Computational Science and Engineering in Python

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Outline I

Outline II

First steps with the Python prompt

The Python prompt

- Spyder (or IDLE, or `python` or `python.exe` from shell/Terminal/MS-Dos prompt, or `IPython`)
- Python prompt waits for input:

```
>>>
```

- Interactive Python prompt waits for input:

```
In [1]:
```

- Read, Evaluate, Print, Loop $\rightarrow$ REPL

Hello World program

Standard greeting:

```python
print("Hello World!")
```

Entered interactively in Python prompt:

```
>>> print("Hello World!")
Hello World!
```

Or in IPython prompt:

```
In [1]: print("Hello world")
Hello world
```

A calculator

```
>>> 2 + 3
5
>>> 42 - 15.3
26.7
>>> 100 * 11
1100
>>> 2400 / 20
120
>>> 2 ** 3                          # 2 to the power of 3
8
>>> 9 ** 0.5                        # sqrt of 9
3.0
```

Create variables through assignment

```
>>> a = 10
>>> b = 20
>>> a
10
>>> b
20
>>> a + b
30
>>> ab2 = (a + b) / 2
>>> ab2
15
```

Important data types / type()

```
>>> a = 1
>>> type(a)
<type 'int'>                    # integer

>>> b = 1.0
>>> type(b)
<type 'float'>                  # float

>>> c = '1.0'
>>> type(c)
<type 'str'>                    # string

>>> d = 1 + 3j
>>> type(d)
<type 'complex'>                # complex number
```

Beware of integer division

This is the problem:

```
>>> 1 / 2
0                               # expected 0.5, not 0
```

Solution: change (at least) one of the integer numbers into a floating point number (i.e. `1` → `1.0`).

```
>>> 1.0 / 2
0.5
>>> 1 / 2.0
0.5
```

Summary useful commands (introspection)

- `print(x)` to display the object `x`
- `type(x)` to determine the type of object `x`
- `help(x)` to obtain the documentation string
- `dir(x)` to display the methods and members of object `x`, or the current name space (`dir()`).

Example:

```
>>> help("abs")
Help on built-in function abs:

abs(...)
    abs(number) -> number

    Return the absolute value of the argument.
```

Interactive documentation, introspection

```
>>> word = 'test'
>>> print(word)
test
>>> type(word)
<type 'str'>
>>> dir(word)
['__add__', '__class__', '__contains__', ...,
'__doc__', ..., 'capitalize', <snip>,
'endswith', ..., 'upper', 'zfill']
>>> word.upper()
'TEST'
>>> word.capitalize()
'Test'
>>> word.endswith('st')
True
>>> word.endswith('a')
False
```

Functions

Example 1:

```
def mysum(a, b):
    return a + b

#main program starts here
print "The sum of 3 and 4 is", mysum(3, 4)
```

Functions should be documented

```python
def mysum(a,b):
    """Return the sum of parameters a and b.
    Hans Fangohr, fangohr@soton.ac.uk,
    last modified 24/09/2013
    """
    return a + b

# main program starts here
print "The sum of 3 and 4 is", mysum(3, 4)
```

Can now use the help function for our new function:

```
>>> help(mysum)
Help on function mysum in module __main__:

mysum(a, b)
    Return the sum of parameters a and b.
    Hans Fangohr, fangohr@soton.ac.uk,
    last modified 24/09/2013
```

Function terminology

```
x = -1.5
y = abs(x)
```

- `x` is the *argument* given to the function
- `y` is the *return value* (the result of the function's computation)
- Functions may expect zero, one or more arguments
- Not all functions (seem to) return a value. (If no `return` keyword is used, the special object `None` is returned.)

Function example

```
def plus42(n):
    """Add 42 to n and return""" # docstring
    l = n + 42                   # body of
                                 # function
    return l

a = 8
b = plus42(a)    # not part of function definition
```

After execution, b carries the value 50 (and a $= 8$).

Summary functions

- Functions provide (black boxes of) functionality: crucial building blocks that hide complexity
- interaction (input, output) through input arguments and return values (*printing* and *returning* values is not the same!)
- docstring provides the specification (contract) of the function's input, output and behaviour
- a function must not modify input arguments (watch out for lists, dicts, more complex data structures as input arguments)

Functions printing vs returning values I

Given the following two function definitions:

```
def print42():
    print(42)

def return42():
    return 42
```

we use the Python prompt to explore the difference:

```
>>> b = return42()    # return 42, is assigned
>>> print(b)          # to b
42

>>> a = print42()     # return None, and
42                    # print 42 to screen
>>> print(a)
None                  # special object None
```

Functions printing vs returning values II

If we use IPython, it shows whether a function returns something (i.e. not None) through the `Out [ ]` token:

```
In [1]: return42()
Out[1]: 42                # Return value of 42


In [2]: print42()
42                        # No 'Out [ ]', so no
                          # returned value
```

About Python

Python

What is Python?

- High level programming language
- interpreted
- Quite similar to MATLAB
- supports three main programming styles (imperative=procedural, object-oriented, functional)
- General purpose tool, yet good for numeric work with extension libraries

Availability

- Python is free
- Python is platform independent (works on Windows, Linux/Unix, Mac OS, ...)

Python documentation

There is lots of documentation that you should learn to use:

- Teaching materials on website, including these slides and a text-book like documents
  - Online documentation, for example
    - Python home page (http://www.python.org)
    - Pylab/Matplotlib (plotting as in Matlab)
    - Numpy (fast vectors and matrices, (NUMerical PYthon)
    - SciPy (scientific algorithms, `odeint`)
    - Visual Python (3d visualisation)
    - SymPy (Symbolic calculation)
- interactive documentation

Which Python version

- There are currently two versions of Python:
  - Python 2.x and
  - Python 3.x
- We will use version 2.7 (compatible with numerical extension modules scipy, numpy, pylab).
- Python 2.x and 3.x are incompatible although the changes only affect very few commands.
- See webpages for notes on installation of Python on computers.

The math module (`import math`)

```
>>> import math
>>> math.sqrt(4)
2.0
>>> math.pi
3.141592653589793
>>> dir(math)          #attributes of 'math' object
['__doc__', '__file__', < snip >
'acos', 'acosh', 'asin', 'asinh', 'atan', 'atan2',
'atanh', 'ceil', 'copysign', 'cos', 'e', 'erf',
'exp', <snip>, 'sqrt', 'tan', 'tanh', 'trunc']

>>> help(math.sqrt)          #ask for help on sqrt
sqrt(...)
    sqrt(x)
    Return the square root of x.
```

Name spaces and modules

Three (good) options to access a module:

1. use the full name:

```python
import math
print math.sin(0.5)
```

2. use some abbreviation

```python
import math as m
print m.sin(0.5)
print m.pi
```

3. import all objects we need explicitly

```python
from math import sin, pi
print sin(0.5)
print pi
```

Integer division (revisited) I

Reminder

```
>>> 1 / 2
0                              # expected 0.5, not 0
```

Solutions:

- change (at least) one of the integer numbers into a floating point number (i.e. `1` → `1.0`).

```
>>> 1.0 / 2
0.5
```

- Or use `float` function to convert variable to float

```
>>> a = 1
>>> b = 2
>>> 1 / float(b)
0.5
```

Integer division (revisited) II

- Or make use of Python's future division:

```
>>> from __future__ import division
>>> 1 / 2
0.5
```

If you really want integer division, use `//`:
`1//2` returns 0 (now and in future).

Coding style

Coding style

- Python programs *must* follow Python syntax.
- Python programs *should* follow Python style guide, because
  - readability is key (debugging, documentation, team effort)
  - conventions improve effectiveness

Common style guide: PEP8

See http://www.python.org/dev/peps/pep-0008/

- This document gives coding conventions for the Python code comprising the standard library in the main Python distribution.
- This style guide evolves over time as additional conventions are identified and past conventions are rendered obsolete by changes in the language itself.
- Many projects have their own coding style guidelines. In the event of any conflicts, such project-specific guides take precedence for that project.
- One of Guido's key insights is that code is read much more often than it is written. The guidelines provided here are intended to improve the readability of code and make it consistent across the wide spectrum of Python code. *"Readability counts"*.
- When not to follow this style guide:
  - When applying the guideline would make the code less readable, even for someone who is used to reading code that follows this PEP.
  - To be consistent with surrounding code that also breaks it (maybe for historic reasons) – although this is also an opportunity to clean up someone else's mess (in true XP style).
  - Because the code in question predates the introduction of the guideline and there is no other reason to be modifying that code.

PEP8 Style guide

- Indentation: use 4 spaces
- One space around `=` operator: `c = 5` and not `c=5`.
- Spaces around arithmetic operators can vary: `x = 3*a + 4*b` is okay, but also okay to write `x = 3 * a + 4 * b`.
- No space before and after parentheses: `x = sin(x)` but not `x = sin( x )`
- A space after comma: `range(5, 10)` and not `range(5,10)`.
- No whitespace at end of line
- No whitespace in empty line
- One or no empty line between statements within function
- Two empty lines between functions
- One import statement per line
- import first standand Python library, then third-party packages (numpy, scipy, ...), then our own modules.

PEP8 Style Summary

- Try to follow PEP8 guide, in particular for new code
- Use tools to help us, for example Spyder editor can show PEP8 violations
- `pep8` program available to check source code.

Conditionals, if-else

Truth values I

The python values `True` and `False` are special inbuilt objects:

```
>>> a = True
>>> print(a)
True
>>> type(a)
<type 'bool'>
>>> b = False
>>> print(b)
False
>>> type(b)
<type 'bool'>
```

We can operate with these two logical values using boolean logic, for example the logical and operation (`and`):

Truth values II

```
>>> True and True            #logical and operation
True
>>> True and False
False
>>> False and True
False
>>> True and True
True
```

There is also logical or (`or`) and the negation (`not`):

```
>>> True or False
True
>>> not True
False
>>> not False
True
>>> True and not False
True
```

Truth values III

In computer code, we often need to evaluate some expression that is either true or false (sometimes called a “predicate”). For example:

```
>>> x = 30              # assign 30 to x
>>> x >= 30   # is x greater than or equal to 30?
True
>>> x > 15              # is x greater than 15
True
>>> x > 30
False
>>> x == 30             # is x the same as 30?
True
>>> not x == 42         # is x not the same as 42?
True
>>> x != 42             # is x not the same as 42?
True
```

if-then-else I

The `if-else` command allows to branch the execution path depending on a condition. For example:

```
>>> x = 30                    # assign 30 to x
>>> if x > 30:                # predicate: is x > 30
...     print("Yes")              # if True, do this
... else:
...     print("No")               # if False, do this
...
No
```

The general structure of the `if-else` statement is

```
if A:
    B
else:
    C
```

where `A` is the predicate.

if-then-else II

- If `A` evaluates to `True`, then all commands `B` are carried out (and `C` is skipped).
- If `A` evaluates to `False`, then all commands `C` are carried out (and `B`) is skipped.
- `if` and `else` are Python keywords.

`A` and `B` can each consist of multiple lines, and are grouped through indentation as usual in Python.

if-else example

```
def slength1(s):
    """Returns a string describing the
    length of the sequence s"""
    if len(s) > 10:
        return 'very long'
    else:
        return 'normal'
```

```
>>> slength1("Hello")
'normal'
>>> slength1("HelloHello")
'normal'
>>> slength1("Hello again")
'very long'
```

if-elif-else example I

If more cases need to be distinguished, we can use the additional keyword `elif` (standing for ELse IF) as many times as desired:

```python
def slength2(s):
    if len(s) == 0:
        return 'empty'
    elif len(s) > 10:
        return 'very long'
    elif len(s) > 7:
        return 'normal'
    else:
        return 'short'
```

if-elif-else example II

```
>>> slength2("")
'empty'
>>> slength2("Good Morning")
'very long'
>>> slength2("Greetings")
'normal'
>>> slength2("Hi")
'short'
```

LAB2

Sequences

Sequences overview

Different types of sequences

- strings
- lists (mutable)
- tuples (immutable)
- arrays (mutable, part of numpy)

They share common commands.

Strings

```
>>> a = "Hello World"
>>> type(a)
<type 'str'>
>>> len(a)
11
>>> print(a)
Hello World
```

Different possibilities to limit strings

```
'A string'
"Another string"
"A string with a ' in the middle"
"""A string with triple quotes can
extend over several
lines"""
```

Strings 2 (exercise)

- Enter this line on the Python prompt:
  `>>> a="One"; b="Two"; c="Three"`
- Exercise: What do the following expressions evaluate to?
  1. `d = a + b + c`
  2. `5 * d`
  3. `d[0], d[1], d[2]` (indexing)
  4. `d[-1]`
  5. `d[4:]` (slicing)

Strings 3 (exercise)

```
>>> s="""My first look at Python was an
... accident, and I didn't much like what
... I saw at the time."""
```

- count the number of (i) letters 'e' and (ii) substrings 'an' s
- replace all letters 'a' with '0'
- make all letters uppercase
- make all capital letters lowercase, and all lower case letters to capitals

Lists

```
[]                          # the empty list
[42]                        # a 1-element list
[5, 'hello', 17.3]          # a 3-element list
[[1, 2], [3, 4], [5, 6]]    # a list of lists
```

- Lists store an ordered sequence of Python objects
- Access through index (and slicing) as for strings.
- Important function: `range()` (`xrange`)
- use `help()`, often used list methods is `append()`

(In general computer science terminology, vector or array might be better name as the actual implementation is not a linked list, but direct $\mathcal{O}(1)$ access through the index is possible.)

Example program: using lists

```
>>> a = []                # creates a list
>>> a.append('dog')       # appends string 'dog'
>>> a.append('cat')       # ...
>>> a.append('mouse')
>>> print(a)
['dog', 'cat', 'mouse']
>>> print(a[0])           # access first element
dog                       # (with index 0)
>>> print(a[1])           # ...
cat
>>> print(a[2])
mouse
>>> print(a[-1])          # access last element
mouse
>>> print(a[-2])          # second last
cat
```

Example program: lists containing a list

```
>>> a=['dog', 'cat', 'mouse', [1, 10, 100, 1000]]
>>> a
['dog', 'cat', 'mouse', [1, 10, 100, 1000]]
>>> a[0]
dog
>>> a[3]
[1, 10, 100, 1000]
>>> max(a[3])
1000
>>> min(a[3])
1
>>> a[3][0]
1
>>> a[3][1]
10
>>> a[3][3]
1000
```

Sequences – more examples

```
>>> a = "hello world"
>>> a[4]
'o'
>>> a[4:7]
'o w'
>>> len(a)
11
>>> 'd' in a
True
>>> 'x' in a
False
>>> a + a
'hello worldhello world'
>>> 3 * a
'hello worldhello worldhello world'
```

Tuples I

- tuples are very similar to lists
- tuples are usually written using parentheses (↔ “round brackets”):

```
>>> t = (3, 4, 50)
>>> t
(3, 4, 50)
>>> type(t)
<type 'tuple'>
>>> l = [3, 4, 50]    # compare with list object
>>> l
[3, 4, 50]
>>> type(l)
<type 'list'>
```

- normal indexing and slicing (because tuple is a sequence)

Tuples II

```
>>> t[1]
4
>>> t[:-1]
(3, 4)
```

- tuples are defined by the comma (!)

```
>>> a = 10, 20, 30
>>> type(a)
<type 'tuple'>
```

- the parentheses are usually optional (but should be written anyway):

```
>>> a = (10, 20, 30)
>>> type(a)
<type 'tuple'>
```

Tuples III

So why do we need tuples (in addition to lists)?

1. use tuples if you want to make sure that a set of objects doesn't change.
2. allow to assign several variables in one line (known as *tuple packing* and *unpacking*)

   ```
   x, y, z = 0, 0, 1
   ```

   - This allows 'instantaneous swap' of values:

     ```
         a, b = b, a
     ```

3. functions return tuples if they return more than one object

   ```
   def f(x):
       return x**2, x**3

   a, b = f(x)
   ```

Tuples IV

4. tuples can be used as keys for dictionaries as they are immutable

(Im)mutables

- Strings — like tuples — are immutable:

```
>>> a = 'hello world'          # String example
>>> a[4] = 'x'
Traceback (most recent call last):
  File "<stdin>", line 1, in ?
TypeError: object doesn't support
           item assignment
```

- strings can only be 'changed' by creating a new string, for example:

```
>>> a = a[0:3] + 'x' + a[4:]
>>> a
'helxo world'
```

Summary sequences

- lists, strings and tuples (and arrays) are sequences. For example
  - list `a = [1, 10, 42, 400]` or
  - string `a = 'hello world'`
- sequences share the following operations

`a[i]`	returns i-th element of `a`
`a[i:j]`	returns elements i up to $j-1$
`len(a)`	returns number of elements in sequence
`min(a)`	returns smallest value in sequence
`max(a)`	returns largest value in sequence
`x in a`	returns `True` if `x` is element in `a`
`a + b`	concatenates `a` and `b`
`n * a`	creates `n` copies of sequence `a`

In the table above, `a` and `b` are sequences, `i`, `j` and `n` are integers.

Loops

Example programmes: for-loops I

```python
animals = ['dog', 'cat', 'mouse']

for animal in animals:
    print("This is the {}".format(animal))
```

produces this output:

```
This is the dog
This is the cat
This is the mouse
```

The `range(n)` command is used to create lists with increasing integer values up to (but not including) `n`:

Example programmes: for-loops II

```
>>> range(6)
[0, 1, 2, 3, 4, 5]
>>> range(3)
[0, 1, 2]
```

```
for i in range(6):
    print("the square of {} is {}"
          .format(i, i ** 2))
```

produces this output:

```
the square of 0 is 0
the square of 1 is 1
the square of 2 is 4
the square of 3 is 9
the square of 4 is 16
the square of 5 is 25
```

The range function

- `range([start,] stop [,step])` returns a list of integers from start to *but not including* stop. Example

```
>>> range(1,4)
[1, 2, 3]
```

`start` defaults to 0 and `step` defaults to 1.

Iterating: for-loop

`for` loop iterates over sequence

Examples:

```
for i in range(5):
    print(i)

for i in [0, 3, 4, 19]:
    print(i)

for animal in ['dog', 'cat', 'mouse']:
    print(animal)

for letter in "Hello World":
    print(letter)
```

Branching: If-then-else

- Example 1 (if-then-else)

```
a = 42
if a > 0:
    print("a is positive")
else:
    print("a is negative or zero")
```

- Example 2 (if-then-elif-else)

```
a = 42
if a > 0:
    print("a is positive")
elif a == 0:
    print("a is zero")
else:
    print("a is negative")
```

Another iteration example

- combine for-loop and if:

```python
def skip13(a,b):
    for k in range (a,b):
        if k == 13:
            pass            #do nothing
        else:
            print(k)
```

This generates a sequence of numbers often used in hotels to label floors (more info)

- As above, but *return* list of numbers (instead of print)

```python
def skip13(a,b):
    result = []
    for k in range (a,b):
        if k == 13:
            pass                #do nothing
        else:
            result.append(k)
    return result
```

Exercise range_double

Write a function `range_double(n)` that behaves in the same way as the in-built python function `range(n)` but which returns twice the number for every entry. For example:

```
>>> range_double(4)
[0, 2, 4, 6]
>>> range_double(10)
[0, 2, 4, 6, 8, 10, 12, 14, 16, 18]
```

For comparison the behaviour of `range`:

```
>>> range(4)
[0, 1, 2, 3]
>>> range(10)
[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
```

LAB3

Exercise: First In First Out (FIFO) queue

Write a *First-In-First-Out* queue implementation, with functions:

- `add(name)` to add a customer with name `name` (call this when a new customer arrives)
- `next()` to be called when the next customer will be served. This function returns the name of the customer
- `show()` to print all names of customers that are currently waiting
- `length()` to return the number of currently waiting customers

Suggest to use a global variable `q` and define this in the first line of the file by assigning an empty list: `q = []`.

While loops

- a `for` loop iterates over a given sequence
- a `while` loop iterates while a condition is fulfilled

Example:

```
x=64
while x>1:
    x = x/2
    print(x)
```

produces

```
32
16
8
4
2
1
```

While loop example 2

Determine ϵ:

```
eps = 1.0

while eps + 1 > 1:
    eps = eps / 2.0
print("epsilon is {}".format(eps))
```

identical to

```
eps = 1.0
while True:
    if eps + 1 == 1:
        break          # leaves innermost loop
    eps = eps / 2.0
print("epsilon is {}".format(eps))
```

Output:

```
epsilon is 1.11022302463e-16
```

Some things revisited

What are variables?

In Python, variables are references to objects.
This is why in the following example, a and b represent the same list: a and b are two *different references* to the *same object*:

```
>>> a = [0, 2, 4, 6]  # bind name 'a' to list
>>> a                 # object [0,2,4,6].
[0, 2, 4, 6]
>>> b = a             # bind name 'b' to the same
>>> b                 # list object.
[0, 2, 4, 6]
>>> b[1]              # show second element in list
2                     # object.
>>> b[1] = 10         # modify 2nd elememnt (via b).
>>> b                 # show b.
[0, 100, 4, 6]
>>> a                 # show a.
[0, 100, 4, 6]
```

id, == and is

- Two objects `a` and `b` are the *same object* if they live in the same place in memory (`id()`). We check with `id(a) == id(b)` or `a is b`.
- Two different objects can have the *same value*. We check with `==` See “Equality and identify“, section 3.5

```
>>> a = 1
>>> b = 1.0
>>> id(a); id(b)
4298187624              #not in the same place
4298197712              #in memory
>>> a is b              #i.e. not the same objects
False
>>> a == b              #but carry the same value
True
>>> a = [1, 2, 3]
>>> b = a               #b is reference to object of a
>>> a is b              #thus they are the same
True
```

Functions - side effect

- If we carry out some activity A, and this has an (unexpected) effect on something else, we speak about *side effects*. Example:

```
def sum(xs):
    s = 0
    for i in range(len(xs)):
        s = s + xs.pop()
    return s

xs = [0, 1, 2, 3]
print "xs =", xs,
print "sum(xs)=", sum(xs)
print "xs =", xs,
print "sum(xs)=", sum(xs)
```

Output:

```
xs = [0, 1, 2, 3] sum(xs)= 6
xs = [] sum(xs)= 0
```

Functions - side effect 2

Better ways to compute the sum of a list `xs` (or sequence in general)

- use in-built command `sum(xs)`
- use indices to iterate over list

```
def sum(xs):
    s=0
    for i in range(len(xs)):
        s = s + xs[i]
    return s
```

- or (better): iterate over list elements directly

```
def sum(xs):
    s=0
    for elem in xs
        s = s + elem
    return s
```

To print or to return?

- A function that returns the control flow through the `return` keyword, will return the object given after `return`.
- A function that does not use the `return` keyword, returns the special object `None`.
- Generally, functions should return a value
- Generally, functions should not print anything
- Calling functions from the prompt can cause some confusion here: if the function returns a value and the value is not assigned, it will be printed.

Reading and writing data files

File input/output

It is a (surprisingly) common task to

- read some input data file
- do some calculation/filtering/processing with the data
- write some output data file with results

Writing a text file I

```
>>> fout = open('test.txt', 'w')   # Write
>>> fout.write("first line\nsecond line")
>>> fout.close()
```

creates a file `test.txt` that reads

```
first line
second line
```

- To write data, we need to use the `'w'` mode:

  ```
      f = open('mydatafile.txt', 'w')
  ```

- If the file exists, it will be overridden with an empty file when the open command is executed.
- The file object `f` has a method `f.write` which takes a string as in input argument.
- Must close file at the end of writing process.

Reading a text file I

We create a file object f using

```
>>> f = open('test.txt', 'r')        # Read
```

and have different ways of reading the data:

- Example 1 (`readlines()`)
  `f.readlines()` returns a list of strings (each being one line)

```
>>> f = open('test.txt', 'r')
>>> lines = f.readlines()
>>> f.close()
>>> lines
['first line\n', 'second line']
```

Reading a text file II

- Example 2 (`read()`)
  `f.read()` returns one long string for the whole file

```
>>> f = open('test.txt', 'r')
>>> data = f.read()
>>> f.close()
>>> data
'first line\nsecond line'
```

- Advanced: `f` is also an iterable object (important for large files)

```
>>> f = open('test.txt', 'r')
>>> for line in f:
...     print(line),
...
first line
second line
>>> f.close()
```

Reading a text file III

- Advanced: Could use a context:

```
>>> with open('test.txt', 'r') as f:
...     data = f.read()
...
>>> data
'first line\nsecond line'
```

Reading a file, iterating over lines

- Often we want to process line by line. Typical code fragment:

```
f = open('myfile.txt', 'r')
lines = f.readlines()
f.close()
# Then do some processing with the
# lines object
```

  `lines` is a list of strings, each representing one line of the file.
- It is good practice to close a file as soon as possible.

Splitting a string

- We often need to split a string into smaller parts: use string method `split()`:
  (try `help("".split)` at the Python prompt for more info)

Example: Take a string and display each word on a separate line:

```
>>> c = 'This is my string'
>>> c.split()
['This', 'is', 'my', 'string']
>>> c.split('i')
['Th', 's ', 's my str', 'ng']
```

Exercise: Shopping list

Given a list

```
bread       1  1.39
tomatoes    6  0.26
milk        3  1.45
coffee      3  2.99
```

Write program that computes total cost per item, and writes to `shopping_cost.txt`:

```
bread       1.39
tomatoes    1.56
milk        4.35
coffee      8.97
```

One solution

One solution is `shopping_cost.py`

```
fin = open('shopping.txt')
lines = fin.readlines()
fin.close()

fout = open('shopping_cost.txt', 'w')
for line in lines:
    words = line.split()
    itemname = words[0]
    number = int(words[1])
    cost = float(words[2])
    totalcost = number * cost
    fout.write("{:20} {}\n".format(itemname,
                                   totalcost))
fout.close()
```

Exercise

Write function `print_line_sum_of_file(filename)` that reads a file of name `filename` containing numbers separated by spaces, and which computes and prints the sum for each line. A data file might look like

```
1 2 4 67 -34 340
0 45 3 2
17
```

LAB4

Exceptions

Exceptions

- Errors arising during the execution of a program result in "exceptions".
- We have seen exceptions before, for example when dividing by zero:

```
>>> 4.5 / 0
Traceback (most recent call last):
  File "<stdin>", line 1, in ?
ZeroDivisionError: float division
```

  or when we try to access an undefined variable:

```
>>> print(x)
Traceback (most recent call last):
  File "<stdin>", line 1, in ?
NameError: name 'x' is not defined
```

- Exceptions are a modern way of dealing with error situations
- We will now see how
  - what exceptions are coming with Python
  - we can "catch" exceptions
  - we can raise ("throw") exceptions in our code

In-built Python exceptions I

Python's inbuilt exceptions can be found in the `exceptions` module.

Users can provide their own exception classes (by inheriting from `Exception`).

```
>>> import exceptions
>>> help(exceptions)
       BaseException
            Exception
                StandardError
                    ArithmeticError
                        FloatingPointError
                        OverflowError
                        ZeroDivisionError
                    AssertionError
                    AttributeError
                    BufferError
                    EOFError
                    EnvironmentError
                        IOError
                        OSError
                    ImportError
                    LookupError
                        IndexError
                        KeyError
                    MemoryError
                    NameError
                        UnboundLocalError
                    ReferenceError
```

In-built Python exceptions II

```
          RuntimeError
              NotImplementedError
          SyntaxError
              IndentationError
                  TabError
          SystemError
          TypeError
          ValueError
              UnicodeError
                  UnicodeDecodeError
                  UnicodeEncodeError
                  UnicodeTranslateError
      StopIteration
      Warning
          BytesWarning
          DeprecationWarning
          FutureWarning
          ImportWarning
          PendingDeprecationWarning
          RuntimeWarning
          SyntaxWarning
          UnicodeWarning
          UserWarning
  GeneratorExit
  KeyboardInterrupt
  SystemExit
```

Catching exceptions (1)

- suppose we try to read data from a file:

```
f = open('myfilename.dat', 'r')
for line in f.readlines():
    print(line)
```

- If the file doesn't exist, then the `open()` function raises an Input-Output Error (`IOError`):

```
IOError: [Errno 2] No such file or directory: 'myfilename.dat'
```

- We can modify our code to catch this error:

```
try:
    f = open('myfilename.dat', 'r')
except IOError:
    print("The file couldn't be opened."),
    print("This program stops here.")
    import sys
    sys.exit(1)        #a way to exit the program

for line in f.readlines():
    print(line)
```

which produces this message:

```
The file couldn't be opened. This program stops here.
```

Catching exceptions (2)

- The `try` branch (line 2) will be executed.
- Should an `IOError` exception be raised the the except branch (starting line 4) will be executed.
- Should no exception be raised in the `try` branch, then the `except` branch is ignored, and the program carries on starting in line 9.

- Catching exceptions allows us to take action on errors that occur
  - For the file-reading example, we could ask the user to provide another file name if the file can't be opened.
- Catching an exception once an error has occurred may be easier than checking beforehand whether a problem will occur ("*It is easier to ask forgiveness than get permission*".)

Raising exceptions I

- Because exceptions are Python's way of dealing with runtime errors, we should use exceptions to report errors that occur in our own code.
- To raise a ValueError exception, we use

  ```
  raise ValueError("Message")
  ```

  and can attach a message "Message" (of type string) to that exception which can be seen when the exception is reported or caught.
  For example

  ```
  >>> raise ValueError("Some problem occured")
  Traceback (most recent call last):
    File "<stdin>", line 1, in <module>
  ValueError: Some problem occured
  ```

Raising exceptions II

- Often used is the `NotImplementedError` in incremental coding:

```
def my_complicated_function(x):
    message = "Function called with x={}".format(x))
    raise NotImplementedError(msg)
```

If we call the function:

```
>>> my_complicated_function(42)
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
  File "<stdin>", line 2, in my_complicated_function
NotImplementedError: Function called with x=42
```

Exercise

Extend `print_line_sum_of_file(filename)` so that if the data file contains non-numbers (i.e. strings), these evaluate to the value 0. For example

```
1 2 4         -> 7
1 cat 4       -> 5
coffee        -> 0
```

LAB5

Printing

Printing: print without parentheses I

- Option 1: list the variables to be printed, separated by comma, no parentheses. Convenient, but not flexible.
- This way of using `print` will not work with python 3.x

```
>>> a = 10
>>> print a
10
>>> print "The number is", a
The number is 10
>>> s = "hello"
>>> print "The number is", a, "and s is", s
The number is 10 and s is hello
>>> print a, s         # the comma adds a space
10 "hello"
```

Printing: print with parentheses I

- Option 2: construct some string s, then print this string using the print function
- Works with Python 2.7 and future python versions

```
>>> s = "I am the string to be printed"
>>> print(s)
I am the string to be printed
```

- The question is, how can we construct the string s? We talk about string formatting.

String formatting: the percentage (%) operator I

% operator syntax

Syntax: `A % B`

where `A` is a string, and `B` a Python object, or a tuple of Python objects.
The format string `A` needs to contain k format specifiers if the tuple has length k. The operation returns a string.

Example: basic formatting of one number

```
>>> import math
>>> p = math.pi
>>> "%f" % p          # format p as float (%f)
'3.141593'            # returns string
>>> "%d" % p          # format p as integer (%d)
'3'
>>> "%e" % p          # format p in exponential style
```

String formatting: the percentage (%) operator II

```
'3.141593e+00'
>>> "%g" % p        # format using fewer characters
'3.14159'
```

The format specifiers can be combined with arbitrary characters in string:

```
>>> 'the value of pi is approx %f' % p
'the value of pi is approx 3.141593'
>>> '%d is my preferred number' % 42
'42 is my preferred number'
```

Printing multiple objects

```
>>> "%d times %d is %d" % (10, 42, 10 * 42)
'10 times 42 is 420'
>>> "pi=%f and 3*pi=%f is approx 10" % (p, 3*p)
'pi=3.141593 and 3*pi=9.424778 is approx 10'
```

Fixing width and/or precision of resulting string I

```
>>> '%f' % 3.14        # default width and precision
'3.140000'

>>> '%10f' % 3.14      # 10 characters long
'  3.140000'

>>> '%10.2f' % 3.14 # 10 long, 2 post-dec digits
'      3.14'

>>> '%.2f' % 3.14      # 2 post-dec digits
'3.14'

>>> '%.14f' % 3.14    # 14 post-decimal digits
'3.14000000000000'
```

Can also use format specifier %s to format strings (typically used to align columns in tables, or such).

Common formatting specifiers

A list of common formatting specifiers, with example output for the astronomical unit (AU) which is the distance from Earth to Sun [in metres]:

```
>>> AU = 149597870700   # astronomical unit [m]
>>> "%f" % AU           # line 1 in table
'149597870700.000000'
```

specifier	style	Example output for AU
`%f`	floating point	149597870700.000000
`%e`	exponential notation	1.495979e+11
`%g`	shorter of %e or %f	1.49598e+11
`%d`	integer	149597870700
`%s`	`str()`	149597870700
`%r`	`repr()`	149597870700L

Formatted printing (% operator) I

The key idea is to create the string using the % operator, and then to pass this string to the print command. Very similar syntax exists in C and Matlab, amongst others for formatted data output to screen and files.
Example (valid in Python 2.7 and Python 3.x) using the print *function*:

```
>>> import math
>>> print("My pi = %.2f." % math.pi)
My pi = 3.14.
```

Print multiple values:

```
>>> print("a=%d b=%d" % (10, 20))
a=10 b=20
```

New style string formatting (format method) I

A new system of built-in formatting has been proposed and is meant to replace the old-style percentage operator formatting (%) in the long term.
Basic ideas in examples:

- Pairs of curly braces are the placeholders.

```
>>> "{} needs {} pints".format('Peter', 4)
'Peter needs 4 pints'
```

- Can *index* into the list of objects:

```
>>> "{0} needs {1} pints".format('Peter',4)
'Peter needs 4 pints'
>>> "{1} needs {0} pints".format('Peter',4)
'4 needs Peter pints'
```

- We can refer to objects through a name:

New style string formatting (format method) II

```
>>> "{name} needs {number} pints".format(\
...                     name='Peter',number=4)
'Peter needs 4 pints'
```

- Formatting behaviour of %f can be achieved through {:f}, (same for %d, %e, etc)

```
>>> "Pi is approx {:f}.".format(math.pi)
'Pi is approx 3.141593.'
```

- Width and post decimal digits can be specified as before:

```
>>> "Pi is approx {:6.2f}.".format(math.pi)
'Pi is approx   3.14.'
>>> "Pi is approx {:.2f}.".format(math.pi)
'Pi is approx 3.14.'
```

New style string formatting (`format` method) III

This is a powerful and elegant way of string formatting.

Further Reading

- Examples http://docs.python.org/library/string.html#format-examples
- Python Enhancement Proposal 3101

What formatting should I use? I

- The `.format` method most elegant and versatile
- `%` operator style okay, links to Matlab, C, ...
- Choice partly a matter of taste
- Should be aware (in a passive sense) of different possible styles (so we can read code from others)
- try to use print with parenthesis (i.e. compatible with Python 3.x) for code you write

Changes from Python 2 to Python 3: print I

One (maybe the most obvious) change going from Python 2 to Python 3 is that the `print` command loses its special status. In Python 2, we could print "Hello World" using

```
print "Hello World"          #valid in Python 2.x
```

Effectively, we call the function `print` with the argument `"Hello World"`. All other functions in Python are called such that the argument is enclosed in parentheses, i.e.

```
print("Hello World")         #valid in Python 3.x
```

This is the new convention *required* in Python 3 (and *allowed* for recent version of Python 2.x.)

Advanced: “str“ and “repr“: “str“ I

All objects in Python should provide a method `__str__` which returns a nice string representation of the object. This method `a.__str__()` is called when we apply the `str` function to object `a`:

```
>>> a = 3.14
>>> a.__str__()
'3.14'
>>> str(a)
'3.14'
```

The `str` function is extremely convenient as it allows us to print more complicated objects, such as

```
>>> b = [3, 4.2, ['apple', 'banana'], (0, 1)]
>>> str(b)
"[3, 4.2, ['apple', 'banana'], (0, 1)]"
```

Advanced: “str“ and “repr“: “str“ II

The string method `x.__str__` of object `x` is called implicitly, when we

- use the "%s" format specifier in %-operator formatting to print `x`
- use the "{}" format specifier in `.format` to print `x`
- pass the object `x` directly to the print command

```
>>> print(b)
[3, 4.2, ['apple', 'banana'], (0, 1)]
>>> "%s" % b
[3, 4.2, ['apple', 'banana'], (0, 1)]
>>> "{}".format(b)
[3, 4.2, ['apple', 'banana'], (0, 1)]
```

Advanced: “str“ and “repr“: “repr“ I

- The `repr` function, should convert a given object into an *as accurate as possible* string representation
- so that (ideally) this string can be used to re-create the object using the `eval` function.
- The `repr` function will generally provide a more detailed string than `str`.
- Applying `repr` to the object `x` will attempt to call `x.__repr__()`.

Advanced: “str“ and “repr“: “repr“ II

Example:

```
>>> import math
>>> p = math.pi
>>> s = str(p)            # str representation of pi
>>> p2 = eval(s)          # convert string to float
>>> p2
3.14159265359
>>> p2 - p                # p2 the same as p?
2.0694557179012918e-13       # -> No
>>> p3 = eval(repr(p))
>>> p3 - p                   # -> Yes
0.0
```

Advanced: “str“ and “repr“: “repr“ III

We can convert an object to its `str()` or `repr()` presentation using the format specifiers `%s` and `%r`, respectively.

```
>>> import math
>>> "%s" % math.pi
'3.14159265359'
>>> "%r" % math.pi
'3.141592653589793'
```

Higher Order Functions

Motivational exercise: function tables

- Write a function `print_x2_table()` that prints a table of values of $f(x) = x^2$ for $x = 0, 0.5, 1.0, ..2.5$, i.e.

```
0.0 0.0
0.5 0.25
1.0 1.0
1.5 2.25
2.0 4.0
2.5 6.25
```

- Then do the same for $f(x) = x^3$
- Then do the same for $f(x) = \sin(x)$

Can we avoid code duplication?

- Idea: Pass function $f(x)$ to tabulate to tabulating function

Example: (`print_f_table.py`)

```
def print_f_table(f):
    for i in range(6):
        x = i * 0.5
        print("{} {}".format(x, f(x)))

def square(x):
    return x ** 2

print_f_table(square)
```

produces

```
    0.0 0.0
    0.5 0.25
    1.0 1.0
    1.5 2.25
    2.0 4.0
```

Can we avoid code duplication (2)?

```
def print_f_table(f):
    for i in range(6):
        x = i * 0.5
        print("{} {}".format(x, f(x)))

def square(x): return x ** 2
def cubic(x): return x ** 3

print("Square"); print_f_table(square)
print("Cubic");  print_f_table(cubic)
```

produces:

```
Square
0.0 0.0
0.5 0.25
1.0 1.0
1.5 2.25
2.0 4.0
2.5 6.25
```

```
Cubic
0.0 0.0
0.5 0.125
1.0 1.0
1.5 3.375
2.0 8.0
2.5 15.625
```

Functions are first class objects

- Functions are *first class objects* $\leftrightarrow$ functions can be given to other functions as arguments
- Example (trigtable.py):

```
import math
funcs = (math.sin, math.cos)
for f in funcs:
    for x in [0, math.pi / 2]:
        print("{}({:.3f}) = {:.3f}".format(
            f.__name__, x, f(x)))
```

```
sin(0.000) = 0.000
sin(1.571) = 1.000
cos(0.000) = 1.000
cos(1.571) = 0.000
```

Module files

Writing module files

- Motivation: it is useful to bundle functions that are used repeatedly and belong to the same subject area into one module file (also called "library")
- Every Python file can be imported as a module.
- If this module file has a main program, then this is executed when the file is imported. This can be desired but sometimes it is not.
- We describe how a main program can be written which is only executed if the file is run on its own but not if is imported as a library.

The internal __name__ variable (1)

- Here is an example of a module file saved as `module1.py`:

```
def someusefulfunction():
    pass

print("My name is {}".format(__name__))
```

We can execute this module file, and the output is

```
My name is __main__
```

- The internal variable `__name__` takes the (string) value `"__main__"` if the program file `module1.py` is executed.
- On the other hand, we can *import* `module1.py` in another file, for example like this:

```
import module1
```

The output is now:

```
My name is module1
```

The internal `__name__` variable (2)

- In summary
  - `__name__` is `"__main__"` if the module file is run on its own
  - `__name__` is the name (type string) of the module if the module file is imported.
- We can therefore use the following `if` statement in `module1.py` to write code that is *only run* when the module is executed on its own:

```
def someusefulfunction():
    pass

if __name__ == "__main__":
    print("I am running on my own.")
```

- This is useful to keep test programs or demonstrations of the abilities of a library module in this “conditional” main program.

Default and Keyword function arguments

Default argument values (1)

- Motivation:
  - suppose we need to compute the area of rectangles and
  - we know the side lengths `a` and `b`.
  - Most of the time, `b=1` but sometimes `b` can take other values.
- Solution 1:

```python
def area(a, b):
    return a * b

print("the area is {}".format(area(3, 1)))
print("the area is {}".format(area(2.5, 1)))
print("the area is {}".format(area(2.5, 2)))
```

Working perfectly.

Default argument values (2)

- We can reduce our efforts by providing a *default* value for b. We then only have to specify b if it is different from this default value:
- Solution 2:

```
def area(a, b=1):
    return a * b

print("the area is {}".format(area(3)))
print("the area is {}".format(area(2.5)))
print("the area is {}".format(area(2.5, 2)))
```

- If a default value is defined, then this parameter (here b) is optional when the function is called.
- Warning: default parameters have to be at the end of the argument list in the function definition.

Keyword argument values (1)

- We can call functions with a "keyword" and a value. (The keyword is the name of the variable in the function.)
- Here is an example

```
def f(a, b, c):
    print("a = {}, b = {}, c = {}"
          .format(a, b, c))

f(1, 2, 3)
f(c=3, a=1, b=2)
f(1, c=3, b=2)
```

which produces this output:

```
a = 1, b = 2, c = 3
a = 1, b = 2, c = 3
a = 1, b = 2, c = 3
```

- If we use *only* keyword arguments in the function call, then we don't need to know the *order* of the arguments. (This is good.)

Keyword argument values (2)

- Can combine default value arguments and keyword arguments
- Example: we use 100 subdivisions unless the user provides a number

```
def trapez(function, a, b, subdivisions=100):
    #code missing here

import math
int1 = trapez(a=0, b=10, function=math.sin)
int2 = trapez(b=0, function=math.exp, \
              subdivisions=1000, a=-0.5)
```

- Note that choosing meaningful variable names in the function definition makes the function more user friendly.

Keyword argument values (3)

You may have met default arguments and keyword arguments before, for example

- the string method `split` uses white space as the default value for splitting
- the `open` function uses `r` (for Reading) as a default value

LAB6

Global and local variables, Name spaces

Name spaces — what can be seen where? (1)

- We distinguish between
  - global variables (defined in main program) and
  - local variables (defined for example in functions), could be several nested layers
  - built-in functions
- The same variable *name* can be used in a function and in the main program but they can refer to different objects and do not interfere:

```
def f():
    x = 'I am local'
    print(x)

x = 'I am global'
f()
print(x)
```

  which produces this output

```
I am local
I am global
```

Name spaces (2)

...so global and local variables can't see each other?

- not quite. Let's read the small print:
  - If — within a function – we try to access a variable, then Python will look for this variable
    - first in the local name space (*i.e.* within that function)
    - then in the global name space (!)

  If the variable can't be found, a `NameError` is raised.
- This means, we can *read* global variables from functions. Example:

```
def f():
    print(x)

x = 'I am global'
f()
```

Output:

```
I am global
```

Name spaces (3)

- but local variables “shadow” global variables:

```
def f():
    y = 'I am local y'
    print(x)
    print(y)

x = 'I am global x'
y = 'I am global y'
f()
print("back in main:")
print(y)
```

Output:

```
I am global x
I am local y
back in main:
I am global y
```

- To *modify* global variables within a local namespace, we need to use the `global` keyword.

Why should I care about global variables?

- Generally, the use of global variables is not recommended:
  - functions should take all necessary input as arguments and
  - return all relevant output.
  - This makes the functions work as independent modules which is good engineering practice.
- However, sometimes the same constant or variable (such as the mass of an object) is required throughout a program:
  - it is not good practice to define this variable more than once (it is likely that we assign different values and get inconsistent results)
  - in this case — in small programs — the use of (read-only) global variables may be acceptable.
  - Object Oriented Programming provides a somewhat neater solution to this.

Python's look up rule

- When coming across an identifier, Python looks for this in the following order in
  - the local name space (L)
  - (if appropriate in the next higher level local name space), (L^2, L^3, ...)
  - the global name space (G)
  - the set of built-in commands (B)
- This is summarised as "LGB" or "L^nGB".
- If the identifier cannot be found, a `NameError` is raised.

Python shells and IDE

Integrated Development Environment: combine editor and prompt: IDLE

- IDLE http://en.wikipedia.org/wiki/IDLE_(Python)__ (comes with Python)
- two windows: program and python prompt
- F5 to execute Python program
- Simple, (written in Python $\rightarrow$ portable)

IPython (interactive python)

- Interactive Python (`ipython` from DOS/Unix-shell)
- command history (across sessions), auto completion,
- special commands:
  - `%run test` will execute file `test.py` in current name space (in contrast to IDLE this does not remove all existing objects from global name space)
  - `%reset` can delete all objects if required
  - `%edit` will open an editor
  - use `range?` instead of `help(range)`
  - `%logstart` will log your session
  - `%prun` will profile code
  - `%timeit` can measure execution time
  - `%load` loads file for editing
- Much (!) more (read at http://ipython.scipy.org)

IPython's QT console

- Prompt as IPython (with all it's features): running in a *graphics console* rather than in *text console*
- but allows multi-line editing of command history
- provides on-the-fly syntax highlighting
- can inline matplotlib figures
- Read more at http://ipython.org/ipython-doc/dev/interactive/qtconsole.html

... and many others

Including

- IPython notebook (http://ipython.org/ipython-doc/dev/interactive/htmlnotebook.html). See video demo at http://youtu.be/HaS4NXxL5Qc
- Eclipse
- vi, vim
- Kate
- Sublime Text
- Spyder

List comprehension

List comprehension I

- List comprehension follows the mathematical "set builder notation"
- Convenient way to process a list into another list (without for-loop).

Examples

```
>>> [2 ** i for i in range(10)]
[1, 2, 4, 8, 16, 32, 64, 128, 256, 512, 1024]

>>> [x ** 2 for x in range(10)]
[0, 1, 4, 9, 16, 25, 36, 49, 64, 81]

>>> [x for x in range(10) if x > 5]
[6, 7, 8, 9]
```

Can be useful to populate lists with numbers quickly

List comprehension II

- Example 1:

```
>>> xs = [i for i in range(10)]
>>> xs
[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
>>> ys = [x ** 2 for x in xs]
>>> ys
[0, 1, 4, 9, 16, 25, 36, 49, 64, 81]
```

- Example 2:

```
>>> import math
>>> xs = [0.1 * i for i in range(5)]
>>> ys = [math.exp(x) for x in xs]
>>> xs
[0.0, 0.1, 0.2, 0.3, 0.4]
>>> ys
[1.0, 1.1051709180756477, 1.2214027581601699,
 1.3498588075760032, 1.4918246976412703]
```

List comprehension III

- Example 3

```
>>> words = 'The quick brown fox jumps \
... over the lazy dog'.split()
>>> print words
['The', 'quick', 'brown', 'fox', 'jumps',
 'over', 'the', 'lazy', 'dog']

>>> stuff = [[w.upper(), w.lower(), len(w)]
             for w in words]
>>> for i in stuff:
...     print(i)
...
['THE', 'the', 3]
['QUICK', 'quick', 5]
['BROWN', 'brown', 5]
['FOX', 'fox', 3]
['JUMPS', 'jumps', 5
['OVER', 'over', 4]
```

List comprehension IV

```
['THE', 'the', 3]
['LAZY', 'lazy', 4]
['DOG', 'dog', 3]
```

List comprehension with conditional

- Can extend list comprehension syntax with `if CONDITION` to include only elements for which `CONDITION` is true.
- Example:

```
>>> [i for i in range(10)]
[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]

>>> [i for i in range(10) if i > 5]
[6, 7, 8, 9]

>>> [i for i in range(10) if i ** 2 > 5]
[3, 4, 5, 6, 7, 8, 9]
```

Dictionaries

Dictionaries I

- Python provides another data type: the dictionary.

  Dictionaries are also called "associative arrays" and "hash tables".

- Dictionaries are *unordered* sets of *key-value pairs*.
- An empty dictionary can be created using curly braces:

```
>>> d = {}
```

- Keyword-value pairs can be added like this:

```
>>> d['today'] = '22 deg C' #'today' is key
                            #'22 deg C' is value
>>> d['yesterday'] = '19 deg C'
```

- `d.keys()` returns a list of all keys:

```
>>> d.keys()
['yesterday', 'today']
```

Dictionaries II

- We can retrieve values by using the keyword as the index:

```
>>> print d['today']
22 deg C
```

Dictionaries III

Here is a more complex example:

```
order = {}          # create empty dictionary

#add orders as they come in
order['Peter'] = 'Pint of bitter'
order['Paul'] = 'Half pint of Hoegarden'
order['Mary'] = 'Gin Tonic'

#deliver order at bar
for person in order.keys():
    print("{} requests {}".format(person, order[perso
```

which produces this output:

```
Paul requests Half pint of Hoegarden
Peter requests Pint of bitter
Mary requests Gin Tonic
```

Dictionaries IV

Some more technicalities:

- The keyword can be any (immutable) Python object. This includes:
  - numbers
  - strings
  - tuples.
- dictionaries are very fast in retrieving values (when given the key)

Dictionaries V

- What are dictionnaries good for? Consider this example:

```python
dic = {}
dic["Hans"]    = "room 1033"
dic["Andy C"] = "room 1031"
dic["Ken"]     = "room 1027"

for key in dic.keys():
    print("{} works in {}"
          .format(key, dic[key]))
```

Output:

```
Hans works in room 1033
Andy C works in room 1031
Ken works in room 1027
```

- Without dictionary:

Dictionaries VI

```
people = ["Hans", "Andy C", "Ken"]
rooms  = ["room 1033", "room 1031", \
     "room 1027"]

# possible inconsistency here since we have
# two lists
if not len(people) == len(rooms):
    raise ValueError("people and rooms " +
                     "differ in length")

for i in range(len(rooms)):
    print ("{} works in {}".format(people[i],
                                  rooms[i]))
```

Iterating over dictionaries

Iterate over the dictionary itself is equivalent to iterating over the keys. Example:

```
order = {}           # create empty dictionary

order['Peter'] = 'Pint of bitter'
order['Paul'] = 'Half pint of Hoegarden'
order['Mary'] = 'Gin Tonic'

#iterating over keys:
for person in order.keys():
    print person, "requests", order[person]

#is equivalent to iterating over the dictionary:
for person in order:
    print person, "requests", order[person]
```

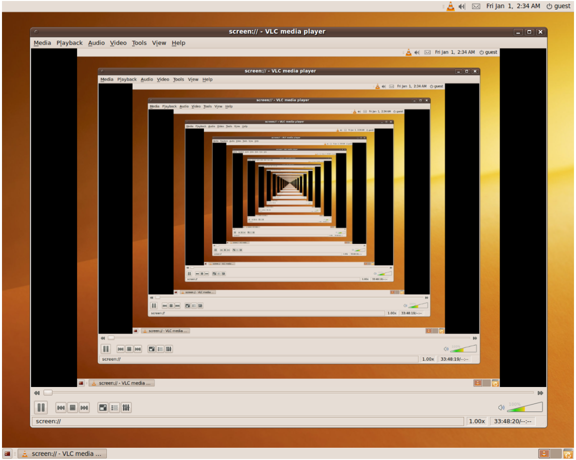
Summary dictionaries

What to remember:

- Python provides dictionaries
- very powerful construct
- a bit like a data base (and values can be dictionary objects)
- fast to retrieve value
- likely to be useful if you are dealing with two lists at the same time (possibly one of them contains the keyword and the other the value)
- useful if you have a data set that needs to be indexed by strings or tuples (or other immutable objects)

Recursion

Recursion



Recursion in a screen recording program, where the smaller window contains a snapshot of the entire screen. Source: http://en.wikipedia.org/wiki/Recursion

Recursion example: factorial

- Computing the factorial (i.e. $n!$) can be done by computing $(n-1)!n$“, i.e. we reduce the problem of size n to a problem of size $n-1$.
- For recursive problems, we always need a base case. For the factorial we know that “0! $=$ 1“
- For n=4:

$$\begin{aligned}
4! &= 3! \cdot 4 && (1)\\
&= 2! \cdot 3 \cdot 4 && (2)\\
&= 1! \cdot 2 \cdot 3 \cdot 4 && (3)\\
&= 0! \cdot 1 \cdot 2 \cdot 3 \cdot 4 && (4)\\
&= 1 \cdot 1 \cdot 2 \cdot 3 \cdot 4 && (5)\\
&= 24. && (6)
\end{aligned}$$

Recursion example

Python code to compute the factorial recursively::

```
def factorial(n):
    if n == 0:
        return 1
    else:
        return n * factorial(n-1)
```

Usage output:

```
>>> factorial(0)
factorial(0)
1
>>> factorial(2)
2
>>> factorial(4)
24
```

Recursion example Fibonacci numbers

Defined (recursively) as: $f(n) = f(n-1) + f(n-2)$ for integers n, and $n > 0$, and $f(1) = 0$ and $f(2) = 1$
Python implementation (fibonacci.py):

```
def f(n):
    if n == 1:
        return 0
    elif n == 2:
        return 1
    else:
        return f(n - 2) + f(n - 1)
```

Recursion exercises

- Write a function `recsum(n)` that sums the numbers from 1 to n *recursively*
- Study the recursive Fibonacci function:
  - what is the largest number n for which we can reasonable compute $f(n)$ within a minutes?
  - Can you write faster versions of Fibonacci? (There are faster versions with and without recursion.)

Common Computational Tasks

Common Computational Tasks

- Data file processing, python & numpy (array processing)
- Random number generation and fourier transforms (numpy)
- Linear algebra (numpy)
- Interpolation of data (`scipy.interpolation.interp`)
- Fitting a curve to data (`scipy.optimize.curve_fit`)
- Integrating a function numerically (`scipy.integrate.quad`)
- Integrating a ordinary differential equation numerically (`scipy.integrate.odeint`)
- Finding the root of a function (`scipy.optimize.fsolve,scipy.optimize.brentq`)
- Minimising a function (`scipy.optimize.fmin`)
- Symbolic manipulation of terms, including integration and differentiation (`sympy`)

Root finding

Rootfinding

Root finding

Given a function $f(x)$, we are searching an x_0 so $f(x_0) = 0$. We call x_0 a root of $f(x)$.

Why?

- Often need to know when a particular function reaches a value, for example the water temperature $T(t)$ reaching 373 K. In that case, we define

$$f(t) = T(t) - 373$$

  and search the root t_0 for $f(t)$

Two methods:

- Bisection method
- Newton method

The bisection algorithm

- Function: `bisect(f, a, b)`
- Assumptions:
  - Given: a (float)
  - Given: b (float)
  - Given: $f(x)$, continuous with single root in $[a, b]$, i.e. $f(a)f(b) < 0$
  - Given: ftol (float), for example ftol=1e-6

The bisection method returns x so that $|f(x)| <$ftol

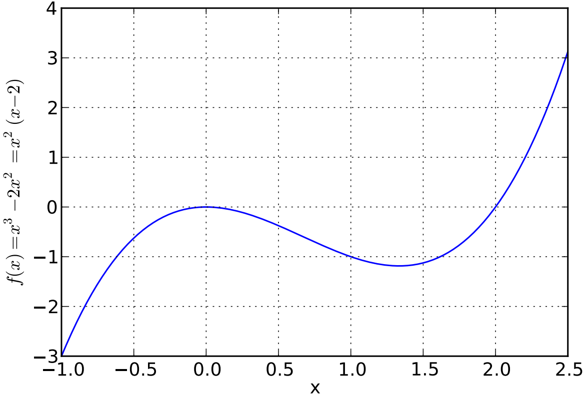
1. $x = (a + b)/2$
2. while $|f(x)| >$ ftol do
   - if $f(x)f(a) > 0$
     then $a \leftarrow x$ #throw away left half
     else $b \leftarrow x$ #throw away right half
   - $x = (a + b)/2$
3. return x

The bisection function from scipy

- Scientific Python provides an interface to the "Minpack" library. One of the functions is
- `scipy.optimize.bisect(f, a, b[, xtol])`
  - `f` is the function for which we search x such that $f(x) = 0$
  - `a` is the lower limit of the bracket [a,b] around the root
  - `b` is the upper limit of the bracket [a,b] around the root
  - `xtol` is an *optional* parameter that can be used to modify the default accuracy of `xtol`$= 10^{-12}$
- the `bisect` function stops 'bisecting' the interval around the root when $|b - a| <$`xtol`.

Example

- Find root of function $f(x) = x^2(x-2)$
- f has a double root at $x = 0$, and a single root at $x = 2$.
- Ask algorithm to find single root at $x = 2$.



Using bisection algorithm from scipy

```
from scipy.optimize import bisect

def f(x):
    """returns f(x)=x^3-2x^2. Has roots at
    x=0 (double root) and x=2"""
    return x ** 3 - 2 * x ** 2

#main program starts here
x = bisect(f, a=1.5, b=3, xtol=1e-6)

print("Root x is approx. x={:14.12g}.".format(x))
print("The error is less than 1e-6.")
print("The exact error is {}.".format(2 - x))
```

generates this:

```
Root x is approx. x= 2.00000023842.
The error is less than 1e-6.
The exact error is -2.38418579102e-07.
```

The Newton method

- Newton method for root finding: look for x_0 so that $f(x_0) = 0$.
- Idea: close to the root, the tangent of $f(x)$ is likely to point to the root. Make use of this information.
- Algorithm:
  while $|f(x)| >$ftol, do

$$x = x - \frac{f(x)}{f'(x)}$$

  where $f'(x) = \frac{\mathrm{d}f}{\mathrm{d}x}(x)$.
- Much better convergence than bisection method
- but not guaranteed to converge.
- Need a good initial guess x for the root.

Using Newton algorithm from scipy

```
from scipy.optimize import newton

def f(x):
    """returns f(x)=x^3-2x^2. Has roots at
    x=0 (double root) and x=2"""
    return x ** 3 - 2 * x ** 2

#main program starts here
x = newton(f, x0=1.6)

print("Root x is approx. x={:14.12g}.".format(x))
print("The error is less than 1e-6.")
print("The exact error is {}.".format(2 - x))
```

generates this:

```
Root x is approx. x=             2.
The error is less than 1e-6.
The exact error is 9.7699626167e-15.
```

Comparison Bisection & Newton method

Bisection method

- Requires root in bracket $[a, b]$
- guaranteed to converge (for single roots)
- Library function: `scipy.optimize.bisect`

Newton method

- Requires good initial guess x for root x_0
- may never converge
- but if it does, it is quicker than the bisection method
- Library function: `scipy.optimize.Newton`

Root finding summary

- Given the function f(x), applications for root finding include:
  - to find x_1 so that $f(x_1) = y$ for a given y (this is equivalent to computing the inverse of the function f).
  - to find crossing point x_c of two functions $f_1(x)$ and $f_2(x)$ (by finding root of difference function $g(x) = f_1(x) - f_2(x)$)
- Recommended method: `scipy.optimize.brentq` which combines the safe feature of the bisect method with the speed of the Newton method.
- For multi-dimensional functions $f(\mathbf{x})$, use `scipy.optimize.fsolve`.

Using BrentQ algorithm from scipy

```
from scipy.optimize import brentq

def f(x):
    """returns f(x)=x^3-2x^2. Has roots at
    x=0 (double root) and x=2"""
    return x ** 3 - 2 * x ** 2

#main program starts here
x = brentq(f, a=1.5, b=3, xtol=1e-6)

print("Root x is approx. x={:14.12g}.".format(x))
print("The error is less than 1e-6.")
print("The exact error is {}.".format(2 - x))
```

generates this:

```
Root x is approx. x= 2.00000001896.
The error is less than 1e-6.
The exact error is -1.89582864962e-08.
```

Using fsolve algorithm from scipy

```
from scipy.optimize import fsolve
        # multidimensional solver

def f(x):
    """returns f(x)=x^2-2x^2. Has roots at
    x=0 (double root) and x=2"""
    return x ** 3 - 2* x ** 2

#main program starts here
x = fsolve(f, x0=1.6)

print("Root x is approx. x={}.".format(x))
print("The error is less than 1e-6.")
print("The exact error is {}.".format(2 - x[0]))
```

generates this:

```
Root x is approx. x=[ 2.].
The error is less than 1e-6.
The exact error is 0.0.
```

Computing derivatives numerically

Overview

- Motivation:
  - We need derivatives of functions for some optimisation and root finding algorithms
  - Not always is the function analytically known (but we are usually able to compute the function numerically)
  - The material presented here forms the basis of the finite-difference technique that is commonly used to solve ordinary and partial differential equations.
- The following slides show
  - the forward difference technique
  - the backward difference technique and the
  - central difference technique to approximate the derivative of a function.
  - We also derive the accuracy of each of these methods.

The 1st derivative

- (Possible) Definition of the derivative (or "*differential* operator" $\frac{\mathrm{d}}{\mathrm{d}x}$)

$$\frac{\mathrm{d}f}{\mathrm{d}x}(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

- Use *difference* operator to approximate differential operator

$$f'(x) = \frac{\mathrm{d}f}{\mathrm{d}x}(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \approx \frac{f(x+h) - f(x)}{h}$$

- $\Rightarrow$ can now compute *an approximation* of f' simply by evaluating f.
- This is called the *forward difference* because we use $f(x)$ and $f(x+h)$.
- Important question: How accurate is this approximation?

Accuracy of the forward difference

- Formal derivation using the Taylor series of f around x

$$
\begin{aligned}
f(x+h) &= \sum_{n=0}^{\infty} h^n \frac{f^{(n)}(x)}{n!} \\
&= f(x) + hf'(x) + h^2 \frac{f''(x)}{2!} + h^3 \frac{f'''(x)}{3!} + \dots
\end{aligned}
$$

- Rearranging for $f'(x)$

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

$$
\begin{aligned}
f'(x) &= \frac{1}{h}\left(f(x+h) - f(x) - h^2 \frac{f''(x)}{2!} - h^3 \frac{f'''(x)}{3!} - \dots \right) \\
&= \frac{f(x+h) - f(x)}{h} - \frac{h^2 \frac{f''(x)}{2!} - h^3 \frac{f'''(x)}{3!}}{h} - \dots \\
&= \frac{f(x+h) - f(x)}{h} - h \frac{f''(x)}{2!} - h^2 \frac{f'''(x)}{3!} - \dots
\end{aligned}
$$

Accuracy of the forward difference (2)

$$f'(x) = \frac{f(x+h) - f(x)}{h} \underbrace{- h\frac{f''(x)}{2!} - h^2\frac{f'''(x)}{3!} - \ldots}_{E_{\text{forw}}(h)}$$

$$f'(x) = \frac{f(x+h) - f(x)}{h} + E_{\text{forw}}(h)$$

- Therefore, the error term $E_{\text{forw}}(h)$ is

$$E_{\text{forw}}(h) = -h\frac{f''(x)}{2!} - h^2\frac{f'''(x)}{3!} - \ldots$$

- Can also be expressed as

$$f'(x) = \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h)$$

The 1st derivative using the backward difference

- Another definition of the derivative (or "differential operator" $\frac{\mathrm{d}}{\mathrm{d}x}$)

$$\frac{\mathrm{d}f}{\mathrm{d}x}(x) = \lim_{h \to 0} \frac{f(x) - f(x-h)}{h}$$

- Use difference operator to approximate differential operator

$$\frac{\mathrm{d}f}{\mathrm{d}x}(x) = \lim_{h \to 0} \frac{f(x) - f(x-h)}{h} \approx \frac{f(x) - f(x-h)}{h}$$

- This is called the *backward difference* because we use $f(x)$ and $f(x-h)$.
- How accurate is the backward difference?

Accuracy of the backward difference

- Formal derivation using the Taylor Series of f around x

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

- Rearranging for $f'(x)$

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

$$\begin{aligned}
f'(x) &= \frac{1}{h}\left(f(x) - f(x-h) + h^2\frac{f''(x)}{2!} - h^3\frac{f'''(x)}{3!} - \dots\right) \\
&= \frac{f(x) - f(x-h)}{h} + \frac{h^2\frac{f''(x)}{2!} - h^3\frac{f'''(x)}{3!}}{h} - \dots \\
&= \frac{f(x) - f(x-h)}{h} + h\frac{f''(x)}{2!} - h^2\frac{f'''(x)}{3!} - \dots
\end{aligned}$$

Accuracy of the backward difference (2)

$$
\begin{aligned}
f'(x) &= \frac{f(x) - f(x-h)}{h} + \underbrace{h\frac{f''(x)}{2!} - h^2\frac{f'''(x)}{3!} - \dots}_{E_{\text{back}}(h)} \\
f'(x) &= \frac{f(x) - f(x-h)}{h} + E_{\text{back}}(h) \qquad (7)
\end{aligned}
$$

- Therefore, the error term $E_{\text{back}}(h)$ is

$$E_{\text{back}}(h) = h\frac{f''(x)}{2!} - h^2\frac{f'''(x)}{3!} - \dots$$

- Can also be expressed as

$$f'(x) = \frac{f(x) - f(x-h)}{h} + \mathcal{O}(h)$$

Combining backward and forward differences (1)

The approximations are

- forward:

$$f'(x) = \frac{f(x+h) - f(x)}{h} + E_{\text{forw}}(h) \tag{8}$$

- backward

$$f'(x) = \frac{f(x) - f(x-h)}{h} + E_{\text{back}}(h) \tag{9}$$

$$\begin{aligned}
E_{\text{forw}}(h) &= -h\frac{f''(x)}{2!} - h^2\frac{f'''(x)}{3!} - h^3\frac{f''''(x)}{4!} - h^4\frac{f'''''(x)}{5!} - \dots \\
E_{\text{back}}(h) &= h\frac{f''(x)}{2!} - h^2\frac{f'''(x)}{3!} + h^3\frac{f''''(x)}{4!} - h^4\frac{f'''''(x)}{5!} + \dots
\end{aligned}$$

$\Rightarrow$ Add equations (8) and (9) together, then the error cancels partly.

Combining backward and forward differences (2)

Add these lines together

$$
\begin{aligned}
f'(x) &= \frac{f(x+h) - f(x)}{h} + E_{\text{forw}}(h) \\
f'(x) &= \frac{f(x) - f(x-h)}{h} + E_{\text{back}}(h)
\end{aligned}
$$

$$
2f'(x) = \frac{f(x+h) - f(x-h)}{h} + E_{\text{forw}}(h) + E_{\text{back}}(h)
$$

Adding the error terms:

$$
E_{\text{forw}}(h) + E_{\text{back}}(h) = -2h^2 \frac{f'''(x)}{3!} - 2h^4 \frac{f'''''(x)}{5!} - \dots
$$

The combined (central) difference operator is

$$
f'(x) = \frac{f(x+h) - f(x-h)}{2h} + E_{\text{cent}}(h)
$$

with

$$
E_{\text{cent}}(h) = -h^2 \frac{f'''(x)}{3!} - h^4 \frac{f'''''(x)}{5!} - \dots
$$

Central difference

- Can be derived (as on previous slides) by adding forward and backward difference
- Can also be interpreted geometrically by defining the differential operator as

$$\frac{\mathrm{d}f}{\mathrm{d}x}(x) = \lim_{h\to 0} \frac{f(x+h) - f(x-h)}{2h}$$

  and taking the finite difference form

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

- Error of the central difference is only $\mathcal{O}(h^2)$, *i.e.* better than forward or backward difference

> It is generally the case that symmetric differences are more accurate than asymmetric expressions.

Example (1)

Using forward difference to estimate the derivative of $f(x) = \exp(x)$

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

Since we compute the difference using values of f at x and $x + h$, it is natural to interpret the numerical derivative to be taken at $x + \frac{h}{2}$:

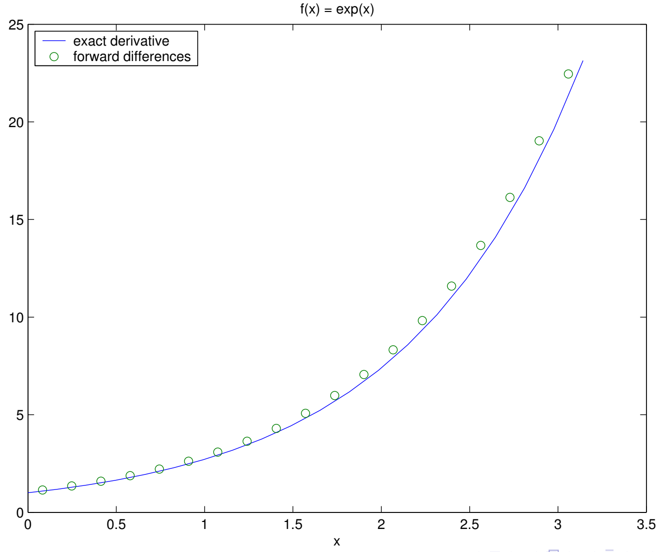
$$f'\left(x + \frac{h}{2}\right) \approx \frac{f(x+h) - f(x)}{h} = \frac{\exp(x+h) - \exp(x)}{h}$$

Numerical example:

- $h = 0.1$, $x = 1$
- $f'(1.05) \approx \frac{\exp(1.1) - \exp(1)}{0.1} = 2.8588$
- Exact answers is $f'(1.05) = \exp(1.05) = 2.8577$

Example (2)

Comparison: forward difference and exact derivative of $\exp(x)$



Summary

- Can approximate derivatives of f numerically
- need only function evaluations of f
- three different difference methods

name	formula	error
forward	$f'(x) = \frac{f(x+h)-f(x)}{h}$	$\mathcal{O}(h)$
backward	$f'(x) = \frac{f(x)-f(x-h)}{h}$	$\mathcal{O}(h)$
central	$f'(x) = \frac{f(x+h)-f(x-h)}{2h}$	$\mathcal{O}(h^2)$

- central difference is most accurate
- Euler's method (ODE) can be derived from forward difference
- Newton's root finding method can be derived from forward difference

LAB7

Note: Euler's (integration) method — derivation using finite difference operator

- Use forward difference operator to approximate differential operator

$$\frac{\mathrm{d}y}{\mathrm{d}x}(x) = \lim_{h\to 0} \frac{y(x+h)-y(x)}{h} \approx \frac{y(x+h)-y(x)}{h}$$

- Change differential to difference operator in $\frac{\mathrm{d}y}{\mathrm{d}x} = f(x,y)$

$$\begin{aligned} f(x,y) = \frac{\mathrm{d}y}{\mathrm{d}x} &\approx \frac{y(x+h)-y(x)}{h} \\ hf(x,y) &\approx y(x+h)-y(x) \\ \Longrightarrow y_{i+1} &= y_i + hf(x_i, y_i) \end{aligned}$$

- $\Rightarrow$ Euler's method (for ODEs) can be derived from the forward difference operator.

Note: Newton's (root finding) method — derivation from Taylor series

- We are looking for a root, *i.e.* we are looking for a x so that $f(x) = 0$.
- We have an initial guess x_0 which we refine in subsequent iterations:

$$x_{i+1} = x_i - h_i \quad \text{where} \quad h_i = \frac{f(x_i)}{f'(x_i)}. \tag{10}$$

.

- This equation can be derived from the Taylor series of f around x. Suppose we guess the root to be at x and $x + h$ is the actual location of the root (so h is unknown and $f(x + h) = 0$):

$$\begin{aligned} f(x+h) &= f(x) + hf'(x) + \dots \\ 0 &= f(x) + hf'(x) + \dots \\ \implies 0 &\approx f(x) + hf'(x) \\ \iff h &\approx -\frac{f(x)}{f'(x)}. \end{aligned} \tag{11}$$

Numpy

numpy

numpy

- is an interface to high performance linear algebra libraries (ATLAS, LAPACK, BLAS)
- provides
  - the `array` object
  - fast mathematical operations over arrays
  - linear algebra, Fourier transforms, Random Number generation
- Numpy is NOT part of the Python standard library.

numpy arrays (vectors)

- An array is a sequence of objects
- all objects in one array are of the same type

Here are a few examples:

```
>>> from numpy import array
>>> a = array([1, 4, 10])
>>> type(a)
<type 'numpy.ndarray'>
>>> a.shape
(3,)
>>> a ** 2
array([  1,  16, 100])
>>> numpy.sqrt(a)
array([ 1.        ,  2.        ,  3.16227766])
>>> a > 3
array([False,  True,  True], dtype=bool)
```

Array creation

Can create from other sequences through `array` function:

- 1d-array (vector)

```
>>> a = array([1, 4, 10])
>>> a
array([ 1,  4, 10])
>>> print(a)
[ 1  4 10]
```

- 2d-array (matrix):

```
>>> B = array([[0, 1.5], [10, 12]])
>>> B
array([[  0. ,   1.5],
       [ 10. ,  12. ]])
>>> print(B)
[[  0.    1.5]
 [ 10.   12. ]]
```

Array shape I

The shape is a tuple that describes

- (i) the dimensionality of the array (that is the length of the shape tuple) and
- (ii) the number of elements for each dimension.

Example:

```
>>> a.shape
(3,)
>>> B.shape
(2, 2)
```

Can use shape attribute to change shape:

Array shape II

```
>>> B
array([[  0. ,    1.5],
       [ 10. ,   12. ]])
>>> B.shape
(2, 2)
>>> B.shape = (4,)
>>> B
array([  0. ,    1.5,   10. ,   12. ])
```

Array size

The total number of elements is given through the `size` attribute:

```
>>> a.size
3
>>> B.size
4
```

The total number of bytes used is given through the `nbytes` attribute:

```
>>> a.nbytes
12
>>> B.nbytes
32
```

Array type

- All elements in an array must be of the same type
- For existing array, the type is the `dtype` attribute

```
>>> a.dtype
dtype('int32')
>>> B.dtype
dtype('float64')
```

- We can fix the type of the array when the create the array, for example:

```
>>> a2 = array([1, 4, 10], numpy.float64)
>>> a2
array([  1.,   4.,  10.])
>>> a2.dtype
dtype('float64')
```

Important array types

- For numerical calculations, we normally use double floats which are knows as *float64* or short `float` in this text.:

```
>>> a2 = array([1, 4, 10], numpy.float)
>>> a2.dtype
dtype('float64')
```

- This is also the default type for `zeros` and `ones`.
- A full list is available at http://docs.scipy.org/doc/numpy/user/basics.types.html

Array creation II

- Other useful methods are `zeros` and `ones` which accept a desired matrix shape as the input:

```
>>> numpy.zeros((3, 3))
array([[ 0.,  0.,  0.],
       [ 0.,  0.,  0.],
       [ 0.,  0.,  0.]])
>>> numpy.zeros((4,))          # (4,) is tuple
array([ 0.,  0.,  0.,  0.])
>>> numpy.zeros(4)             # works as well,
                               # although 4 is
                               # not tuple.
array([ 0.,  0.,  0.,  0.])

>>> numpy.ones((2, 7))
array([[ 1.,  1.,  1.,  1.,  1.,  1.,  1.],
       [ 1.,  1.,  1.,  1.,  1.,  1.,  1.]])
```

Array indexing (1d arrays)

```
>>> x = numpy.array(range(0, 10, 2))
>>> x
array([0, 2, 4, 6, 8])
>>> x[3]
6
>>> x[4]
8
>>> x[-1]
```

Can query length as for any sequence:

```
>>> len(x)
5
>>> x.shape
(5,)
```

Array indexing (2d arrays)

```
>>> C = numpy.arange(12)
>>> C
array([ 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11])
>>> C.shape = (3, 4)
>>> C
array([[ 0,  1,  2,  3],
       [ 4,  5,  6,  7],
       [ 8,  9, 10, 11]])

>>> C[0, 0]
0
>>> C[2, 0]
8
>>> C[2, -1]
11
>>> C[-1, -1]
11
```

Array slicing (1d arrays)

New double colon operator `::`: Read as `START:END:INDEX STEP`

If either START or END are omitted, the end of the array is used:

```
>>> y = numpy.arange(10)
>>> y
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
>>> y[0:5]                    #slicing as we know it
array([0, 1, 2, 3, 4])
>>> y[0:5:1]                  #slicing with index step 1
array([0, 1, 2, 3, 4])
>>> y[0:5:2]                  #slicing with index step 2
array([0, 2, 4])
>>> y[:5:2]                   #from the beginning
array([0, 2, 4])
```

Array slicing (1d arrays continued) continued

Can also use a negative step size:

```
>>> y[0:5:1]              # positive index step size
array([0, 1, 2, 3, 4])
>>> y[0:5:-1]             # negative index step size
array([], dtype=int32)
>>> y[5:0:-1]
array([5, 4, 3, 2, 1])
>>> y[5:0:-2]
array([5, 3, 1])
>>> y[:0:-2]
array([9, 7, 5, 3, 1])
>>> y[:0:-1]
array([9, 8, 7, 6, 5, 4, 3, 2, 1])
>>> y[::-1]               # reverses array elements
array([9, 8, 7, 6, 5, 4, 3, 2, 1, 0])
```

Creating copies of arrays

Create copy of 1d array:

```
>>> copy_y = y[:]
```

Could also use `copy_y = y[::]` to create a copy.
To create a copy with reverse order of elements, we can use:

```
>>> y[::-1]
array([9, 8, 7, 6, 5, 4, 3, 2, 1, 0])
```

To create new array `z` of the same size as `y` (filled with zeros, say) we can use (for example):

```
>>> y
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
>>> z=numpy.zeros(y.shape)
>>> z
array([0., 0., 0., 0., 0., 0., 0., 0., 0., 0.])
```

Array slicing (2d)

Slicing for 2d (or higher dimensional arrays) is analog to 1-d slicing, but applied to each component. Common operations include extraction of a particular row or column from a matrix:

```
>>> C
array([[ 0,  1,  2,  3],
       [ 4,  5,  6,  7],
       [ 8,  9, 10, 11]])
>>> C[0, :]             # row with index 0
array([0, 1, 2, 3])
>>> C[:, 1]             # column with index 1
                       # (i.e. 2nd col)
array([1, 5, 9])
```

Other linear algebra tools

`help(numpy.linalg)` provides an overview, including

- `pinv` to compute the inverse of a matrix
- `svd` to compute a singular value decomposition
- `det` to compute the determinant
- `eig` to compute eigenvalues and eigenvectors

Curve fitting

- We typically fit lower order polynomials or other functions (which are the model that we expect the data to follow) through a number of points (often measurements).
- We typically have many more points than degrees of freedom, and would employ techniques such as least squared fitting.
- The function `numpy.polyfit` provides this functionality for polynomials.
- The function `scipy.optimize.curve_fit` provides curve fitting for generic functions (not restricted to polynomials).

Solving linear systems of equations

- `numpy.linealg.solve(A, b)` solves $A\mathbf{x} = \mathbf{b}$ for a square matrix A and given vector $\mathbf{b}$, and returns the solution vector $\mathbf{x}$ as an array object:

```
>>> A=numpy.array([[1, 0], [0, 2]])
>>> b=numpy.array([1, 4])
>>> from numpy import linalg as LA
>>> x = LA.solve(A, b)
>>> x
array([ 1.,  2.])
>>> numpy.dot(A, x)          #Computing A*x
array([ 1.,  4.])            #this should be b
```

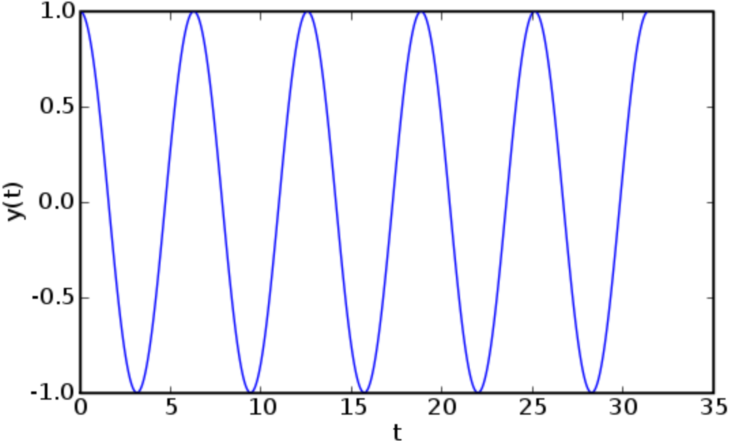
Other comments

- numpy provides fast array operations (comparable to Matlab's matrices)
- fast if number of elements is large: for an array with one element, `numpy.sqrt` will be slower than `math.sqrt`
- speed-ups of up to factor 300 are possible using numpy instead of lists
- Consult Numpy documentation if used outside this course.
- Matlab users may want to read Numpy for Matlab Users

Plotting arrays (vectors) I

```
import pylab
import numpy as N

t = N.arange(0, 10 * N.pi, 0.01)
y = N.cos(t)

pylab.plot(t, y)
pylab.xlabel('t')
pylab.ylabel('y(t)')
pylab.show()
```

Plotting arrays (vectors) II



Matplotlib / Pylab I

- Matplotlib tries to make easy things easy and hard things possible
- a python 2D plotting library which produces publication quality figures (increasingly also 3d)
- can be fully scripted but interactive interface available

Within the IPython console (for example in Spyder), use

- `%matplotlib inline` to see plots inside the console window, and
- `%matplotlib qt` to create pop-up windows with the plot when the `matplotlib.show()` command is used.

Matplotlib / Pylab II

Pylab is a Matlab-like (state-driven) plotting interface (to matplotlib).

- Convenient for 'simple' plots
- Check examples in lecture note text book and
- Make use of `help(pylab.plot)` to remind you of line styles, symbols etc.
- Check gallery at http://matplotlib.org/gallery.html#pylab_examples

Matplotlib.pyplot is an object oriented plotting interface.

- Very fine grained control over plots
- Check gallery at Matplotlib gallery
- Try Matplotlib notebook (on module's home page) as an introduction and useful reference.

LAB8

Higher Order Functions 2

More list processing and functional programming

- So far, have processed lists by iterating through them using for-loop
- perceived to be conceptually simple (by most learners) but
- not as compact as possible and not always as fast as possible
- Alternatives:
  - list comprehension
  - `map`, `filter`, `reduce`, often used with `lambda`

Anonymous function lambda

- lambda: anonymous function (function literal)

```
>>> lambda a: a
<function <lambda> at 0x319c70>
>>> lambda a: 2 * a
<function <lambda> at 0x319af0>
>>> (lambda a: 2 * a)
<function <lambda> at 0x319c70>
>>> (lambda a: 2 * a)(10)
20
>>> (lambda a: 2 * a)(20)
40
>>> (lambda x, y: x + y)(10,20)
30
>>> (lambda x, y, z: (x+y) * z )(10,20,2)
60
>>> type(lambda x, y: x + y)
<type 'function'>
```

- Useful to define a small helper function that is only needed once

Lambda usage example 1

Integrate $f(x) = x^2$ from 0 to 2, without lambda

lambda1.py:

```
from scipy.integrate import quad
def f(x):
    return x * x

y, abserr = quad(f, 0, 2)
print("Int f(x)=x^2 from 0 to 2 = {:f} +- {:g}"
      .format(y, abserr))
```

With lambda lambda1b.py:

```
from scipy.integrate import quad
y, abserr = quad(lambda x: x * x, 0, 2)
print("Int f(x)=x^2 from 0 to 2 = {:f} +- {:g}"
      .format(y, abserr))
```

Both programs produce the same output:

```
Int f(x)=x^2 from 0 to 2 = 2.666667 +- 2.96059e-14
```

Higher order functions

Roughly: "Functions that take or return functions" (see for example (Wikipedia entry))

Rough summary (check `help(COMMAND)` for details)

- `map(function, sequence)` → `list`:
  apply function to all elements in sequence
- `filter(function, sequence)` → `list`:
  return items of sequence for which function(item) is true.
- `reduce(function, sequence, initial)` → `value`:
  apply function(x,y) from left to right to reduce sequence to a single value.

Map

- `map(function, sequence)` → `list`: apply function to all elements in sequence
- Example:

```
>>> def f(x): return x ** 2
...
>>> map(f, [0, 1, 2, 3, 4])
[0, 1, 4, 9, 16]
```

Equivalent operation using list comprehension:

```
>>> [ x ** 2 for x in [0, 1, 2, 3, 4]]
[0, 1, 4, 9, 16]
```

Examples map

- Example:

```
>>> import math
>>> map(math.exp, [0,0.1,0.2,1.,10,100])
[1.0, 1.1051709180756477, 1.2214027581601699,
2.7182818284590451,22026.465794806718,
2.6881171418161356e+43]
```

- Example (slug):

```
>>> news="Python programming occasionally \
... more fun than expected"
>>> slug = "-".join( map( lambda w: w[0:6],
...                          news.split()))
>>> slug
'Python-progra-proves-more-fun-than-expect'
```

Equivalent list comprehension expression:

```
>>> slug = "-".join( [ w[0:6] for w
...                    in news.split() ])
```

Filter

- `filter(function, sequence)` → `list`: return items of sequence for which function(item) is true.
- Example:

```
>>> c="The quick brown fox jumps".split()
>>> print c
['The', 'quick', 'brown', 'fox', 'jumps']
>>> def len_gr_4(s):
...     return len(s) > 4
>>> map( len_gr_4, c)
[False, True, True, False, True]
>>> filter( len_gr_4, c)
['quick', 'brown', 'jumps']
>>> filter( lambda w: len(w) > 4, c)
['quick', 'brown', 'jumps']
```

Equivalent operation using list comprehension:

```
>>> [ s for s in c if len(s)>4 ]
['quick', 'brown', 'jumps']
```

Examples filter

- Example:

```
>>> def is_positive(n):
...     return n > 0
>>> filter(is_positive,
...          [-5,-4,-3,-2,-1,0,1,2,3,4])
[1, 2, 3, 4]
>>> filter(lambda n:n>0,
...          [-5,-4,-3,-2,-1,0,1,2,3,4])
[1, 2, 3, 4]
```

List comprehension equivalent:

```
>>> [ x for x in
...          [-5,-4,-3,-2,-1,0,1,2,3,4] if x>0]
[1, 2, 3, 4]
```

Reduce

- `reduce(function, sequence, initial)` → `value`: apply function(x,y) from left to right to reduce sequence to a single value.
- Examples:

```
>>> def f(x,y):
...     print "Called with x={}, y={}".format(x, y
...     return x + y
...
>>> reduce(f, [1, 3, 5], 0)
Called with x=0, y=1
Called with x=1, y=3
Called with x=4, y=5
9
>>> reduce(f, [1, 3, 5], 100)
Called with x=100, y=1
Called with x=101, y=3
Called with x=104, y=5
109
```

Reduce

```
>>> def f(x,y):
...     print "Called with x=%s, y=%s" % (x,y)
...     return x+y
...
>>> reduce(f,"test","")
Called with x=, y=t
Called with x=t, y=e
Called with x=te, y=s
Called with x=tes, y=t
'test'
>>> reduce(f,"test","FIRST")
Called with x=FIRST, y=t
Called with x=FIRSTt, y=e
Called with x=FIRSTte, y=s
Called with x=FIRSTtes, y=t
'FIRSTtest'
```

Operator module

- operator module contains functions which are typically accessed not by name, but via some symbols or special syntax.
- For example `3 + 4` is equivalent to `operator.add(3, 4)`. Thus:

```
def f(x, y): return x + y
reduce(f, range(10), 0)
```

can also be written as:

```
reduce(operator.add, range(10), 0)
```

Note: could also use:

```
reduce(lambda a, b: a + b, range(10), 0)
```

but use of `operator` module is preferred (faster).

Functional programming

- Functions like `map`, `reduce` and `filter` are found in just about any lanugage supporting functional programming.
- provide functional abstraction for commonly written loops
- Use those instead of writing loops, because
  - Writing loops by hand is quite tedious and error-prone.
  - The functional version is often clearer to read.
  - The functions result in faster code (if you can avoid `lambda`)

What command to use when?

- `lambda` allows to define a (usually simple) function "in-place"
- `map` transforms a sequence to another sequence (of same length)
- `filter` filters a sequence (reduces number of elements)
- `reduce` carries out an operation that "collects" information (sum, product, ...), for example reducing the sequence to a single number.
- `list comprehension` transforms a list (can include filtering).
- Hint: if you need to use a `lambda` in a `map`, you are probably better off using list comprehension.

Standard example: squaring elements in list

Some alternatives:

```
>>> res = []
>>> for x in range(5):
...     res.append(x ** 2)
...
>>> res
[0, 1, 4, 9, 16]

>>> [ x ** 2 for x in range(5) ]
[0, 1, 4, 9, 16]

>>> map( lambda x: x ** 2, range(5))
[0, 1, 4, 9, 16]
```

Returning function objects

We have seen that we can pass function objects as arguments to a function. Now we look at functions that return function objects.

Example closure_adder42.py:

```
def make_add42():
    def add42(x):
        return x + 42
    return add42

add42 = make_add42()
print(add42(2))              # output is '44'
```

Closures

A closure (Wikipedia) is a function with bound variables. We often create closures by calling a function that returns a (specialised) function. For example closure_adder.py:

```
import math

def make_adder(y):
    def adder(x):
        return x + y
    return adder

add42 = make_adder(42)
addpi = make_adder(math.pi)
print(add42(2))          # output is 44
print(addpi(-3))         # output is 0.14159265359
```

LAB9

Object Orientation and all that

Object Orientation and Closures

Earlier, we did an exercise for a first-in-first-out queue. At the time, we used a global variable to keep the state of the queue. The following slides show:

- the original FIFO-queue solution (using a global variable, generally not good)
- a modified version where the queue variable is passed to every function ($\rightarrow$ this is OO orientation without objects)
- a object orient version (where the queue data is part of the queue object)
- a version based on closures (where the state is part of the closures)

Original FIFO solution

Original FIFO solution fifoqueue.py

```
queue = []

def length():
    """Returns number of waiting customers"""
    return len(queue)

def show():
    """SHOW queue: print list of waiting customers. Customer
    waiting longest are shown at the end of the list."""
    for name in queue:
        print("waiting customer: {}".format(name))

def add(name):
    """Customer with name 'name' joining the queue"""
    queue.insert(0, name)

def next():
    """Returns name of next customer to serve, removes
    customer from queue"""
    return queue.pop()

add('Spearing'); add('Fangohr'); add('Takeda')
show(); next()
```

Improved FIFO solution fifoqueue2.py

```
def length(queue):
    return len(queue)

def show(queue):
    for name in queue:
        print("waiting customer: {}".format(name))

def add(queue, name):
    queue.insert(0, name)

def next(queue):
    return queue.pop()

q1 = []
q2 = []
add(q1, 'Spearing'); add(q1, 'Fangohr'); add(q1, 'Takeda')
add(q2, 'John'); add(q2, 'Peter')
print("{} customers in queue1:".format(length(q1)); show(q1)
print("{} customers in queue2:".format(length(q2)); show(q2)
```

Object-Oriented FIFO solution

Object-Oriented improved FIFO solution fifoqueueOO.py

```
class Fifoqueue:
    def __init__(self):
        self.queue = []

    def length(self):
        return len(self.queue)

    def show(self):
        for name in self.queue:
            print("waiting customer: {}".format(name))

    def add(self, name):
        self.queue.insert(0, name)

    def next(self):
        return self.queue.pop()

q1 = Fifoqueue()
q2 = Fifoqueue()
q1.add('Spearing'); q1.add('Fangohr'); q1.add('Takeda')
q2.add('John'); q2.add('Peter')
print("{} customers in queue1:".format(q1.length()); q1.show()
print("{} customers in queue2:".format(q2.length()); q2.show()
```

Functional FIFO solution

Functional (closure-based) FIFO solution fifoqueue_closure.py

```
def make_queue():
    queue = []

    def length():
        return len(queue)

    def show():
        for name in queue: print("waiting customer: {}".format(nam

    def add(name):
        queue.insert(0, name)

    def next():
        return queue.pop()

    return add, next, show, length

q1_add, q1_next, q1_show, q1_length = make_queue()
q2_add, q2_next, q2_show, q2_length = make_queue()
q1_add('Spearing');  q1_add('Fangohr');  q1_add('Takeda')
q2_add('John');  q2_add('Peter')
print("{} customers in queue1:".format(q1_length()); q1_show()
print("{} customers in queue2:".format(q2_length()); q2_show()
```

Lessons (Object Orientation)

Object orientation (OO):

- one import ideas is to combine data and functions operating on data (in objects),
- objects contain data but
- access to data through interface (implementation details irrelevant to user)
- can program in OO style without OO-programming language:
  - as in FIFO2 solution
  - as in closure based approach

Numerical Integration

Numerical Integration 1— Overview

Different situations where we use integration:

(A) solving (definite) integrals

(B) solving (ordinary) differential equations
  - more complicated than (A)
  - Euler's method, Runge-Kutta methods

Both (A) and (B) are important.

We begin with the numeric computation of integrals (A).

(A) Definite Integrals

Often written as

$$I = \int_a^b f(x)\mathrm{d}x \tag{12}$$

- example: $I = \int_0^2 \exp(-x^2)\mathrm{d}x$
- solution is $I \in \mathbb{R}$ (*i.e.* a number)
- right hand side $f(x)$ depends only on x
- if $f(x) > 0 \quad \forall x \in [a, b]$, then we can visualise I as the area underneath $f(x)$
  - Note that the integral is *not* necessarily the same as the area enclosed by $f(x)$ and the x-axis:
    - $\int_0^{2\pi} \sin(x)\mathrm{d}x = 0$
    - $\int_0^1 (-1)\mathrm{d}x = -1$

(B) Ordinary Differential Equations (ODE)

Often written as

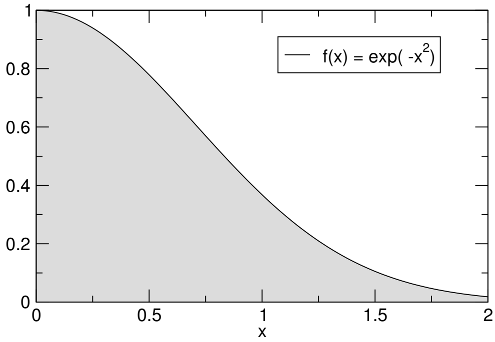
$$y' \equiv \frac{\mathrm{d}y}{\mathrm{d}x} = f(x, y) \tag{13}$$

- example: $\frac{\mathrm{d}v}{\mathrm{d}t} = \frac{1}{m}(g - cv^2)$
- solution is $\begin{aligned} y(x) : \quad & \mathbb{R} \to \mathbb{R} \\ & x \mapsto y(x) \end{aligned}$ (*i.e.* a function)
- right hand side $f(x, y)$ depends on x and on solution y
- Can write (13) formally as $y = \int \frac{\mathrm{d}y}{\mathrm{d}x} \mathrm{d}x = \int f(x, y) \mathrm{d}x$. That's why we "integrate differential equations" to solve them.

Numeric computation of definite integrals

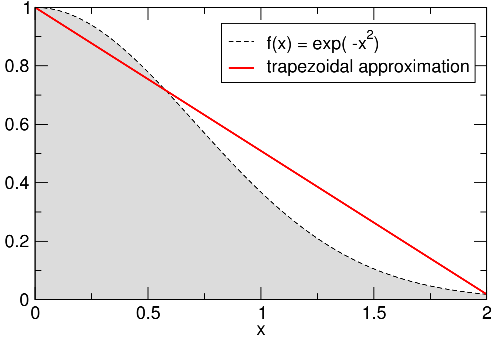
Example:

$$I = \int_0^2 \exp(-x^2)\mathrm{d}x$$



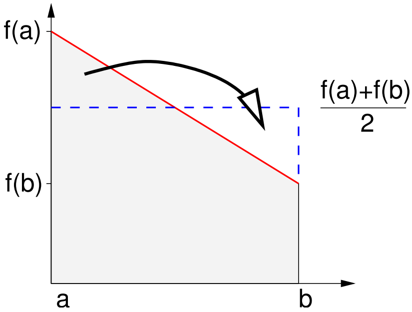
Simple trapezoidal rule

- Approximate function by straight line



Simple trapezoidal rule (2)

- Compute area underneath straight line $p(x)$



- Result

$$A = \int_a^b p(x)\mathrm{d}x = (b-a)\frac{f(a)+f(b)}{2}$$

Simple trapezoidal rule (3)

Aim: compute

$$I = \int_a^b f(x)\mathrm{d}x$$

Strategy:

- approximate $f(x)$ with a linear function $p(x)$:

$$p(x) \approx f(x)$$

- compute the area A underneath that function $p(x)$:

$$A = \int_a^b p(x)\mathrm{d}x = (b-a)\frac{f(a)+f(b)}{2}$$

- approximate

$$I = \int_a^b f(x)\mathrm{d}x \approx \int_a^b p(x)\mathrm{d}x = A = (b-a)\frac{f(a)+f(b)}{2}$$

Simple trapezoidal rule (4) Example

- Integrate $f(x) = x^2$

$$I = \int_0^2 x^2 \mathrm{d}x$$

- What is the (correct) analytical answer?
  Integrating polynomials:

$$I = \int_a^b x^k \mathrm{d}x = \left[\frac{1}{k+1} x^{k+1}\right]_a^b$$

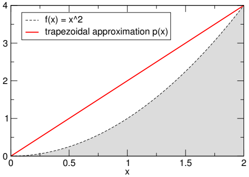
- for $a = 0$ and $b = 2$ and $k = 2$

$$I = \left[\frac{1}{2+1} x^{2+1}\right]_0^2 = \frac{1}{3} 2^3 = \frac{8}{3} \approx 2.6667$$

- Using the trapezoidal rule

$$A = (b-a)\frac{f(a)+f(b)}{2} = 2\frac{0+4}{2} = 4$$

- The correct answer is $I = 8/3$ and the approximation is $A = 4$. We thus *overestimate* I by $\frac{A-I}{I} \approx 50\%$.
- Plotting $f(x) = x^2$ together with the approximation reveals why we overestimate I



- The linear approximation, $p(x)$, overestimates $f(x)$ everywhere (except at $x = a$ and $x = b$).

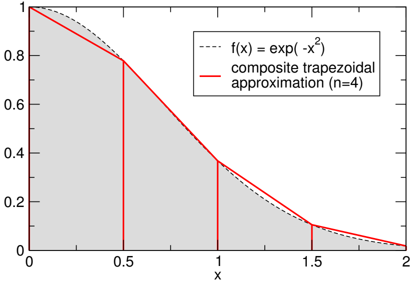
  Therefore, the integral of $p(x)$ is greater than the integral of $f(x)$.

  (More formally: $f(x)$ is convex on $[a, b]$ $\iff$ $f''(x) \geq 0 \quad \forall x \in [a, b]$.)

Composite trapezoidal rule

Example $f(x) = \exp(-x^2)$:

$$I = \int_0^2 f(x)\mathrm{d}x = \int_0^2 \exp(-x^2)\mathrm{d}x$$



$$I = \int_0^{0.5} f(x)\mathrm{d}x + \int_{0.5}^{1} f(x)\mathrm{d}x + \int_{1}^{1.5} f(x)\mathrm{d}x + \int_{1.5}^{2} f(x)\mathrm{d}x$$

General composite trapezoidal rule

For n subintervals the formulae for the composite trapezoidal rule are

$$\begin{aligned} h &= \frac{b-a}{n} \\ x_i &= a + ih \quad \text{with} \quad i = 1, \ldots, n-1 \end{aligned}$$

$$\begin{aligned} A &= \frac{h}{2}\Big(f(a) + 2f(x_1) + 2f(x_2) + \ldots \\ &\qquad +2f(x_{n-2}) + 2f(x_{n-1}) + f(b)\Big) \\ &= \frac{h}{2}\Big(f(a) + \sum_{i=1}^{n-1} 2f(x_i) + f(b)\Big) \end{aligned}$$

Error of composite trapezoidal rule

One of the important (and difficult) questions in numerical analysis and computing is:

- How accurate is my approximation?

For integration methods, we are interest in how much the error decreases when we decrease h (by increasing the number of subintervals, n).

For the composite trapezoidal rule it can be shown that:

$$\int_a^b f(x)\mathrm{d}x = \frac{h}{2}\left(f(a) + f(b) + 2\sum_{i=1}^{n-1} f(x_i)\right) + \mathcal{O}(h^2)$$

The symbol $\mathcal{O}(h^2)$ means that the error term is (smaller or equal to an upper bound which is) proportional to h^2:

- If we take 10 times as many subintervals then h becomes 10 times smaller (because $h = \frac{b-a}{n}$) and the error becomes 100 times smaller (because $\frac{1}{10^2} = \frac{1}{100}$).

Error of composite trapezoidal rule, example

- The table below shows how the error of the approximation, A, decreases with increasing n for

$$I = \int_0^2 x^2 \mathrm{d}x.$$

n	h	A	I	$\Delta = A – I$	rel.err.$=\Delta/I$
1	2.000000	4.000000	2.666667	1.333333	50.0000%
2	1.000000	3.000000	2.666667	0.333333	12.5000%
3	0.666667	2.814815	2.666667	0.148148	5.5556%
4	0.500000	2.750000	2.666667	0.083333	3.1250%
5	0.400000	2.720000	2.666667	0.053333	2.0000%
6	0.333333	2.703704	2.666667	0.037037	1.3889%
7	0.285714	2.693878	2.666667	0.027211	1.0204%
8	0.250000	2.687500	2.666667	0.020833	0.7813%
9	0.222222	2.683128	2.666667	0.016461	0.6173%
10	0.200000	2.680000	2.666667	0.013333	0.5000%
50	0.040000	2.667200	2.666667	0.000533	0.0200%
100	0.020000	2.666800	2.666667	0.000133	0.0050%

Summary trapezoidal rule for numerical integration

- Aim: to find an approximation of

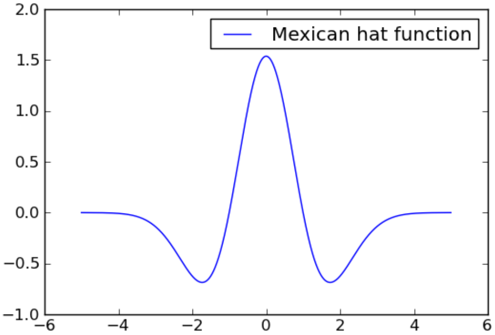
$$I = \int_a^b f(x)\mathrm{d}x$$

- Simple trapezoidal method:
  - approximate $f(x)$ by a simpler (linear) function $p(x)$ and
  - integrate the approximation $p(x)$ exactly.
- Composite trapezoidal method:
  - divides the interval $[a, b]$ into n equal subintervals
  - employs the simple trapezoidal method for each subinterval
  - has an error term of order h^2.

Numpy usage examples

Making calculations fast with numpy

- Calculations using numpy are faster (up to about 300 times) than using pure Python (see example next slide).
- Imagine we need to compute the mexican hat function with many points



Making calculations fast with numpy I

```python
"""Demo: practical use of numpy (mexhat-numpy.py)"""

import time
import math
import numpy as np

N = 10000


def mexhat_py(t, sigma=1):
    """Computes Mexican hat shape, see
    http://en.wikipedia.org/wiki/Mexican_hat_wavelet for
    equation (13 Dec 2011)"""
    c = 2. / math.sqrt(3 * sigma) * math.pi ** 0.25
    return c * (1 - t ** 2 / sigma ** 2) * \
        math.exp(-t ** 2 / (2 * sigma ** 2))


def mexhat_np(t, sigma=1):
    """Computes Mexican hat shape using numpy, see
    http://en.wikipedia.org/wiki/Mexican_hat_wavelet for
    equation (13 Dec 2011)"""
```

Making calculations fast with numpy II

```
    c = 2. / math.sqrt(3 * sigma) * math.pi ** 0.25
    return c * (1 - t ** 2 / sigma ** 2) * \
        np.exp(-t ** 2 / (2 * sigma ** 2))


def test_is_really_the_same():
    """Checking whether mexhat_np and mexhat_py produce
    the same results."""
    xs1, ys1 = loop1()
    xs2, ys2 = loop2()
    deviation = math.sqrt(sum((ys1 - ys2) ** 2))
    print "error:", deviation
    assert deviation < 1e-15


def loop1():
    """Compute arrays xs and ys with mexican hat function
    in ys(xs), returns tuple (xs,ys)"""
    xs = np.linspace(-5, 5, N)
    ys = []
    for x in xs:
        ys.append(mexhat_py(x))
    return xs, ys
```

Making calculations fast with numpy III

```
def loop2():
    """As loop1, but uses numpy to be faster."""
    xs = np.linspace(-5, 5, N)
    return xs, mexhat_np(xs)


def time_this(f):
    """Call f, measure and return number of seconds
    execution of f() takes"""
    starttime = time.time()
    f()
    stoptime = time.time()
    return stoptime - starttime


def make_plot(filenameroot):
    import pylab
    pylab.figure(figsize=(6, 4))
    xs, ys = loop2()
    pylab.plot(xs, ys, label='Mexican hat function')
    pylab.legend()
```

Making calculations fast with numpy IV

```
    pylab.savefig(filenameroot + '.png')
    pylab.savefig(filenameroot + '.pdf')


def main():
    test_is_really_the_same()
    make_plot('mexhat1d')
    time1 = time_this(loop1)
    time2 = time_this(loop2)
    print "Numpy version is %.1f times faster" %\
        (time1 / time2)

if __name__ == "__main__":
    main()
```

Produces this output:

```
error: 1.57009245868e-16
Numpy version is 248.4 times faster
```

Making calculations fast with numpy V

A lot of the source code above is focussed on measuring the execution time. Within IPython, we could just have used `%timeit loop1` and `%timeit loop2` to get to the same timing information.

Array objects of shape () behave like scalars I

```
>>> import numpy as np
>>> np.sqrt(4.)        #apply numpy-sqrt to scalar
2.0                      # looks like float
>>> type(np.sqrt(4.))  # but is numpy-float
<type 'numpy.float64'>
>>> float(np.sqrt(4.)) #but can convert to float
2.0
>>> a = np.sqrt(4.)      # what shape is the
                         # numpy-float?
>>> a.shape
()
>>> type(a)              # just to remind us
<type 'numpy.float64'> # of the type
>>>
```

So numpy-scalars (i.e. arrays with shape ()) can be converted to float. In fact, this happens implicitly:

Array objects of shape () behave like scalars II

```
>>> import numpy as np
>>> import math
>>> math.sqrt(np.sqrt(81))
3.0
```

Conversion to float fails if array has more than one element:

```
>>> import numpy as np
>>> a = np.array([10., 20., 30.])
>>> a
array([ 10.,  20.,  30.])
>>> print(a)
[ 10.  20.  30.]
>>> type(a)
<type 'numpy.ndarray'>
>>> a.shape
(3,)
>>> float(a)
Traceback (most recent call last):
```

Array objects of shape () behave like scalars III

```
  File "<stdin>", line 1, in <module>
TypeError: only length-1 arrays can be converted
           to Python scalars
>>> math.sqrt(a)
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
TypeError: only length-1 arrays can be converted
           to Python scalars
```

However, if the array contains only one number, then the conversion is possible:

```
>>> b = np.array(4.0)
>>> type(b)
<type 'numpy.ndarray'>
>>> b.shape
()
>>> b
array(4.0)
```

Array objects of shape `()` behave like scalars IV

```
>>> float(b)
4.0
>>> math.sqrt(b)
2.0
```

Note: an array with shape `(1,)` can also be converted to a float:

```
>>> c = np.array([3])
>>> c.shape
(1,)
>>> float(c)
3.0
```

This allows us to write functions `f(x)` that can take an input argument `x` which can either be a `numpy.array` or a scalar. The `mexhat_np(t)` function is such an example:

Array objects of shape () behave like scalars V

```
>>> a = mexhat_np(3.)
>>> type(a)
<type 'numpy.float64'> #essentially a float
>>> a
-0.13662231969702732
>>> float(a)              #converts to python float
-0.13662231969702732
>>> b = mexhat_np(np.arange(0, 11, 2))
>>> type(b)
<type 'numpy.ndarray'>
>>> b
array([  1.53729366e+00,  -6.24150219e-01,
        -7.73556857e-03,  -8.19453296e-07,
        -1.22651811e-12,  -2.93540437e-20])
```

Scientific Python

SciPy (SCIentific PYthon)

(Partial) output of `help(scipy)`:

```
    stats       --- Statistical Functions
    sparse      --- Sparse matrix
    lib         --- Python wrappers to external
                    libraries
    linalg      --- Linear algebra routines
    signal      --- Signal Processing Tools
    misc        --- Various utilities that don't
                    have another home.
    interpolate --- Interpolation Tools
    optimize    --- Optimization Tools
    cluster     --- Vector Quantization / Kmeans
    fftpack     --- Discrete Fourier Transform
    io          --- Data input and output
    integrate   --- Integration routines
    lib.lapack  --- Wrappers to LAPACK library
    special     --- Special Functions
    lib.blas    --- Wrappers to BLAS library
```

Interpolation of data

Given a set of N points (x_i, y_i) with $i = 1, 2, \dots N$, we sometimes need a function $\hat{f}(x)$ which returns $y_i = f(x_i)$ and interpolates the data between the x_i.

- $\rightarrow$ `y0 = scipy.interpolate.interp1d(x,y)` does this interpolation. Note that the function
- `interp1d` returns *a function* `y0` which will interpolate the x-y data for any given x when called as $y0(x)$
- Data interpolation of $y_i = f(x_i)$ may be useful to
  - Create smoother plots of $f(x)$
  - find minima/maxima of $f(x)$
  - find x_c so that $f(x_c) = y_c$, provide inverse function $x = f^{-1}(y)$
  - integrate $f(x)$
- Need to decide how to interpolate (nearest, linear, quadratic or cubic splines, ...)

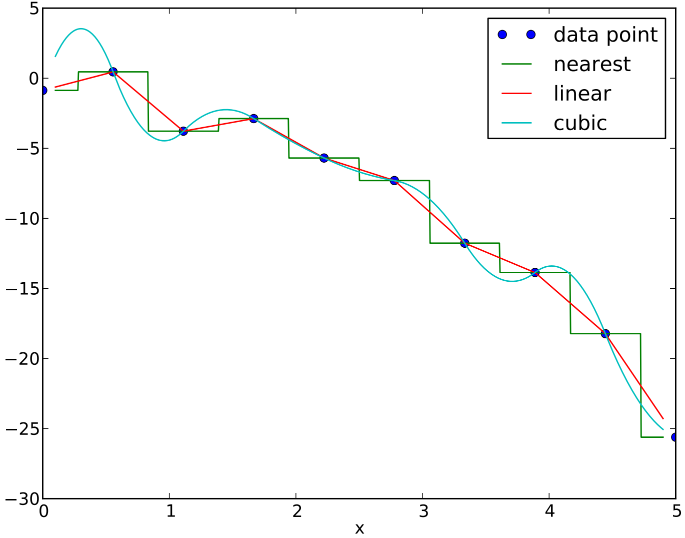
Interpolation of data example I

```
import numpy as np
import scipy.interpolate
import pylab

def create_data(n):
    """Given an integer n, returns n data points
    x and values y as a numpy.array."""
    xmax = 5.
    x = np.linspace(0, xmax, n)
    y = - x**2
    #make x-data somewhat irregular
    y += 1.5 * np.random.normal(size=len(x))
    return x, y

#main program
n = 10
x, y = create_data(n)

#use finer and regular mesh for plot
xfine = np.linspace(0.1, 4.9, n * 100)
#interpolate with piecewise constant function (p=0)
y0 = scipy.interpolate.interp1d(x, y, kind='nearest')
```

Interpolation of data example II

```
#interpolate with piecewise linear func (p=1)
y1 = scipy.interpolate.interp1d(x, y, kind='linear')
#interpolate with piecewise constant func (p=2)
y2 = scipy.interpolate.interp1d(x, y, kind='quadratic')

pylab.plot(x, y, 'o', label='data point')
pylab.plot(xfine, y0(xfine), label='nearest')
pylab.plot(xfine, y1(xfine), label='linear')
pylab.plot(xfine, y2(xfine), label='cubic')
pylab.legend()
pylab.xlabel('x')
pylab.savefig('interpolate.pdf')
pylab.show()
```

Interpolation of data example III



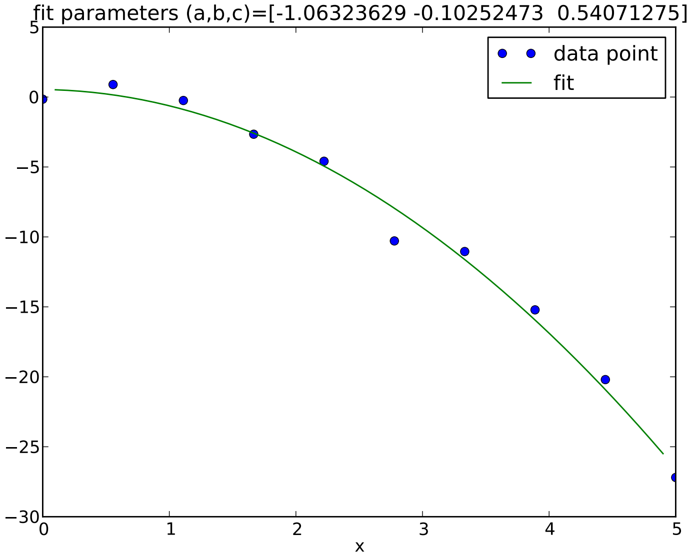
Curve fitting example I

```
import numpy as np
import scipy.optimize
import pylab

def create_data(n):
    """Given an integer n, returns n data points
    x and values y as a numpy.array."""
    xmax = 5.
    x = np.linspace(0, xmax, n)
    y = - x**2
    #make x-data somewhat irregular
    y += 1.5 * np.random.normal(size=len(x))
    return x, y

def model(x, a, b, c):  # Equation for fit
    return a * x ** 2 + b * x + c
```

Curve fitting example II

```
# main program
n = 10
x, y = create_data(n)
# do curve fit
p, pcov = scipy.optimize.curve_fit(model, x, y)
a, b, c = p
# plot fit and data
xfine = np.linspace(0.1, 4.9, n * 5)
pylab.plot(x, y, 'o', label='data point')
pylab.plot(xfine, model(xfine, a, b, c), \
    label='fit')
pylab.title('fit parameters (a,b,c)=%s' % p)
pylab.legend()
pylab.xlabel('x')
pylab.savefig('curvefit2.pdf')
pylab.show()
```

Curve fitting example III



Function integration example I

```python
from math import exp, pi
from scipy.integrate import quad


#function we want to integrate
def f(x):
    return exp(math.cos(-2 * x * pi)) + 3.2

#call quad to integrate f from -2 to 2
res, err = quad(f, -2, 2)

print("The numerical result is {:f} (+-{:g})"
    .format(res, err))
```

which produces this output:

```
The numerical result is 17.864264 (+-1.55117e-11)
```

LAB10

Optimisation (Minimisation)

- Optimisation typically described as:
  given a function $f(x)$, find x_m so that $f(x_m)$ is the (local) minimum of f.
- To maximise $f(x)$, create a second function $g(x) = -f(x)$ and minimise $g(x)$.
- Optimisation algorithms need to be given a starting point (initial guess x_0 as close as possible to x_m)
- Minimum position x obtained may be local (not global) minimum

Optimisation example I

```
from scipy import arange, cos, exp
from scipy.optimize import fmin
import pylab

def f(x):
    return cos(x) - 3 * exp( -(x - 0.2) ** 2)

# find minima of f(x),
# starting from 1.0 and 2.0 respectively
minimum1 = fmin(f, 1.0)
print "Start search at x=1., minimum is",minimum1
minimum2 = fmin(f, 2.0)
print "Start search at x=2., minimum is",minimum2

# plot function
x = arange(-10, 10, 0.1)
y = f(x)
```

Optimisation example II

```
pylab.plot(x, y, label='$\cos(x)-3e^{-(x-0.2)^2}$')
pylab.xlabel('x')
pylab.grid()
pylab.axis([-5, 5, -2.2, 0.5])

# add minimum1 to plot
pylab.plot(minimum1, f(minimum1), 'vr',
           label='minimum 1')
# add start1 to plot
pylab.plot(1.0, f(1.0), 'or', label='start 1')

#add minimum2 to plot
pylab.plot(minimum2,f(minimum2),'vg',\
           label='minimum 2')
#add start2 to plot
pylab.plot(2.0,f(2.0),'og',label='start 2')

pylab.legend(loc='lower left')
```

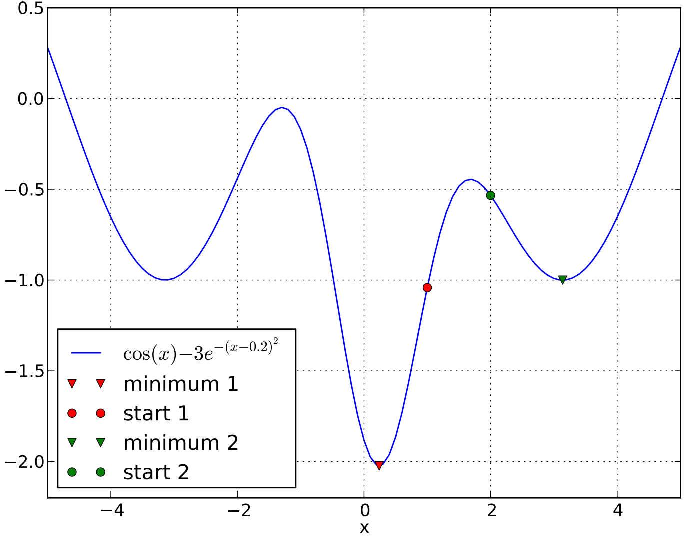
Optimisation example III

```
pylab.savefig('fmin1.pdf')
pylab.show()
```

Code produces this output:

```
Optimization terminated successfully.
         Current function value: -2.023866
         Iterations: 16
         Function evaluations: 32
Start search at x=1., minimum is [ 0.23964844]
Optimization terminated successfully.
         Current function value: -1.000529
         Iterations: 16
         Function evaluations: 32
Start search at x=2., minimum is [ 3.13847656]
```

Optimisation example IV



LAB11

Ordinary Differential Equations (ODEs)

Ordinary Differential Equations I

- Many processes, in particular *time-dependent* processes, can be described as Ordinary Differential Equations (ODEs). This includes dynamics of engineering systems, quantum physics, chemical reactions, biological systems modelling, population dynamics, and many other models.
- ODEs have *exactly one* independent variable, and we assume for simplicity this is the time t.
- The easiest ODE type has one degree of freedom, y, which depends on the time t, i.e. $y = y(t)$. (Thinks of temperature as a function of time, the distance a car has moved as function of time, the angular velocity of a rotating motor, etc.)

Ordinary Differential Equations II

- (In general, a vector $\mathbf{y}$ with k components can depend on the independent variable, in which case we are looking at a *system* of ordinary differential equations with k degrees of freedom.)
- We are seeking the function $y(t)$ – this is *the solution* of the ODE.
- We are typically being given an initial value y_0 of $y(t)$ at some time t_0 and
- the ODE itself which relates the change of y with t to some function $f(t, y)$, i.e.

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f(y, t) \tag{14}$$

Interface odeint

- aim: solve

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f(y,t)$$

- get access to "odeint":
  `from scipy.integrate import odeint`
- `odeint` has the following input and output parameters:

```
ys = odeint(f, y0, ts)
```

Input:

- `f` is function `f(y, t)` that returns the right-hand side
- `y0` is the initial value of the solution at time t_0
- `ts` is a numpy `array` containing times t_i for which we would like to know the solution $y(t_i)$
  - the first value in the array has to be t_0 (with $y(t_0) = y_0$)

Output:

- `ys` is the numpy `array` that contains the solution

Using `odeint` – example 1

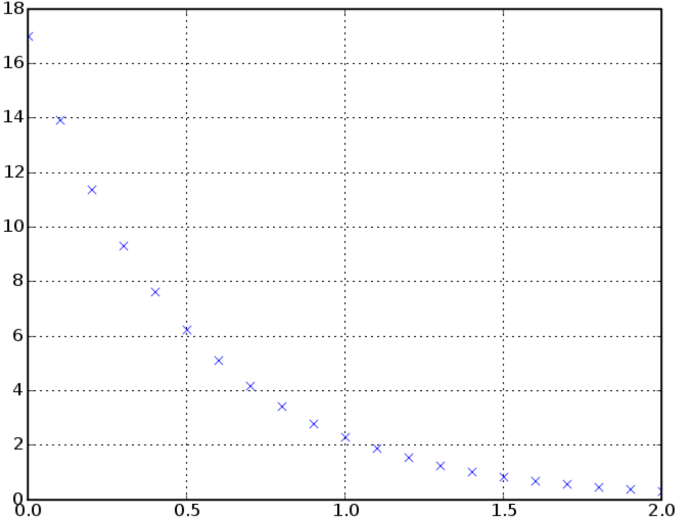
- require solution $y(t)$ from $t = 0$ to $t = 2$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = -2y \quad \text{with} \quad y(0) = 17$$

```python
import numpy as np
from scipy.integrate import odeint

def f(y,t):
    return -2 * y

ts = np.arange(0, 2.1, 0.1)
y0 = 17
ys = odeint(f, y0, ts)

import pylab
pylab.plot(ts, ys, 'x')
pylab.grid()
pylab.savefig('odeintexample1.pdf')
pylab.show()
```

Using `odeint` – example 1

Solution:



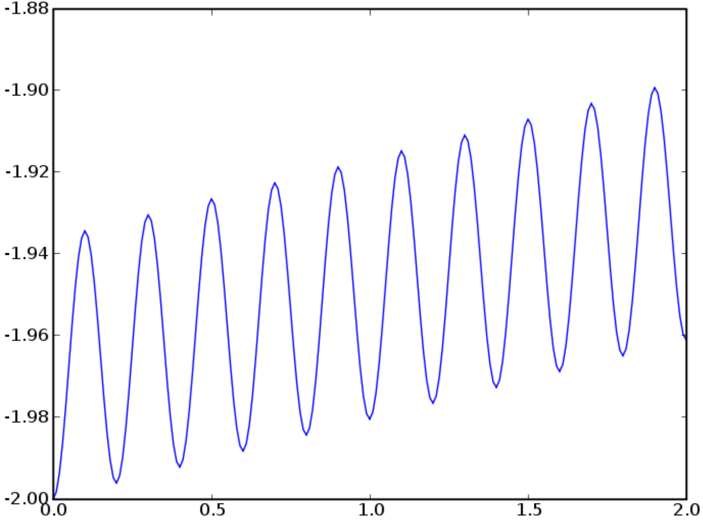
Using odeint – example 2

- require solution $y(t)$ from $t = 0$ to $t = 2$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = -\frac{1}{100}y + \sin(10\pi t) \quad \text{with} \quad y(0) = -2$$

```
import math
import numpy as np
from scipy.integrate import odeint

def f(y, t):
    return -0.01 * y + \
        math.sin(10 * math.pi * t)

ts = np.arange(0, 2.01, 0.01)
y0 = -2
ys = odeint(f, y0, ts)

import pylab
pylab.plot(ts, ys)
pylab.savefig('odeintexample2.pdf')
pylab.show()
```

Solution:



2nd order ODE

- Any second order ODE can be re-written as two coupled first order ODE
- Example: Harmonic Oscillator (HO)
  - Differential equation $\frac{\mathrm{d}^2 r}{\mathrm{d}t^2} = -\omega^2 r$ or short $r'' = -\omega^2 r$
  - Introduce $v = r'$
  - rewrite equation as two first order equations

$$r'' = -\omega^2 r \qquad \longrightarrow \qquad \begin{aligned} v' &= -\omega^2 r \\ r' &= v \end{aligned}$$

- General strategy:
  - convert higher order ODE into a set of (coupled) first order ODE
  - use computer to solve set of 1st order ODEs

2nd order ODE – using `odeint`

- One 2nd order ODE $\rightarrow$ 2 coupled 1st order ODEs
- Integration of *system* of 1st order ODEs:
  - "pretty much like integrating one 1st order ODE" but
  - y is now a vector (and so is f):

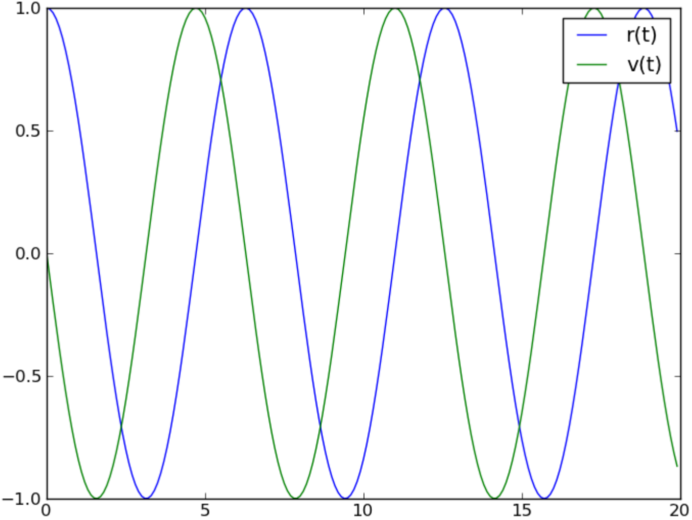
$$\frac{\mathrm{d}\mathbf{y}}{\mathrm{d}t} = \mathbf{f}(\mathbf{y}, t) \quad \Longleftrightarrow \quad \begin{pmatrix} \frac{\mathrm{d}y_1}{\mathrm{d}t} \\ \frac{\mathrm{d}y_2}{\mathrm{d}t} \end{pmatrix} = \begin{pmatrix} f_1(\mathbf{y}, t) \\ f_2(\mathbf{y}, t) \end{pmatrix}$$

  - need to pack and unpack variables into the *state vector* $\mathbf{y}$:
  - Example harmonic oscillator:
    - decide to use this packing: $\mathbf{y} = (r, v)$
    - then $\mathbf{f}$ needs to return $\mathbf{f} = \left(\frac{\mathrm{d}r}{\mathrm{d}t}, \frac{\mathrm{d}v}{\mathrm{d}t}\right)$
  - `odeint` returns a vector $\mathbf{y}$ for every time step $\rightarrow$ a matrix
    - need to extract results for r and v from that matrix (rows are time, first column is r, second column is v) $\rightarrow$ see next slide

2nd order ODE – Python solution HO

```
from numpy import array, arange
from scipy.integrate import odeint

def f(y, t):                    # right hand side, takes array(!) y
    omega = 1
    r = y[0]                    # extract r from array y
    v = y[1]                    # extract v from array y
    drdt = v                    # compute right hand side
    dvdt = -omega ** 2 * r
    return array([drdt, dvdt])  # return array

ts = arange(0, 20, 0.1)    # required times for solution
r0 = 1                      # initial r
v0 = 0                      # initial v
y0 = array([r0, v0])        # combine r and v into y

ys = odeint(f, y0, ts)      # solve ODEs

rs = ys[:, 0]               # extract results: r(t)
vs = ys[:, 1]               # extract results: v(t)

import pylab                # plot results
pylab.plot(ts, rs, label='r(t)')
pylab.plot(ts, vs, label='v(t)'); pylab.legend()
pylab.savefig('odeintexample1dHO.pdf')
```

Solution (not annotated):



Summary 2nd order system

- Strategy:
  - transform one 2nd order ODE into 2 (coupled) first order ODEs
  - solve both first order ODEs simultaneously
- nothing conceptually complicated
- but need to use matrices ("arrays") in Python to shuffle the data around.
- Warning: the meaning of y, x depends on context: often $x = t$ and $y = x$. It helps to write down equations before coding them.
- Use example on previous slides as guidance.

2 Coupled ODEs: Predator-Prey problem I

- Predator and prey. Let
  - $p_1(t)$ be the number of rabbits
  - $p_2(t)$ be the number of foxes
- Time dependence of p_1 and p_2:
  - Assume that rabbits proliferate at a rate a. Per unit time a number ap_1 of rabbits is born.
  - Number of rabbits is reduced by collisions with foxes. Per unit time cp_1p_2 rabbits are eaten.
  - Assume that birth rate of foxes depends only on food intake in form of rabbits.
  - Assume that foxes die a natural death at a rate b.
- Numbers
  - rabbit birth rate $a = 0.7$
  - rabbit-fox-collision rate $c = 0.007$
  - fox death rate $b = 1$

Predator-Prey problem (2) I

- Put all together in predator-prey ODEs

$$
\begin{aligned}
p_1' &= ap_1 - cp_1p_2 \\
p_2' &= cp_1p_2 - bp_2
\end{aligned}
$$

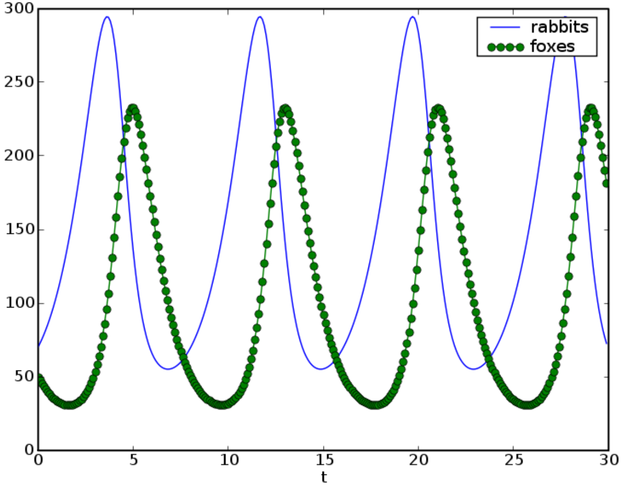
- Solve for $p_1(0) = 70$ and $p_2(0) = 50$ for 30 units of time:

```
import numpy as N
from scipy.integrate import odeint

def rhs(y, t):
    a = 0.7;      c = 0.007;    b = 1
    p1 = y[0]
    p2 = y[1]
    dp1dt = a * p1 - c * p1 * p2
    dp2dt = c * p1 * p2 - b * p2
    return N.array([ dp1dt, dp2dt ])
```

Predator-Prey problem (2) II

```
p0 = N.array([70, 50])    #initial condition
ts = N.arange(0, 30, 0.1)

res = odeint( rhs, p0, ts )#compute solution

p1 = res[:, 0]                   #extract p1 and
p2 = res[:, 1]                   #p2

import pylab                    #plot result
pylab.plot(ts, p1,label='rabbits')
pylab.plot(ts, p2,'-og',label='foxes')
pylab.legend()
pylab.xlabel('t')
pylab.savefig('predprey.eps')
pylab.savefig('predprey.png')
pylab.show()
```

Predator-Prey problem (2) III



Outlook I

- Suppose we want to solve a (vector) ODE based on Newton's equation of motion in three dimensions:

$$\frac{\mathrm{d}^2\mathbf{r}}{\mathrm{d}t^2} = \frac{\mathbf{F}(\mathbf{r}, \mathbf{v}, t)}{m}$$

- Rewrite as two first order (vector) ODEs:

$$\begin{aligned} \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} &= \frac{\mathbf{F}(\mathbf{r}, \mathbf{v}, t)}{m} \\ \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} &= \mathbf{v} \end{aligned}$$

- Need to pack 6 variables into "$\mathbf{y}$": for example

$$\mathbf{y} = (r_x, r_y, r_z, v_x, v_y, v_z)$$

Outlook II

- Right-hand-side function $\mathbf{f}(\mathbf{y}, t)$ needs to return:

$$\mathbf{f} = \left(\frac{\mathrm{d}r_x}{\mathrm{d}t}, \frac{\mathrm{d}r_y}{\mathrm{d}t}, \frac{\mathrm{d}r_z}{\mathrm{d}t}, \frac{\mathrm{d}v_x}{\mathrm{d}t}, \frac{\mathrm{d}v_y}{\mathrm{d}t}, \frac{\mathrm{d}v_z}{\mathrm{d}t}\right) \tag{15}$$

- Example: Molecular dynamics simulations have one set of degrees of freedom as in equation 15 *for every atom* in their simulations.
- Example: Material simulations discretise space into finite elements, and for dynamic simulations the number of degrees of freedom are proportional to the number of nodes in the mesh.
- Very sophisticated time integration schemes fore ODEs available (such as "sundials" suite).
- The tools in `scipy.integrate` are pretty useful already (`odeint` and `ode`).

Symbolic Python (sympy)

Symbolic Python I

```
>>> import sympy
>>> x = sympy.Symbol('x')   # define symbolic
>>> y = sympy.Symbol('y')   # variables
>>> x + x
2*x
>>> t = (x + y)**2
>>> print t
(x + y)**2
>>> sympy.expand(t)
x**2 + 2*x*y + y**2
>>> sympy.pprint(t)       #PrettyPRINT
       2
(x + y)
>>> sympy.printing.latex(t) #Latex export
'\\left(x + y\\right)^{2}'
```

Symbolic Python II

```
>>> t
(x + y)**2
>>> t.subs(x, 3)           #substituting variables
(y + 3)**2                 #or values
>>> t.subs(x, 3).subs(y, 1)
16
>>> n=t.subs(x, 3).subs(y, sympy.pi)
>>> print n
(3 + pi)**2
>>> n.evalf()              #evaluate to float
37.7191603226281
>>> p = sympy.pi
>>> p
pi
>>> p.evalf()
3.14159265358979
>>> p.evalf(47)            #request 47 digits
3.1415926535897932384626433832795028841971693993
```

Symbolic Python III

```
>>> from sympy import limit, sin, oo
>>> limit(1/x, x, 50)
1/50
>>> limit(1/x, x, oo)          ##oo is infinity
0
>>> limit(sin(x) / x, x, 0)
1
>>> limit(sin(x)**2 / x, x, 0)
0
>>> limit(sin(x) / x**2, x, 0)
oo

>>> from sympy import integrate
>>> a, b = sympy.symbols('a,b')
>>> integrate(2*x, (x, a, b))
-a**2 + b**2
>>> integrate(2*x, (x, 0.1, b))
b**2 - 0.01
```

Symbolic Python IV

```
>>> integrate(2*x, (x, 0.1, 2))
3.99000000000000

>>> from sympy import series
>>> taylorseries = series(sin(x), x, 0)
>>> taylorseries
x - x**3/6 + x**5/120 + O(x**6)
>>> sympy.pprint(taylorseries)
     3     5
    x     x
x - -- + --- + O(x**6)
    6    120
>>> taylorseries = series(sin(x), x, 0, n=10)
>>> sympy.pprint(taylorseries)
     3     5      7        9
    x     x      x        x
x - -- + --- - ---- + ------ + O(x**10)
    6    120   5040   362880
```

Symbolic Python V

Finally, we can solve non-linear equations, for example:

```
>>> (x + 2)*(x - 3)      # define quadratic equation
                         # with roots x=-2, x=3
(x - 3)*(x + 2)
>>> r = (x + 2)*(x - 3)
>>> r.expand()
x**2 - x - 6
>>> sympy.solve(r, x)   # solve r = 0
[-2, 3]                 # solution is x = -2, 3
```

Sympy summary

- Sympy is purely Python based
- fairly powerful (although better open source tools are available if required)

Symbolic Python VI

- we should use computers for symbolic calculations routinely alongside pen and paper, and numerical calculations
- can produce latex output
- can produce C and fortran code (and wrap this up as a python function automatically ("autowrap"))

```
changeset:   320:e36c68f84379
tag:         tip
user:        Hans Fangohr [MBA] <fangohr@soton.ac.uk>
date:        Tue Sep 24 23:42:15 2013 +0100
```