

theory

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outline

key scientific computing rules to get your started

elaboration, details, in other words; general rules

and yet one more variation on general rules

the zen of Python

Know Your Data!

- simply cant use it well if you dont know it well
 - (not just data; the field: theory, lit, method, etc)
 - this is where you beat IT folks (MS/PhD just in IT)
- again, be prepared to invest a lot of time into your data
 - use data that you're passionate about
 - or that can make \$ (now or in future career)
 - or ideally both!
- don't forget to think about it! don't be mindless!
 - ask questions, be investigative, be critical
- double check, cross check, give to others to check

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Wilson put it well

- print out Box 1 from these 2 art
- hang it at your office, home, and elsewhere
- <https://journals.plos.org/plosbiology/article?id=10.1371/journal.pbio.1001745>
- <https://journals.plos.org/ploscompbiol/article?id=10.1371/journal.pcbi.1005510>
- and Know Your Data (2nd slide)
- and variations on these, and other general rules follow

simplicity, cleanliness, and organization!

- keep it as simple as possible
 - especially if overwhelmed or struggling
- say retain only 5vars and 25obs
 - much easier to understand such data
- simplicity transparency clarity:
 - use fancy code: eg loops iff they simplify
- have chunks of code only once
- code it all from raw to final (replication principle)
- organize: sections, comments, and logical order (eg rewrite, move code around)

be fast/efficient

- the fancier the code, the more time/effort to write it
- don't do fancy things unless they save time in the long run
- it's all about managing complexity
- automate as much as you can
- simplify and be clear
- have general modules (sections or separate files)
 - that can be reused for different projects
- be lazy: don't reinvent the wheel—google often

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accuracy / correctness

- ◇ it's fundamental and obvious: bad if wrong
- double check
- especially at the beginning do not assume things
- double/triple check the whole code once finished
- go public, present, give it to others
- its human to err, there will be mistakes

1.write; 2.rewrite/reorganize; 3.optimize/improve

- 1. dump it, do “free writing” with code, too (i often come up with some idea out of sudden, and just write it down)
 - start simple and keep on adding things
- 2. rewrite/reorganize your code
- 3. optimize/improve
 - dont optimize too early, first make it work
 - (there is often a tendency to over optimize, ie spending days on small chunk of code that does not really matter that much)
- (then can rewrite/reorganize again)

rewrite and reorganize

- efficiency: few lines of code do many things
 - do more in fewer lines, drop unnecessary things
- reorganize and rewrite!
 - just like your papers: you print them out
 - and move paragraphs and words around
 - and you simplify and strike out unnecessary words
- do the same with code! drop everything you can!
- ◇ code should be “tight”
 - as few lines as possible to perform given task
- use wrappers on more laborious functions, google it, stack-overflow, etc
 - instead of lists: pandas, etc

efficiency: on the other hand

- but you also want to be extensive in a way
- in a good way...
- like with free writing, so with code
 - do “free writing”
- be expressive and dump your ideas into notebook
- just be organized so that you know what is going on!
- yes, by all means, be efficient—drop unnecessary things
- but do not drop things that may be useful
 - say in the future or other projects
 - may comment them out, move to LATER sec, etc

optimize/improve/get fancy

- think how to optimize
- related to efficiency: do more in fewer lines
 - but here instead of dropping unnecessary stuff
 - we get fancy: loop, list comprehension, your own function
- but first: dont reinvent the wheel, search for existing functions
 - only then optimize yourself, eg loop, write your own function

simplicity: different, often opposite, from

optimization

- ◇ people don't realize this!
- be as simple as possible in writing the code (papers, too)
- ◇ the more code you have (always try to get less) and the more complicated (optimized) it is:
 - the more likely you have mistakes
 - and the more difficult it is to find them
- do not complicate (optimize) your code for the sake of fanciness
- yes simpler is better

standardize

- ◇ standardize— >fewer mistakes (eg make fewer decisions, like a template, on autopilot)
- standardize— >code more transparent, easier to find weird stuff, errors
- like have a template for some vis: say always hist for all key vars; scatterplot matrix for all continuous vars, etc
- and then have the creative part, vis for specific project

modularity

- break large tasks into small (manageable) blocks/components
 - (like in dissertation—don't overwhelm yourself doing everything at once)
- the components are like sections in a paper, step-by-step
- it is easy then to reuse these components
- so have separate ipynb for different tasks; and have sec and subsec within ipynb

automation (closely related to standardization)

- everything should be coded
- no copy-paste, point-and-click, etc
- dont use excel for anything!
- ◇ automate as much as possible!
- ◇ practical reason: faster! (in the long run)
- ◇ technical reason: computers **never** make mistakes
- ◇ eg pull automatically from database, upload to github
etc

document

- have text fields in ipynb and `#` comments in code fields
- meaningful commit messages in git
- may have changelog (version, date and explain what changed, eg: 0.1 dumped raw ideas; 0.2 loaded X data; 0.21 loaded Y, Z data)
- difficult to overestimate importance of documentation
- note: typically, i underdocument, too

singularity

- have only one chunk of code and one file in one place, ideally in git
- as projects grow, get complex and maybe branch off, do have parents-children, and possibly branches
- elaborate: eg i do a lot with gss, draw flow-chart
- at first it was a first paper
- then i write 2nd paper, and realize most of dat man is the same
- so i create one root/parent with common code for all gss papers

portability

- import libs at the beginning, the fewer the better
 - i overdid, i need to cut down
- you could get version of key libs, ie pandas and mpl and save info
- but just 2 libs, can easily trace it back if sth doesnt run in couple years
- but do always save raw data! likely in couple years dataset may disappear or change
- also keep in mind magics (%matplotlib) for running in different environments eg spyder

tradeoffs: life is difficult

- ◇ simplicity is sometimes inversely (positively) related to efficiency (amount of code/being verbose) (as you cut stuff down, it may take longer to figure it out (parsimonious is sometimes complicated))
- simplicity usually inversely related to optimization (eg loops)
- ◇ simplicity often inversely related to automation (eg complicated code with if else)

cont

- ◇ so make choices, the more serious you are about coding, the more work you do:
- the more you should care for automation, efficiency, and optimization
- the more automation/efficiency/optimization actually simplifies
- like Py v excel: excel simpler for simple tasks
- but Py is simpler for complicated tasks
- stick with one soft! [i think i'm quitting stata]

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more principles

- from 2 books about general programming (classics and free!)
 - <http://catb.org/esr/writings/taoup/>
 - <http://www.htdp.org/2003-09-26/Book/curriculum-Z-H-1.html>

clarity

- “design for transparency and discoverability”
 - write clean code [eg split 1 fn over many l for readability]
 - avoid fancy code
 - fancy code is buggier
 - clarity is better than cleverness
- eg:
 - group logical chunks together
 - more than twice nested loops gets confusing
 - if your code is mostly loops, consider functions

modularity

- “write simple parts that are cleanly connected”
- “controlling complexity is the essence of computer programming”
- debugging dominates development
- eg:
 - better many small loops that each does one thing, than one huge (>100 lines) loop that does everything
 - clear sections of one file
 - or many files instead of one file without sections

modularity

- code should be organized logically not chronologically
 - do free writing, but then reorganize
 - like with papers, code should be rewritten, eg:
 - no data management in data vis part
 - move rename, replace, etc earlier

composition

- “design programs to be connected to other programs”
- notebook or its sec will produce output for another notebook or sec
- eg: you clean up data in one file to make data ready for another one to vis
 - or just have one big file
- but the workflow needs to be logically organized

optimization (fancier, fewer lines)

- yes, but “get it working before optimizing” !
- eg:
 - first make mpl hist for one var, make it working
 - and then deploy it for 10 vars with a loop

extensibility

- “design for the future because it will be sooner than you think”
 - you will reuse your code in the near future
 - so write it clean
 - have sections, etc
 - use lots of comments
 - reorganize, rewrite
 - optimize

silence

- “when a program has nothing surprising to say, it should say nothing”
- drop unnecessary code
 - if you think it may be useful in the future comment it out
- do not generate unnecessary output, do not lose your reader in unnecessary clutter
 - if the output has nothing useful to say it should be dropped
 - (or commented out)

automation (again)

- “rule of generation: avoid hand-hacking”
- because humans make mistakes and computers don't, computers should replace humans wherever possible
- automate anything that you can
- but stay human, focus on fun creative part, eg vis
- dont automate everything; eg dont crank out bunch of vis mindlessly

save time: reuse (copy-paste), don't reinvent the wheel

- if someone has already solved a problem once, reuse it!
- it is very unlikely you are doing something completely new
 - eg google 'student data analysis python'
- if anything, the problem is that people do not share their code
- usually all you need to do is to adjust somebody else's code or your old code
 - its like doing lit rev, but with code
 - and with data too, eg google scholar psid biking to find out how people use biking var in psid

save time: reuse, don't reinvent the wheel

- ask people for code:
 - your supervisor
 - journal article authors
 - your colleagues, friends, etc
- share your code
 - you may want to protect some parts of it
 - (critical, innovative research ideas, etc)
 - but share as much as possible
- acknowledge others' work

defensive programing

- “people are dumb-make program bullet-proof”
 - you will find negative income, age over 200
- think of likely possibilities/instances; especially if you suspect some specific problems
- thats also why its so important to interpret critically your vis, if something looks funny or unlikely, maybe there's a mistake

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- Beautiful is better than ugly.
- Explicit is better than implicit.
- Simple is better than complex.
- Complex is better than complicated.
- Flat is better than nested.
- Sparse is better than dense.
- Readability counts.
- Special cases aren't special enough to break the rules.
- Although practicality beats purity.
- Errors should never pass silently.
- Unless explicitly silenced.
- In the face of ambiguity, refuse the temptation to guess.

- There should be one— and preferably only one —obvious way to do it.
- Although that way may not be obvious at first unless you're Dutch.
- Now is better than never.
- Although never is often better than **right** now.
- If the implementation is hard to explain, it's a bad idea.
- If the implementation is easy to explain, it may be a good idea.
- Namespaces are one honking great idea — let's do more of those!