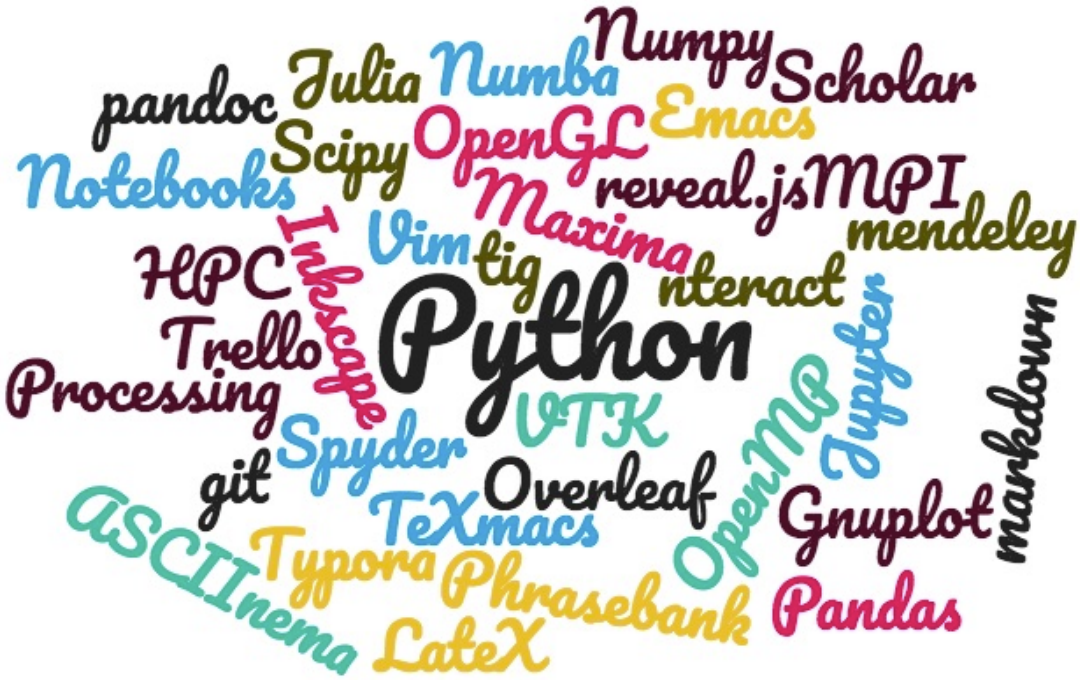
The efficient toolbox of the Computational Scientist



Dr. Gábor Závodszky - *Computational Science Lab* https://github.com/gzavo/CS_Assignment

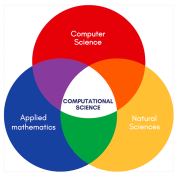
> "Never do a live demo" -- Every presenter ever

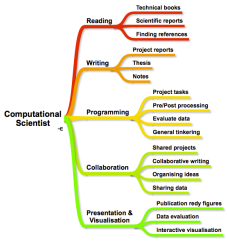
Structure of the lecture

- Domains of "The Computational Scientist"
- Scientific writing and reading
- Programming and visualization basics
- Software development in a collaborative environment
- Homework assingment

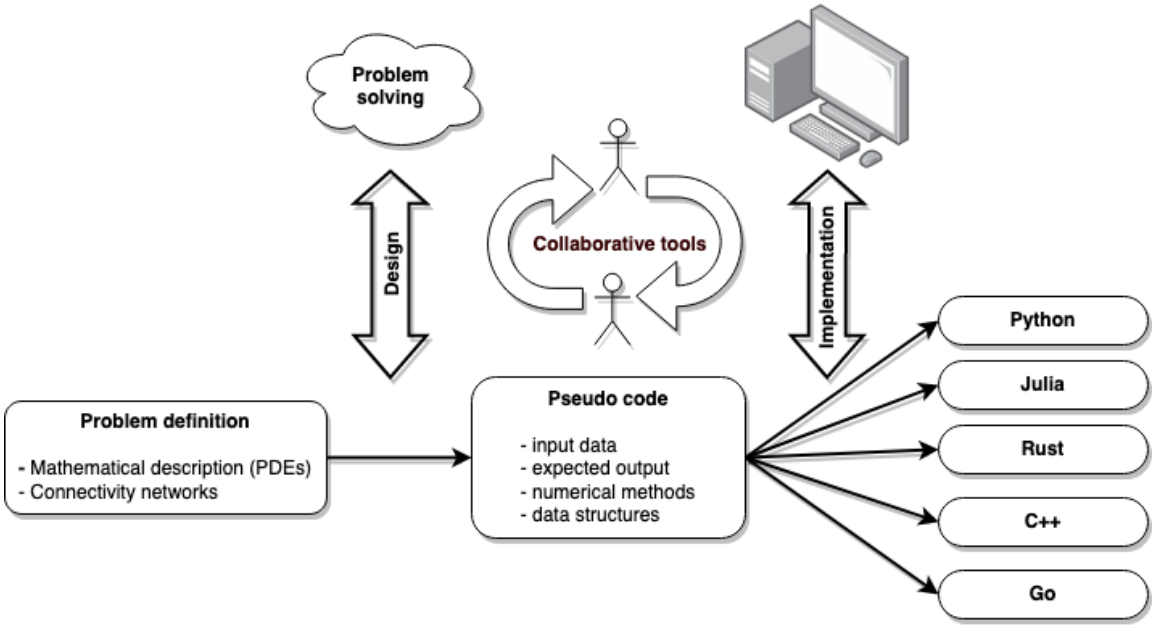
- Can be an information overload!
- The slides contain the very basics.
- Due to the structure of this MSc programme, you might not need *everything*.
- The most important things are marked: **(!)**.
- Some things are there to hear at least once.
- You can use the pdf version as a list of useful tools.

Who is the Computational Scientist? - Domains and fundamental skills





General workflow of the Computational Scientist



CLS Activities - Reading

- UvA Library (!) (http://uba.uva.nl/en)
- You can also use it to get access to non-open access journal papers.

- Google Scholar (!) - https://scholar.google.com
  - Search for papers
  - export references
  - look at researcher profiles
  - E.g.: "Carbon monoxide, boldly goes where..."
- Web of Science, Scopus, ...

- Managing references: Mendeley, Zotero (!), Papers, etc.
  - Sync. paper database
  - Annotate pdfs, add notes and sync them as well
- Most students use Zotero (I use it as well).
- Mendeley gives more cloud space, but its less flexible.

CLS Activities - Writing

- LaTeX
  - Overleaf (!) - https://www.overleaf.com/
  - TexMaker
  - TeXmacs
  - latex2png - http://latex2png.com/

-> Why is LaTeX useful?

- Not a WYSIWYG solution
- But often WYGIWYN
- Literally a programming language for word processing

from IPython.display import IFrame

IFrame("https://www.nature.com/news/scientific-writing-the-online-cooperative-1.16039", "100%", 600)

- Markdown (!)
  - Use Pandoc (!) to turn it to .doc, .pdf, .html, you name it (https://pandoc.org/)
  - Zettlr (!) (https://www.zettlr.com/)
  - Typora (https://typora.io/)
  - Mark Text (https://github.com/marktext/marktext)
  - Basically everywhere (websites, forums, editors...really, everywhere)
  - Supersets / alternatives (ASCIIDOC, ...)

Markdown

Write equations: $e^{i\pi} + 1 = 0$

Embed code:

```
def f(x):
    """docstring of this very useful function"""
    return x**2
```

Add tables:

This	is
a	table

Create lists:

- list item 1
- list item 2
- list item 3

Markdown is a simple way to format text that looks great on any device. It doesn't do anything fancy like change the font size, color, or type — just the essentials, using keyboard symbols you already know.

TRY OUR 10 MINUTE MARKDOWN TUTORIAL

Type	Or	... to Get
`*Italic*`	`_Italic_`	*Italic*
`**Bold**`	`__Bold__`	**Bold**
`# Heading 1`	`Heading 1` `=========`	Heading 1
`## Heading 2`	`Heading 2` `---------`	Heading 2

`[Link](http://a.com)`	`[Link][1]`
	⋮
	`[1]: http://b.org`
		Link

`![Image](http://url/a.png)`	`![Image][1]`
	⋮
	`[1]: http://url/b.jpg`
		

`> Blockquote`		Blockquote
`* List` `* List` `* List`	`- List` `- List` `- List`	• List • List • List
`1. One` `2. Two`	`1) One` `2) Two`	1. One 2. Two

```
from IPython.display import IFrame

IFrame("http://commonmark.org/help/", "100%", 600)
```

CLS Activities - Writing - cont.

Pandoc a universal document converter

Donate Flattr

About
Installing
Getting started
Demos
Documentation
Help
Extras
Releases

About pandoc

If you need to convert files from one markup format into another, pandoc is your swiss-army knife. Pandoc can convert documents in (several dialects of) Markdown, reStructuredText, textile, HTML, DocBook, LaTeX, MediaWiki markup, TWiki markup, TikiWiki markup, Creole 1.0, Vimwiki markup, OPML, Emacs Org-Mode, Emacs Muse, txt2tags, Microsoft Word docx, LibreOffice ODT, EPUB, or Haddock markup to

HTML formats

XHTML, HTML5, and HTML slide shows using Slidy, reveal.js, Slideous, S5, or DZSlides

Word processor formats

Microsoft Word docx, OpenOffice/LibreOffice ODT, OpenDocument XML, Microsoft PowerPoint.

Ebooks

EPUB version 2 or 3, FictionBook2

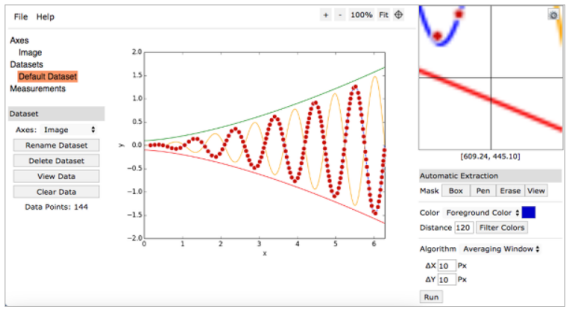
https://automeris.io/WebPlotDigitizer/

WebPlotDigitizer

Web based tool to extract data from plots, images, and maps

English Launch Download

Home Blog Tutorials Citation Privacy



Web Application

English

Launch Now!

Desktop Version

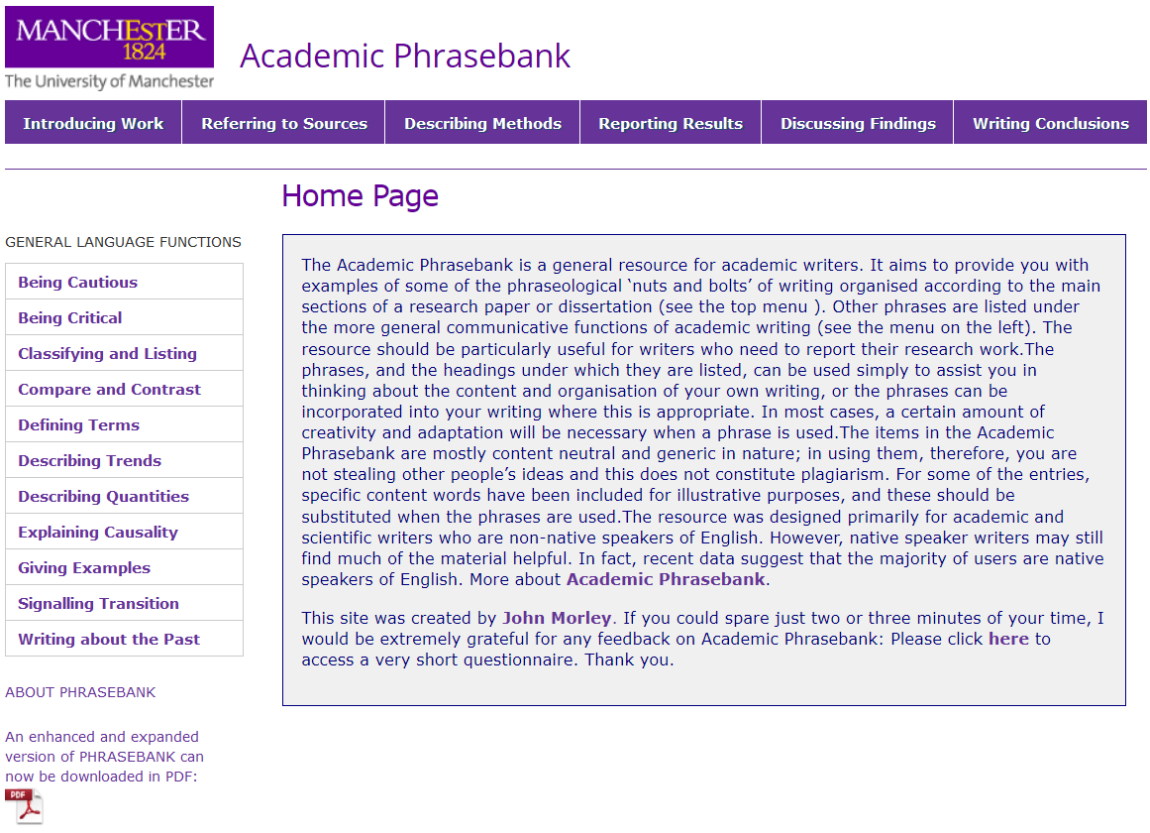
View Source

GitHub

It is often necessary to reverse engineer images of data visualizations to extract the underlying numerical data. WebPlotDigitizer is a semi-automated tool that makes this process extremely easy:

- Works with a wide variety of charts (XY, bar, polar, ternary, maps etc.)
- Automatic extraction algorithms make it easy to extract a large number of data points
- Free to use, opensource and cross-platform (web and desktop)
- Used in hundreds of published works by thousands of users
- Also useful for measuring distances or angles between various features
- More to come soon...

http://www.phrasebank.manchester.ac.uk/



CLS Activities - Programming

- programming languages
- editors
- examples

Programming languages

- Python (!)
- C (!) (performance, hardware access)
- C++ (!) (If you need performance + OO)
- Julia (!) (C + Python + Lisp structures)
- Rust (!) (performance and safety)
- Kotlin (the new popular kid, mobile development)
- Nim (Python, but C)
- R (statistics)
- Scala (data science)
- Go (Google's try)
- Javascript (too popular to leave out)
- Racket (for the gourmet)
- +1 Lobster lang. (http://strlen.com/lobster/)

> Application domains can overlap, choose 2-3 and learn them well!
>
> For instance, C/C++ and Python is a quite versatile combination.
>
> Computer Language Benchmark Game (https://benchmarksgame-team.pages.debian.net/benchmarksgame/index.html)
>
> Rosetta Code (http://www.rosettacode.org)

In [ ]:

General editors

- Visual Studio Code (!)
- Sublime Text
- **Jupyter** / **JupyterLab**
- NVim
- Emacs (Spacemacs)
- micro
- Note++
- ... wide palett of other editors ...

Specific editors / IDEs

- Spyder (!)
- **Pluto** (for Julia) (!)
- PyCharm
- Juno (VSCode, Julia)
- Lazarus (UI for desktop)
- Code::Blocks

Why is Jupyter important?

- HTML5 platform (kernel as backend, can run remotely on a different machine)
- Compatible with several languages (C++, Python, Julia, Haskell, ...)
- Important step in hosting and sharing codes (reproducability)
- Towards reproducable science! (also see Jupyter Lab)

> Careful: non-linear state, see next example! (Check out Pluto for linear state solution)

- Additional benefits of the separate backend: parallel execution, cluster management

In [51]:
```
b=2
print(b)
```

```
2
```

In [52]:
```
print(b)
b=3
```

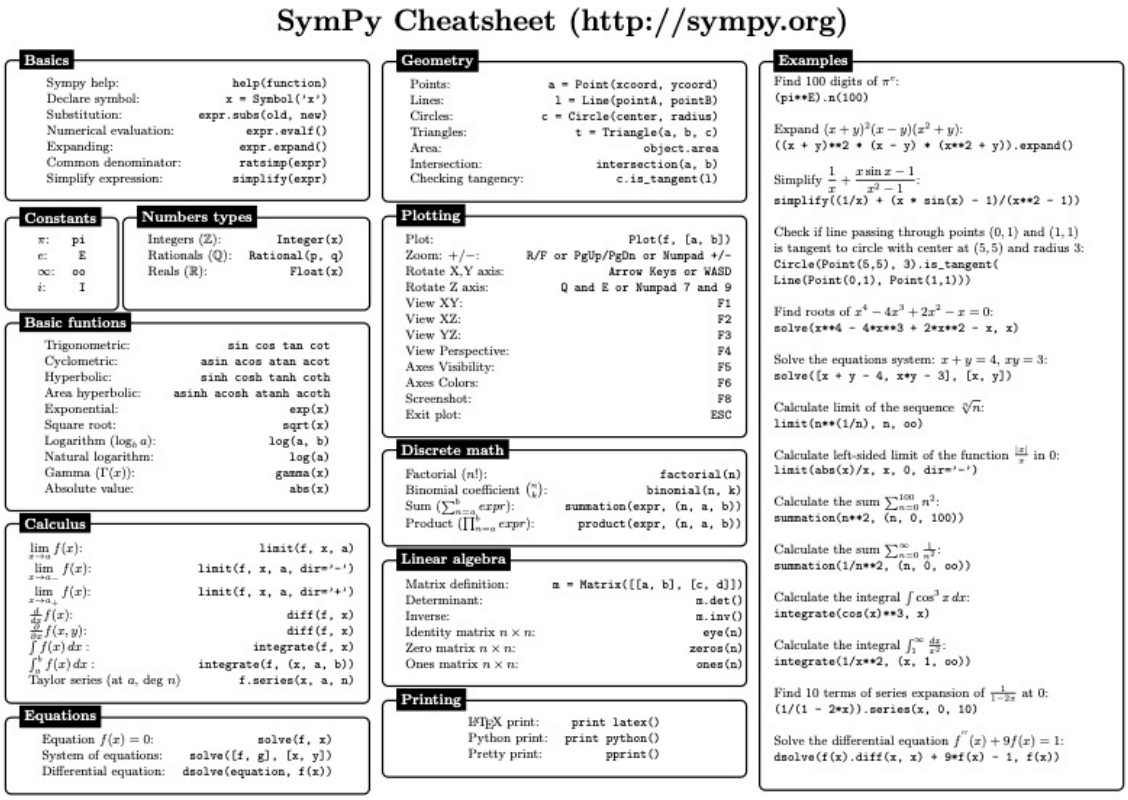
```
2
```

In [53]:
```
import sympy as sp
sp.init_printing(use_latex='mathjax')
x,y,z = sp.symbols('x,y,z')
f = sp.sin(x*y)+sp.cos(y*z)
sp.integrate(f,x)
```

Out[53]:

$$x \cos\left(yz\right) + \begin{cases} -\frac{\cos\left(xy\right)}{y} & \text{for } y \neq 0 \\ 0 & \text{otherwise} \end{cases}$$

Sympy



SymPy Cheatsheet (http://sympy.org)

Basics

Sympy help:	`help(function)`
Declare symbol:	`x = Symbol('x')`
Substitution:	`expr.subs(old, new)`
Numerical evaluation:	`expr.evalf()`
Expanding:	`expr.expand()`
Common denominator:	`ratsimp(expr)`
Simplify expression:	`simplify(expr)`

Constants

π:	`pi`
e:	`E`
∞:	`oo`
i:	`I`

Numbers types

Integers ($\mathbb{Z}$):	`Integer(x)`
Rationals ($\mathbb{Q}$):	`Rational(p, q)`
Reals ($\mathbb{R}$):	`Float(x)`

Basic funtions

Trigonometric:	`sin cos tan cot`
Cyclometric:	`asin acos atan acot`
Hyperbolic:	`sinh cosh tanh coth`
Area hyperbolic:	`asinh acosh atanh acoth`
Exponential:	`exp(x)`
Square root:	`sqrt(x)`
Logarithm ($\log_a a$):	`log(a, b)`
Natural logarithm:	`log(a)`
Gamma ($\Gamma(x)$):	`gamma(x)`
Absolute value:	`abs(x)`

Calculus

$\lim_{x\to a} f(x)$:	`limit(f, x, a)`
$\lim_{x\to a-} f(x)$:	`limit(f, x, a, dir='-')`
$\lim_{x\to a+} f(x)$:	`limit(f, x, a, dir='+')`
$\frac{d}{dx} f(x)$:	`diff(f, x)`
$\frac{d}{dx} f(x, y)$:	`diff(f, x)`
$\int f(x)\,dx$:	`integrate(f, x)`
$\int_a^b f(x)\,dx$:	`integrate(f, (x, a, b))`
Taylor series (at a, deg n)	`f.series(x, a, n)`

Equations

Equation $f(x) = 0$:	`solve(f, x)`
System of equations:	`solve([f, g], [x, y])`
Differential equation:	`dsolve(equation, f(x))`

Geometry

Points:	`a = Point(xcoord, ycoord)`
Lines:	`l = Line(pointA, pointB)`
Circles:	`c = Circle(center, radius)`
Triangles:	`t = Triangle(a, b, c)`
Area:	`object.area`
Intersection:	`intersection(a, b)`
Checking tangency:	`c.is_tangent(l)`

Plotting

Plot:	`Plot(f, [a, b])`
Zoom: +/−:	`R/F or PgUp/PgDn or Numpad +/-`
Rotate X,Y axis:	`Arrow Keys or WASD`
Rotate Z axis:	`Q and E or Numpad 7 and 9`
View XY:	`F1`
View XZ:	`F2`
View YZ:	`F3`
View Perspective:	`F4`
Axes Visibility:	`F5`
Axes Colors:	`F6`
Screenshot:	`F8`
Exit plot:	`ESC`

Discrete math

Factorial ($n!$):	`factorial(n)`
Binomial coefficient $\binom{n}{k}$:	`binomial(n, k)`
Sum ($\sum_{n=a}^{b} expr$):	`summation(expr, (n, a, b))`
Product ($\prod_{n=a}^{b} expr$):	`product(expr, (n, a, b))`

Linear algebra

Matrix definition:	`m = Matrix([[a, b], [c, d]])`
Determinant:	`m.det()`
Inverse:	`m.inv()`
Identity matrix $n \times n$:	`eye(n)`
Zero matrix $n \times n$:	`zeros(n)`
Ones matrix $n \times n$:	`ones(n)`

Printing

LaTeX print:	`print latex()`
Python print:	`print python()`
Pretty print:	`pprint()`

Examples

Find 100 digits of π^e:
`(pi**E).n(100)`

Expand $(x+y)^2(x-y)(x^2+y)$:
`((x + y)**2 * (x - y) * (x**2 + y)).expand()`

Simplify $\frac{1}{x} + \frac{x \sin x - 1}{x^2 - 1}$:
`simplify((1/x) + (x * sin(x) - 1)/(x**2 - 1))`

Check if line passing through points $(0,1)$ and $(1,1)$ is tangent to circle with center at $(5,5)$ and radius 3:
`Circle(Point(5,5), 3).is_tangent(Line(Point(0,1), Point(1,1)))`

Find roots of $x^4 - 4x^3 + 2x^2 - x = 0$:
`solve(x**4 - 4*x**3 + 2*x**2 - x, x)`

Solve the equations system: $x + y = 4$, $xy = 3$:
`solve([x + y - 4, x*y - 3], [x, y])`

Calculate limit of the sequence $\sqrt[n]{n}$:
`limit(n**(1/n), n, oo)`

Calculate left-sided limit of the function $\frac{|x|}{x}$ in 0:
`limit(abs(x)/x, x, 0, dir='-')`

Calculate the sum $\sum_{n=0}^{100} n^2$:
`summation(n**2, (n, 0, 100))`

Calculate the sum $\sum_{n=0}^{\infty} \frac{1}{n^2}$:
`summation(1/n**2, (n, 0, oo))`

Calculate the integral $\int \cos^3 x\,dx$:
`integrate(cos(x)**3, x)`

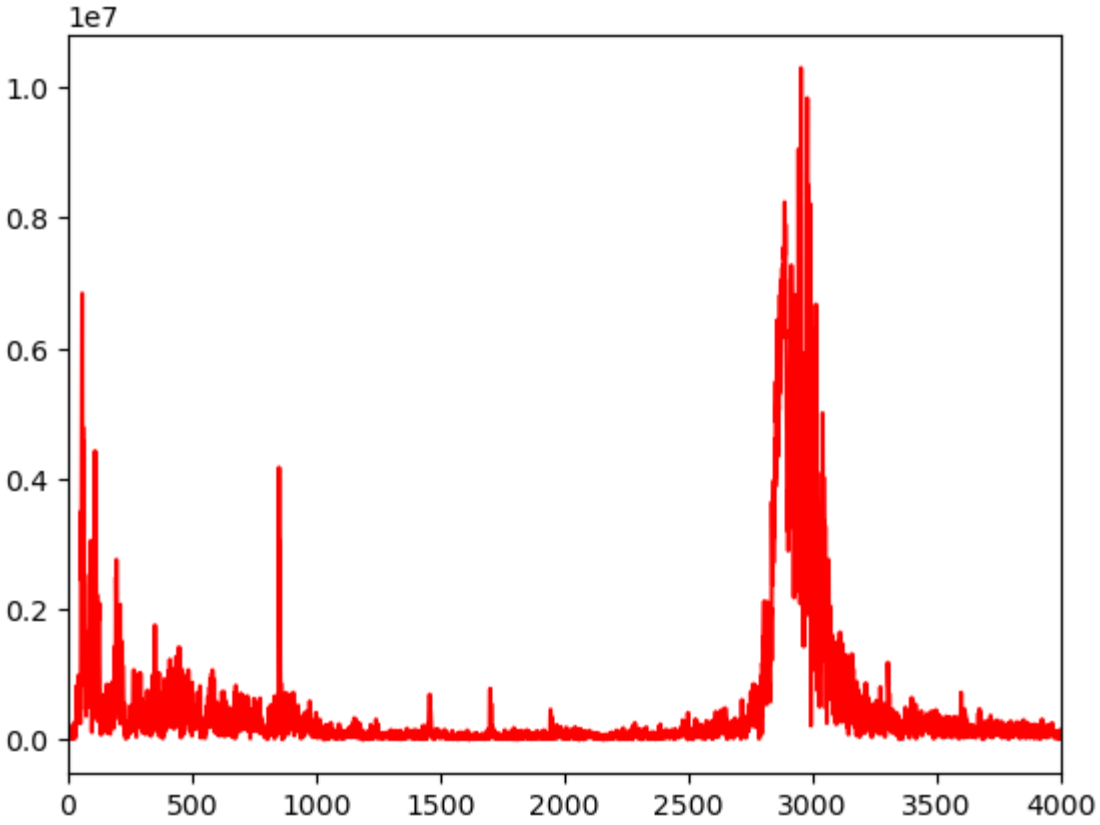
Calculate the integral $\int_1^\infty \frac{dx}{x^2}$:
`integrate(1/x**2, (x, 1, oo))`

Find 10 terms of series expansion of $\frac{1}{1-2x}$ at 0:
`(1/(1 - 2*x)).series(x, 0, 10)`

Solve the differential equation $f''(x) + 9f(x) = 1$:
`dsolve(f(x).diff(x, x) + 9*f(x) - 1, f(x))`

In [54]:
```
import matplotlib.pyplot as plt
%matplotlib inline
from scipy.fftpack import fft; from scipy.io import wavfile
fs, data = wavfile.read('sound/try2.wav') # load the data, 16 bit, 44.1 kHz
c = fft(data.T) # calculate fourier transform (complex numbers list)
d = len(c)//2  # you only need half of the fft list (real signal symmetry)
plt.plot(abs(c[:(d-1)]),'r'); plt.xlim((0,4000))
```

Out[54]: (0.0, 4000.0)

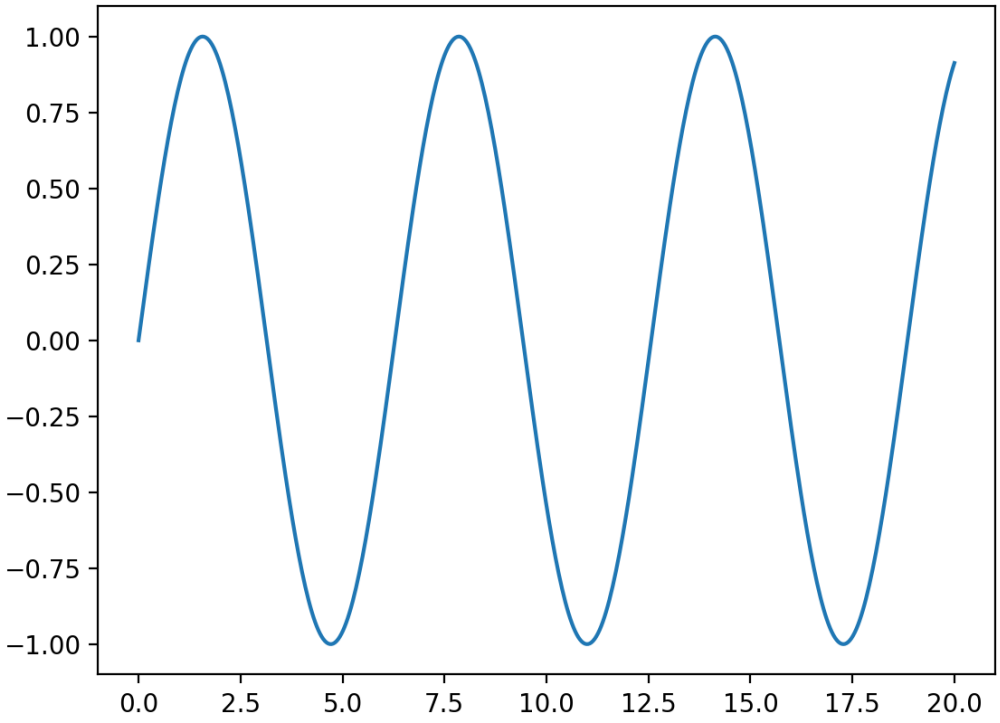


In [55]:
```
import IPython
IPython.display.Audio('sound/sample440.wav')
# IPython.display.Audio('sound/sample.wav')
```

Out[55]:

0:00 / 0:01

In [56]:
```
import matplotlib.pyplot as plt
%matplotlib notebook
import numpy as np
x = np.linspace(0,20,500)
plt.plot(x, np.sin(x))
```



Out[56]:
```
[<matplotlib.lines.Line2D at 0x1476cf070>]
```

In [57]:
```
import matplotlib.pyplot as plt
%matplotlib inline
from ipywidgets import interact, IntSlider
from IPython.display import display,clear_output

def f(freq):
    x = np.linspace(0,20,500)
    plt.plot(x, np.sin(x*freq))
    plt.show()
    #display(plt.figure)

interact(f, freq=IntSlider(min=1,max=5,step=1,value=1));
```

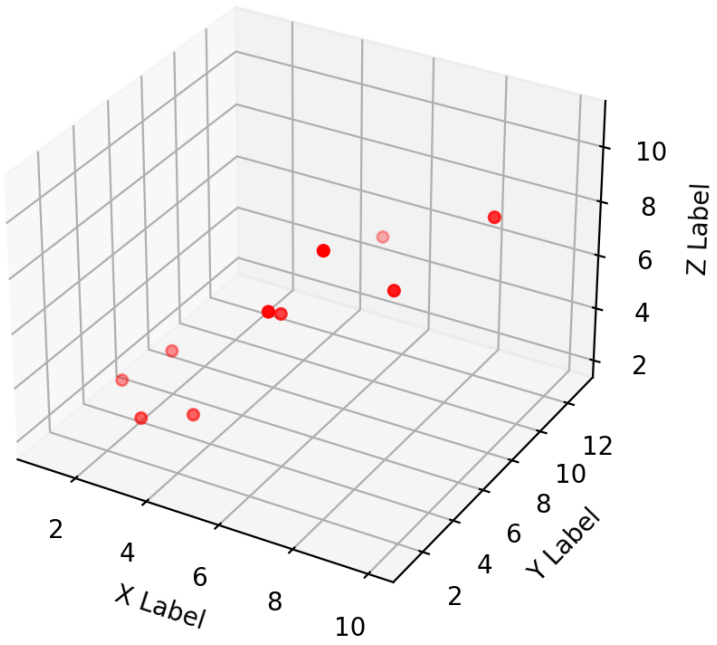
```
interactive(children=(IntSlider(value=1, description='freq', max=5, min=1),
Output()), _dom_classes=('widget-i…
```

In [58]:
```
from IPython.display import display, Javascript
import ipywidgets as widgets

L = widgets.Label("Hello World")
display(L)
```

```
Label(value='Hello World')
```

In [59]:
```
L.value = "Howdy World"
```

In [60]:
```
from mpl_toolkits.mplot3d import Axes3D; import matplotlib.pyplot as plt;
%matplotlib notebook

fig = plt.figure(); ax = fig.add_subplot(111, projection='3d')
x =[1,2,3,4,5,6,7,8,9,10]; y =[5,6,2,3,13,4,1,2,4,8]; z =[2,3,3,3,5,7,9,11,9
ax.scatter(x, y, z, c='r', marker='o'); ax.set_xlabel('X Label'); ax.set_yla
```



Out[60]:
```
Text(0.5, 0, 'Z Label')
```

In [61]:
```
import ipyvolume as ipv
import numpy as np
import ipyvolume.datasets
stream = ipyvolume.datasets.animated_stream.fetch()
fig = ipv.figure()
# instead of doing x=stream.data[0], y=stream.data[1], ... vz=stream.data[5]
# limit to 50 timesteps to avoid having a huge notebook
q = ipv.quiver(*stream.data[:,0:50,:200], color="red", size=7)
ipv.style.use("dark") # looks better
ipv.animation_control(q, interval=200)
ipv.show()
```

```
Container(children=[HBox(children=(Play(value=0, interval=200, max=49), Int
Slider(value=0, max=49)))], figure=…
```

In [62]:
```
import matplotlib.pyplot as plt
%matplotlib notebook
import pandas as pd
import seaborn as sns
df = sns.load_dataset("anscombe") #Anscombe's quartet, there are others (Tit
df.head()
```

Out[62]:

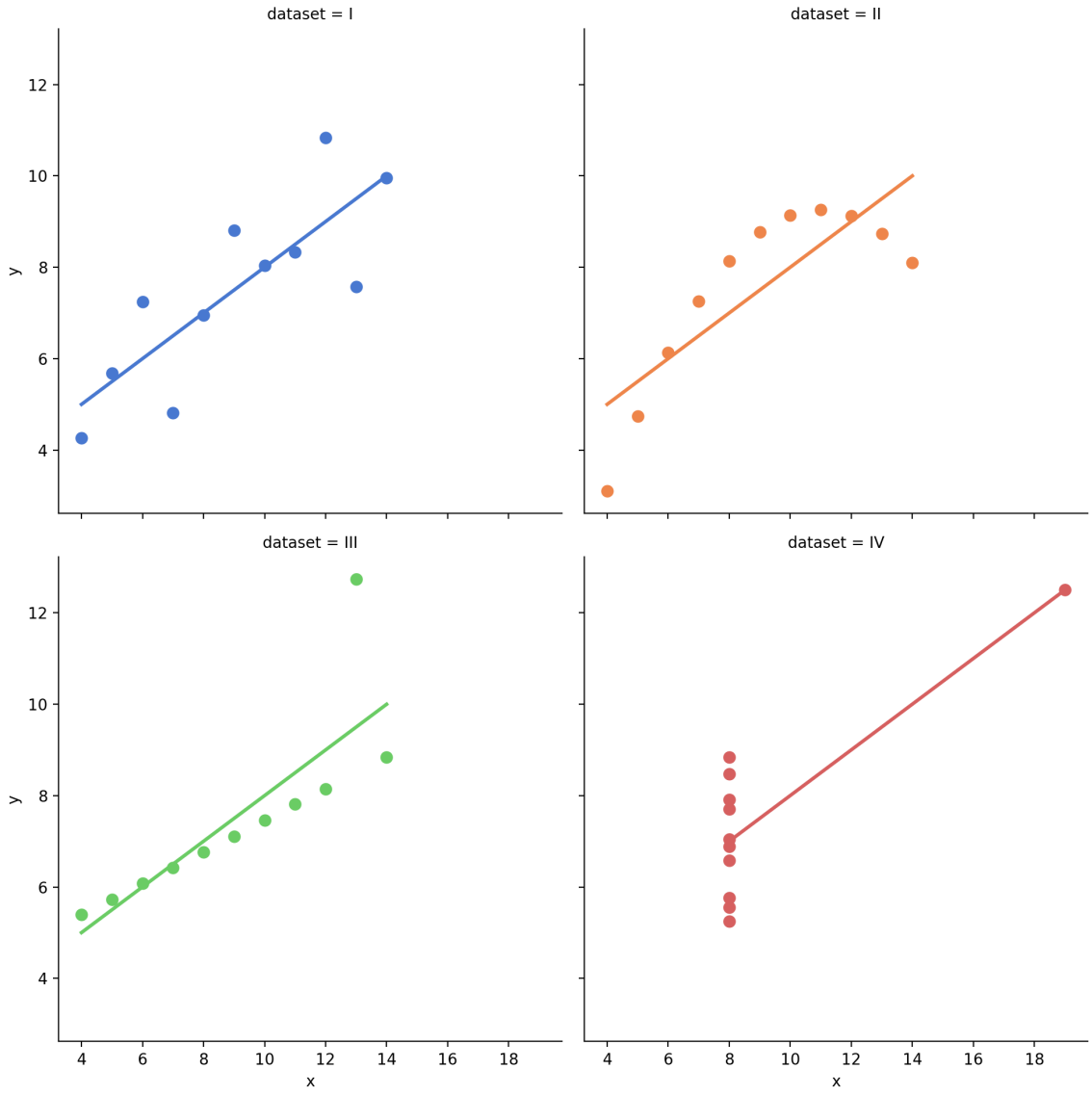
	dataset	x	y
0	I	10.0	8.04
1	I	8.0	6.95
2	I	13.0	7.58
3	I	9.0	8.81
4	I	11.0	8.33

In [63]:
```
df.groupby(df.dataset).describe()
```

Out[63]:

	x										
	count	mean	std	min	25%	50%	75%	max	count	mean	std	r
dataset												
I	11.0	9.0	3.316625	4.0	6.5	9.0	11.5	14.0	11.0	7.500909	2.031568	4
II	11.0	9.0	3.316625	4.0	6.5	9.0	11.5	14.0	11.0	7.500909	2.031657	3
III	11.0	9.0	3.316625	4.0	6.5	9.0	11.5	14.0	11.0	7.500000	2.030424	5
IV	11.0	9.0	3.316625	8.0	8.0	8.0	8.0	19.0	11.0	7.500909	2.030579	5

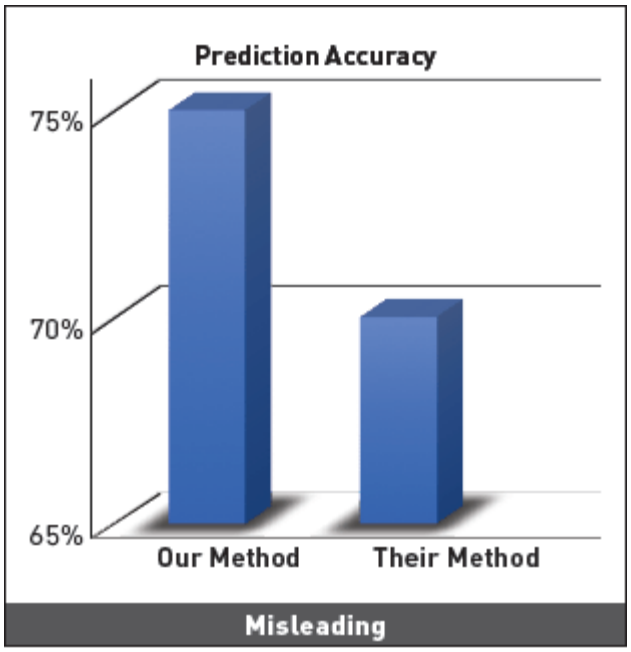
In [66]:
```
%matplotlib notebook # To put any warning below
sns.lmplot(x="x", y="y", col="dataset", hue="dataset", data=df, col_wrap=2,
           scatter_kws={"s": 50, "alpha": 1}); plt.show()
```

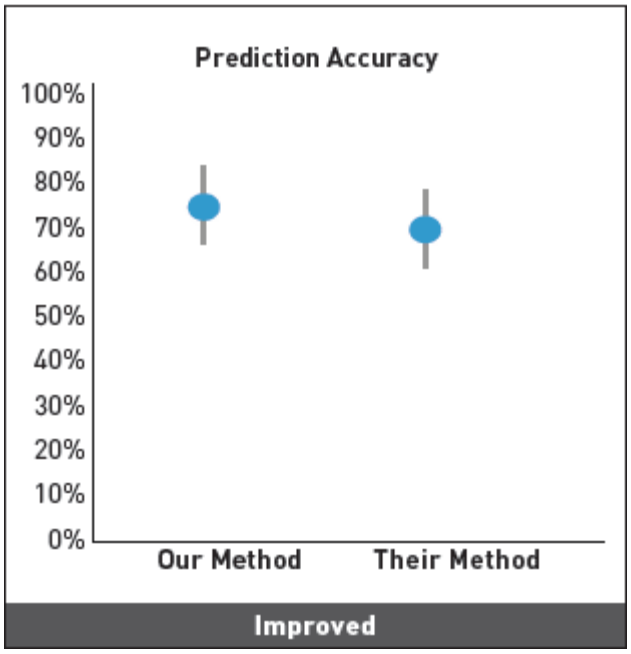


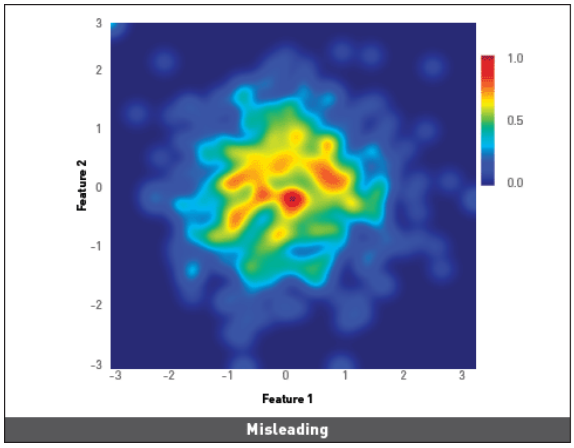

```
/Users/gzavo/anaconda3/envs/cstoolbox/lib/python3.10/site-packages/seaborn/
axisgrid.py:118: UserWarning: The figure layout has changed to tight
  self._figure.tight_layout(*args, **kwargs)
```

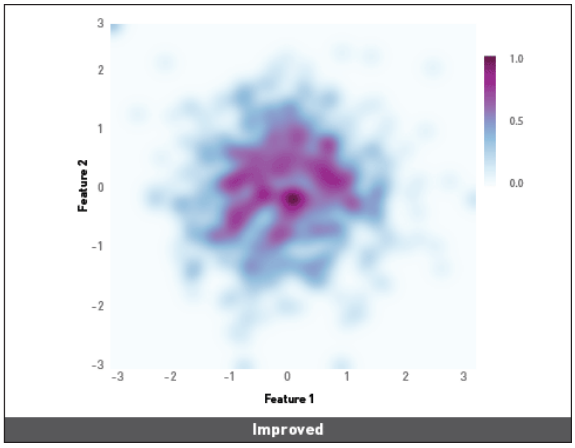
Visualization practices

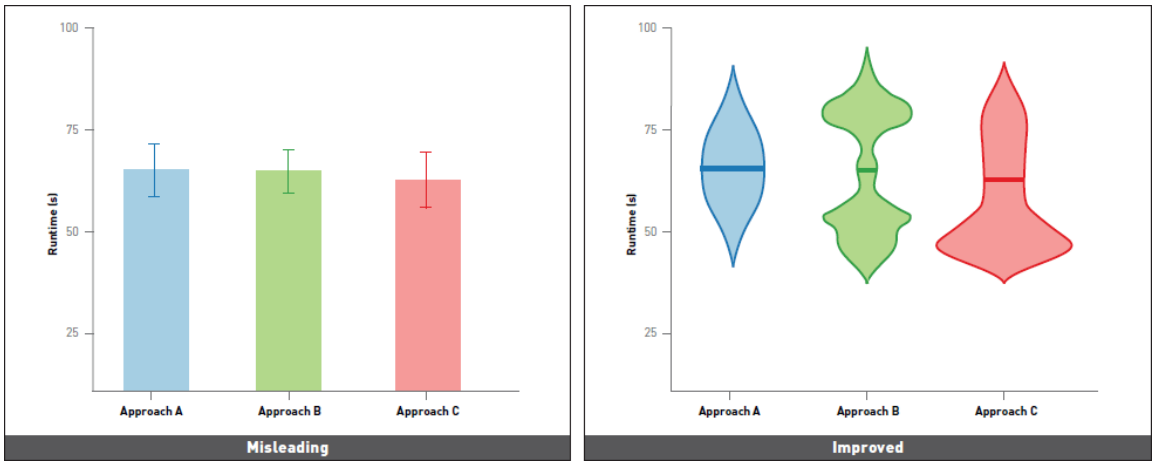
https://interactions.acm.org/archive/view/july-august-2018/the-good-the-bad-and-the-biased


Prediction Accuracy
75%
70%
65%
Our Method
Their Method
Misleading


Prediction Accuracy
100%
90%
80%
70%
60%
50%
40%
30%
20%
10%
0%
Our Method
Their Method
Improved


Feature 2
Feature 1
1.0
0.5
0.0
Misleading


Feature 2
Feature 1
1.0
0.5
0.0
Improved



Further visualization tools

Because our simulations produce a lot of data (big data?!), but the purpose of the computation is not numbers, but insight.

- python matplotlib (!) - (https://matplotlib.org/)
- ParaView (!) - VTK based parallel 3D visualization tool (https://www.paraview.org/)
- MayaVi - ParaView alternative, written in python (embeddable!) (https://docs.enthought.com/mayavi/mayavi/)
- gnuplot (!) - Swiss army knif of plotters (http://www.gnuplot.info/)
- vedo - Simple visualization 2D/3D, simulation friendly (https://github.com/marcomusy/vedo)
- Processing - Programming language designed for 3D visualizations (https://processing.org/)
- Inkscape - For that nice poster. (https://inkscape.org/)
- Blender - (https://www.blender.org/)

Presentation tools

- MS PowerPoint (!)
- LaTex (!) (e.g. Beamer)
- Reveal.js (https://github.com/hakimel/reveal.js/)
- Jupyter Notebook (sort of works...)
- TexMacs, LyX, ...

Further things to look at in the Python world

- https://github.com/barbagroup/CFDPython
- http://mbakker7.github.io/exploratory_computing_with_python
- https://github.com/vinta/awesome-python

Other tools to mention

- Desktop Jupyter: nteract (https://nteract.io/)
- Desktop JupyterLab: (https://github.com/jupyterlab/jupyterlab-desktop)
- Calculator: SpeedCrunch (https://speedcrunch.org/)
- CAS: Sympy (!) (www.sympy.org), Maxima (http://maxima.sourceforge.net/)
- Worksheet: SMathStudio (https://en.smath.com/view/SMathStudio/summary)
- Recording terminal session: ASCIInema (https://asciinema.org/)
- Collection of command line terminal tools (https://www.wezm.net/technical/2019/10/useful-command-line-tools/)

Software development in a collaborative environment

- Student-ware ('agile' method? - https://www.atlassian.com/agile)
- Guidelines PEP8
- Version control
- Tests

Software development as a student

The boundary conditions are a bit different compared to 'real' development, but still aim to adopt good practices!

The typical situation:

- most often no preliminary design
- "let's see what happens" first version
- then the code is "grown" in incremental steps
- "backups" is some old version on a pendrive, or sent in email
- patchworky design in team development
- this is a natural process given the boundary conditions

Pro.:

- nothing really
- maybe time efficiency on the short-run (*maybe*)

Con.:

- difficult collaboration with unnecessary friction
- quickly leads to decaying efficiency
- resulting code is not robust or future proof
- often difficult to extend (aka. rewrite to add a feature)

What can be improved?

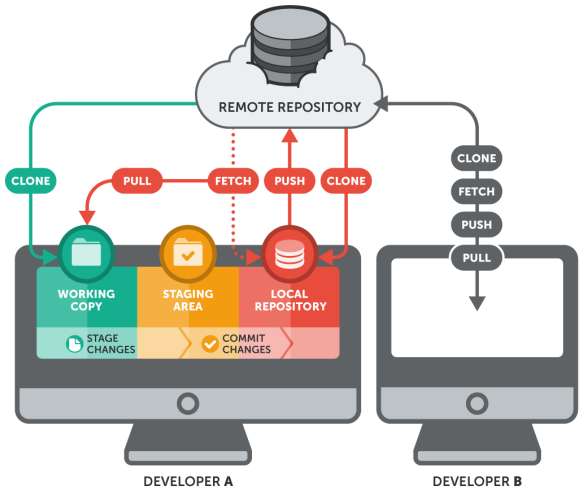
Coding style (!)

- Style guides:
  - Python PEP8 (https://www.python.org/dev/peps/)
  - C++ Google Style guide (https://google.github.io/styleguide/cppguide.html)
  - C - Many, e.g. Rob Pike's (https://www.maultech.com/chrislott/resources/cstyle/pikestyle.html)
  - Most IDEs have builtin support for this.
- Documentation (proper README.md)
- Code comments and function documentation (e.g. docstring).

In [71]:
```
print("".join(map(lambda x: chr((lambda p, x: int(sum(map(lambda i: p[i]*x**
```

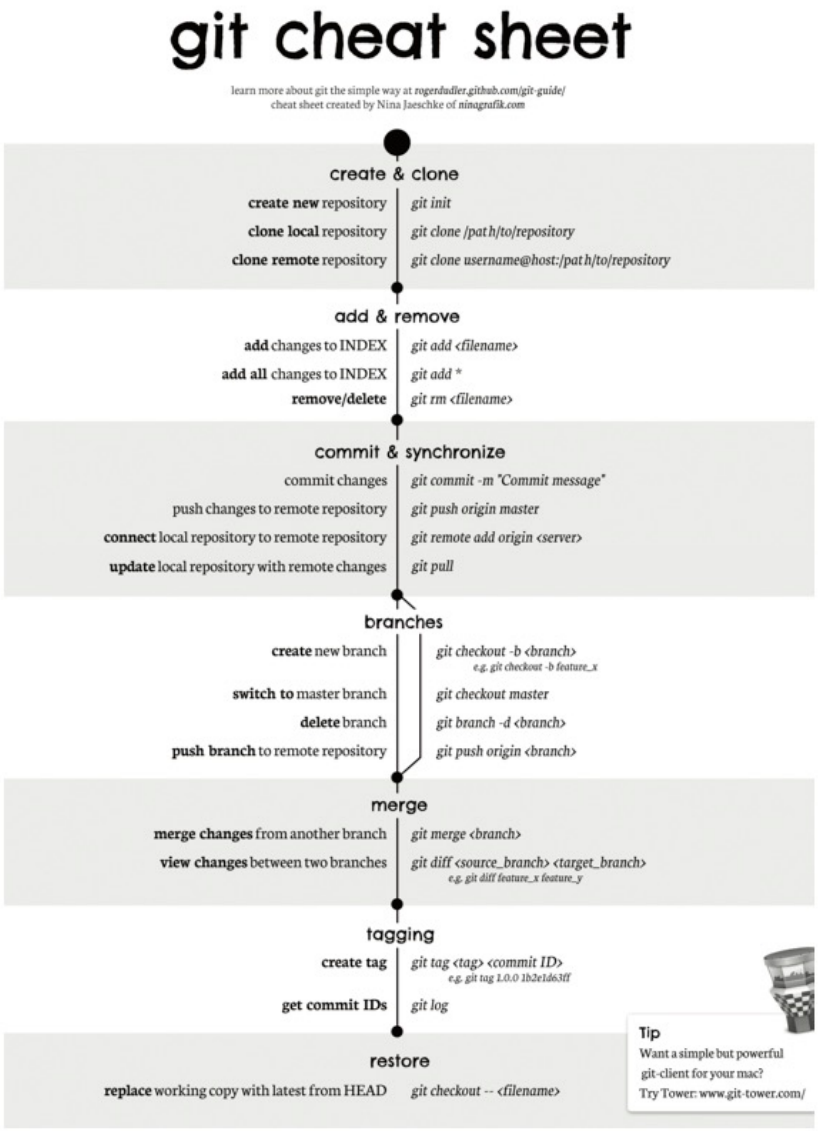
```
Hello world!
```

Version control - git (!)



In [68]:
```
from IPython.display import IFrame
IFrame("doc/git_cheat_sheet.jpg", width=800, height=600) # from http://roger
```

Out[68]:



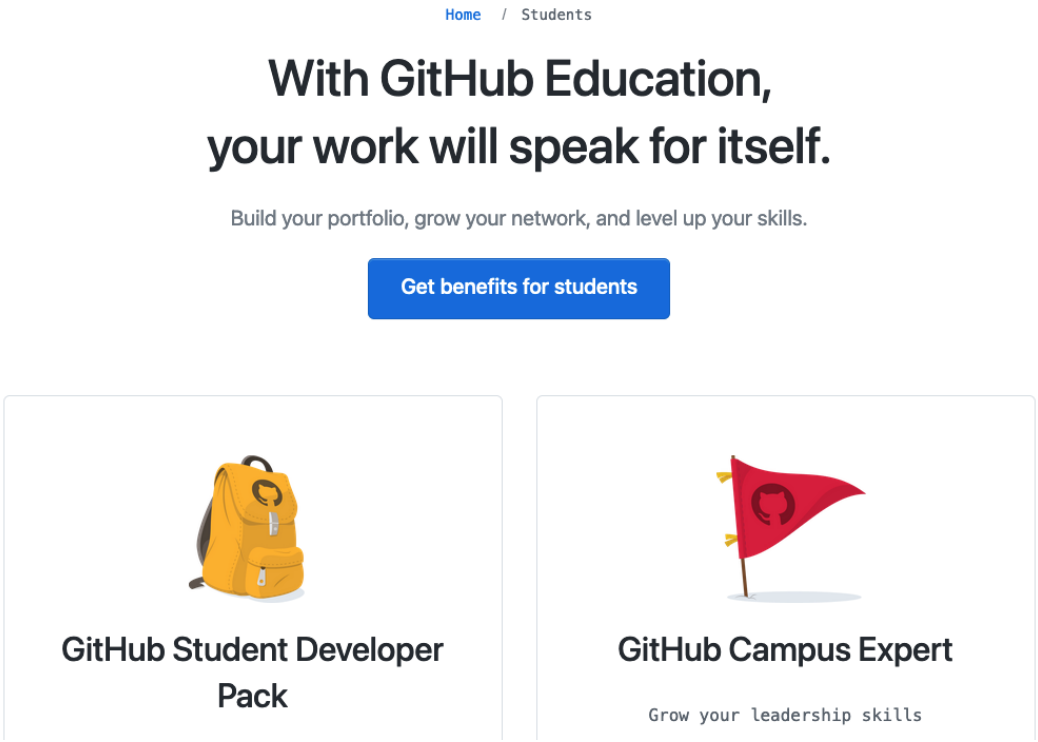
Tools for git

- tig (!) (https://github.com/jonas/tig)
- sourcetree (https://www.sourcetreeapp.com/)
- GitUp (mac only :/) (https://gitup.co/)
- gitKraken (not free, but part of GitHub Education :/) (https://www.gitkraken.com/)
- most IDEs have built in support for git
- Free git service: github, bitbucket, gitlab

GitHub

https://education.github.com/students

Access to additional tools: GitHub Copilot, Copilot Chat, Git Kraken, Termius....




I AM GOING TO USE GIT LIKE A PRO FROM NOW ON!
@GARABATOKID
ONE HOUR LATER
Main.js
_Main.js
__Main.js
Main_prev.js
Main_old.js

Git fame

https://github.com/casperdcl/git-fame

```
~$ git fame --cost hour,month --loc ins
Processing: 100%|████████████████████████| 1/1 [00:00<00:00,  2.16repo/s]
Total commits: 1775
Total ctimes: 2770
Total files: 461
Total hours: 449.7
Total loc: 41659
Total months: 151.0
| Author               |   hrs |   mths |   loc |   coms |   fils | distribution    |
|:---------------------|------:|-------:|------:|-------:|-------:|:----------------|
| Casper da Costa-Luis |   228 |    108 | 28572 |   1314 |    172 | 68.6/74.0/37.3  |
| Stephen Larroque     |    28 |     18 |  5243 |    203 |     25 | 12.6/11.4/ 5.4  |
| pgajdos              |     2 |      9 |  2606 |      2 |     18 | 6.3/ 0.1/ 3.9   |
| Martin Zugnoni       |     2 |      5 |  1656 |      3 |      3 | 4.0/ 0.2/ 0.7   |
| Kyle Altendorf       |     7 |      2 |   541 |     31 |      7 | 1.3/ 1.7/ 1.5   |
| Hadrien Mary         |     5 |      1 |   469 |     31 |     17 | 1.1/ 1.7/ 3.7   |
| Richard Sheridan     |     2 |      1 |   437 |     23 |      3 | 1.0/ 1.3/ 0.7   |
| Guangshuo Chen       |     3 |      1 |   321 |     18 |      7 | 0.8/ 1.0/ 1.5   |
| Noam Yorav-Raphael   |     4 |      1 |   229 |     11 |      6 | 0.5/ 0.6/ 1.3   |
| github-actions[bot]  |     2 |      1 |   186 |      1 |     51 | 0.4/ 0.1/11.1   |
...
```

Testing

- Unit tests (!)
- doc tests
- CI (continuous integration) / CD (continuous delivery)

In [69]:
```
import unittest

def fun(x):
    return x + 1

class MyTest(unittest.TestCase):
    def test(self):
        self.assertEqual(fun(3), 4)

# Testing
# Normally: unittest.main()
unittest.main(argv=['first-arg-is-ignored'], exit=False)
```

```
.
----------------------------------------------------------------------
Ran 1 test in 0.002s

OK
```

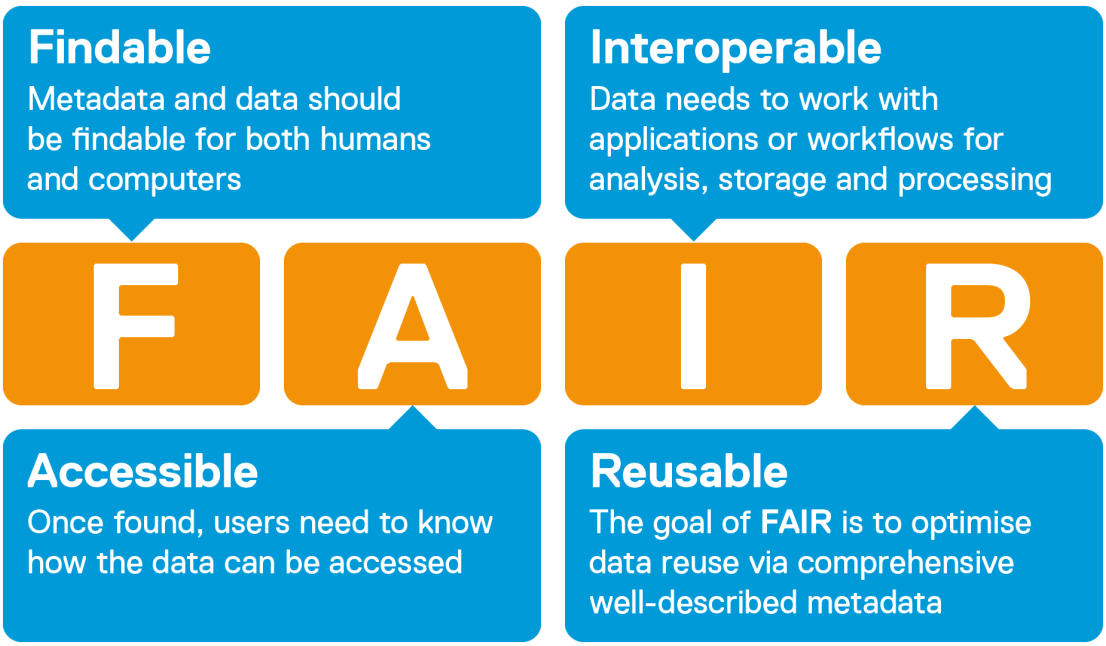
Out[69]:
```
<unittest.main.TestProgram at 0x1446df010>
```

In [70]:
```
def square(x):
    """Return the square of x.

    >>> square(3)
    9
    >>> square(-2)
    4
    """

    return x * x

# Testing
import doctest
doctest.testmod()
```

Out[70]:
```
TestResults(failed=0, attempted=2)
```

Data handling - FAIR principles

Publication in Nature Data Science - https://doi.org/10.1038/sdata.2016.18



Use case - HemoCell (www.hemocell.eu)

Some highlights:

HemoCell is a high-cost code, it is in continuous development for 8 years. >20 developers, >20 associated scientific publications, largest distributed execution in Europe.

Tools and techniques of interest:

- Developped in C++ with processing scripts in Python and Bash.
- The source code is version controlled under git (GitHub).
- Uses 2 CI/CD servers to test commits.
- Edited mostly in Visual Studio Code, Sublime Text, and NetBeans.
- The documentation is written in Markdown(-ish) text.
- The publications are written in Overleaf.
- Data visualization through ParaView and Blender.
- Data evaluation through Python (+ HDF5, VTK, ...).
- Presentations, posters done in PowerPoint.
- Illustrative graphics in Inkscape.

Take home message

1. Always aim for work quality suitable for collaboration!
2. Write tidy, well commented code. I.e.: "Will I understand my code completely by reading this 2 years from now?"
3. Write documentation! You'll be glad you did few years down the line.
4. Use version control, even if you are the only developer.
5. Try to cover with tests as much as possible.
6. Visualize whenever possible, develop fast pipelines for visualization.
7. Use multiple visualization, observe it from different angles before you decide how will you present it.
8. Every statement you write down requires evidence! I.e., data produced by you or references (scientific ones, not wikipedia).

Homework assignement

https://github.com/gzavo/CS_Assignment

1. Create a free github account if you don't already have one.
2. Fork this repository.
3. Create a markdown (.md) named "solution_.md" file that will contain the following:
4. The title of the following papers pivotal to our knowledge:
    - MCC Van Dyke et al., 2019
    - JT Harvey, Applied Ergonomics, 2002
    - DW Ziegler et al., 2005
5. Create 1 plot from the dataset "istherecorrelation.csv", with DPI=300. The objective is to visualize the data as you see fit. Include the resulting image in the markdown file (and you can also write a few lines of interpretation if you like).
6. Commit and push these two files to your fork.
7. Create a pull request for me to this (original) repo. (Hint: use "compare across forks").

Thank you for your attention!

Questions?