Principles of Programming in Econometrics

Introduction, structure, and advanced programming techniques

Charles S. Bos

Vrije Universiteit Amsterdam

c.s.bos@vu.nl

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Lecture slides

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Target of course

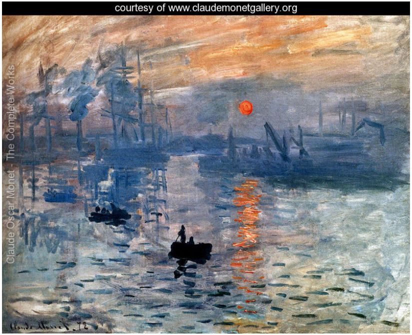
- Learn
- structured
- programming
- and organisation
- (in Python/Julia/Matlab/Ox or other language)

Not only: Learn more syntax... (mostly today)
Remarks:

- Structure: Central to this course
- Small steps, simplifying tasks
- Hopefully resulting in: Robustness!
- Efficiency: Not of first interest... (Value of time?)
- Language: Theory is language agnostic

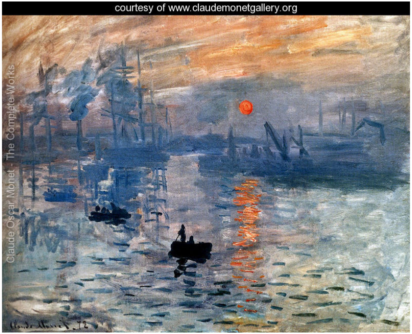
Target of course II

... Or move from

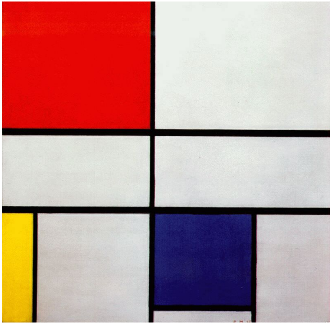


Target of course II

... Or move from



to



(Maybe discuss at end of first day?...)

Syntax

What is 'syntax'?

- Set of rules
- Define how program 'functions'
- Should give clear, non-ambiguous, description of steps taken
- Depends on the language

Today:

- Learn basic Python syntax
- Learn to read manual/web/google for further syntax!

Syntax II

What is not 'syntax'?

- Rule-book on how to program
- Choice between packages
- Complete overview

For clarity:

- We will *not* cover all of Python
- We make a (conservative) *choice* of packages (numpy, scipy, pandas, matplotlib)
- We focus on structure, principle, guiding thoughts
- ... and then you should be able to do the hard work

Overview

Principles of Programming in Econometrics

D0: Syntax, example 2^8

D1: Structure, scope

D2: Numerics, packages

D3: Optimisation, speed

Day 0: Syntax

- Introduction
- Example: 2^8
- Elements
- Main concepts
- Closing thoughts
- Revisit E0
- Practical
  - Checking variables, types, conversion and functions
  - Implementing Backsubstitution

Day 1: Structure

- Introduction
  - Programming in theory
  - Science, data, hypothesis, model, **estimation**
- Structure & Blocks (Droste)
- Further concepts of
  - Data/Variables/Types
  - Functions
  - Scope, globals
- Practical
  - Regression: Simulate data
  - Regression: Estimate model

Day 2: Numerics and flow

- Numbers and representation
- Steps, flow and structure
- Floating point numbers
- Practical Do's and Don'ts
- Packages
- Graphics
- Practical
  - Cleaning OLS program
  - Loops
  - Bootstrap OLS estimation
  - Handling data: Inflation

Day 3: Optimisation

- Optimization (`minimize`)
  - Idea behind optimization
  - Gauss-Newton/Newton-Raphson
  - Stream/order of function calls
- Standard deviations
- Restrictions
- Speed
- Practical
  - Regression: Maximize likelihood
  - GARCH-M: Intro and likelihood

Evaluation

- No old-fashioned exam
- Range of exercises, to try out during course
- Short final exercise (see VU Canvas), obligatory for TI/BDS (and voluntary for DHPQRM). Hand it in, I'll mark it (pass/fail), plus you may receive some comments/hints on programming style.

Main message: Work for your own interest, later courses will be simpler if you make good use of this course...

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Day 0: Syntax

- Introduction
- Example: 2^8
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Programming by example

Let's start simple

- Example: What is 2^8?
- Goal: Simple situation, program to solve it
- Broad concepts, details follow

Power: Steps

First steps:

- Get a first program (pow0.py)
- Initialise, provide (incorrect) output (pow1.py)
- `for`-loop (pow2.py)
- Introduce function (pow3.py)
- Use a while loop (pow4.py)
- Recursion (pow5.py)
- Check output (pow6.py)

Power: First program

Listing 1: pow0.py

```
"""
pow0.py
Purpose:
    Calculate 2^8
Version:
    0       Outline of a program
Date:
    2023/7/29
Author:
    Charles Bos
"""
################################
### Imports
# import numpy as np

################################
### main
print ('Hello world')
```

To note:

- Explanation of program, in triple quotes """ ((docstring))
- Comments #
- Possible imports
- Main code at bottom

Power: Initialise

Listing 2: pow1.py

```
# Magic numbers
dBase= 2
iC= 8
# Initialisation
dRes= 1
# Estimation
# Not done yet...
# Output
print (f'The result of {dBase}^{iC}= {dRes}')
```

To note:

- Each line is a command
- Distinction between 'magics', 'initialisation', 'estimation' and 'output'
- **F**ormatted print function `print(f'a= {a}')` is used, printing *value* of elements in {}

Power: Estimate

Listing 3: pow2.py

```
#########################
### main
# Magic numbers
...
# Estimation
for i in range(iC):
    dRes= dRes * dBase

# Output
...
```

To note:

- For loop, counts in extra variable `i`
- Function `range(iStop)`, counts from 0, . . . , iStop-1
- Executes `indented commands` after `for i in range(iC):`
- Mind the `:` after the `for` statement

Intermezzo 1: Check output
Intermezzo 2: Check The for and while loops.
Intermezzo 3: Discuss why the `range()` function (and indexing, later), is upper-bound exclusive.

Power: Functions

Listing 4: pow3.py

```
def Pow(dBase, iPow):
    """
    Purpose:
      Calculate dBase^iPow
    Inputs:
      dBase     double, base
      iPow      integer, power
    Return value:
      dRes
double, dBase^iPow
    """
    dRes= 1
    for i in range(iPow):
        # print (f'i= {i}')
        dRes= dRes * dBase
    return dRes
### Main
dRes= Pow(dBase, iC)
```

To note:

- Function has own docstring
- Function defines two arguments `dBase, iPow`
- Function *indents one tab forward*
- Uses local `dRes, i`
- `returns` the result
- And `dRes= Pow(dBase, iC)` catches the result `dRes= 256`.

- Allows to re-use functions for multiple purposes
- Could also be called as `dRes= Pow(4, 7)`
- Here, only one output

Power: While

Listing 5: pow3.py

```
dRes= 1
for i in range(iC):
    dRes= dRes*dBase
```

Listing 6: pow4.py

```
dRes= 1
i= 0
while (i < iPow):
    dRes= dRes*dBase
    i+= 1
```

To note:

- The `for i in range(iter)` loop corresponds to a `while` loop
- Look at the order: First init, then check, then action, then increment, and check again.
- The for-loop is slightly simpler, as beforehand the number of iterations is fixed.
- A loop command can be a *compound* command, multiple commands all indented equally.

Power: Recursion

Listing 7: pow5.py

```
def Pow_Recursion(dBase, iPow):
    # print (f'In Pow_Recursion, with iPow= {iPow}')
    if (iPow == 0):
        return 1

    return dBase * Pow_Recursion(dBase, iPow-1)
```

To note:

- $2^8 \equiv 2 \times 2^7$
- $2^0 \equiv 1$
- Use this in a recursion
- New: If statement

Intermezzo: Check Python manual on if statement, or a simpler Wiki on the same topic.

Q: What is *wrong*, or maybe just *non-robust* in this code?

Power: Recursion

Listing 8: pow5.py

```
def Pow_Recursion(dBase, iPow):
    # print (f'In Pow_Recursion, with iPow= {iPow}')
    if (iPow == 0):
        return 1

    return dBase * Pow_Recursion(dBase, iPow-1)
```

To note:

- $2^8 \equiv 2 \times 2^7$
- $2^0 \equiv 1$
- Use this in a recursion
- New: If statement

Intermezzo: Check Python manual on if statement, or a simpler Wiki on the same topic.

Q: What is *wrong*, or maybe just *non-robust* in this code?

A: Rather use `if (iPow <= 0)`, do not continue for non-positive `iPow`!

Power: Check outcome

Always, (*always...!*) check your outcome

Listing 9: pow6.py

```
import math
...
# Output
print (f'The result of {dBase}^{iC}=')
print (f'  - Using Pow(): {Pow(dBase, iC)}')
print (f'  - Using Pow_Recursion(): {Pow_Recursion(dBase, iC)}')
print (f'  - Using **: {dBase ** iC}')
print (f'  - Using math.pow: {math.pow(dBase, iC)}')
```

Listing 10: output

```
 The result of  2^8 =
   - Using Pow():  256
   - Using Pow_Recursion():  256
   - Using **:  256
   - Using math.pow:  256.0
```

Power: Check outcome II

To note:

- Yes, indeed, Python has (multiple…) power operators readily available.
- Always check for available functions…
- And carefully check the manual, for difference between `x**y`, `pow(x,y)`, `math.pow()`.

Q: And what is this difference between the powers?

Power: Check outcome II

To note:

- Yes, indeed, Python has (multiple…) power operators readily available.
- Always check for available functions…
- And carefully check the manual, for difference between x**y, pow(x,y), math.pow().

Q: And what is this difference between the powers?

A: According to the manual, `math.pow()` transforms first to floats, then computes. The others leave integers intact.

Elements to consider

- Comments: `# (until end of line)`
- Docstring: `""" Docstring """`
- `import` statements: At front of each code file
- Spacing: Important for routines/loops/conditional statements
- Variables, types and naming (subset):

boolean	`bX=True`
scalar integer	`iN= 20`
scalar double/float	`dC= 4.5`
string	`sName= 'Beta1'`
list	`lX= [1, 2, 3]`, `lY= ['Hello', 2, True]`
tuple	`tX= (1, 2, 3)`
vector	`vX= np.array([1, 2, 3, 4])`
matrix	`mX= np.array([[1, 2.5], [3, 4]])`
function	`fnFunc = print`

Elements: Comments

Use: `# (until end of line)`

- To explain reasoning behind code
- ... but sparingly: Code should be self-explanatory(?)
- ... while maintaining readability: Will you, or someone else, understand after three ~~years~~months?
- ... Hence use for quick additions to code
- **and** ... for temporarily turning off parts of the code (e.g., checks?)

Important, very...

Elements: Docstrings

Use:

- To explain the functions/modules you write
- Either single-line (`"""Return the iPow'th power of dBase."""`),
- or multi-line, after function defintion:

```
def Pow_Recursion(dBase, iPow):
    """
    Purpose:
      Calculate dBase^iPow through recursion

    Inputs:
      dBase     double, base
      iPow      integer, power

    Return value:
      dRes      double, dBase^iPow
    """
```

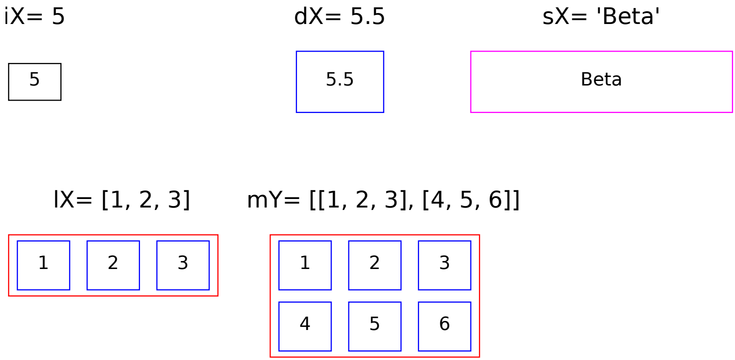
- . . . and at start of module, explaining name/purpose/version/date/author

Important, indeed...

Elements: Docstrings II

```
IPython 8.12.0 -- An enhanced Interactive Python. Type '?' for help.

In [1]: run pow6
The result of 2^8=
  - Using Pow(): 256
  - Using Pow_Recursion(): 256
  - Using **: 256
  - Using math.pow: 256.0

In [2]: ?Pow_Recursion
Signature: Pow_Recursion(dBase, iPow)
Docstring:
Purpose:
  Calculate dBase^iPow through recursion

Inputs:
  dBase     double, base
  iPow      integer, power

Return value:
  dRes      double, dBase^iPow
File:      ~/vu/ppectr23/lists_py/power/pow6.py
Type:      function
```

Elements: Imagine variables



Every element has its representation in memory — no magic

Try out variables

Listing 11: variables.py

```
bX= True
type(bX)

iN= 20
type(iN)

dC= 4.5
type(dC)

sX='Beta1'
type(sX)

lX= [1, 2, 3]
type(lX)

mY= [[1, 2, 3], [4, 5, 6]]
type(mY)

mZ= np.array(mY)
type(mZ)

fnX= print
type(fnX)

rX= range(4)
type(rX)
print ('Range rX= ', rX)
print ('List of contents of range rX= ', list(rX))
```

Hungarian notation prefixes

prefix	type	example
`i`	integer	`iX`
`b`	boolean	`bX`
`d`	double	`dX`
`m`	matrix	`mX`
`v`	vector	`vX`
`s`	string	`sX`
`fn`	Function	`fnX`
`l`	list	`lX`
`g_`	variable with global scope	`g_mX`

Use them *everywhere, always*.

Possible exception: Counters `i`, `j`, `k` etc.

Hungarian 2

Python does not force Hungarian notation. Why would you?

- Forces you to think: What should each object be?
- Improves readability of code
- Helps (tremendously) in debugging

Drawbacks:

- Python recognizes many different types; in 'EOR/QRM/PhD', not all are useful to track
- Hungarian notation best used for 'intention': vector `vX` for 1-dimensional list or array or a $n \times 1$ or $1 \times n$ matrix, matrix `mX` for 2-dimensional list/array

Hungarian 3

Correct but *very* ugly is

Listing 12: nohun.py

```
def main():
    iX= 'Hello'
    sX= 5
```

Instead, *always* use

Listing 13: hun.py

```
def main():
    sX= 'Hello'
    iX= 5
```

Recap

But let us recap the first lessons, and extend the knowledge...

All work in functions

All work is done in functions (or at least, that's what we'll do!)

Listing 14: recap1.py

```
def main():
    dX= 5.5
    dX2= dX ** 2

    print ("The square of ", dX, " is ", dX2)

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

Note:

- This function `main()` takes no arguments
- ... but Python only executes the first line outside a function
- ... which is an `if` statement, calling `main()`
- ... only if we call this routine as a separate program (allows us to `import` files later)

Quiz-time: Main

Listing 15: recap_quiz.py

```
def main():
    print ('Hello world')

##############################################################
### start main
print ('This is an orphan statement')
if __name__ == "__main__":
    main()
```

Q1 What is the output of this program?

Q2 Would anything change if the line starting with `if` is skipped?

Q3 And why does one use the conditional statement?

Quiz-time: Main

Listing 16: recap_quiz.py

```
def main():
    print ('Hello world')

###########################################################
### start main
print ('This is an orphan statement')
if __name__ == "__main__":
    main()
```

Q1 What is the output of this program?

Q2 Would anything change if the line starting with `if` is skipped?

Q3 And why does one use the conditional statement?

Answer: Deep Python philosophy. But follow the custom...

Squaring and printing

Use other functions to do your work for you

Listing 17: recap2.py

```
import math

def printsquare(dIn):
    dOut= math.pow(dIn, 2)
    print (f'The square of {dIn} is {dOut}')

def main():
    dX= 5.5
    printsquare(dX)

    printsquare(6.3)
```

Here, `printsquare` does not give a return value, only screen output.

`printsquare` takes in one argument, with a value locally called `dIn`. Can either be a true variable (`dX`), a constant (6.3), or even the outcome of a calculation (`dX-5`).

Note the usage of `import math` for the `math.pow()` function.

Return

Use `return a` to give one value back to the calling function (as e.g. the `math.pow()` function also gives a value back).

Listing 18: recap_return.py

```
def createones(iR, iC):
    mX= np.ones((iR, iC))    # Use numpy, handing over Tuple (iR, iC)
    return mX

def main():
    iR= 2                        # Magic numbers
    iC= 5
    mX= createones(iR, iC)       # Estimation, catch output of createones
    print ("Matrix mX=\n", mX)   # Output
```

Alternative: See below, altering pre-defined mutable (= matrix) argument

Return: A tuple

Alternatively, return a *tuple* if multiple values should be handed back to the calling routine:

Listing 19: recap_return_tuple.py

```
def createones_size(iR, iC):
    mX= np.ones((iR, iC))   # Use numpy, handing over Tuple (iR, iC)
    iSize= iR*iC
    return (mX, iR*iC)

def main():
    iR= 2        # Magic numbers
    iC= 5
    (mX, iSize)= createones_size(iR, iC)              # Estimation
    print (f'Matrix mX=\n{mX}\nof size {iSize}') # Output
```

Alternative: See below, altering pre-defined mutable (= matrix) argument

Q: Why is this example rather stupid/non-robust?

Return: A tuple

Alternatively, return a *tuple* if multiple values should be handed back to the calling routine:

Listing 20: recap_return_tuple.py

```
def createones_size(iR, iC):
    mX= np.ones((iR, iC))   # Use numpy, handing over Tuple (iR, iC)
    iSize= iR*iC
    return (mX, iR*iC)

def main():
    iR= 2        # Magic numbers
    iC= 5
    (mX, iSize)= createones_size(iR, iC)             # Estimation
    print (f'Matrix mX=\n{mX}\nof size {iSize}') # Output
```

Alternative: See below, altering pre-defined mutable (= matrix) argument

Q: Why is this example rather stupid/non-robust?

A: Rather use `mX.size`, no space for errors

Indexing

A matrix is a NumPy array of multiple doubles, a string consists of multiple characters, a list of multiple elements. Get to those elements by using indices (starting at 0):

Listing 21: recap3.py

```
def index(mA, sB, lC):
  print ('Element [0,1] of\n', mA, f'\nis {mA[0,1]}')
  print (f'Elements [0:5] of {sB} are {sB[0:5]}')
  print (f'Element [4] of {sB} is letter {sB[4]}')
  print (f'Element [1] of\n{lC}\nis {lC[1]}')
############################################################
### main
def main():
    mX= np.random.randn(2, 3)      # Some random numbers
    sY= 'Hello world'              # A string
    lZ= [mX, sY, 6.3]              # A list of items
    index(mX, sY, lZ)
```

Warnings:

- Indexing starts at [0] (as in C, Java, Julia, Ox etc, fine)
- Selecting a range indicates [start:end+1]... **Extremely dangerous, if you use other languages... And ugly, according to Prof E.W. Dijkstra**

Indexing matrices

Python indexes 'logically'. . . , but sometimes counterintuitively.

- A matrix is effectively an array of an array
- A one-dimensional array can (often) be used as both row/column vector, `vX1d= np.array([1,2,3])`.
- Though sometimes an explicitly *two*-dimensional array is more useful, `vX2d= np.array([1, 2, 3]).reshape(-1, 1)` (depends on the situation, be careful)
- But then check the difference between `vX1d[0]`, `vX2d[0]`, `vX2d[0,0]`, `vX2d[0:1]` and `vX2d[0:1,0]`

See `recap4.py`. . .

Indexing matrices II

Listing 22: recap4.py

```
import numpy as np

###########################################################
### main
def main():
    vX= np.array([1, 2, 3]).reshape(-1, 1)    # A column vector

    print ('vX=\n', vX)
    print ('Note how vX is a lists-of-lists, cast to a two-dimensional array\n')

    print ('vX[0]= ', vX[0], '(a one-dimensional array)')
    print ('vX[0,0]= ', vX[0,0], '(a scalar)')
    print ('vX[0:1]= ', vX[0:1], '(a 1 x 1 matrix)')
###########################################################
### start main
if __name__ == "__main__":
    main()
```

Stepwise Indexing

An index may also take a step:

Listing 23: recap4b.py

```
import numpy as np

##########################################################
### main
def main():
    vX= np.random.randn(10)

    print ('Full vX:\n', vX)
    print ('Every second element:\n', vX[::2])
    print ('Every second element, starting at second:\n', vX[1::2])
```

Convenient for selecting subsets!

Boolean Indexing

One can also index using (a vector of) booleans, to select only the rows/columns/elements where the boolean is `True`:

Listing 24: recap4c.py

```
import numpy as np

###########################################################
### main
def main():
    vX= np.random.randn(10)
    vI= vX >= 0

    print ('vX:', vX)
    print ('vI:', vI)

    vXP= vX[vI]
    print ('Non-negative elements:\n', vXP)
    print ('(Careful with resulting type/size!)')
```

Convenient for selecting subsets!

Matrices

A matrix:

- ...is the work-horse of most econometric work (data, linear algebra, likelihoods and derivatives etc)
- ...is not natively included in Python
- ...hence we'll take the `numpy` array instead
- (Note: We'll choose nòt to use the `numpy` matrix)
- Matrices tend to be two-dimensional
- ...hence we'll often force our matrices/vectors into such shape:

```
vX= [1, 2, 3]            # A one-dimensional list
vX= np.array(vX)         # ... transformed into a one-dimensional array
vX= vX.reshape(3, 1)     # ... and made into a two-dimensional matrix
vX= vX.reshape(-1, 1)    # ... same thing (or more robust), Python checks r
```

- Important: Check your matrices, make sure you distinguish matrix/one-dimensional array/scalar!

Matrices II

Matrices can be used, after starting with e.g. `mX= np.random.randn(3, 4)`,

- as *arguments* of functions: `dSum= np.sum(mX)`
- or applying a function on a matrix directly, `dSum= mX.sum(); vSum= mX.sum(axis=0); vX= mX.reshape(1, -1)`
- looking at its *characteristics*, `(iR, iC)= mX.shape`
- changing its characteristics even: `mX.shape= (1, iR*iC)`

(see `recap4d.py`)

Q: What is difference between `dSum` and `vSum`?

Matrices II

Matrices can be used, after starting with e.g. `mX= np.random.randn(3, 4)`,

- as *arguments* of functions: `dSum= np.sum(mX)`
- or applying a function on a matrix directly, `dSum= mX.sum(); vSum= mX.sum(axis=0); vX= mX.reshape(1, -1)`
- looking at its *characteristics*, `(iR, iC)= mX.shape`
- changing its characteristics even: `mX.shape= (1, iR*iC)`

(see `recap4d.py`)

Q: What is difference between `dSum` and `vSum`?

Hint: Always, *always* keep track of what your matrix is, and check yourself...

Indexing and non-matrices

There is more than matrices...

- Strings, lists, . . .

Listing 25: recap5.py

```
def showelement(sElem, aElem):
  print (sElem, '= ', aElem, ' with type ', type(aElem),
           ' with shape ', np.shape(aElem), ', size ', np.size(aElem),
           ' and len ', len(aElem))

def main():
    lX= [[1, 2, 'hello'],
         ['there', 'A', 4.5]]
    print ('Show the full list:')
    showelement('lX', lX)                  # a two-dimensional list
    print ('Reference first list:')
    showelement('lX[0]', lX[0])            # a one-dimensional list
    print ('Reference the third element [2] of the first list lX[0]:')
    showelement('lX[0][2]', lX[0][2])     # a string

    print ('It would be incorrect to reference lX[0,2]')
    # showelement('lX[0,2]', lX[0,2])     # an error...
```

Q1: How do I get 'here' by referencing a part of `lX`?

Q2: What is difference in `np.shape()`, `np.size()`, `len()`?

Scope

Each variable has a *scope*, a part of the program where it is known. The scope is either

- local: The variable is known within the present function only
- global: ...

Listing 26: recap6.py

```
def localfunc(aX):
    sX= 'local var'
    print ('In localfunc: Local arg aX: ', aX)
    print ('In localfunc: Local var sX: ', sX)
    # Next line gives an error
    # print ('Double dY: ', dY)

def main():
    dY= 5.5
    localfunc('a variable from main')
    print ('In main: Double dY= ', dY)
    # Next line gives an error
    # print ('In main: sX= ', sX)
```

Q: What variable is known where exactly?

Scope II

Each function (including main)

- can create/use at will new local variables
- can receive through arguments variables from other functions

Additionally, each function can

- share a global variable
- where the global variable shall be prefixed by `g_`, as in `g_mX`
- ... where the variable is declared `global` within a function, before its use, see `recap7.py`

Scope III

Listing 27: recap7.py

```
##############################################################
### localfunc(iX)
def localfunc(iX):
    global g_lX
    print ('In localfunc: argument iX: ', iX)
    print ('In localfunc: g_lX: ', g_lX)

    g_lX[1]= iX        # Change a single element in global
    print ('In localfunc: g_lX after changing an element: ', g_lX)

    g_lX= list(range(iX, 2*iX))    # Change the full variable
    print ('In localfunc: g_lX, after changing all: ', g_lX)

##############################################################
### main
def main():
    global g_lX

    iY= 5
    g_lX= [1, 2, 3]
    localfunc(iY)
    print ('In main: Global var= ', g_lX)
```

Scope IV

Each function (including main)

- can create/use at will new local variables
- can receive through arguments variables from other functions
- can use global variables (but please forget them...)

Additionally, each function can

- change *part* of the *mutable* variable (list/array/matrix) ... Then *the variable does not change*, only part of the *contents*

[Example: See `recap8.py` below]

Function arguments

In Python, functions can alter contents of variables, but not the full variable itself:

Listing 28: recap8.py

```
def func_nochange(mX):
    mX= np.random.randn(3, 4)
    print ('In func_nochange, changing mX locally to mX=\n', mX)

def func_change(mX):
    iR, iC= mX.shape
    mX[:,:]= np.random.randn(iR, iC)
    print ('In func_change, changing mX locally to mX=\n', mX)

def main():
    mX= np.array([[1.0,2,3],[4,5,6]])
    func_nochange(mX)
    print ('In main, after func_nochange: mX=\n', mX)
    func_change(mX)
    print ('In main, after func_change: mX=\n', mX)
```

Function arguments II

Limitations: Changing function arguments

- works with *mutable* variables (i.e. lists, arrays, NumPy matrices, Pandas dataframes),
- does not work with *immutable* variables (i.e. strings, tuples, doubles, integers)
- allows for changes in value, (generally (...)) not in size of argument
- which implies that arguments have to be pre-assigned at the correct size

Example:

Listing 29: e0_elim.py

```
def ElimElement(mC, i, j):
    ...
    mC[i,j:]= mC[i,j:] - dF*mC[j,j:]
    return True
```

Function arguments III

Notes (**IMPORTANT**):

- If you are going to change an input argument to a function *MENTION IT IN THE DOCSTRING*, listing the variable under the `Outputs`
- General rule of thumb: A function argument can be changed when you assign to *a part of* the argument, as in `mC[1,2]= 5`. The moment you do a full `mC= np.random.rand(3,4)` the full variable is overwritten, and the result is *not* available to the outside routine.
- Exception to size changing argument: In Pandas, you are allowed to extend an existing dataframe with additional columns.

Closing thoughts

Almost enough for today...

Missing are:

- Operators for ndarrays
- Precise definition of compound statements
  - if-elif-else
  - while
  - for
- Corresponding concepts in Matlab
- Many, many details. . .

During this course,

Open the Python/NumPy documentation

and learn to find your way

Installation of Python

Many ways... Here:

- AnaConda (https://www.anaconda.com/download/): This installs the base Python 3.X+packages+Spyder, with minimal fuss.
- At Conda command prompt (= terminal on OSX/Linux), install missing packages (hardly ever needed, most was included already)

```
conda install numpy
```

- Once in a while, update it all from Conda command prompt, using

```
conda update --all
conda clean --all
```

Editor/IDE

For editing/running programs, several options again:

- Whatever editor of choice, run from command line (go ahead)
- Spyder: Install (if needed) through

```
conda install spyder
```

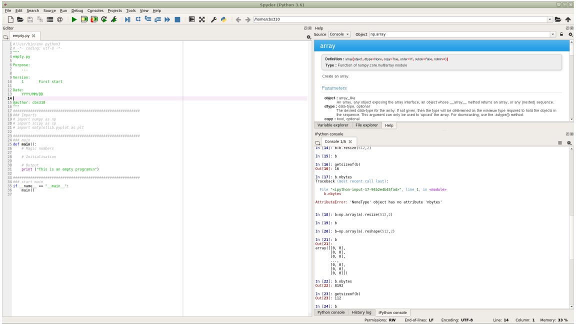
- ~~Atom: Install from https://atom.io with packages Hydrogen, Autocomple-python~~ (**Deprecated**), and add

```
conda install jupyter
```

- VSCode: Install from https://code.visualstudio.com/, with Python extension
- PyCharm: Install from https://www.jetbrains.com/pycharm/
- IPython: Install (if needed) through

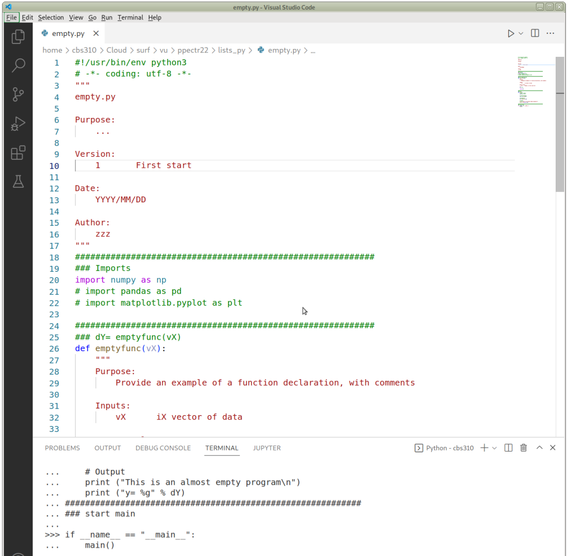
```
conda install ipython
```

Spyder

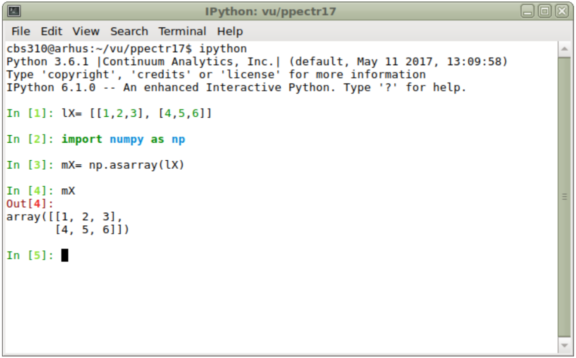


Spyder environment

VSCode


empty.py - Visual Studio Code
File Edit Selection View Go Run Terminal Help
empty.py
home > cbs310 > Cloud > surf > vu > ppectr22 > lists_py > empty.py > ...
#!/usr/bin/env python3
-*- coding: utf-8 -*-
"""
empty.py
Purpose:
...
Version:
1 First start
Date:
YYYY/MM/DD
Author:
zzz
"""
###
Imports
import numpy as np
# import pandas as pd
# import matplotlib.pyplot as plt
###
dY= emptyfunc(vX)
def emptyfunc(vX):
"""
Purpose:
Provide an example of a function declaration, with comments
Inputs:
vX iX vector of data
PROBLEMS OUTPUT DEBUG CONSOLE TERMINAL JUPYTER
Python - cbs310
... # Output
... print ("This is an almost empty program\n")
... print ("y= %g" % dY)
... ###
... ### start main
...
>>> if __name__ == "__main__":
... main()

IPython



IPython environment

Overview

Principles of Programming in Econometrics

D0: Syntax, example 2^8

D1: Structure, scope

D2: Numerics, packages

D3: Optimisation, speed

Day 1: Structure

- Introduction
  - Programming in theory
  - Science, data, hypothesis, model, **estimation**
- Structure & Blocks (Droste)
- Further concepts of
  - Data/Variables/Types
  - Functions
  - Scope, globals
- Practical
  - Regression: Simulate data
  - Regression: Estimate model

Target of course

- Learn
- structured
- programming
- and organisation
- (in Python/Julia/Matlab/Ox or other language)

Not: Just learn more syntax...
Remarks:

- Structure: Central to this course
- Small steps, simplifying tasks
- Hopefully resulting in: Robustness!
- Efficiency: Not of first interest... (Value of time?)
- Language: Theory is language agnostic

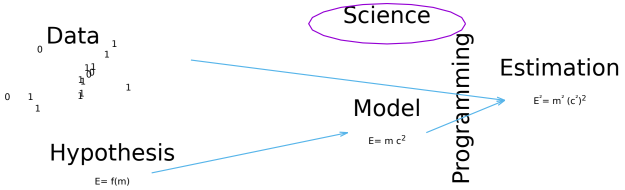
What? Why?

Wrong answer:

For the fun of it

A correct answer

To get to the results we need, in a fashion that is controllable, where we are free to implement the newest and greatest, and where we can be 'reasonably' sure of the answers



Aims and objectives

- Use computer power to enhance productivity
- Productive Econometric Research:
  combination of interactive modules and programming tools
- Data Analysis, Modelling, Reporting
- Accessible Scientific Documentation (no black box)
- Adaptable, Extendable and Maintainable (object oriented)
- Econometrics, statistics and numerical mathematics procedures
- Fast and reliable computation and simulation

Options for programming

	GUI	CLI	Program	Speed	QuanEcon	Comment
EViews	+	-	-	±	+	Black box, TS
Stata	±	+	-	-	-	Less programming
Matlab	+	+	+	+	±	Expensive, other audience
Gauss	±	±	+	±	+	'Ugly' code, unstable
S+/R	±	+	+	-	±	Very common, many packages
Ox	+	±	+	+	+	Quick, links to C, ectrics
Python	+	+	+	+	±	Neat syntax, common
Julia	+	+	+	++	+	General/flexible/difficult, quick
C(++)/Fortran	-	-	+	++	-	Very quick, difficult

Here: Use ~~Ox~~ ~~Matlab~~ Python as environment, apply theory elsewhere

History

There was once...
Apple II, CPU 6502, 1Mhz, 48kB of memory...
Now: More possibilities, also computationally:

Timings for OLS (30 observations, 4 regressors):

2020	R5 2500U 2.0Ghz	64b	1.318.000† /sec
2017	I5-7Y54 1.2Ghz	64b	1.047.000† /sec
2014	I5-4460S 2.9Ghz	64b	1.100.000† /sec
2012	Xeon E5-2690 2.9Ghz	64b	950.000† /sec
2009	Xeon X5550 2.67Ghz	64b	670.000† /sec
2008	Xeon 2.8Ghz	OSX	392.000† /sec
2006	AMD3500+	64b	320.000† /sec
2004	PM-1200		147.000† /sec
2001	PIII-1000		104.000† /sec
1996	PPro200		30.000/sec
1993	P5-90		6.000/sec
1989	386/387		300/sec
1981	86/87 (est.)		30/sec

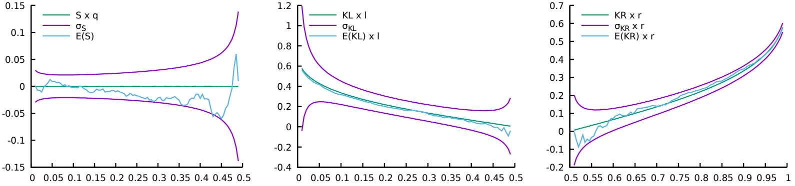
Increase:
$\approx \times$ 1000 in 15 years
$\approx \times$ 10000 in 25 years.

Note: For further speed increase, use multi-cpu.

Speed increase — but keep thinking

$$x \sim \mathrm{NIG}(\alpha, \beta, \delta, \mu) \quad P(X < x) = \int_0^x f(z)dz = F(x) \quad x_q = F^{-1}(q)$$

$$\mathcal{S}(q) = \frac{x_{1-q} + x_q - 2x_{\frac{1}{2}}}{x_{1-q} - x_q} \quad \mathcal{K}^L(q) = \frac{x_{\frac{1-q}{2}} + x_{\frac{q}{2}} - 2x_{\frac{1}{4}}}{x_{\frac{1-q}{2}} - x_{\frac{q}{2}}} \quad \mathcal{K}^R(q) = \ldots$$

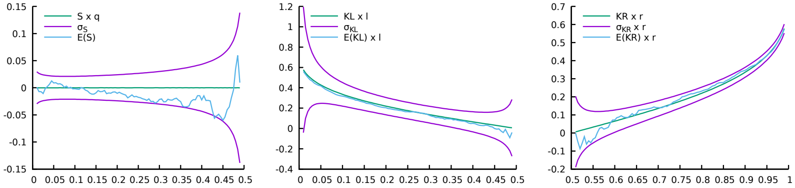


Direct calculation of graph: > 40 min

Speed increase — but keep thinking

$$x \sim \text{NIG}(\alpha, \beta, \delta, \mu) \quad P(X < x) = \int_0^x f(z)dz = F(x) \quad x_q = F^{-1}(q)$$

$$\mathcal{S}(q) = \frac{x_{1-q} + x_q - 2x_{\frac{1}{2}}}{x_{1-q} - x_q} \quad \mathcal{K}^L(q) = \frac{x_{\frac{1-q}{2}} + x_{\frac{q}{2}} - 2x_{\frac{1}{4}}}{x_{\frac{1-q}{2}} - x_{\frac{q}{2}}} \quad \mathcal{K}^R(q) = \ldots$$



Direct calculation of graph: > 40 min
Pre-calc quantiles (=*memoization*): 5 sec

Programming in Theory

Plan ahead

- Research question: What do I want to know?
- Data: What inputs do I have?
- Output: What kind of output do I expect/need?
- Modelling:
  - What is the structure of the problem?
  - Can I write it down in equations?
- Estimation: What procedure for estimation is needed (OLS, ML, simulated ML, GMM, nonlinear optimisation, Bayesian simulation, etc)?

Closer to practice

Blocks:

- Is the project separable into blocks, independent, or possibly dependent?
- What separate routines could I write?
- Are there any routines available, in my own old code, or from other sources?
- Can I check intermediate answers?
- How does the program flow from routine to routine?

... names:

- How can I give functions and variables names that I am sure to recognise later (i.e., also after 3 months)?
  Use (always) sensible **Hungarian notation**

Even closer to practice

Define, **on paper**, for each routine/step/function:

- What inputs it has (shape, size, type, meaning), exactly
- What the outputs are (shape, size, type, meaning), also exactly...
- What the purpose is...

Also for your main program:

- Inputs can be *magic numbers*, (name of) *data file*, but also specification of model
- Outputs could be screen output, file with cleansed data, estimation results etc. etc.

Elements to consider

- Explanation: Be generous (enough)
- Initialise from main
- Then do the estimation
- ... and give results

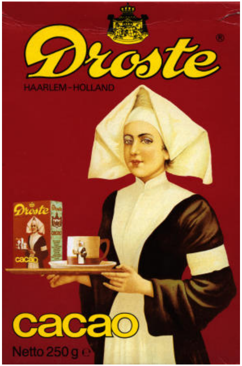
Listing 30: stack/stackols.py

```
def main():
    # Magic numbers
    sData= 'data/stackloss.csv'
    sY= 'Air Flow'
    asX= ['Water Temperature', 'Acid Concentration', 'Stack Loss']

    # Initialisation
    ...

    # Estimation
    ...

    # Output
    ...
```

NB: These steps are usually split into separate functions

The 'Droste effect'

- The program performs a certain function
- The main function is split in three (here)
- Each subtask is again a certain function that has to be performed



Apply the Droste effect:

- Think in terms of functions
- Analyse each function to split it
- Write in smallest building blocks

Preparation of program

What do you do for preparation of a program?

1. Turn off computer
2. On paper, analyse your inputs
3. Transformations/cleaning needed? Do it in a separate program...
4. With input clear, think about output: What do you want the program to do?
5. Getting there: What steps do you recognise?
6. Algorithms
7. Available software/routines
8. Debugging options/checks

Work it all out, before starting to type...

KISS

KISS

Keep it simple, stupid

Implications:

- Simple functions, doing one thing only
- Short functions (one-two screenfuls)
- With commenting on top
- Clear variable names (but not too long either; Hungarian)
- Consistency everywhere
- Catch bugs before they catch you

See also:

- `https://www.kernel.org/doc/Documentation/process/coding-style.rst` (General Kernel)
- `https://www.python.org/dev/peps/pep-0008/` (PEP 8: Python coding guide)

,

What is programming about?

> *Managing* DATA, *in the form of* VARIABLES, *usually through a set of predefined* FUNCTIONS *or* ACTIONS

Of central importance: Understand *variables*, *functions* at all times...

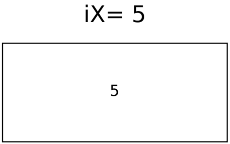
So let's exagerate

Variable

- A *variable* is an item which can have a certain *value*.
- Each variable has *one* value at each point in time.
- The value is of a specific *type*.
- A program works by managing *variables*, changing the *values* until reaching a final *outcome*

[Example: Paper integer 5]

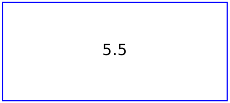
Integer



- An integer is a number without fractional part, in between -2^{31} and $2^{31} - 1$ (C/Ox/Matlab) or limitless (Python 3.X)
- Distinguish between the *name* and *value* of a variable.
- A variable can usually *change value*, but never *change its name*

Double

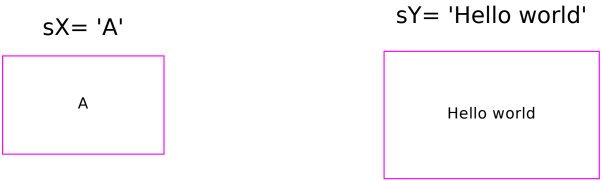
dX= 5.5



- A double (aka float) is a number with possibly a fractional part.
- Note that 5.0 is a double, while 5 is an integer.
- A computer is not ‘exact’, careful when comparing integers and doubles
- If you add a double to an integer, the result is double (in Python 3/Ox at least, language dependent)

[Example: `dAdd= 1/3; iD= 0; dD= iD + dAdd; type(dD)`]

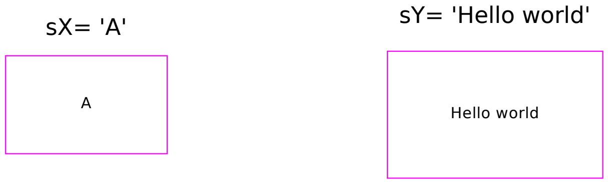
String



- A character is a string of length one.
- A string is a collection of characters.
- The ' are not part of the string, they are the *string delimiters*.
- One or multiple characters of a string are a string as well, `sY[0:4]`, `sY[1]`, `sY[1:2]` are strings.

[Example: `sY= 'Hello world'`]
Q: Trick question: What is difference between `sY[1]` and `sY[1:2]`?

String



- A character is a string of length one.
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- One or multiple characters of a string are a string as well, `sY[0:4]`, `sY[1]`, `sY[1:2]` are strings.

[Example: `sY= 'Hello world'`]

Q: Trick question: What is difference between `sY[1]` **and** `sY[1:2]`**?**

A: Check `sY[1] == sY[1:2]`

'Simple' types

- Boolean
- Integer
- Double/float
- String

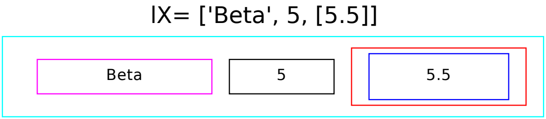
Check type using

```
bX= True
type(bX)
```

‘Difficult’ types

- List
- Tuple
- Matrix
- Function
- Lambda function
- DataFrame
- ...

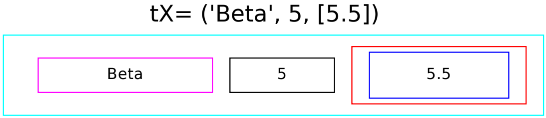
List



- A *list* is a collection of *other objects*.
- A list itself has one *dimension*, but can contain lists.
- An element of a list can be of any type (integer, double, function, matrix, list etc)
- A list of a list of a list has *three* dimensions etc.
- One may replace elements of a list (*a list is mutable*)

[Example: `lX= ['Beta', 5, [5.5]]; lX[0]= 'Alpha'`]

Tuple



- A *tuple* is a collection of *other objects*.
- A tuple itself has one *dimension*, but can contain lists.
- An element of a tuple can be of any type (integer, double, function, matrix, list, tuple etc)
- A tuple of a tuple of a tuple has *three* dimensions etc.
- One may **NOT** replace elements of a tuple (*a tuple is immutable*)

[Example:

```
tX= ('Beta', 5, [5.5]); # Error: tX[0]= 'Alpha' ]
```

Matrix

mX= np.array([[1.0, 2, 3], [4, 5, 6]])

1.0	2.0	3.0
4.0	5.0	6.0

- A *matrix* (to an Econometrician at least) is a collection of *doubles*; in Python a matrix may also contain other types.
- A matrix has (generally) two *dimensions*.
- A matrix of size $k \times 1$ or $1 \times k$ we tend to call a *vector*, `vX`
- Watch out: NumPy allows single-dimensional k vectors, different from $k \times 1$ matrices.
- Later on we'll see how matrix operations can simplify/speed up calculations.

Matrix II

mX= np.array([[1.0, 2, 3], [4, 5, 6]])

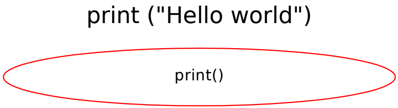
1.0	2.0	3.0
4.0	5.0	6.0

In Python:

- we'll use a list-of-lists as input into a NumPy array
- ensure we have doubles by making at least one of the entries a double (here: 1.0), `type(mX[1,2])`, or use `mX= np.array([[1,2,3], [4, 5, 6]]).astype(float)`
- if needed force it into a 2-dimensional shape, `mX.shape= (6, 1)`

[Example: `mX= np.array([[1.0, 2, 3], [4, 5, 6]])`]

Function



- A *function* performs a certain task, usually on a (number of) variables
- Hopefully the name of the function helps you to understand its task
- You can assign a function to a variable, `fnMyPrintFunction= print`

[Example: `fnMyPrintFunction('Hello world')`]

Function II

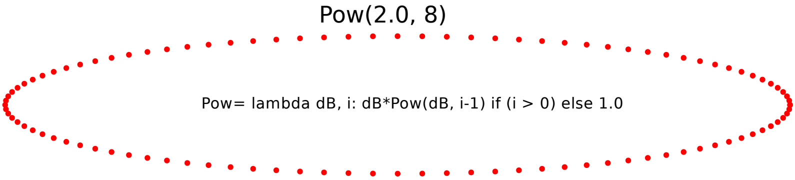
Listing 31: pow6.py

```
def Pow(dBase, iPow):
    dRes= 1
    i= 0
    while (i < iPow):
        # print ('i= ', i)
        dRes= dRes * dBase
        i+= 1
    return dRes
```

- You can define your own routines/functions
- You decide the output
- You tend to `return` the output
- (later: You may alter mutable arguments)

[Example: `dPow= Pow(2.0, 8)`]

Lambda Function



- A *lambda function* is a single line locally declared function
- It can access the present value of variables in the *scope*
- Hence it can *hide* passing of variables
- More details in the last lecture, when useful for optimising
- Syntax:

  `name=` **lambda** `arguments:  expression(arguments)`

Listing 32: pow_lambda.py

```
Pow= lambda dB,i: dB*Pow(dB,i-1) if (i > 0) else 1.0
dPow= Pow(2.0, 8)
```

List comprehension

Alternative to a *Lambda* function can be a *list comprehension*, in certain cases. A *list comprehension*

- applies a function successively on all items in a list
- and returns the list of results

Structure:

```
List = [ func(i) for i in somelist]
```

Examples:

```
[i for i in range (10)]
[i for i in range (10) if i%2 == 0]
[i**2 for i in range(10)]
[np.sqrt(mS2[i,i]) for i in range(iK)]
```

Q: Can you predict the outcome of each of these statements?

DataFrame

- A Pandas *dataframe* is an object made for input/output of data
- It can be used to read/store/show your data
- And has plenty more options
- Very useful for data handling!

[Example: `import pandas as pd; lc= list('ABC');`
`df= pd.DataFrame(np.random.randn(4,3), columns=lc); df`]

DataFrame II

Listing 33: stackols.py

```
sData= 'data/stackloss.csv'
sY= 'Air Flow'
asX= ['Water Temperature', 'Acid Concentration', 'Stack Loss']

# Initialisation
df= pd.read_csv(sData)          # Read csv into dataframe
vY= df[sY].values               # Extract y-variable
mX= df[asX].values              # Extract x-variables
iN= vY.size                     # Check number of observations
mX= np.hstack([np.ones((iN, 1)), mX])          # Append a vector of 1s
asX= ['constant']+asX

# Estimation
vBeta= np.linalg.lstsq(mX, vY)[0]              # Run OLS y= X beta + e

# Output
print ('Ols estimates')
print (pd.DataFrame(vBeta, index=asX, columns=['beta']))
```

View or copy

What does assignment do in Python? Check out this code:

view_copy.py

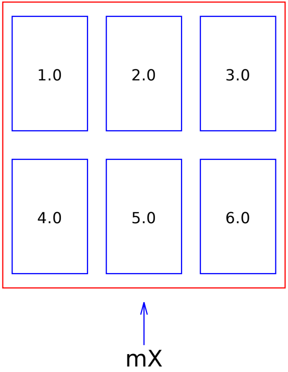
```
mX= np.arange(6)+1.0    # Get vector of numbers 1.0, 2.0, .., 6.0
print ('Shape :', mX.shape)
mX.shape= (2, 3)        # Assign TO shape characteristic
print ('Shape :', mX.shape)
print ('What is mX now?\n', mX)

mY= mX                  # New view of mX
mY[0, 0]= 0             # Change element of Y
print ('What is mX now, after changing element of Y?\n', mX)

mY= np.copy(mX)         # New copy of mX
mY[0, 0]= -1
print ('What is mX now, after re-copying y, putting a -1 in first location?\n', mX)
print ('What is mY now?\n', mY)
```

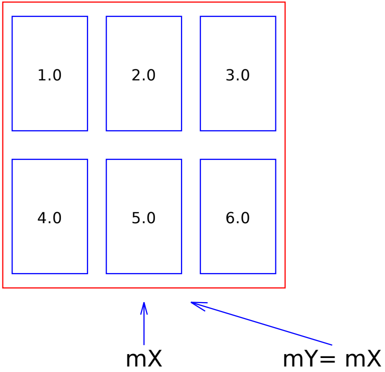
What happens here?

View or copy II



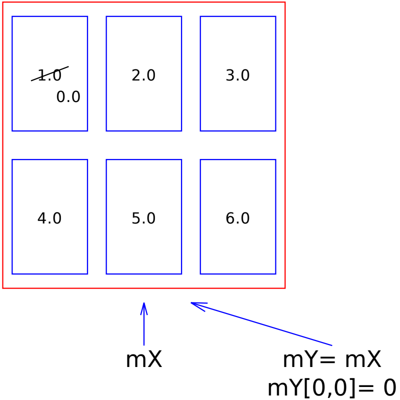
Step 1: Creating `mX`

View or copy II



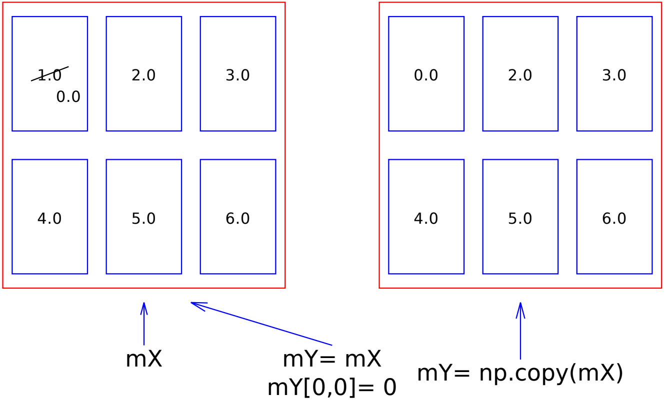
Step 2: Creating `mY= mX`, new *view* of *same matrix*

View or copy II



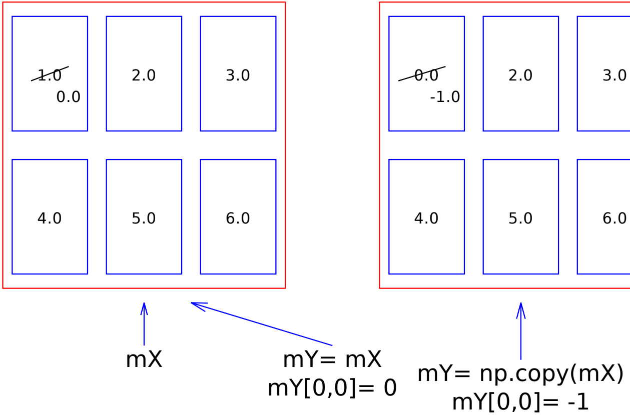
Step 3: Alter `mY[0,0]= 0` changes `mX` as well...

View or copy II



Step 4: Now explicitly copy over `mY= np.copy(mX)`

View or copy II



Step 5: Change `mY[0,0]= -1` leaves `mX` unaltered

View or copy III

How can I know whether I get a view or a copy?

```
print ('Is mX the same as mY? ', id(mX) == id(mY))
print ('id(mX)=%i, id(mY)=%i' % (id(mX), id(mY)))
```

Check the id...

View or copy III

How can I know whether I get a view or a copy?

```
print ('Is mX the same as mY? ', id(mX) == id(mY))
print ('id(mX)=%i, id(mY)=%i' % (id(mX), id(mY)))
```

Check the id...

What is the advantage of the 'view' of an object, not copying?

- Save memory, not having multiple copies of same (large) object
- Pass a (view to) a mutable object (ndarray/matrix/vector/dataframe) to a function, change *part* of it

View or copy IV

Change part of a matrix, output value through argument:

view_copy2.py

```
def FillRes(mRes):
    """
    Purpose:
        Perform (fake) calculating, filling mRes column by column

    Inputs:
        mRes    iR x iC matrix, to be overwritten

    Outputs:
        mRes    iR x iC matrix, filled by column

    Return value:
        dR      double, sum of all results
    """
    (iR, iC)= mRes.shape
    dR= 0.0
    for c in range(iC):
        vC= np.random.randn(iR)      # Do computations. Here: Get R random outcomes
        mRes[:,c]= vC
        dR+= vC.sum()

    return dR
```

Passing a ‘basket’ to function, allow change of contents of basket...

Basket: Mutable vs immutable

Python hands over a new 'view' of a list to a function. This implies:

- The function can access *the same* list/matrix/array/dataframe
- As long as it is careful not to replace the list, it can alter elements
- Replaced elements will be handed back to the main program, as such

Examples:

- `lX[1]= 'hello'`: Replace second list item by a new string
- `mX[0,4]= 3.14`: Replace element in row 1, column 5, by 3.14
- `mX[:,:]= mX * mX`: Replace all elements of existing matrix `mX` by their squares, keeping same 'basket'

Q: What is difference of last example, `mX[:,:]= mX * mX`, with `mX= mX * mX`?

Python and other languages

Concepts are similar

- Python (and e.g. Ox/Gauss/Matlab) have automatic typing. Use it, but carefully...
- C/C++/Fortran need to have types and sizes specified at the start. More difficult, but still same concept of variables.
- Precise manner for specifying a matrix differs from language to language. Python needs some getting used to, but is (very...) flexible in the end
- Remember: An element has a value and a name
- A program moves the elements around, hopefully in a smart manner

Keep track of your variables,
know what is their *type*, *size*, and *scope*

Python and other languages II

Concepts similar, implementation different:

- Python (and e.g. R, Julia) have object-like variables: Each variable has *characteristics*
- Python uses views of the data, often without copying, dangerous
- Powerful but sometimes confusing (see before)

Warning: Too much to discuss here, but dangerous implications... See e.g. https://medium.com/@larmalade/python-everything-is-an-object-and-some-objects-are-mutable-4f55eb2b468b

All languages

Programming is exact science

- Keep track of your variables
- Know what is their scope
- Program in small bits
- Program *extremely* structured
- Document your program wisely
- Think about algorithms, data storage, outcomes etc.

Further topics: Scope

Any variable is available only within the block in which it is declared.
In practice:

1. Arguments to a function, e.g. `mX` in `fnPrint( mX)`, are available within this function
2. A local variable `mY` is only known *below* its first use, within the present function
3. A global variable, indicated with `global g_mZ` at the start of a function, and retains its value between functions.

Further topics: Scope

Any variable is available only within the block in which it is declared.

In practice:

1. Arguments to a function, e.g. `mX` in `fnPrint( mX)`, are available within this function
2. A local variable `mY` is only known *below* its first use, within the present function
3. A global variable, indicated with `global g_mZ` at the start of a function, and retains its value between functions.

(but forget about globals... or use them the absolute minimum?)

Further topics: Scope II

Listing 34: scope_global.py

```
def localfunc():
    global g_sX
    print ("In localfunc: g_sX= ", g_sX)

    g_sX= "and goodbye"    # Change the full global variable

############################################################
### main
def main():
    global g_sX

    g_sX= "Hello"
    localfunc()
    print ("In main, after localfunc: g_sX= ", g_sX)
```

Rules for globals:

- Only use them when absolutely necessary (dangerous!)
- Annotate them, g_
- Fill them at *last possible moment*
- Do not change them afterwards (unless absolutely necessary)

Overview

Principles of Programming in Econometrics

D0: Syntax, example 2^8

D1: Structure, scope

D2: Numerics, packages

D3: Optimisation, speed

Day 2: Numerics and flow

- Numbers and representation
- Steps, flow and structure
- Floating point numbers
- Practical Do's and Don'ts
- Packages
- Graphics
- Practical
  - Cleaning OLS program
  - Loops
  - Bootstrap OLS estimation
  - Handling data: Inflation

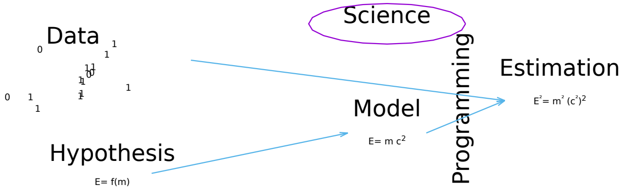
Reprise: What? Why?

Wrong answer:

For the fun of it

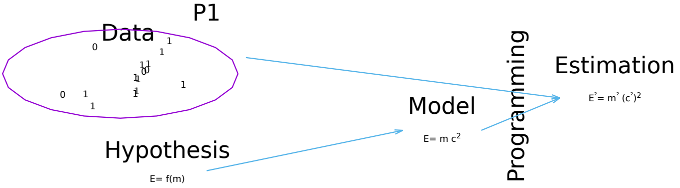
A correct answer

To get to the results we need, in a fashion that is controllable, where we are free to implement the newest and greatest, and where we can be 'reasonably' sure of the answers



Step P1: Analyse the data

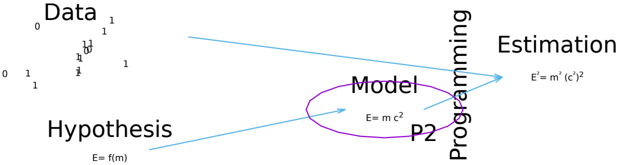
- Read the original data file
- Make a first set of plots, look at it
- Transform as necessary (aggregate, logs, first differences, combine with other data sets)
- Calculate statistics
- Save a file in a convenient format for later analysis




```
mData= np.hstack([vDate, mFX])
df= pd.DataFrame(mData, columns=["Date", "UKUS", "EUUS", "JPUS"])
df.to_csv("data/fx9709.csv")
df.to_csv("data/fx9709.csv.gz", compression="gzip")
df.to_excel("data/fx9709.xlsx")
```

Step P2: Analyse the model

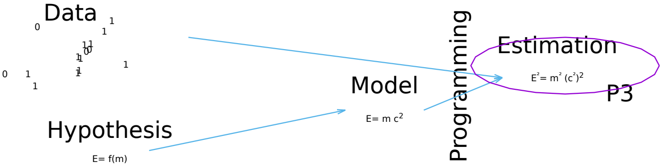
- Can you simulate data from the model?
- Does it look 'similar' to empirical data?
- Is it 'the same' type of input?




```
mU= np.random.randn(iT, 4);    # Log-returns US, UK, EU, JP factors
mF= np.cumsum(mU, axis=0);     # Log-factors
mFX= np.exp(mF[:,1:]-mF[:.0]);     # FX UK EU JP wrt US
```

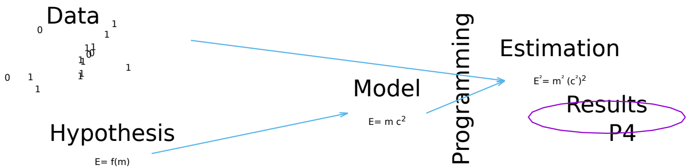
Step P3: Estimate the model

- Take input (either simulated or empirical data)
- Implement model estimation
- Prepare useful outcome



Step P4: Extract results

- Use estimated model parameters
- Calculate policy outcome etc.



Step P5: Output

- Create tables/graphs
- Provide relevant output

Often this is the hardest part: What exactly did you want to know? How can you look at the results? How can you go back to original question, is this really the (correct) answer?

Result of steps

```
def main():
    # Magic numbers
    sData= "data/fx0017.csv"             # Or use "data/sim0017.csv"
    asFX= ["EUR/USD","GBP/USD","JPY/USD"]
    vYY= [2000, 2015]                    # Years to analyse

    # Initialise
    (vDate, mRet)= ReadFX(asFX, vYY, sData)

    # Estimate
    (vP, vS, dLnPdf)= Estimate(mRet, asFX)
    mFilt= ExtractResults(vP, mRet)

    #Output
    Output(vP, vS, dLnPdf, mFilt, asFX)
```

- Short `main`
- Starts off with setting items that might be changed: Only up front in main (*magic numbers*)
- Debug one part at a time (`t.py`)!
- Easy for later re-use, if you write clean small blocks of code
- Input for estimation is *prepared* data file, not raw data (...).

Program flow

Programming is (should be) no magic:

- Read your program. There is only one route the program will take. You can follow it as well.
- Statements are executed in order, starting at `main()`
- A statement can call a function: The statements within the function are executed in order, until encountering a `return` statement or the end of the function
- A statement can be a *looping* or *conditional* statement, repeating or skipping some statements. See below.
- (The order can also be broken by `break` or `continue` statements. Don't use, ugly.)

And that is all, any program follows these lines.
(Sidenote: Objects/parallel programming etc)

Flow 2: Reading easily

As a general hint:

- Main .py file:
  - `import` packages
  - `import` your routines (see next page)
  - Contains only `main()`
  - Preferably only contains calls to routines (`Initialise, Estimate, Output`)
- Each routine: Maximum 30 lines / one page. If longer, split!

Flow 3: Using modules

A module *is a file containing a set of functions*

All content from module `incstack.py` in directory `lib` can be imported by

```
from lib.incstack import *
```

Result: Nice short `stackols3.py`

```
##########################################################
### main
def main():
    # Magic numbers
    ...
    # Initialisation
    (vY, mX)= ReadStack(sData, sY, asX, True)
    ...
```

Q: What would be the difference between `from lib.incstack import *` and `import lib.incstack`?

In Spyder:

- check current directory (`pwd`), make sure that you are in your working directory (use `cd` if need be)
- add general directory with modules to the `PYTHONPATH`, using Tools-PYTHONPATH manager

Flow 4: Cleaning out directory structure

Use structure for programming, and for storing results:

```
stack/stackols3.py            # Main routine
stack/lib/incstack.py         # Included functions
stack/data/stackloss.csv      # Data
stack/output/                 # Space for numerical output
stack/graphs/                 # Space for graphs
```

Ensure you program cleanly, make sure you can find routines/results/graphs/etc...

Precision

Not all numbers are made equal...
Example: What is $1/3 + 1/3 + 1/3 + ...$?

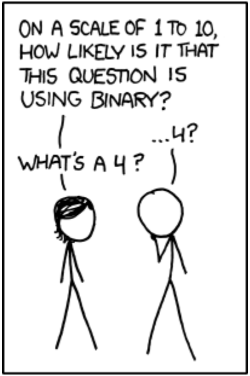
Listing 35: precision/onethird.py

```
def main():
    # Magic numbers
    dD= 1/3

    # Estimation
    print ("i j sum diff");
    dSum= 0.0
    for i in range(10):
        for j in range(3):
            print (i, j, dSum, (dSum-i))
            dSum+= dD       # Successively add a third
```

See outcome: It starts going wrong after 16 digits...

Decimal or Binary



1-to-10 (Source: XKCD, http://xkcd.com/953/)

Representation: Int

In many languages...

- Integers are represented exactly using 4 bytes/32 bits (or more, depending on system)
- 1 bit is for sign, usually 31 for number
- Hence range is `[-2147483648, 2147483647]`= `[-2^31, 2^31-1]`

Q: Afterwards, when `i= 2^31-1 + 1`, what happens?

Representation: Int

In many languages...

- Integers are represented exactly using 4 bytes/32 bits (or more, depending on system)
- 1 bit is for sign, usually 31 for number
- Hence range is `[-2147483648, 2147483647]=` `[-2^31, 2^31-1]`

Q: Afterwards, when `i= 2^31-1 + 1`**, what happens?** Answer:

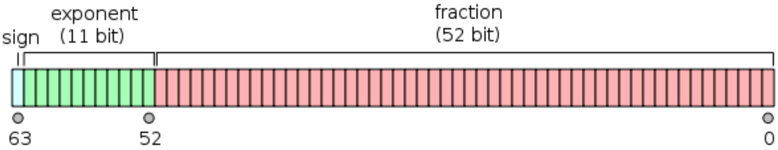
- Ox: Circles around to a negative integer, without warning...
- Matlab: Gets stuck at `2^31-1`...
- Python2: Uses 8 bytes, 64 bits. After $2^{63} - 1$, moves to *long* type, without limit
- Python3: *long* is the standard integer type, without any limit!

See `precision/intmax.py`, or `http://xkcd.com/571/`

Representation: Double

- Doubles are represented in 64 bits. This gives a total of $2^{64} \approx 1.84467 \times 10^{19}$ different numbers that can be represented.

How?



Double floating point format (Graph source: Wikipedia)

Split double in

- Sign (one bit)
- Exponent (11 bits)
- Fraction or mantissa (52 bits)

Representation: Double II

$$x = \begin{cases} (-1)^{\text{sign}} \times 2^{\text{exponent}-1023} \times \left(1 + \sum_{i=1}^{52} b_{52-i} 2^{-i}\right) & \text{Generally} \\ (-1)^{\text{sign}} \times 2^{1-1023} \times 0.\text{mantissa} & \text{if exp=0x.000} \\ (-1)^{\text{sign}} \times \infty & \text{if exp=0x.7ff, mant} = 0 \\ \text{NaN} & \text{if exp} = \text{0x.7ff, mant} \neq 0 \end{cases}$$

Note: Base-2 arithmetic

Sign	Expon	Mantissa	Result
0	0x.3ff	$0000\ 0000\ 0000_{16}$	$-1^0 \times 2^{(1023-1023)} \times 0.0$ $= 0$
0	0x.3ff	$0000\ 0000\ 0001_{16}$	$-1^0 \times 2^{(1023-1023)} \times 1.0000000000000000222$ $= 1.0000000000000000222$
0	0x.400	$0000\ 0000\ 0000_{16}$	$-1^0 \times 2^{(1024-1023)} \times 1.0$ $= 2$
0	0x.400	$0000\ 0000\ 0001_{16}$	$-1^0 \times 2^{(1024-1023)} \times 1.0000000000000000222$ $= 2.0000000000000000444$

Bit weird...

Consequence: Addition

Let's work in Base-10 arithmetic, assuming 4 significant digits:

Sign	Exponent	Mantissa	Result	x
$+$	4	0.1234	0.1234×10^4	1234
$+$	3	0.5670	0.5670×10^3	567

What is the sum?

Consequence: Addition

Let's work in Base-10 arithmetic, assuming 4 significant digits:

Sign	Exponent	Mantissa	Result	x
$+$	4	0.1234	0.1234×10^4	1234
$+$	3	0.5670	0.5670×10^3	567

What is the sum?

Sign	Exponent	Mantissa	Result	x
$+$	4	0.1234	0.1234×10^4	1234
$+$	4	0.0567	0.0567×10^4	567
$+$	4	0.1801	0.1801×10^4	1801

Shift to same exponent, add mantissas, perfect

Consequence: Addition II

Let's use dissimilar numbers:

Sign	Exponent	Mantissa	Result	x
$+$	4	0.1234	0.1234×10^4	1234
$+$	1	0.5670	0.5670×10^1	5.67

What is the sum?

Consequence: Addition II

Let's use dissimilar numbers:

Sign	Exponent	Mantissa	Result	x
$+$	4	0.1234	0.1234×10^4	1234
$+$	1	0.5670	0.5670×10^1	5.67

What is the sum?

Sign	Exponent	Mantissa	Result	x
$+$	4	0.1234	0.1234×10^4	1234
$+$	4	$0.0005\cancel{67}$	0.0005×10^4	5
$+$	4	0.1239	0.1239×10^4	1239

Shift to same exponent, add mantissas, lose precision...

Further consequence:

Add numbers of similar size together, preferably!

In Python/Ox/C/Java/Matlab/Octave/Gauss: 16 digits ($\approx$ 52 bits) available instead of 4 here

Consequence: Addition III

Check what happens in practice:

Listing 36: precision/accuracy.py

```
def main():
    dA= 0.123456 * 10**0
    dB= 0.471132 * 10**15
    dC= -dB

    print ("a: ", dA, ", b: ", dB, ", c: ", dC)
    print ("a + b + c: ", dA+dB+dC)
    print ("a + (b + c): ", dA+(dB+dC))
    print ("(a + b) + c: ", (dA+dB)+dC)
```

Consequence: Addition III

Check what happens in practice:

Listing 37: precision/accuracy.py

```
def main():
    dA= 0.123456 * 10**0
    dB= 0.471132 * 10**15
    dC= -dB

    print ("a: ", dA, ", b: ", dB, ", c: ", dC)
    print ("a + b + c: ", dA+dB+dC)
    print ("a + (b + c): ", dA+(dB+dC))
    print ("(a + b) + c: ", (dA+dB)+dC)
```

results in

```
a:  0.123456 , b:  471132000000000.0 , c:  -471132000000000.0
a + b + c:  0.125
a + (b + c):  0.123456
(a + b) + c:  0.125
```

Other hints

- Adding/subtracting tends to be better than multiplying
- Hence, log-likelihood $\sum \log \mathcal{L}_i$ is better than likelihood $\prod \mathcal{L}_i$
- Use true integers when possible
- Simplify your equations, minimize number of operations
- Don't do $x = \exp(\log(z))$ if you can escape it

Other hints

- Adding/subtracting tends to be better than multiplying
- Hence, log-likelihood $\sum \log \mathcal{L}_i$ is better than likelihood $\prod \mathcal{L}_i$
- Use true integers when possible
- Simplify your equations, minimize number of operations
- Don't do $x = \exp(\log(z))$ if you can escape it

(Now forget this list... use your brains, just remember that a computer is not exact...)

Do's and Don'ts

The do's:

+ Use commenting through DocString for each routine, consistent style, and inline comments elsewhere if necessary
+ Use consistent indenting
+ Use Hungarian notation throughout (exception: counters i, j, k, l etc)
+ Define clearly what the purpose of a function is: *One* action per function for clarity
+ Pass only necessary arguments to function
+ Analyse on paper before programming
+ Define debug possibilities, and use them
+ Order: Header – DocString – Code
+ Debug each bit (line...) of code after writing

Do's and Don'ts

The don'ts:

- Multipage functions
- Magic numbers in middle of program
- Use globals `g_vY` when not necessary
- Unstructured, spaghetti-code
- Program using 'write – write – write – debug'...
- Replicate code for similar tasks

import

Enlarging the capabilities of Python beyond basic capabilities: `import` Use through:

- `import package`: You'll have to use `package.func()` to access function `func()` from the package
- `import package as p`: You may use `p.func()` as shorthand
- `from package import func`: You can use `func()` directly, but no other functions from the package
- `from package import *`: You can use all functions from the package directly

Custom use:

```
import numpy as np                  # Shorten numpy to np
import pandas as pd                 # Etc...
import matplotlib.pyplot as plt
from lib.incmyfunc import *         # Get all my own functions directly
```

Python packages

Package	Purpose
numpy	Central, linear algebra and statistical operations
scipy	Additional scientific python routines
matplotlib.pyplot	Graphical capabilities
pandas	Input/output, data analysis
...	Many others...

Warning: Use packages, but with care. How can you ascertain that the package computes exactly what you expect? Do you understand?

Private modules

- Convenient to package routines into modules, for use from multiple (related) programs
- Stored in local project/lib directory, if only related to current project
- ... or stored at central python/lib directory: Use environment variable `PYTHONPATH` to tell Python where modules may be found; see Spyder – Tools – PYTHONPATH Manager

A module: matplotlib.pyplot

Several options available, here we focus on pyplot.

Listing 38: matplotlib/plot1.py

```
import matplotlib.pyplot as plt
import numpy as np

# Initialisation
mY= np.random.randn(100, 3)

# Output
plt.figure(figsize=(8,4))        # Choose alternate size (def= (6.4,4.8))
plt.subplot(2, 1, 1)             # Work with 2x1 grid, first plot
plt.plot(mY)                     # Simply plot the white noise
plt.legend(["a", "b", "c"])      # Add a legend
plt.title("White noise")         # ... and a title

plt.subplot(2, 1, 2)             # Start with second plot
plt.plot(mY[:,0], mY[:,1:], ".")  # Plot here some cross-plots
plt.ylabel("b,c")
plt.xlabel("a")
plt.title("Unrelated data")      # ... and name the graph
plt.savefig("graphs/plot1.png");    # Save the result
plt.show()                       # Done, show it
```

Details: matplotlib documentation, or e.g. Kevin Sheppard's Python Introduction

A module: matplotlib.pyplot II

Basic plot:

- Initialise the plot with `plt.figure()`
- (Optionally) also set the size with `plt.figure(figsize=(8,4))` (I prefer a wider shape)
- Graphing appears in *subplots*, choose i'th plot out of $R \times C$ using `plt.subplot(iR, iC, i)` (counting starts at 1, following matlab customs)
- Plot either y values against x-axis (`plt.plot(mY)`)
- ... or plot x against y, `plt.plot(mY[:,0], mY[:,1:])`

A module: matplotlib.pyplot III

Embellish plot:

- Place a legend for multiple lines using `plt.legend(['a', 'b', 'c'])`
- Alternatively, specify the label with the plot, `plt.plot(vY, label='y'); plt.legend()`. In the latter case, don't forget to turn on the legend.
- Plot takes extra arguments specifying line types, colours etc: `plt.plot(vX, vY, 'r+')` for red crosses
- *After* drawing the graph, and before showing it, possibly save the figure, as `.eps`, `.png`, `.pdf`, `.jpg`, `.svg` or others, `plt.savefig('graphs/plot1.png')`

A module: matplotlib.pyplot IV

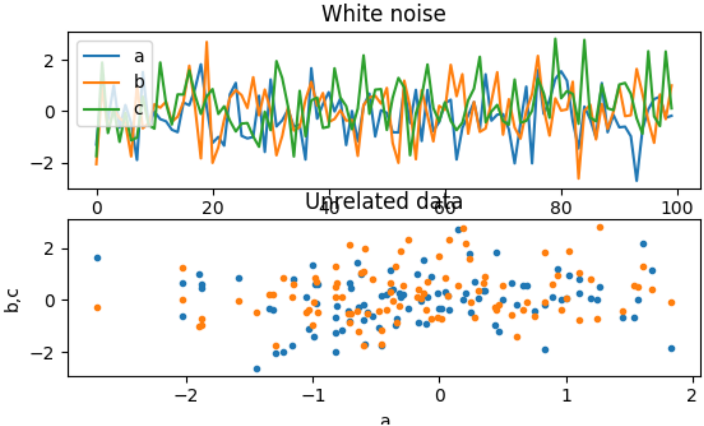


Figure: The resulting `plot1.png`

A module: matplotlib.pyplot V

All plotting is done against the last *figure* and/or *axes*. This one can make explicit as well:

Listing 39: matplotlib/plot1b.py

```
fig= plt.figure(figsize=(8, 6))          # Choose alternate size
ax=fig.add_subplot(2, 1, 1)              # Work with 2x1 grid, first plot
ax.plot(mY)                              # Simply plot the white noise
ax.legend(["a", "b", "c"])               # Add a legend
ax.set_title("White noise")              # ... and a title

ax2=fig.add_subplot(2, 1, 2)             # Start with second plot
ax2.plot(mY[:,0], mY[:,1:], ".")         # Plot here some cross-plots
ax2.set_ylabel("b,c")
ax2.set_xlabel("a")
ax2.set_title("Unrelated data")          # ... and name the graph
fig.savefig("graphs/plot1b.png")         # Save the result
fig.show()                               # Done, show figure
```

A module: matplotlib.pyplot + LaTeX

For inclusion in LaTeX, true formulas might be nice.
Example:

Listing 40: plot_latex.py

```
plt.rc('text', usetex=True)     # Start using latex text

plt.figure()
plt.plot(mY, '.')                    # Simply plot the white noise, with dots
plt.legend([r'$E=m C^2$', r'$s=\sum_{i=1}^n y_j$'])          # Add a legend
plt.title(r'Use \textbf{(most)} \LaTeX\ commands {\em at will}')
plt.savefig('graphs/plot_latex1.png')
plt.show()
```

Note: Without the `usetex=True`, you can still use simple LaTeX commands, but get different fonts.

A module: matplotlib.pyplot + LaTeX II

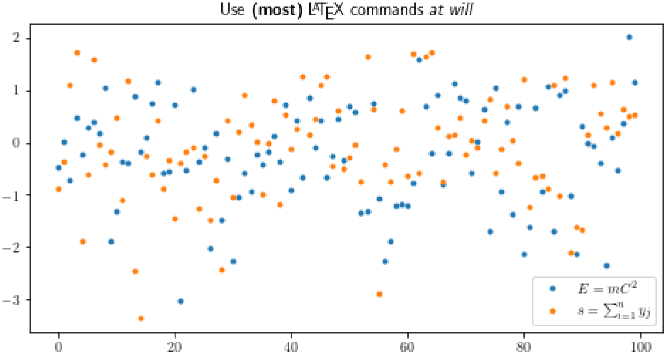


Figure: The resulting `plot_latex1.png`

A module: matplotlib.pyplot + ???

Other options:

- Zillions...
- Check the examples
- Use google, get some practice!

A module: Pandas

Extensive set of data analytics and data handling routines, Pandas.
Goal:

- Loading/saving
- Indexing/selecting
- Manipulating
- ...

A module: Pandas

Extensive set of data analytics and data handling routines, Pandas.
Goal:

- Loading/saving
- Indexing/selecting
- Manipulating
- ...
- Printing nicely
- Plotting
- and other?

Initialisation:

```
import pandas as pd
```

Pandas Types

From Pandas we'll use two types:

- `DataFrame`: matrix-like format, with row `index` and `columns` names
- `Series`: vector-like format, with row `index` and `name`

```
import pandas as pd

sData= 'shoesize_bk2020'

# Initialisation
df= pd.read_csv('data/%s.csv' % sData)      # DataFrame
sf= df['Gender']                            # Series

print ('Type df: %s\nType sf: %s' % (type(df), type(sf)))
```

NB: Normally, work with the DataFrame itself... Not much use to extract the separate series

Pandas Types II

Instead of reading data into a DataFrame, we can also create one based on data:

```
dfR= pd.DataFrame(np.random.randn(10,4), columns=['a', 'b', 'c', 'd'])
print (dfR)
print (dfR.to_latex(float_format='%.4f'))
```

Why?

- To store a set of results, in a convenient dataframe
- Also, to print them in a clean format (even as LaTeX)

Pandas Input files

Reading files: Use `df= pd.read_...` with

- `csv`: Clean input, easy to check in editor or excel, but large in size
- `excel`: Convenient, but a bit dangerous as each version of excel behaves differently
- `csv.gz`: Gzipped csv, smaller
- `hdf, pickle, ...`: Many formats available

Extra options (and many others):

- CSV: `skiprows=8`, `sep=';'`, for choosing to skip some input, or indicate the separator
- Excel: `sheet_name='Sheet 2'`, `usecols=[0, 3, 4]`, for choosing specific sheet, or only some columns
- with both: `index_col=['Year', 'Period']`, to indicate what column(s) will be the index

Pandas elements

Check the contents of the DataFrame and Series, either printing all, or only the `.head()` or `.tail()`:

```
print ('Head of df: \n', df.head(), sep='')
print ('Tail of sf:\n', sf.tail(), sep='')
```

resulting in

```
Head of df:
    Shoesize  Length  Gender
0       45.0   187.0    Male
1       40.0   180.0  Female
2       45.0   185.0    Male
3       43.0   185.0    Male
4       43.0   174.0    Male
```

```
Tail of sf:
114     Male
115     Male
116     Male
117     Male
118     Male
Name: Gender, dtype: object
```

Notice: `index 0, .., 118`, columns `Shoesize, Length, Gender`, `Name: Gender`

Pandas: Information

Check out the contents of the data with e.g.

- `df.head()`, `df.tail()`, `df`: Either show a part, or the full data frame (or a limited number of rows and columns, that is)
- `df.mean()`, `df.var()`, `df.min()`, `df.max()`: Find the mean/var/min/max over the columns
- `df.info()`, `df.describe()`: More detailed information on the contents
- `df.shape`, `df.size`: What shape (rows $\times$ columns) or size (number of elements) is it?
- `df.index`, `df.columns`: What are the row/column indices?
- ...

and especially:

- `df.values`: Extract the *values* from the dataframe, as a numpy matrix...!

Pandas: Indexing

Different methods:

`asC= ['Shoesize', 'Length']; asR= range(4, 8)`

`df[asC]`	Select *columns* by name
`vI= df['Gender'] == 'Male'; df[vI]`	Select *rows* by boolean masking
`df.loc[asR,:]`	Select rows by index, all columns
`df.loc[asR, asC]`	Subset of rows and columns
`df.iloc[8, 2]`	Read out single element, indexed column location
`df.iloc[vR, vC]`	Subset of rows and columns, in ranges

Remarks:

- Needs practice...
- I regularly move to a `NumPy` matrix/array, leaving DataFrames only for input/output

Pandas: Advanced indexing I

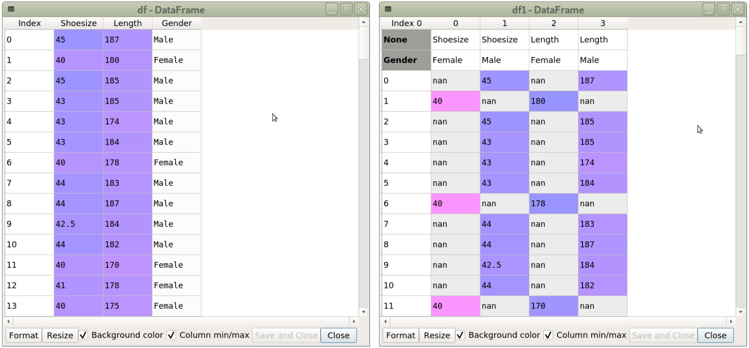
What if I want to find the average length of the males?

a. Index, find only the males: `vI= df['Gender'] == 'Male'; dfM= df[vI]; dfM['Length'].mean()`
b. Move to *wide* instead of *long* table...

Definition:

- Long format: All subjects are placed one below the other, with observations on the necessary variables in a single row
- Wide format: Observations on several types of subjects may be placed next to eachother, for the same *index*

Pandas: Long vs wide



Index	Shoesize	Length	Gender
0	45	187	Male
1	40	180	Female
2	45	185	Male
3	43	185	Male
4	43	174	Male
5	43	184	Male
6	40	178	Female
7	44	183	Male
8	44	187	Male
9	42.5	184	Male
10	44	182	Male
11	40	170	Female
12	41	178	Female
13	40	175	Female

Index 0	0	1	2	3
None	Shoesize	Shoesize	Length	Length
Gender	Female	Male	Female	Male
0	nan	45	nan	187
1	40	nan	180	nan
2	nan	45	nan	185
3	nan	43	nan	185
4	nan	43	nan	174
5	nan	43	nan	184
6	40	nan	178	nan
7	nan	44	nan	183
8	nan	44	nan	187
9	nan	42.5	nan	184
10	nan	44	nan	182
11	40	nan	170	nan

Long vs. wide table

```
df1= df.pivot(columns='Gender', values=['Shoesize', 'Length'])
df1[asC].mean()        # Give means of both values, per Gender
```

Here: Not too useful. But what about data with observations for each month/quarter/half year?

Pandas: Advanced indexing II

With pivoted table, one gets to MultiIndex tables:

```
In [74]:  df1.columns
Out[74]: MultiIndex([('Shoesize', 'Female'),
                      ('Shoesize',   'Male'),
                      (  'Length', 'Female'),
                      (  'Length',   'Male')],
                    names=[None, 'Gender'])
```

Or: Index contains both variable name and pivot value, in a *tuple*.
Hence: Select a single column with a *tuple* etc:

```
df1[('Shoesize', 'Male')].mean()     # Single mean
df1['Shoesize'].mean()               # Both Female and Male means
```

Warning: Do try this at home... Options, way to work with MultiIndex, takes *lots* of practice...

Pandas: Saving

With data, you also want to save... Options: Many...
Personal preference (with e.g. `sData='shoesize_bk2020'`):

1. `df.to_csv('data/%s_out.csv' % sData)`: Clean csv file, easy to read in editor or excel, robust
2. `df.to_csv('data/%s_out.csv.gz' % sData)`: Clean csv file, but gzipped: Smaller, quite easy to read in editor or excel
3. `df.to_excel('data/%s_out.xlsx' % sData)`: Pure excel file (but with limits on number of columns/rows!)
4. `df.to_excel('data/%s_out.ods' % sData)`: Pure OpenDocument format file (but with limits on number of columns/rows!)

Pandas: Saving II

Extra options for saving:

- `df.to_...(sOut, index=False)`: Do not write the index column along (sometimes not informative)
-
  `df.to_excel(sOut, sheet_name='BK2020 shoe sizes vs leng`

(and many others... Do check the excellent reference guide at as well!)

Pandas: Plotting

Plotting is a separate chapter, with too many details to cover here.
Hence an example:

```
df.plot.area(figsize=(8,4))
df.plot.area(subplots=True)
df.plot.density(subplots=True)

plt.figure(figsize=(8,4))
df.plot.box()
plt.savefig('graphs/shoesize_box')
plt.show()
```

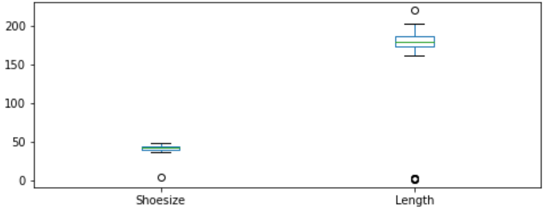


Figure: Shoesize and length of 2020 class of BK Statistics

Pandas: Printing

And at last, the printing: Often, I write results as a DataFrame, as in

Listing 41: pandas_print.py

```
vP0= np.array([0.5, 1, 4])
vP= np.array([0.745, .986, 3.74])
vS= np.array([.045, .062, .254])
asR= ['B0', 'B1', 's2']
asC= ['p0', 'pHat', 'sHat']
mRes= np.vstack([vP0, vP, vS]).T        # Stack underneath, transpose
df= pd.DataFrame(mRes, index=asR, columns=asC)

print ("Simply printing the dataframe:")
print (df)
print ("\nPrinting the dataframe towards LaTeX:")
print (df.to_latex(float_format='%6.3f'))
```

Pandas: Other

And further?

- Unimaginable, what Pandas may do for you
- Do check the manuals, great
- Prediction: Your usage of Pandas may explode, once you get hooked...

Overview

Principles of Programming in Econometrics

D0: Syntax, example 2^8

D1: Structure, scope

D2: Numerics, packages

D3: Optimisation, speed

Day 3: Optimisation

- Optimization (`minimize`)
  - Idea behind optimization
  - Gauss-Newton/Newton-Raphson
  - Stream/order of function calls
- Standard deviations
- Restrictions
- Speed
- Practical
  - Regression: Maximize likelihood
  - GARCH-M: Intro and likelihood

Optimisation

Doing Econometrics $\equiv$ estimating models, e.g.:

1. Optimise likelihood
2. Minimise sum of squared residuals
3. Minimise difference in moments
4. Solving utility problems (macro/micro)
5. Do Bayesian simulation, MCMC

Options 1-3 evolve around

$$\hat{\theta} = \underset{\theta}{\operatorname{argmin}} f(y;\theta), \qquad f(y;\theta) : \Re^p \to \Re$$

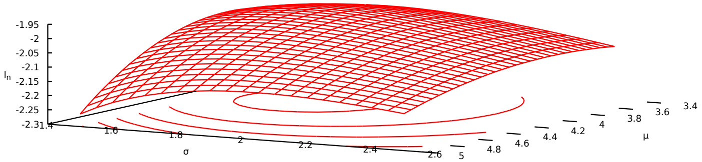
Option 4 evolves around

$$r(y;\hat{\theta}) \equiv \mathbf{0}, \qquad r(y;\theta) : \Re^p \to \Re^p$$

Example

For simplicity: Econometrics example, ...

$$\bar{l}(y;\theta) = -\frac{1}{2n}\sum_{i=1}^{n}\left(\log 2\pi + \log\sigma^2 + \frac{(y_i-\mu)^2}{\sigma^2}\right)$$

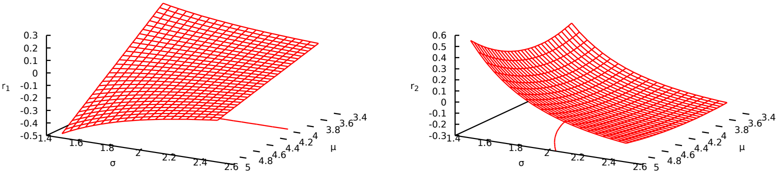


Relatively simple function to optimize, but how?

Example II

... translated to Macro/Micro solving equations

$$r(y;\theta) \equiv \frac{\partial \bar{l}(y;\theta)}{\partial \theta} = \begin{pmatrix} \frac{1}{n\sigma^2}\sum(y_i - \mu) \\ -\frac{1}{\sigma} + \frac{\sum(y_i-\mu)^2}{n\sigma^3} \end{pmatrix}$$



Score = derivative of (avg) loglikelihood $\bar{l}(y;\theta)$, $\Re^2 \to \Re^2$

Crawling up a hill

Step back and concentrate:

- Searching for

$$\hat{\theta} = \text{argmin}_\theta\, f(y;\theta) = \text{argmax}_\theta - f(y;\theta)$$

- How would you do that?

Crawling up a hill

Step back and concentrate:

- Searching for

$$\hat{\theta} = \text{argmin}_\theta\, f(y;\theta) = \text{argmax}_\theta\, -f(y;\theta)$$

- How would you do that?
- Imagine Alps:
  a. Step outside hotel
  b. What way goes up?
  c. Start Crawling up a hill
  d. Continue for a while
  e. If not at top, go to b.

Use function characteristics

Translate to mathematics:

a. Set $j = 0$, start in some point $\theta^{(j)}$
b. Choose a direction s
c. Move distance α in that direction, $\theta^{(j+1)} = \theta^{(j)} + \alpha s$
d. Increase j, and if not at top continue from b

Direction s: Linked to gradient?
Minimum: Gradient 0, second derivative *positive* definite?
(Maximum: Gradient 0, second derivative *negative* definite?)

Ingredients

Inputs are

- f, use (*negative*) *average log* likelihood, or *average* sum-of-squares;
- Starting value $\theta^{(0)}$;
- Possibly $g = f'$, analytical first derivatives of f;
- (and possibly $H = f''$, analytical second derivatives of f).

Ingredients

Inputs are

- f, use (*negative*) *average log* likelihood, or *average* sum-of-squares;
- Starting value $\theta^{(0)}$;
- Possibly $g = f'$, analytical first derivatives of f;
- (and possibly $H = f''$, analytical second derivatives of f).

or

- r, use set of equations, if necessary *scaled*;
- Starting value $\theta^{(0)}$;
- If available $J = r'$, analytical Jacobian of r

Ingredients II (optimize)

$$f(\theta) : \Re^p \rightarrow \Re \qquad \text{Function, scalar}$$

$$f'(\theta) = \left[\frac{\partial f(\theta)}{\partial \theta_1}, \ldots, \frac{\partial f(\theta)}{\partial \theta_p}\right]^T \equiv g \qquad \text{Derivative, gradient, } p \times 1$$

$$f''(\theta) = \left[\frac{\partial^2 f(\theta)}{\partial \theta_i \partial \theta_j}\right]_{i,j=1}^p \equiv H \qquad \text{Second derivative, Hessian, } p \times p$$

If derivatives are continuous (as we assume), then

$$\frac{\partial^2 f(\theta)}{\partial \theta_i \partial \theta_j} = \frac{\partial^2 f(\theta)}{\partial \theta_j \partial \theta_i} \qquad H = H^T$$

Hessian symmetric

Ingredients III (solve)

$$
\begin{aligned}
r(\theta) &: \Re^p \rightarrow \Re^p && \text{Function, } p \times 1 \\
r'(\theta) &= \left[\frac{\partial r(\theta)}{\partial \theta_1}, \ldots, \frac{\partial r(\theta)}{\partial \theta_p}\right] \equiv J && \text{Derivative, Jacobian, } p \times p
\end{aligned}
$$

No reason for Jacobian to be symmetric

Newton-Raphson for minimisation

- Approximate $f(\theta)$ locally with quadratic function

$$f(\theta + h) \approx q(h) = f(\theta) + h^T f'(\theta) + \frac{1}{2} h^T f''(\theta) h$$

- Minimise $q(h)$ (instead of $f(\theta + h)$)

$$q'(h) = f'(\theta) + f''(\theta)h = 0 \Leftrightarrow f''(\theta)h = -f'(\theta) \text{ or } Hh = -g$$

  by solving last expression, $h = -H^{-1}g$
- Set $\theta = \theta + h$, and repeat as necessary

Problems:

- Is H positive definite/invertible, at each step?
- Is step h, of length $||h||$, too big or small?
- Do we converge to true solution?

Newton-Raphson for solving equations

- Approximate $r(y;\theta)$ locally with linear function

$$r(\theta + h) \approx q'(h) = r(\theta) + r'(\theta)h$$

- Solve $q'(h) = \mathbf{0}$ (instead of $r(\theta + h) = \mathbf{0}$)

$$q'(h) = r(\theta) + r'(\theta)h = \mathbf{0} \Leftrightarrow r'(\theta)h = -r(\theta) \text{ or } Jh = -r$$

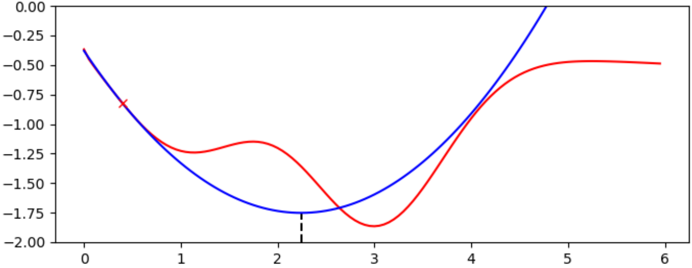
  by solving last expression, $h = -J^{-1}r$

- Set $\theta = \theta + h$, and repeat as necessary

Problems:

- Is J ~~positive definite~~/invertible, at each step?
- Is step h, of length $||h||$, too big or small?
- Do we converge to true solution?

Newton-Raphson II



$$f(\theta) = -e^{-(\theta-1)^2} - 1.5e^{-(\theta-3)^2} - .2\sqrt{\theta}$$

- How does the algorithm converge?
- Where does it converge to?

`ipython np_newton_show2, theta= 5.9/1/0.1/0.4`

Problematic Hessian?

Algorithms based on NR need $H_j = f''(\theta^{(j)})$. Problematic:

- Taking derivatives is not stable (...)
- Needs many function-evaluations
- H not guaranteed to be positive definite

Problem is in step

$$s_j = -{H_j}^{-1} g_j \approx -M_j g_j$$

Replace ${H_j}^{-1}$ by some M_j, positive definite by definition?

BFGS

Broyden, Fletcher, Goldfarb and Shanno (BFGS) thought of following trick:

1. Start with $j = 0$ and positive definite M_j, e.g. $M_0 = I$
2. Calculate $s_j = -M_j g_j$, with $g_j = f'(\theta^{(j)})$
3. Find new $\theta^{(j+1)} = \theta^{(j)} + h_j, h_j = \alpha s_j$
4. Calculate, with $q_j = g_j - g_{j+1}$

$$M_{j+1} = M_j + \left(1 + \frac{q_j' M_j q_j}{h_j' q_j}\right) \frac{h_j h_j'}{h_j' q_j} - \frac{1}{h_j' q_j} \left(h_j q_j' M_j + M_j q_j h_j'\right)$$

Result:

- No Hessian needed
- Still good convergence
- No problems with negative definite H_j

⇒ `scipy.optimize.minimize(method="BFGS", ...)` in Python, similar routines in Ox/Matlab/Gauss/other.

Inputs

Inputs could be

- f, use (*negative*) *average log* likelihood, or *average* sum-of-squares.
- Starting value θ_0
- Possibly f', analytical first derivatives of f.

$$\hat{\theta} = \underset{\theta}{\operatorname{argmin}}\ f(y;\theta), \qquad f(y;\theta) : \Re^p \to \Re$$

Or one could need

- Set of conditions to be solved,
- preferably nicely scaled,

$$r(y;\hat{\theta}) \equiv \mathbf{0}, \qquad r(y;\theta) : \Re^p \to \Re^p$$

Model

$$y_i \sim \mathcal{N}(X_i \beta, \sigma^2)$$

ML maximises (log-)likelihood (other options: Minimise sum-of-squares, optimise utility etc):

$$L_i(y_i; \theta) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_i - X_i\beta)^2}{2\sigma^2}\right)$$
$$L(y; \theta) = \prod_i L_i(y_i; \theta)$$

In this case, e.g. $\theta = (\sigma, \beta)$

Function f

Write towards function f, to *minimise*:

$$\log L_i(y_i;\theta) = -\frac{1}{2}\left(\log 2\pi + \log \sigma^2 + \frac{1}{\sigma^2}(y_i - X_i\beta)^2\right)$$

$$f(y, X;\theta) = -\frac{1}{n}\sum \log L_i(y_i;\theta)$$

For testing:

- Work with generated data, e.g. $n = 100, \beta =< 1, 1, 1 >', \sigma = 1, X = [1, U_2, U_3], y = X\beta + \epsilon, \epsilon \sim \mathcal{N}(0, \sigma^2)$
- Ensure you have the data...

Function r

Remember solving $r(y;\theta) \equiv \mathbf{0}$? One could take $r(y;\theta) = g(y;\theta) = f'(y;\theta)$,

$$
\begin{aligned}
f(y, X;\theta) &= \frac{1}{2}\left(\log 2\pi + \log\sigma^2 + \frac{1}{n\sigma^2}\sum(y_i - X_i\beta)^2\right) \\
e &= y - X\beta \\
\frac{\partial f(y;\theta)}{\partial\beta} &= ... \\
\frac{\partial f(y;\theta)}{\partial\sigma} &= ...
\end{aligned}
$$

- In this case, it matters whether $\theta = (\sigma, \beta)$, or $\theta = (\beta, \sigma)$, or even $\theta = (\beta, \sigma^2)$!
- Find score of NEGATIVE AVERAGE loglikelihood

(and for now, first concentrate of f, afterwards we'll fill in r)

Comments of function

Listing 42: estnorm.py

```
#################################################################
### vLL= LnLRegr(vP, vY, mX)
def LnLRegr(vP, vY, mX):
    """
    Purpose:
        Compute loglikelihood of regression model

    Inputs:
        vP      iK+1 vector of parameters, with sigma and beta
        vY      iN vector of data
        mX      iN x iK matrix of regressors

    Return value:
        vLL     iN vector, loglikelihood
    """
```

Note: Full set of inputs including data. Parameters `vP` and `vY` both in *1D vector*, `mX` as *2D matrix*.

Body of function

Listing 43: estnorm.py

```
def LnLRegr(vP, vY, mX):
    (iN, iK)= mX.shape
    if (np.size(vP) != iK+1):         # Check if vP is as expected
        print ("Warning: wrong size vP= ", vP)

    (dSigma, vBeta)= (vP[0], vP[1:])  # Extract parameters
    ...
    return vLL
```

Body of function II

and fill in the remainder

Listing 44: estnorm.py

```
def LnLRegr(vP, vY, mX):
    ...
    vE= vY - mX @ vBeta
    vLL= -0.5*(np.log(2*np.pi) + 2*np.log(dSigma) + np.square(vE/dSigma))

    print (".", end="")             # Give sign of life

    return vLL
```

Intermezzo: On robustness

WARNING:

- Check sizes of arguments to LL `LnLRegr` function carefully...
- Both y and θ should be *1D* vectors, not *2D* columns
- Calculate LL per observation
- Possibly, alternative: Return `dLL= np.sum(vLL, axis= 0)`, *explicitly along axis 0*, instead.

What could go wrong?

Intermezzo: On robustness II

What could go wrong?

```
iN= 10; dSigma= 1;
vBeta= np.array([1, 1, 1])     # 1D array
iK= vBeta.size
vY= np.random.randn(iN, 1)     # 2D array, breaking rule!
mX= np.random.rand(iN, iK)     # 2D array
vE= vY - mX@vBeta              # 2D array, shape (iN, iN)!
vLL= -0.5*(np.log(2*np.pi) + 2*np.log(dSigma) + np.square(vE/dSigma))
dLL1= np.sum(vLL)            # No error, nice scalar, but WRONG
dLL2= np.sum(vLL, axis=0)    # No error, but 1D (iN,) vector, detectable
print ("Shape dLL1: ", dLL1.shape)
print ("Shape dLL2: ", dLL2.shape)
```

Watch out: The above `np.sum(vLL)` takes, without error, the sum over a full matrix...
Instead, force `np.sum(vLL, axis=0)` to take sum over the first axis! Watch out with shapes/dimensions

... And optimize? NO!

Before you continue: Check the loglikelihood

- Does it work at all?
- Is the total/average LL higher for a ‘good’ set of parameters, low for ‘bad’ parameters?
- Is it reasonably efficient?
- How does it react to incorrect *shape* of parameters/data?
- How does it react to incorrect parameters ($\sigma \leq 0$)?

... And optimize? NO!

Before you continue: Check the loglikelihood

- Does it work at all?
- Is the total/average LL higher for a 'good' set of parameters, low for 'bad' parameters?
- Is it reasonably efficient?
- How does it react to incorrect *shape* of parameters/data?
- How does it react to incorrect parameters ($\sigma \leq 0$)?

Latter question, several options:

1. Don't allow it, set `dSigma= np.fabs(vP[0])`
2. Flag that things go wrong: `if (dSigma <= 0):  return -math.inf * np.ones(iN)`
3. Use *constrained* optimisation, e.g. Sequential Least SQuares Programming (SLSQP)

Minimize: Syntax

(In Python) Function to minimize should have a format

```
dF= fnFunc(vP)
dF= fnFunc(vP, a, b, c)      # Alternative, not used in this document
```

where `a, b, c` are some optional parameters, not used by Python

- Choose your own logical function name
- `vP` is a p **1-dimensional** array with parameters
- `dF` is the function value, or a missing/∞ if function could not be evaluated

See the manual of SciPy's optimize functions

Minimize: Syntax II

No space for data? Negative average LL instead of LL per observation? Use local `Lambda` function, providing the function to minimize as

Listing 45: estnorm.py

```
# Create lambda function returning NEGATIVE AVERAGE LL, as function of vP only
AvgNLnLRegr= lambda vP: -np.mean(LnLRegr(vP, vY, mX), axis=0)
```

Advantage:

- Simply return the negative average of your previously prepared function
- Value of data `vY, mX` at moment of call is passed along
- No globals needed!

Alternative: Construct function `AvgNLnLRegrXY(vP, vY, mX)`, and call `opt.minimize(AvgNLnLRegr, vP0, args=(vY, mX), method="BFGS")`

Minimize: Syntax III

Call `scipy.opt.minimize()` according to

```
import scipy.optimize as opt
...
res= opt.minimize(fnFunc, vP0, method="BFGS")
```

- `fnFunc` is the name of the function
- `vP0` is a 1D array of initial parameters
- `method="BFGS"` indicates we want to use this method for optimisation

The return value `res` is a structure containing results.

Minimize: Syntax IV

After optimisation:

- Always check the outcome:

```
res= opt.minimize(AvgNLnLRegr, vP0, method="BFGS")

vP= np.copy(res.x)         # For safety, make a fresh copy
sMess= res.message
dLL= -iN*res.fun
print ("\nBFGS results in ", sMess, "\nPars: ", vP, "\nLL= ", dLL)
# print ("Full results: ", res)
```

- Possibly start thinking of *using* the outcome (standard errors, predictions, policy evaluation, robustness ...)

Optimisation

Approach for general *criterion function* $f(y;\theta)$: Write

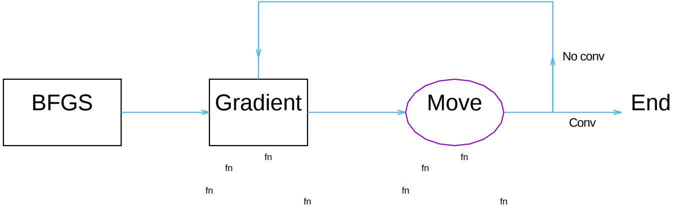
$$
\begin{aligned}
f(\theta+h) \approx q(h) &= f(\theta) + h^T g(\theta) + \frac{1}{2} h^T H(\theta) h \\
g(\theta) &= \frac{\partial}{\partial\theta} f(y;\theta) \\
H(\theta) &= \frac{\partial^2}{\partial\theta\partial\theta'} f(y;\theta)
\end{aligned}
$$

Optimise approximate $q(h)$:

$$
\begin{aligned}
g(\theta) + H(\theta)h &= 0 && \text{First order conditions} \\
\Leftrightarrow \theta^{\text{new}} &= \theta - H(\theta)^{-1} g(\theta)
\end{aligned}
$$

and iterate into oblivion.

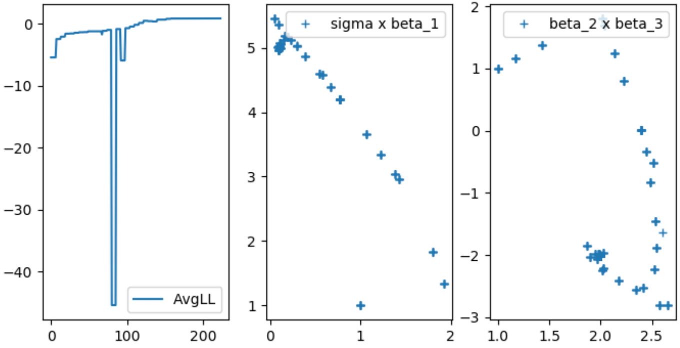
opt.minimize(method="BFGS"): Program flow



Flow:

1. You call `opt.minimize(..., method="BFGS")`
2. ... which calls `Gradient`
3. ... which calls your function, multiple times.
4. Afterwards, it makes a move, choosing a step size
5. ... by calling your function multiple times,
6. ... and decides if it converged.
7. If not, repeat from 2.

BFGS: Program flow II



Check out `estnorm_plot.py` ($p = 3, n = 100$)

Minimize: Average

Why use average loglikelihood?

1. Likelihood function $L(y; \theta)$ tends to have tiny values $\rightarrow$ possible problem with precision
2. Loglikelihood function $\log L(y; \theta)$ depends on number of observations: Large sample may lead to large $|\text{LL}|$, not stable
3. Average loglikelihood tends to be moderate in numbers, well-scaled...

Better from a numerical precision point-of-view.
Warning:

Take care with score and standard errors (see later)

Minimize: Average

Why use average loglikelihood?

1. Likelihood function $L(y;\theta)$ tends to have tiny values $\rightarrow$ possible problem with precision
2. Loglikelihood function $\log L(y;\theta)$ depends on number of observations: Large sample may lead to large $|\text{LL}|$, not stable
3. Average loglikelihood tends to be moderate in numbers, well-scaled...

Better from a numerical precision point-of-view.
Warning:

Take care with score and standard errors (see later)

Warning 2:

Average is only for numerical *reasons — always report full loglikelihood among outcomes*

Minimize: Precision

Optimisation is said to be successfull if (roughly):

1. $||g^{(j)}(\theta^{(j)})|| \leq g_{\text{tol}}$, with $g^{(j)}$ the score at $\theta^{(j)}$, at iteration j: Scores are relatively small.

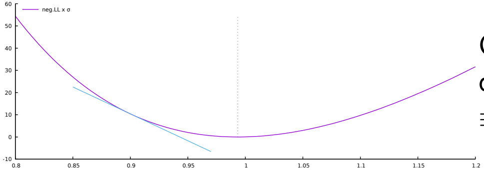
Note: Check 1 also depends on the scale of your function...
Preferably $f(\theta) \approx 1$, not $f(\theta) \approx 1e - 15$!

Adapt the precision with

```
res= opt.minimize(AvgNLnLRegr, vP0, args=(),
method="BFGS", tol= 1e-4),
```

default is `tol=1e-5`.

Minimize: Scores



Optimising ≡ 'going down'
≡ finding gradient.

Numerical gradient, for small h:

$$f'(\theta) = \frac{\partial f(\theta)}{\partial \theta} \approx \frac{f(\theta + h) - f(\theta)}{h} \approx \frac{f(\theta + h) - f(\theta - h)}{2h}$$

Function evaluations: $2 \times \dim(\theta)$

Preferred: Analytical score $f'(\theta)$

Minimize: Scores II

```
# Get a lambda function to return score, for NEGATIVE AVERAGE LL
AvgNLnLRegr_Sc= lambda vP: -np.mean(LnLRegr_Sc(vP, mY, mX))
```

- Provide a score function for loglikelihood vector
- Work out vector of scores, of same size as θ.
- DEBUG! Check your score against `opt.approx_fprime()`

Minimize: Scores IIb

- ...
- DEBUG! Check your score against `opt.approx_fprime()` or `gradient_2sided`

Listing 46: estnorm_score3.py

```
vSc0= AvgNLnLRegr_Sc(vP0, vY, mX)
vSc1= opt.approx_fprime(vP0, AvgNLnLRegr, 1e-5*np.fabs(vP0))
vSc2= gradient_2sided(AvgNLnLRegr, vP0)
print ("Scores, analytical and numerical:\n", np.vstack([vSc0, vSc1, vSc2]))
```

Don't ever forget debugging this
(goes wrong 100% of the time...)

Minimize: Scores III

Let's do it...

$$f(y;\theta) = \frac{1}{2}\left(\log 2\pi + 2\log\sigma + \frac{\sum(y_i - X_i\beta)^2}{n\sigma^2}\right)$$

$$e = y - X\beta$$

$$\frac{\partial f(y;\theta)}{\partial\sigma} = \ldots$$

$$\frac{\partial f(y;\theta)}{\partial\beta} = \ldots$$

- It matters whether $\theta = (\beta, \sigma)$ or $\theta = (\beta, \sigma^2)$ or $\theta = (\sigma, \beta)$!
- Find score of AVERAGE NEGATIVE loglikelihood, in general of function $f()$
- (In `estnorm_score3.py`, for simplicity, score of `vLL` is taken, which later is combined into score of AvgNLnLRegr)

Minimize: Scores Results

Output of estnorm.py:

```
BFGS results in  Optimization terminated successfully.
Pars:  [ 0.09888969  5.01707341  1.9962231  -2.01475073]
LL=  89.48117606217971 , f-eval=  230
```

Output of estnorm_score3.py:

```
BFGS results in  Optimization terminated successfully.
Pars:  [ 0.09888969  5.01707342  1.9962231  -2.01475074]
LL=  89.48117606217936 , f-eval=  40
```

Q: What are the differences?

Solve

Remember:

$$r(y;\theta) = \mathbf{0}$$

Use function scipy.optimize.least_squares, with basic syntax

```
import scipy.optimize as opt

##################################################################
### vF= fnFunc0(vP)
def fnFunc0(vP):
    vF= ...          // k 1D vector, should be 0 at solution
    return vF

res= opt.least_squares(fnFunc0, x0)
print ("Nonlin LS returns ", res.message, "\nParameters ", res.x)
```

Solve II

```
import scipy.optimize as opt
res= opt.least_squares(fnFunc0, x0)
print ("Nonlin LS returns ", res.message, "\nParameters ", res.x)
```

- General idea similar to `minimize`
- Solves *nonlinear* least squares problems
- Again, extra arguments can easily be passed through Lambda function:
  `fnFunc1L= lambda vP: fnFunc1(vP, a1, a2)`,
  where `fnFunc1L(vP)` is the lambda function calling the original `fnFunc1(vP, a1, a2)` which depends on multiple arguments.
- Further options available, check manual.

Example: Solve Macro

Given the parameters $\theta = (p_H, \nu_1)$, depending on input $y = (\sigma_1, \sigma_2)$, a certain system describes the equilibrium in an economy if

$$r(y;\theta) = \begin{pmatrix} p_H^{-\frac{1}{\sigma_1}} \nu_1 + p_H^{-\frac{1}{\sigma_2}} (1 - \nu_1) - 2 \\ p_H^{\frac{\sigma_1 - 1}{\sigma_1}} \nu_1 + \nu_1 - p_H - \frac{1}{2} \end{pmatrix} = \mathbf{0}.$$

For the solution to be sensible, it should hold that $0 < \nu_1 < 1$ and $p_H \neq 0$.
If $y = (2, 2)$, what are the optimal values of $\theta = (p_H, \nu_1)$?

Solution: $\hat{\theta} = (0.25, .5)$

Example: Solve Macro II

Starting point as before: Prepare the restriction function, e.g.

```
###########################################################
### vF= EquilMacro(vP, vS)
def EquilMacro(vP, vS):
    """
    Purpose:
      Check the equilibrium in some specific problem from TI-Macro I

    Inputs:
      vP         2 vector with pH and Nu1
      vS         2 vector, relative risk aversions

    Return value:
      vF         2 vector, with distance from equilibrium
    """
```

It will indeed:

- need the parameters $\theta = (p_H, \nu_1)$
- need the data $y = (\sigma_1, \sigma_2)$
- return the value of the restriction, $r(y; \theta)$

Example: Solve Macro III

Step 2: Read out the parameters, prepare the output:

```
def EquilMacro(vP, vS):
    vF= np.ones_like(vP)

    (dpH, dNu1)= vP
    (dS1, dS2)= vS
    ...
    print (".", end="")         # Give sign of life
    return vF
```

Q: Why would I initially set `vF` to a vector of ones, and not a vector of zeros?

Example: Solve Macro III

Step 3: Then compute the $r(y;\theta)$ function

$$r(y;\theta) = \begin{pmatrix} p_H^{-\frac{1}{\sigma_1}} \nu_1 + p_H^{-\frac{1}{\sigma_2}} (1-\nu_1) - 2 \\ p_H^{\frac{\sigma_1 - 1}{\sigma_1}} \nu_1 + \nu_1 - p_H - \frac{1}{2} \end{pmatrix}$$

```
def EquilMacro(vP, vS):
    ...
    vF[0]= (1.0 / dpH)**(1.0 /dS1)*dNu1 + (1.0 / dpH)**(1.0 / dS2)*(1.0-dNu1)-2
    vF[1]= dpH**( (dS1-1)/dS1)*dNu1+dNu1-dpH-(1/2)
    ...
    return vF
```

Example: Solve Macro IV

Step 4: Try things out, and solve!

Listing 47: solvemacro.py

```
def main():
    # Magic numbers
    vS= [2, 2]          # Data
    vP= [10, .9]        # Initial parameters

    # Estimation
    vF= EquilMacro(vP, vS)
    print ("\nInitial distance vF= ", vF, "at vP= ", vP)

    EquilMacroL= lambda vP: EquilMacro(vP, vS)
    res= opt.least_squares(EquilMacroL, vP)
```

And check the results

Example: Solve Macro V

Results:

```
.
Initial distance vF=  [-1.68377223 -6.75395011] at vP=  [10, 0.9]
solvemacro.py:47: RuntimeWarning: invalid value encountered in double_scalars
  vF[0]= (1.0 / dpH)**(1.0 /dS1)*dNu1 + (1.0 / dpH)**(1.0 / dS2)*(1.0-dNu1)-2
solvemacro.py:48: RuntimeWarning: invalid value encountered in double_scalars
  vF[1]= dpH**( (dS1-1)/dS1)*dNu1+dNu1-dpH-(1/2)
..............................
NLS returns  'gtol' termination condition is satisfied.
Parameters:  [0.25 0.5 ]
The distance to equilibrium is  [ 6.57252031e-14 -3.88578059e-16]
```

Success!

Q: What is your opinion of those warnings? Would you investigate? If yes, how?

Standard deviations

Given a model with

$$
\begin{aligned}
&\mathcal{L}(Y;\theta) && \text{Likelihood function}\\
l(Y;\theta) &= \log \mathcal{L}(Y;\theta) && \text{Log likelihood function}\\
\hat\theta &= \text{argmax}_\theta l(Y;\theta) && \text{ML estimator}
\end{aligned}
$$

what is the vector of standard deviations, $\sigma(\hat\theta)$?
Assuming correct model specification,

$$
\begin{aligned}
\Sigma(\hat\theta) &= -H(\hat\theta)^{-1}\\
H(\hat\theta) &= \left.\frac{\partial^2 l(Y;\theta)}{\partial\theta\partial\theta'}\right|_{\theta=\hat\theta}
\end{aligned}
$$

SD2: Average likelihood

For numerical stability, optimise *average negative* loglikelihood $\bar{l}_n$.

For regression model, with the likelihood approach, one can use

$$l(Y;\theta) = -\frac{(y - X\beta)'(y - X\beta)}{2\sigma^2} - N \log 2\pi\sigma^2 + c$$

$$\bar{l}_n(Y;\theta) = \frac{(y - X\beta)'(y - X\beta)}{2N\sigma^2} + \log 2\pi\sigma^2 - c'$$

$$H_{\bar{l}_n} \equiv \frac{\partial^2 \bar{l}_n(Y;\theta)}{\partial\theta\partial\theta'} = -\frac{1}{N} H_l \qquad H_l \equiv -N H_{\bar{l}_n}$$

Listing 48: estnorm.py

```
res= opt.minimize(AvgNLnLRegr, vP0, method="BFGS")

vP= res.x
mHn= hessian_2sided(AvgNLnLRegr, vP)
mH= -iN*mHn
mS2= -np.linalg.inv(mH)
vS= np.sqrt(np.diag(mS2))
print ("\nBFGS results in ", res.message,
       "\nPars: ", vP,
       "\nStdev: ", vS
       "\nLL= ", -iN*res.fun, ", f-eval= ", res.nfev)
```

SD2: Hessian...

Hessian:

- is numerically unstable
- defines your standard errors
- hence is utterly important
- should be calculated with care!

But first: Check the gradient (simpler)

SD2: Gradient...

Gradient:

$$g = \frac{\partial f(\theta)}{\partial \theta} \approx \frac{f(\theta + h) - f(\theta)}{h} \approx \frac{f(\theta + h) - f(\theta - h)}{2h}$$

- Central difference *far* more precise than forward difference
- Step size h_i should depend on θ_i, different per element
- Rounding errors can become enormous, when h too small
- Python seems to provide `scipy.optimize.approx_fprime`, forward difference
- ... and symbolic differentiation (better, slower, not pursued here)

$\Rightarrow$ `lib/grad.py` contains `gradient_2sided()`

SD2: gradient_2sided

⇒ `lib/grad.py` contains `gradient_2sided()` (simplified here)

Listing 49: lib/grad.py

```
def gradient_2sided(fun, vP, *args):
    iP = np.size(vP)
    vP= vP.reshape(iP)       # Ensure vP is 1D-array

    vh = 1e-8*(np.fabs(vP)+1e-8)   # Find stepsize
    mh = np.diag(vh)         # Build a diagonal matrix

    fp = np.zeros(iP)
    fm = np.zeros(iP)
    for i in range(iP):      # Find f(x+h), f(x-h)
        fp[i] = fun(vP+mh[i], *args)
        fm[i] = fun(vP-mh[i], *args)

    vG= (fp - fm) / (2*vh)  # Get central gradient
    return vG
```

SD2: Gradient II

Listing 50: opt/estnorm_score.py

```
vSc0= AvgNLnLRegr_Jac(vP0, vY, mX)
vSc1= opt.approx_fprime(vP0, AvgNLnLRegr, 1e-5*np.fabs(vP0), vY, mX)
vSc2= gradient_2sided(AvgNLnLRegr, vP0, vY, mX)
print ("\nScores:\n",
       pd.DataFrame(np.vstack([vSc0, vSc1, vSc2]), index=["Analytical", "grad_1sided", "
```

results in

```
Scores:
                    0         1         2         3
Analytical  -7.965135 -2.863504 -1.502223 -1.341437
grad_1sided -7.965005 -2.863499 -1.502222 -1.341435
grad_2sided -7.965135 -2.863504 -1.502223 -1.341437
```

Q: What do you prefer?

SD2: Hessian II

Back to Hessian:

- `lib/grad.py` contains `gradient_2sided()` and `hessian_2sided()` (source: Python for Econometrics, Kevin Sheppard, with minor alterations)
- **DO NOT** use scipy.misc.derivative, as it allows only for a single constant difference *h*, applied in all directions
- DO NOT EVER use the output from `res= opt.minimize()`, where `res.hess_inv` seems to be some inverse hessian estimate. (Indeed, it is *some* estimate, useful for BFGS optimisation, not for computing standard errors)
- (Same result can be obtained from NumDiffTools. However, here you have to understand what you are doing...)

Conclusion:

1. For standard errors: Feel free to copy code
2. Possibly better: Use improved covariance matrix, sandwich form. See Econometrics course

Optimization and restrictions

Take model

$$y = X\beta + \epsilon, \qquad\qquad \epsilon \sim \mathcal{N}(0, \sigma^2)$$

Parameter vector $\theta = (\sigma, \beta')'$ is clearly restricted, as $\sigma \in [0, \infty)$ or $\sigma^2 \in [0, \infty)$

- Newton-based method (BFGS) doesn't know about ranges
- Alternative optimization (SLSQP) *may be*(?) slower/worse convergence, but simpler

Hence: First tricks for `SLSQP`.

Warning: Don't use `SLSQP` (or any optimization...) unless you know what you're doing (the function looks attractive, but isn't always...)

Restrictions: SLSQP

`minimize(method="SLSQP")` is an alternative to `minimize(method="BFGS")`

- Without restrictions, delivers results similar to `BFGS`
- Allows for sequential quadratic programming solution, for *linear* and *non-linear* restrictions.

General call:

```
res= opt.minimize(fun, vP0, method="SLSQP", args=(),
                  bounds=tBounds, constraints=tCon)
```

SLSQP IIa

Restrictions:

1. `bounds`: Tuple of form `tBounds= ((l0, u0), (l1, u1), ...)` with lower and upper bounds per parameter (use `None` if no restriction)
2. ...

Listing 51: estnorm_slsqp.py

```
# Fix sigma > 0, -inf < beta < inf
tBounds= ((0, None),) + iK*((None, None),)    # Concatenate 1 + K tuples
res= opt.minimize(AvgNLnLRegr, vP0, method="SLSQP", bounds=tBounds)
```

SLSQP IIb

Restrictions, alternative:

1. ...
2. `constraints`: Tuple of dictionaries with entry 'type', indicating whether the function indicates an *inequality* ("ineq") or *equality* ("eq"), and entry 'fun', giving a function of a single argument which returns the constrained value. E.g. `tCons= ({'type': 'ineq', 'fun': fngt0}, {'type': 'eq', 'fun': fneq0})`

Listing 52: estnorm_slsqp.py

```
# Or, alternatively
fnsigmapos= lambda vP: vP[0]                    # Function which returns sigma only
tCons= ({'type': 'ineq', 'fun': fnsigmapos})
res= opt.minimize(AvgNLnLRegr, vP0, method="SLSQP", constraints=tCons)
```

See manual for more details...

SLSQP III

Advantages:

- Simple
- Implements restrictions on parameter space (e.g. $\sigma > 0, 0 < \alpha + \delta < 1$)

Disadvantages:

- BFGS is meant for *global* optimisation; `SLSQP` might work worse
- Often better to incorporate restrictions in parameter transformation: Estimate $\theta = \log \sigma, -\infty < \theta < \infty$

So check out transformations...

Transforming parameters

Variance parameter positive?
Solutions:

1. Use σ^2 as parameter, have `AvgLnLiklRegr` return -math.inf when negative σ^2 is found
2. Use $\sigma \equiv |\theta_0|$ as parameter, ie forget the sign altogether (doesn't matter for optimisation, interpret negative σ in outcome as positive value)
3. Transform, optimise $\theta_0^* = \log \sigma \in (-\infty, \infty)$, no trouble for optimisation

Last option most common, most robust, neatest.

Transform: Common transformations

Constraint	θ^*	θ
$[0,\infty)$	$\log(\theta)$	$\exp(\theta^*)$
$[0,1]$	$\log\left(\frac{\theta}{1-\theta}\right)$	$\frac{\exp(\theta^*)}{1+\exp(\theta^*)}$

Of course, to get a range of $[L, U]$, use a rescaled $[0,1]$ transformation.

Note: See also exercise `transpar`

Transform: General solution

Distinguish $\theta = (\sigma, \beta')'$ and $\theta^* = (\log \sigma, \beta')'$. Steps:

- Get starting values θ
- Transform to θ^*
- Optimize θ^*, transforming back within LL routine
- Transform optimal θ^* back to θ

Listing 53: opt/estnorm_tr.py

```
# Prepare wrapping function
def AvgNLnLiklRegrTr(vPTr):
    vP= np.copy(vPTr)        # Remember to COPY vPTr to a NEW variable
    vP[0]= np.exp(vPTr[0])
    return AvgNLnLiklRegr(vP)   # Use old function, of untransformed parameters
...
vP0Tr= np.copy(vP0)          # Remember to COPY vP0 to a NEW variable
vP0Tr[0]= np.log(vP0[0])
res= opt.minimize(AvgNLnLRegrTr, vP0Tr, method="BFGS")
vP= np.copy(res.x)           # Remember to COPY x to a NEW variable
vP[0]= np.exp(vP[0])         # Remember to transform back!
```

Transform: Use functions

Notice code before: Transformations are performed

1. Before `minimize`
2. After `minimize`
3. Within `AvgNLnLiklRegrTr`
4. And probably more often for computing standard errors

Premium source for bugs... (see previous page: Two distinct implementations for back-transform? Why?!?)

Solution: Define

- `vPTr= TransPar(vP)`: $\theta \rightarrow \theta^*$
- `vP= TransBackPar(vPTr)`: $\theta^* \rightarrow \theta$

And test (in a separate program) whether transformation works right. Necessary when using multiple transformed parameters.

Transform: Use functions II

Listing 54: opt/estnorm_tr2.py

```
# Use lambda function to transform back in place
# AvgNLnLRegrTr= lambda vPTr: AvgNLnLRegr(TransBackPar(vPTr))
# Option 1
AvgNLnLRegrTr= lambda vPTr: -np.mean(LnLRegr(TransBackPar(vPTr), vY, mX), axis=0)
# Option 2

vP0Tr= TransPar(vP0)
res= opt.minimize(AvgNLnLRegrTr, vP0Tr, method="BFGS")

vP= TransBackPar(res.x)      # Remember to transform back!
```

Standard deviations

Remember:

$$\Sigma(\hat{\theta}) = -H(\hat{\theta})^{-1}$$
$$H(\hat{\theta}) = \left.\frac{\delta^2 l(Y;\theta)}{\delta\theta\delta\theta'}\right|_{\theta=-\hat{\theta}} = -N \left.\frac{\delta^2 \bar{l}_n(Y;\theta)}{\delta\theta\delta\theta'}\right|_{\theta=\hat{\theta}}$$

Therefore, we need (average negative) loglikelihood in terms of θ, not θ^* for sd's...

Transforming parameters II: SD

Question: How to construct standard deviations?

Answers:

1. Use transformation in estimation, not in calculation of standard deviation. *Advantage*: Simpler. *Disadvantage*: Troublesome when parameter close to border.
2. Use transformation throughout, use Delta-method to compute standard errors. *Advantage*: Fits with theory. *Disadvantage*: Is standard deviation of σ informative, is its likelihood sufficiently peaked/symmetric?
3. After estimation, compute bootstrap standard errors
4. Who needs standard errors? Compute 95% confidence bounds on θ^*, translate those to 95% bounds on parameter θ. *Advantage*: Theoretically nicer. *Disadvantage*: Not everybody understands advantage.

See next slides.

Transforming: Temporary

- Use transformation in estimation,
- Use no transformation in calculation of standard deviation.

Listing 55: opt/estnorm_tr2.py

```
...
vP0Tr= TransPar(vP0)
res= opt.minimize(AvgNLnLRegrTr, vP0Tr, method="BFGS")
vP= TransBackPar(res.x)   # Remember to transform back!

# Get covariance matrix from function of vP, not vPTr!
mHn= hessian_2sided(AvgNLnLRegr, vP)
mH= -iN*mHn
mS2= -np.linalg.inv(mH)
vS= np.sqrt(np.diag(mS2))
```

Transforming: Delta

$$
\begin{aligned}
n^{1/2}(\hat{\theta}^* - \theta_0^*) &\overset{a}{\sim} \mathcal{N}\left(0, V^\infty(\hat{\theta}^*)\right) \\
\hat{\theta} &= g(\hat{\theta}^*) \\
\hat{\theta} &\approx g(\theta_0^*) + g'(\theta_0^*)(\hat{\theta}^* - \theta_0^*) \\
n^{1/2}(\hat{\theta} - \theta_0) &\overset{a}{=} g_0' n^{1/2}(\hat{\theta}^* - \theta_0^*) \overset{a}{\sim} \mathcal{N}(0, (g_0')^2 V^\infty(\hat{\theta}^*)) \quad \text{scalar} \\
n^{1/2}(\hat{\theta} - \theta_0) &\overset{a}{\sim} \mathcal{N}(0, G_0 V^\infty(\hat{\theta}^*) G_0') \quad \text{vector}
\end{aligned}
$$

In practice: Use

$$
\begin{aligned}
\text{var}(\hat{\theta}) &= \hat{G}\,\text{var}(\hat{\theta}^*)\hat{G}' \\
\hat{G} &= \frac{\delta g(\theta^*)}{\delta \theta^{*\prime}} = \begin{pmatrix} \frac{dg(\theta^*)}{d\theta_1^*} & \frac{dg(\theta^*)}{d\theta_2^*} & \cdots & \frac{dg(\theta^*)}{d\theta_k^*} \end{pmatrix} = \text{Jacobian}
\end{aligned}
$$

Transforming: Delta in Python

Listing 56: opt/estnorm_tr2.py

```
vPTr= res.x

# Get standard errors, using delta method
mHnTr= hessian_2sided(AvgNLnLRegrTr, vPTr)
mHTr= -iN*mHnTr
mS2Tr= -np.linalg.inv(mHTr)
mG= jacobian_2sided(TransBackPar, vPTr)  # Evaluate jacobian at vPTr
mS2= mG @ mS2Tr @ mG.T                  # Cov(vP)
vS= np.sqrt(np.diag(mS2))               # s(vP)
```

Transforming: Bootstrap

- Estimate model, resulting in $\hat\theta = g(\hat\theta^*)$
- From the model, generate $j = 1, .., B$ bootstrap samples $y_s^{(j)}(\hat\theta)$
- For each sample, estimate $\hat\theta_s^{(j)} = g({\hat\theta^*}_s^{(j)})$
- Report $\text{var}(\hat\theta) = \text{var}(\hat\theta_s^{(1)}, \ldots, \hat\theta_s^{(B)})$

I.e, report variance/standard deviation among those B estimates of the parameters, assuming your parameter estimates are used in the DGP.

Simple, somewhat computer-intensive?

Transforming: Bootstrap in Ox

```
{
  ...
  for (j= 0; j < iB; ++j)
    {
      // Simulate data Y from DGP, given estimated parameter vP
      GenerateData(&vY, mX, vP);

      TransPar(&vPTr, vP);
      ir= MaxBFGS(fnAvgLnLiklRegrTr, &vPTr, &dLL, 0, TRUE);
      TransBackPar(&vPB, vPTr);

      mG[][j]= vPB;  // Record re-estimated parameters
    }
  mS2= variance(mG');
  avS[0]= sqrt(diagonal(mS2)');
}
```

For the tutorial: Try it out for the normal model, in Python?

Speed

Elements to consider

- Use matrices, avoid loops
- Adapt large matrices in-place (†)
- Use built-in functions (†)
- Pre-declare matrix, do not concatenate
- Use Numba or Cython
- Use multi-processing (smartly)

Speed: Loops vs matrices

Avoid loops like the plague.
Most of the time there is a matrix alternative, like for constructing dummies:

Listing 57: speed_loop2.py

```
iN= 10000
iR= 1000
vY= np.random.randn(iN, 1)
vDY= np.zeros_like(vY)

with Timer("Loop"):
  for r in range(iR):
      for i in range(iN):
          if (vY[i] > 0):
              vDY[i]= 1
          else:
              vDY[i]= -1

with Timer("Matrix"):
  for r in range(iR):
      vDY= np.ones_like(vY)
      vDY[vY <= 0]= -1
```

Speed: Argument vs return

Listing 58: speed_argument.py

```
def funcret(mX):
    (iN, iK)= mX.shape
    mY= np.random.randn(iN, iK)
    return mY

def funcarg(mX):
    (iN, iK)= mX.shape
    mX[:,:]= np.random.randn(iN, iK)

def main():
    ...
    mX= np.zeros((iN, iK))
    with Timer("return"):
      for r in range(iR):
        mX= funcret(mX)

    with Timer("argument"):
      for r in range(iR):
        funcarg(mX)
```

Note: No true difference to be found, good memory management...

Speed: Built-in functions

Listing 59: speed_builtin.py

```
def MyOls(vY, mX):
    vB= np.linalg.inv(mX.T@mX)@mX.T@vY
    return vB

def main():
    ...
    with Timer("MyOls"):
      for r in range(iR):
        vB= MyOls(vY, mX)

    with Timer("lstsq"):
      for r in range(iR):
        vB= np.linalg.lstsq(mX, vY, rcond=None)[0]
```

Note: This function lstsq is even slower... More stable in awkward situations...

Speed: Concatenation or predefine

In a simulation with a matrix of outcomes, predefine the matrix to be of the correct size, then fill in the rows.
The other option, concatenating rows to previous results, takes a lot longer.

Listing 60: speed_concat.py

```
iN= 1000
iK= 1000

mX= np.empty((0, iK))
with Timer("vstack"):
  for j in range(iN):
    mX= np.vstack([mX, np.random.randn(1, iK)])

mX= np.empty((iN, iK))
with Timer("predef"):
  for j in range(iN):
    mX[j,:]= np.random.randn(1, iK)
```

Speed: Using Numba

Numba may help in pre-translating routines using Just-in-Time translation to machine code. After the translation, code will run (much...) faster.

```
def Loop(mX, iR):
    (iN, iK)= mX.shape
    for r in range(iR):
        mXtX= np.zeros((iK, iK))
        for i in range(iK):
            for j in range(i+1):
                for k in range(iN):
                    mXtX[i,j]+= mX[k,i] * mX[k,j]
                mXtX[j, i]= mXtX[i, j]
    return mXtX

def main():
    ...
    # Estimation
    with Timer("Loop, Rx"):
        mXtX= Loop(mX, iR)
```

Speed: Using Numba II

- Add a *decorator* to indicate that a loop should be pre-compiled
- Run the loop once, to allow for the compilation
- Afterwards, loops are *much* quicker

```
@njit()
def Loop_NJit(mX, iR):
    (iN, iK)= mX.shape
    for r in range(iR):
        mXtX= np.zeros((iK, iK))
        for i in range(iK):
            for j in range(i+1):
                for k in range(iN):
                    mXtX[i,j]+= mX[k,i] * mX[k,j]
                mXtX[j, i]= mXtX[i, j]
    return mXtX

def main():
    ...
    # Estimation
    with Timer("Loop_NJit 1x, compiling"):
        mXtX= Loop_NJit(mX, 1)
    with Timer("Loop_NJit Rx"):
        mXtX= Loop_NJit(mX, iR)
```

Speed: Using Numba III

With `@njit()`, code is pushed into machine code; hence vectorisation is no longer needed.
Next step: Allow for parallelisation

```
@njit(parallel= False)      # Do the inner part translated to C, no parallelisation
def Loop_Inner(mX):
    (iN, iK)= mX.shape
    mXtX= np.zeros((iK, iK))
    for i in range(iK):
        for j in range(i+1):
            for k in range(iN):
                mXtX[i,j]+= mX[k,i] * mX[k,j]
            mXtX[j, i]= mXtX[i, j]
    return mXtX

@njit(parallel= True)       # Do the outer loop in parallel
def Loop_parallel(mX, iR):
    (iN, iK)= mX.shape
    mXtXr= np.zeros((iK, iK))
    for r in prange(iR):             # Use prange, indicating a parallel loop
        mXtXr+= Loop_Inner(mX)       # Reduction, by computing the average
    return mXtXr/iR
```

Speed: Using Numba IV

Hints:

- Don't reuse variables in a parallel loop (race condition between threads?)
- If inner loop takes lots of memory, don't do it in parallel either (as it will take multiple copies of memory)
- Combine results smartly
- Don't overdo it, only run explicitly the most outer loop in parallel
- `@njit(parallel= True)` already may parallelise vector operations, test where it is most useful
- Explicit vectorisation + njit is not really useful, simple looping code may be just as quick

Conclusion: It takes practice and trials to find best/quickest combination!

Speed: Using Multiprocessing

Using multiple CPU's in Python is *not* simple:

- Standard *multi-threading* does not help (for CPU tasks), as Python has a *Global Interpreter Lock*: Only one computation at a time. Save it for I/O bound tasks
- Less standard *multi-processing* may help for CPU tasks, but is slightly more difficult to set up.

Basis worker function:

```
def LoopG(r):
    global g_mX
    return Loop(g_mX, 1)
```

Speed: Using Multiprocessing II

```
from multiprocessing import Pool
...
def LoopJ(mX, iR):
    global g_mX              # Prepare a global for passing mX
    g_mX= mX                 # Fill the global with the value of mX

    pool= Pool()             # Open the pool of processors, as many as possible
    lXtX= pool.map(LoopG, range(iR))        # Call LoopG, for each value r= 0, .., iR-1
                        # Store all results in the list lXtX

    # close the pool and wait for the work to finish
    pool.close()
    pool.join()

    return lXtX[0]        # Return only a single of those results
```

Result: Speedup of factor 1.6 for 2-core system, factor 9 for 16-core system...
Background: https://medium.com/@yasufumy/python-multiprocessing-c6d54107dd55

Speed: Overview

Conclusions:

- If your program takes more than a few seconds, optimise
- Track the time spent in functions, optimise what takes longest (hint: inner loop...)
- Don't concatenate/stack
- Use matrix-operations/vectorized code instead of loops
- Look into Numba for loop-heavy code
- Multiprocessing may help (but matrices help more...)
- Use Cython (not covered here), or move to Julia, (not covered here) for computationally intensive stuff

Closing thoughts

And so, the course comes to an end...
Please

- keep concepts, principles of programming, in mind
- structure your programs wisely

On a obligatory (TI/BDS) or voluntary (DHPQRM) basis:

- before Friday September 30 2022, 23.59h
- hand in *your own* solution to
  1. GARCH-ML problem (similar to OLS exercise, minor extensions)
  2. BinTree problem (relevant to QRM students, nice setting for others)

(see Canvas for details)