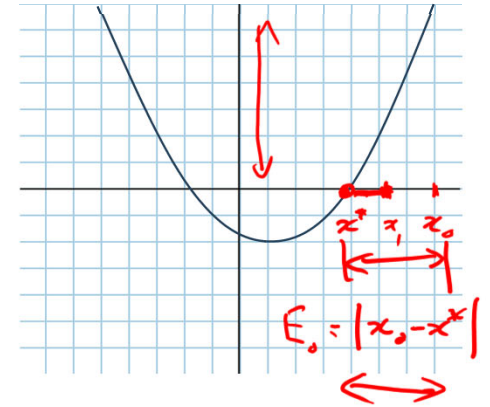
The *true solution* (which is usually not known) is usually denoted  $x^*$ .

## Convergence Plots

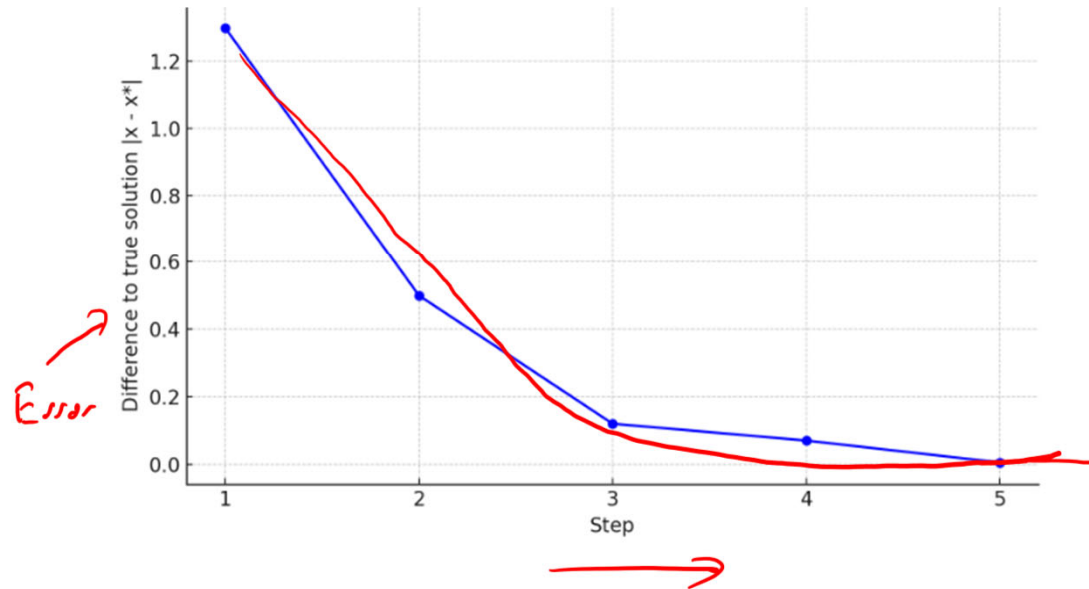
The absolute value of the difference between the current solution  $x$  and the true solution  $x^*$  is known as the *error*.

$$E_n = |x_n - x^*|$$

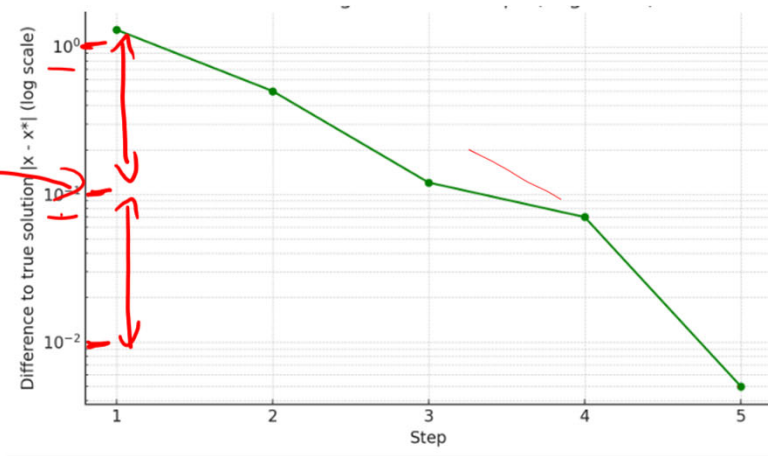
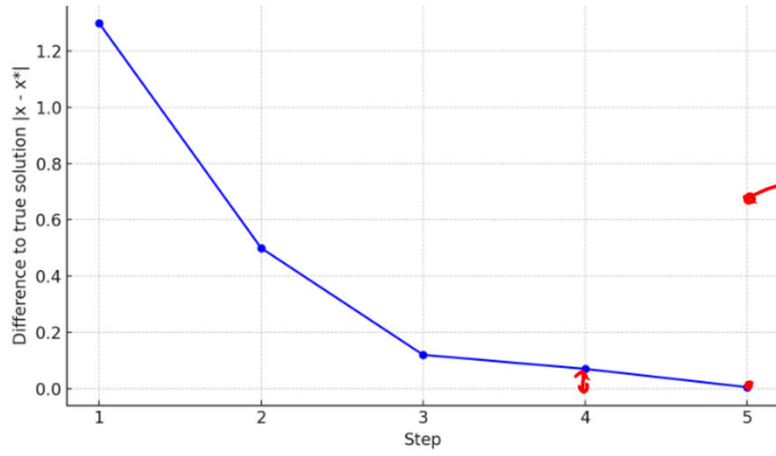
A convergence plot plots the error as the algorithm continues.



Step	Difference to true solution $ x - x^* $
1	1.3
2	0.5
3	0.12
4	0.07
5	0.005



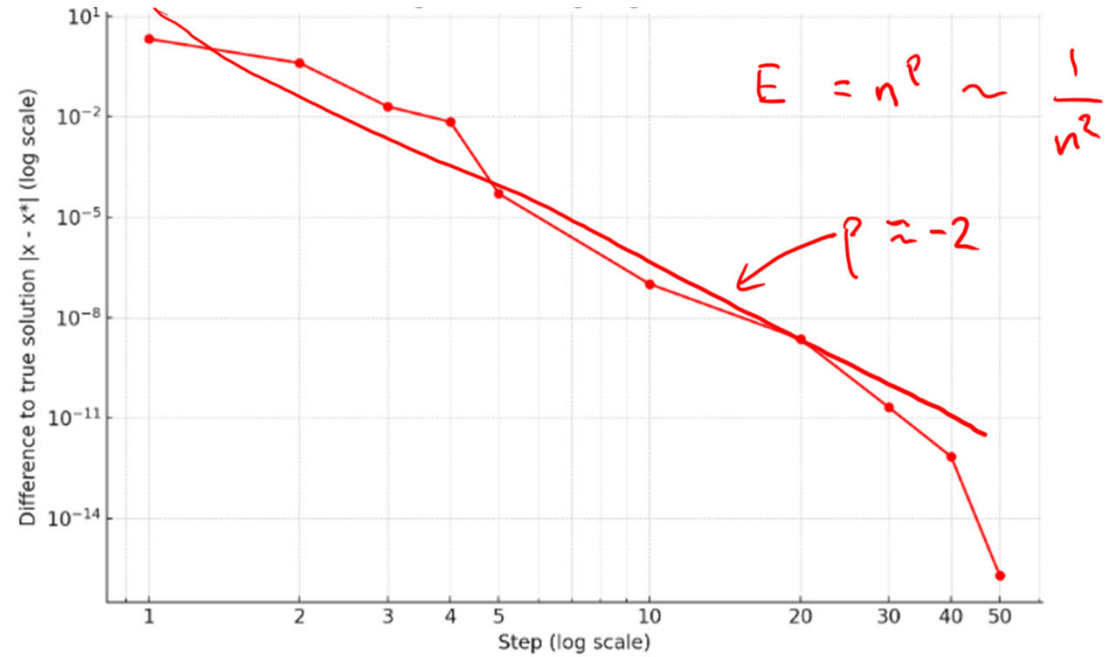
It is usually best to plot the convergence on a *logarithmic* scale.



Even better is to plot the error on a *double-logarithmic* scale.

Step	Difference to true solution $ x-x^* $
1	2.1
2	0.4
3	0.02
4	0.007
5	0.00005

10	1e-7
20	2.3e-9
30	2.1e-11
40	7e-13
50	2e-16



This gives a direct trade-off between accuracy and time/resources.

Question: if we want to know the error we have to know the *true solution*.  
But this is unknown! What do we do?

Answer: we compute the error using the most recent solution.

$$E_n = |x_n - x^*|$$

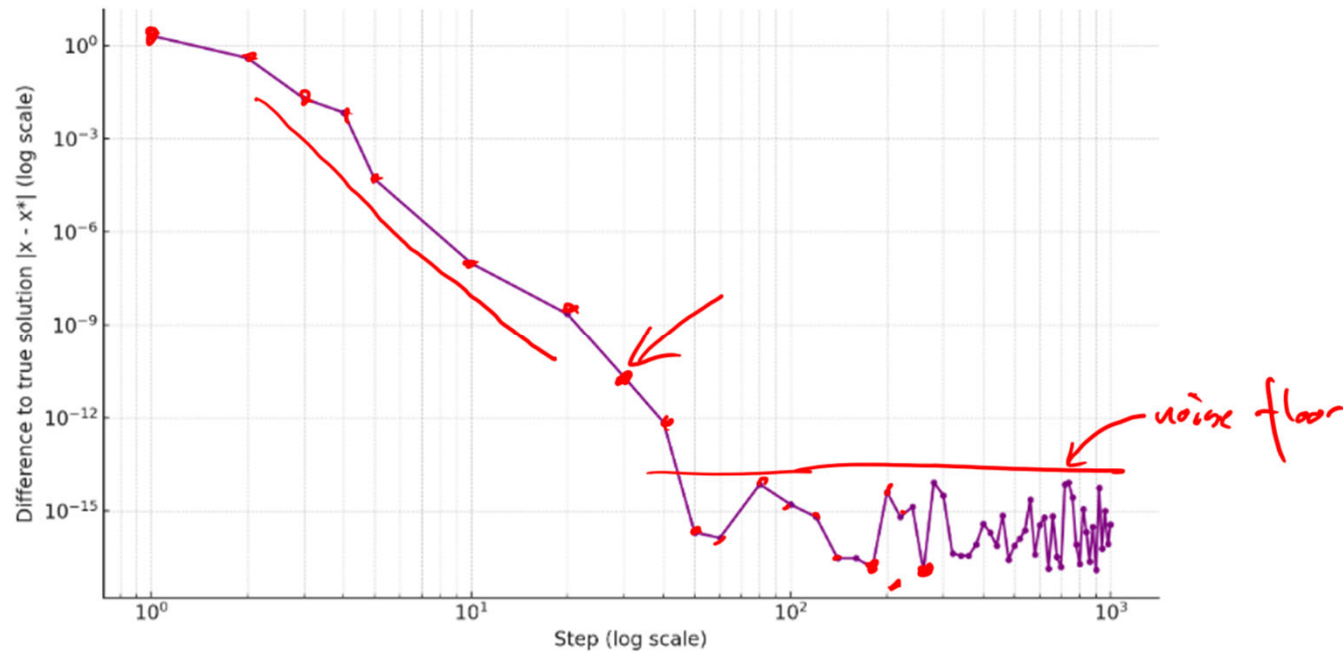
↑            ↑  
                 L?

Step	x	$ x - x^* $
1	4.1340570	2.134057
2	2.4045237	0.404523
3	2.0211838	0.021183
4	2.0073523	0.007352
5	2.0000005	0

↑  
 $\sim x^*$

## The noise floor

When the error gets small (for a good algorithm, this is the machine precision) then it starts bouncing around instead of decreasing. This is called *the noise floor*.



Giving the algorithm more time or resources doesn't improve the error from this point on.

## Topic 1: Numerical Differentiation

First rule of numerical differentiation: Avoid it if at all possible

Discussion question:

Imagine that we have a function  $f(x)$  which we can evaluate only numerically. How can we compute the derivative  $f'(x)$ ?

$$f'(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}$$

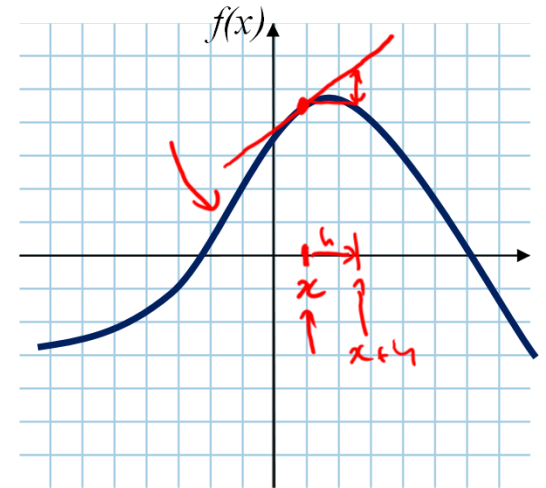
$$\approx \frac{f(x+h) - f(x)}{h} \leftarrow \text{"forward difference"}$$

What is the error? Use Taylor series:

$$f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2f''(x) + \frac{1}{3!}h^3f'''(x) + \dots$$

$$f(x+h) - f(x) = hf'(x) + \frac{1}{2}h^2f''(x)$$

$$\frac{f(x+h) - f(x)}{h} \approx f'(x) + \frac{1}{2}hf''(x) \Rightarrow f'(x) = \frac{f(x+h) - f(x)}{h} + \varepsilon(h)$$



$$f(x) = f(x_0) + f'(x_0)(x-x_0) + \frac{1}{2}f''(x_0)(x-x_0)^2 + \dots$$

$\uparrow$   $x$        $\uparrow$   $h$

The formula for computing the derivative

$$f'(x) \approx \frac{1}{h} (f(x+h) - f(x))$$

is known as a *forward difference method*.

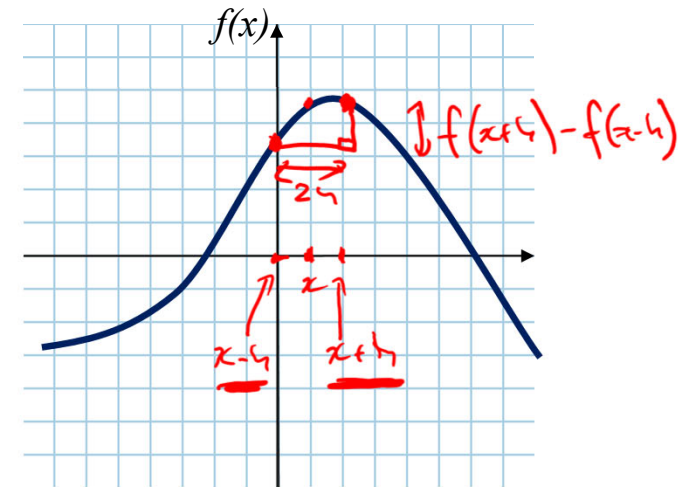
We could also define the backward difference method

$$f'(x) \approx \frac{1}{h} (f(x) - f(x-h))$$

which has the same error.

There are other options: for example, we could also try the balanced difference

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



$$\underline{f'(x)} \approx \frac{1}{2h} (\underline{f(x+h)} - \underline{f(x-h)}) \quad \leftarrow$$

$$\begin{aligned} f(x+h) &= f(x) + \underline{hf'(x)} + \frac{1}{2}h^2f''(x) + \frac{1}{6}h^3f'''(x) + \dots \\ f(x-h) &= f(x) - \underline{hf'(x)} + \frac{1}{2}h^2f''(x) - \frac{1}{6}h^3f'''(x) + \dots \end{aligned}$$

$$\begin{aligned} f(x+h) - f(x-h) &= \cancel{f(x)} - \cancel{f(x)} + 2hf'(x) + \cancel{\frac{1}{2}h^2f''(x)} - \cancel{\frac{1}{2}h^2f''(x)} + \frac{2}{6}f'''(x)h^3 + \dots \\ &= \underline{2hf'(x)} + \frac{1}{3}f'''(x)h^3 + \dots \end{aligned}$$

So

$$f'(x) = \frac{1}{2h} [f(x+h) - f(x-h)] - \underbrace{\frac{1}{3}h^2f'''(x)}_{\substack{\uparrow \\ \Sigma(h) \sim h^2 \\ \uparrow \\ \text{proportional}}}$$

$$\Sigma(h) \sim h \uparrow$$

