Best Practices

A talk for Barcelona Supercomputing Center's Ph.D. students

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Welcome to Ph.D. student's life

Congratulations, by the way

Doing a Ph.D. is an amazing experience

But it can also be stressful

We want to present some ideas on how to survive (and succeed) your Ph.D.

Some of them are personal opinions

(informed by shared experiences)

Some of them are endorsed by research

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- Mathematical Engineer, U. of Chile
- PhD Informatics, INRIA–U Rennes 1, France
- PhD Mathematical Modeling, U. of Chile
- Research in machine learning for metagenomics, and in gene expression analysis for systems biology

Focus on Philosophy, not Tools

Tools will change in time. There will be new tools

You probably use tools that did not exist 10 years ago

And they often are a matter of *personal taste*

So we will focus on the *philosophy* of the tools

(i.e. the part that will not change)

A Ph.D. goal is to produce and communicate new knowledge

(we call it “Doing Science”)

The key word here is *communicate*

What is the value of a result that is not made public?

We communicate with our *collaborators*

Most of research is done in teams

Good practices help teamwork, by:

- Keep track of what was (or was not) done
- Coordinate next steps
- Avoid work duplication

...but I work alone...

Even if we work alone, we are still communicating

- with your **supervisor/advisor**
- with the **referees** of your paper
- with other **scientists** that read (and cite) you
  - including the next Ph.D. student in your lab
- with the **general public**
- with our **future self**

Each one of these interactions can improve following a good practice

Communicate with: your supervisor

Research results are not enough

You must convince your boss (and the jury) that you deserve to be called “Doctor”

Make your work easy to *understand*

Make clear what is your original contribution

...with the **referees** of your paper

Give them all they need to *replicate* and *validate* your work

Referees are busy people and are not paid

Being *clear and transparent* helps them to decide fast

You will get published faster, or at least get good feedback

...with **other scientists** in your field

that will read your paper
(and hopefully cite your work)

The game does not end when you publish

50% of papers are read only by the referee

Make your work easy to *understand* and *replicate*

I forgot where I read it

with the **general public**

Eventually, your work will have an impact outside academia

(the end goal is to make a better world, no?)

We need to be aware of the *ethical* implications

- Licensing
- Privacy
- Truth

This is reflected in the Reproducibility Crisis

with our **future self**

Nothing is more frustrating that reading your old work

“The past is a foreign country”

Undocumented code/protocols are hard to understand…
and you can only blame yourself

We need good practices, because

our mind fools us

We think we will never forget, but we do

> *“I remember it now, therefore I will remember it forever”*

When we see something or learn something, this fact is present in our short-term memory and we feel like we will always remember it

Solution: Use a journal (or lab notebook, or blog)

We think our memories correspond to facts, but often they do not

“Things were exactly as I remember”

Research shows that our memory is not at all a “recorder”

We misremember a lot

Solution: Use a journal

We are bad at estimating projects' complexity

We think that we can finish a project in less time that it will really take

Solution: Write in your journal how much time you worked every day.
Reflect on how did you use your time

We think that everybody knows what we know, so they do not need explanations

> *"I understand it, so everybody understands it"*

This is the *curse of knowledge*

It is **the main reason** why our text is hard to read

Solution: still trying to figure out. Practice.

We think that everything we do is easy

> *“I’m not really that good, and one day they will realize I don’t know anything”*

We learn a little every day, so it never feels hard

But we accumulated learning in a large period,
and it is hard to see how much we have learned

This leads to *Impostor Syndrome*

Solution: Look at your journal and *reflect* on how much have you learned in the last year

We don’t know that we don’t know

“Incompetent, and unaware of it”

This is the Dunning-Kruger effect

It is hard to improve if we don’t know we are bad

Be open to criticism of your work

You are not your work

First idea:

Structured documents

You probably know that using a good *data structure* can dramatically improve an algorithm

And you use *structured programs*

The same applies to structuring our documents

Maybe you have used LaTeX, or Markdown

Maybe you know HTML

Separation of concerns

The key idea is to describe *what things are*, not *how they look*

Describe the role of text, not the “looks”

Separate style from structure

This part is based on the ideas discussed in “LaTeX: A Document Preparation System” by Leslie Lamport (1986).

It is like a house

Structure makes the house solid and comfortable

If you only do decoration, the house looks nice but it is not solid

Structure of the walls come first

Painting the walls in a nice color is secondary

Structural elements

- Sections, subsections, paragraphs
- Figures and Tables
- Lists
- References
- Equations
- Metadata
    - Title
    - Authors
    - Affiliations
    - Dates: submission, acceptance
    - Media/format

Example: writing in LaTeX

A LaTeX document looks like this

```
\documentclass[a4paper]{article}
\title{On computable numbers, with an application to the Entscheidungsproblem}
\author{Alan M. Turing}
\date{28 May, 1936}
\begin{document}
\section{Introduction}
The ``computable'' numbers may be described as the real numbers whose
expression as a decimal are calculable by finite means.
\end{document}
```

LaTeX files are text files. They will never be obsolete.

Changing the `documentclass` will change the document *look*

Advantages of LaTeX

- Write first, compile later
- Do not waste time playing with fonts
- Good journals accept LaTeX submissions
  (they also accept Microsoft Word format)

LaTeX files are *text files*

- Independent of any provider
- Use your favorite text editor (VScode?)
- Version control friendly (GitHub?)
- Can probably be read 20 years from now

We cannot say the same about Microsoft Word

According to the author of LaTeX

> *"[LaTeX] It's easy to use—if you're one of the 2% of the population who thinks logically and can read an instruction manual. The other 98 % of the population would find it very hard or impossible to use.*

So maybe the main advantage is that it *forces* you to think logically and organize your ideas

"How (La)TeX changed the face of Mathematics". An E-interview with Leslie Lamport. http://lamport.azurewebsites.net/pubs/lamport-latex-interview.pdf

3 mistakes that people should stop making

1. Worrying too much about formatting and not enough about content.
2. Worrying too much about formatting and not enough about content.
3. Worrying too much about formatting and not enough about content.

"How (La)TeX changed the face of Mathematics". An E-interview with Leslie Lamport. http://lamport.azurewebsites.net/pubs/lamport-latex-interview.pdf

Bonus: Slides for presentations

After writing your paper, you will probably present it
(or maybe before finishing it)

Using structured document makes it easy to *recycle* your material to presentation slides

In LaTeX you can do that using the `beamer` document class

Writing Math Expressions

LaTeX is favored by people who writes mathematical formulas

```
$$(a+b)^n=\sum_{k=0}^n \frac{n!}{k!(n-k)!} a^k b^{n-k}$$
```

$$(a+b)^n=\sum_{k=0}^n \frac{n!}{k!(n-k)!} a^k b^{n-k}$$

You can use this syntax in Microsoft Word's Equation Editor, and in web pages (using KaTeX or MathJax)

Learning how to write math is a good investment

Bibliographic References

There are *hundreds* of citation styles

Life is too short to sort references *manually*

LaTeX also provides a convenient way to handle references

References are stored in a separate text file, in BiBTeX format

Many tools can create BiBTeX files for you

- Zotero
- Mendeley

Collaborating with other people

Since LaTeX files are *text files*, it can be put under *version control*

In practice this means `git`, and maybe *GitHub* or *GitLab*
(or something in your server)

Several people can edit the same file at the same time
Git will do the right thing when merging

It does not need permanent Internet access
(i.e. you can write while traveling)

Real time collaboration

> *Overleaf is an online collaborative writing and publishing tool*

> *Overleaf provides … an easy-to-use LaTeX editor with real-time collaboration and the compiled output produced automatically … as you type*

You do not need to install anything in your computer

https://www.overleaf.com/

LaTeX disadvantages

- LaTeX is hard to learn
  - This discourages many people
  - Your collaborators may not use it
  - You need to have the Reference Manual at hand
- It is oriented to producing printed material
  - It produces PDF files or equivalents
  - Not suitable for Web or eBook
- Writing tables is hard

Alternative: Markdown

It is a light markup system that can be easily converted into nice presentations

```
% On computable numbers, with an application to the Entscheidungsproblem
% Alan M. Turing
% 28 May, 1936

# Introduction
The "computable" numbers may be described as the real numbers whose
expression as a decimal are calculable by finite means.
```

You probably have seen it in GitHub or Jupyter Notebooks

Same philosophy as LaTeX, but simpler

Markdown's author says:

"The overriding design goal for Markdown's formatting syntax is to make it as readable as possible.

"The idea is that a Markdown-formatted document should be publishable as-is, as plain text, without looking like it's been marked up with tags or formatting instructions."

John Gruber https://daringfireball.net/projects/markdown/

Using Markdown in practice

There are dozens (maybe hundreds) of Markdown editors and compilers

They offer many extensions

They are not always compatible

There is not yet an official standard

Recommendation: pandoc

Pandoc

> *If you need to convert files from one markup format into another, pandoc is your swiss-army knife*

Pandoc can convert between *many* formats, including

- Markdown
- Microsoft Word/Powerpoint
- LaTeX
- Jupyter notebook

Practical pandoc

- You can write your main text in Markdown, and convert it into LaTeX
- Pandoc understands LaTeX math expression, and can convert them to HTML or Microsoft Word
- You can mix Markdown and LaTeX, and pandoc will keep the LaTeX part

Pandoc advantages

- Text files
- It is easy to write tables in Markdown
- It is easy to write lists
- Can be used for slides
    - Several web platforms (like this document)
    - Microsoft Powerpoint
- Handles BiBTeX references

Collaborating using Markdown

Markdown files are text files

Thus, *git* is the way to go

But if you want *real time* collaboration, try https://hackmd.io/

Alternative: Microsoft Word

Depending on your *boundary conditions*, you may choose to use a WYSIWYG word processor

You can still follow the same philosophy:

- Separate style from structure
- Focus on content

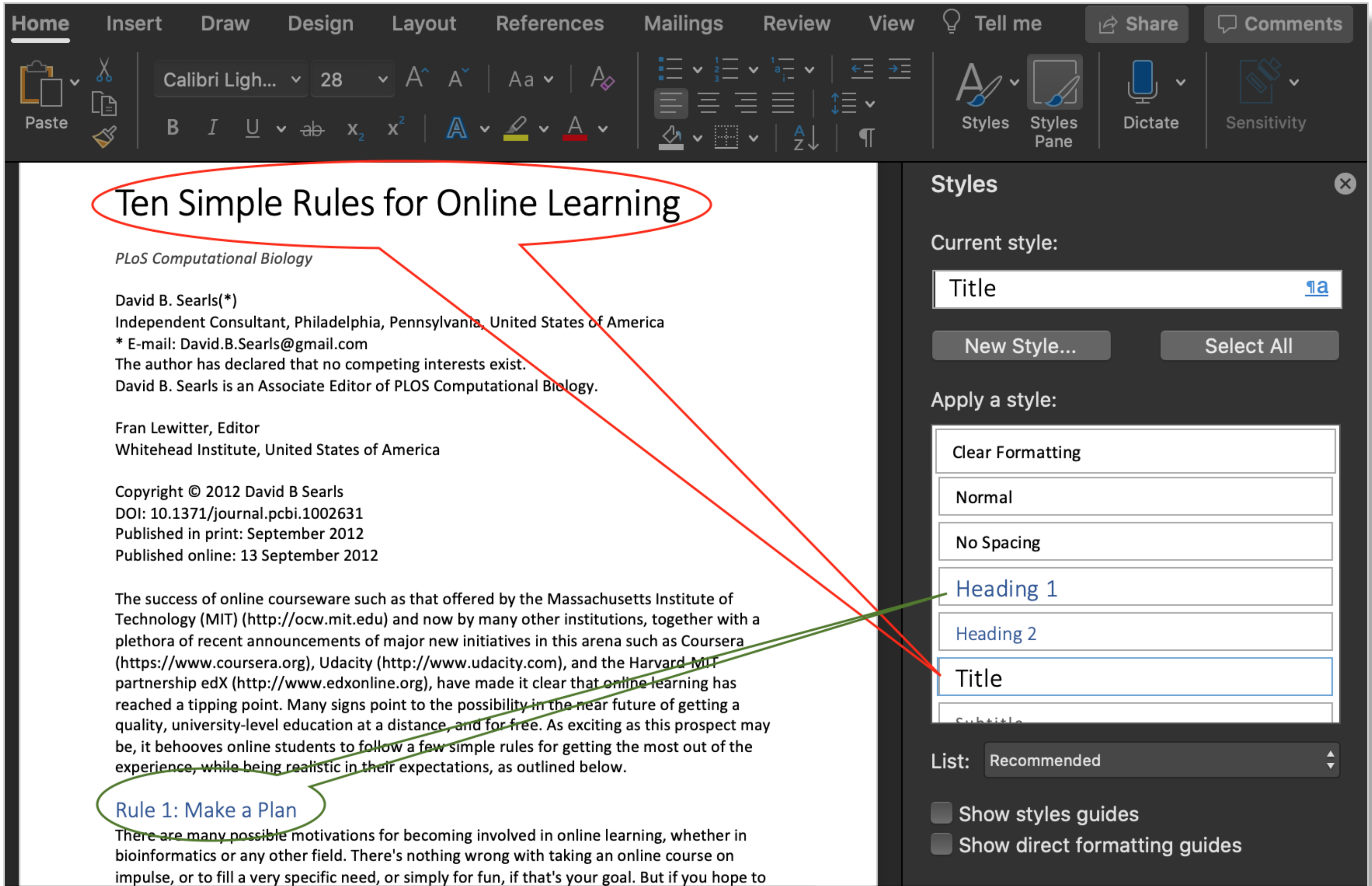
Style is not Structure

In word processors like Word®,
What You See Is What You Get

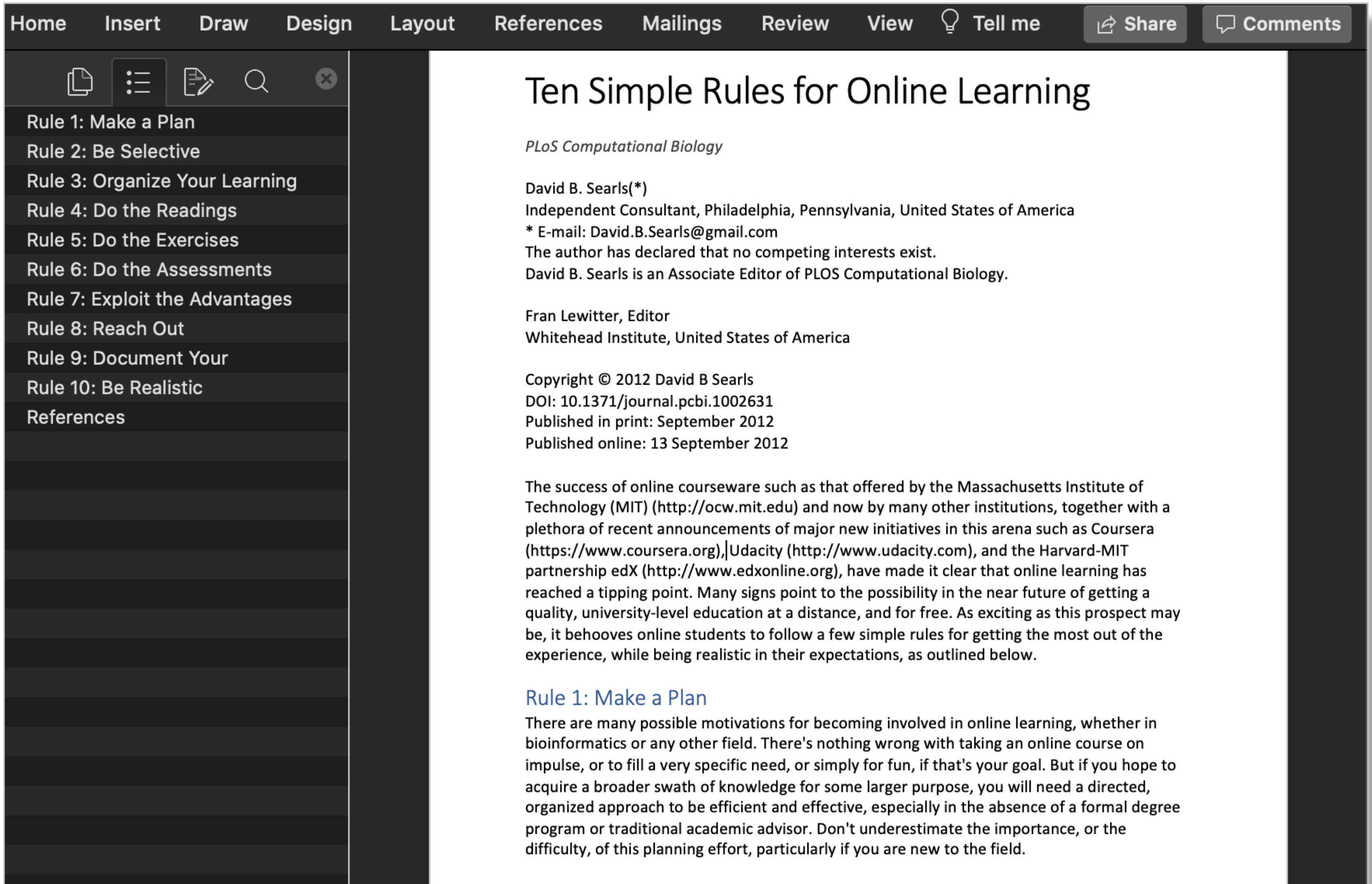
This is sometimes called **WYSIWYG**

It is easy to change fonts, sizes, colors and other visual attributes, without paying attention to *structure*

Structured Word documents



Now the document has structure



Ten Simple Rules for Online Learning

PLoS Computational Biology

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The success of online courseware such as that offered by the Massachusetts Institute of Technology (MIT) (http://ocw.mit.edu) and now by many other institutions, together with a plethora of recent announcements of major new initiatives in this arena such as Coursera (https://www.coursera.org), Udacity (http://www.udacity.com), and the Harvard-MIT partnership edX (http://www.edxonline.org), have made it clear that online learning has reached a tipping point. Many signs point to the possibility in the near future of getting a quality, university-level education at a distance, and for free. As exciting as this prospect may be, it behooves online students to follow a few simple rules for getting the most out of the experience, while being realistic in their expectations, as outlined below.

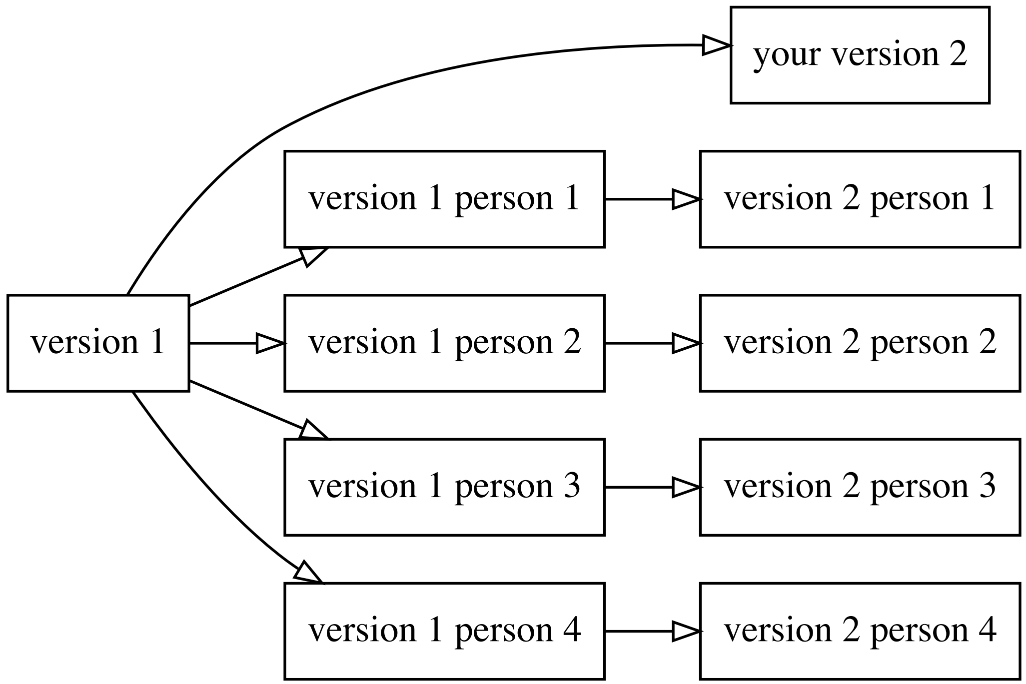
Rule 1: Make a Plan

There are many possible motivations for becoming involved in online learning, whether in bioinformatics or any other field. There's nothing wrong with taking an online course on impulse, or to fill a very specific need, or simply for fun, if that's your goal. But if you hope to acquire a broader swath of knowledge for some larger purpose, you will need a directed, organized approach to be efficient and effective, especially in the absence of a formal degree program or traditional academic advisor. Don't underestimate the importance, or the difficulty, of this planning effort, particularly if you are new to the field.

Collaborating

Sharing Word documents by email is a **VERY BAD IDEA**

It leads to *chaos and confusion*



Use an Online service

You can share your document via Dropbox or Google Drive

You can edit online using Microsoft Office 365 or Google Docs

Several people can work in the same document at the same time

Advantage: better spelling and grammar correction

But they require a permanent internet connection

My protocol

When I collaborate with non-markdown people, we use Google Docs

- We avoid using **bold** and *italics*
    - Exception: scientific names of species (e.g. *Homo sapiens*)
- Instead we use *Styles* to define the structure
- I follow *pandoc* rules for citations
- Once finished, I export a Word file, and I convert it to Markdown using *pandoc*
- We share the *code* to produce every figure and table

My other protocol

If my collaborators know Markdown, I often use RMarkdown

- Developed for R language, but supports Python and other languages
- Syntax is Markdown + code
  - The code for each table and figure is included in the document
  - This is a big step towards *replicability*
- R replaces each *code chunk* with its result, and gives a plain Markdown file
- It uses *pandoc* to make Word/PDF/HTML
- We share using *git*

RMarkdown v/s Jupyter Notebooks

Both are similar in spirit

- Jupyter is like Excel. It is good to explore ideas
  - It is code with a lot of comments
- RMarkdown is like Word. It is good to write a paper
  - It is text with just enough code

Second idea

Prepare your files for the next user… it may be you

Someone unfamiliar with your project should be able to look at your computer files and understand in detail what you did and why

William Stafford Noble. *"A Quick Guide to Organizing Computational Biology Projects."* PLoS Computational Biology 5, no. 7 (2009): 1–5. https://doi.org/10.1371/journal.pcbi.1000424.

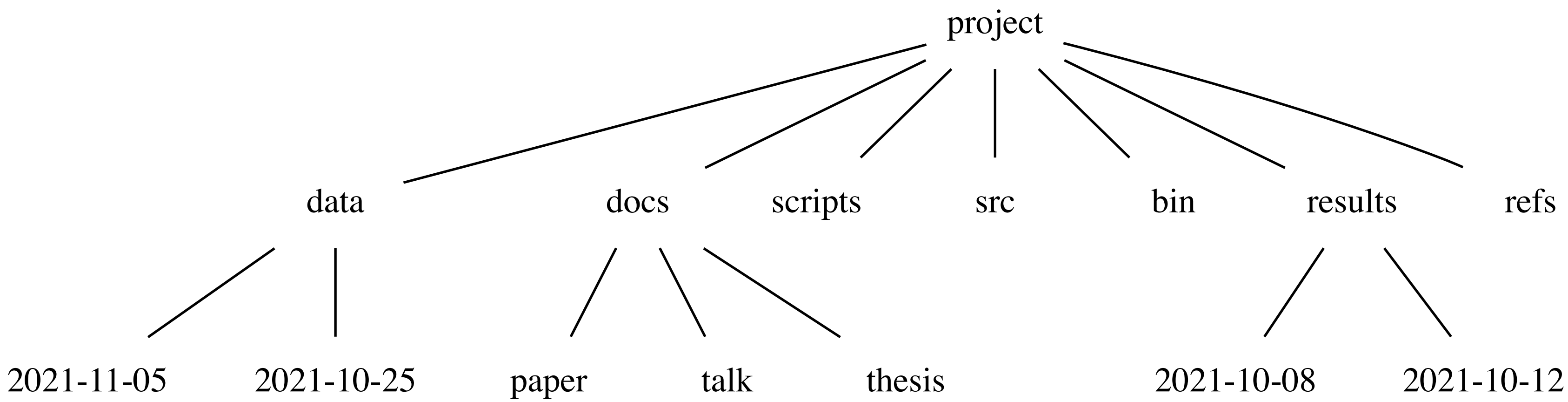
This "someone" could be:

- *someone who read your published article and wants to try to reproduce your work,*
- *a collaborator who wants to understand the details of your experiments,*
- *a future student working in your lab who wants to extend your work after you have moved on to a new job,*
- *your research advisor, who may be interested in understanding your work or who may be evaluating your research skills.*

Most commonly, however, that "someone" is you.

William Stafford Noble. *"A Quick Guide to Organizing Computational Biology Projects."* PLoS Computational Biology 5, no. 7 (2009): 1–5. https://doi.org/10.1371/journal.pcbi.1000424.

Folder structure for every project



- `docs` is where you write your paper/talk/thesis
- `refs` is to store reference documents, like citations
- `data` is anything that you get from outside the computer
- `results` is what your code produces
- `scripts` and `src` is where you write your code
- `bin` is for the compiled code

Data is Sacred

Producing data is expensive and time consuming

You don't want to lose it

Mark it *read only* immediately
(and make backups)

Never modify them

Create cleaned up versions via a script

Filenames Rule 1: Be coherent

Decide when to use `.`, `-`, and `_`

Agree a standard with your collaborators

Check periodically that you are following your standard (maybe with a script)

Rule 2: Write dates as YYYY-MM-DD

- When was 8/3/1965?
- Is today 5/11/2021 or 11/5/2021?

YYYY-MM-DD is an ISO standard

Sorting alphabetically, numerically, and chronologically are the same

There is no ambiguity of meaning

Collaborating

Sharing

- Git
  - GitHub
  - Bitbucket
  - GitLab
  - your own servers
- Online editors
  - Google Docs
  - HackMD.io
  - Overleaf

Choosing roles and protocols

Define who are the authors early

Recommended reading:

“What Makes an Author.” Nature Methods 18, no. 9 (September 3, 2021): 983–983. https://doi.org/10.1038/s41592-021-01271-8.

Gewin, Virginia. “Steer Clear of Conflict.” Nature 594, no. 7863 (2021): 462–63.

More recommendations

Weinberger, Cody J., James A. Evans, and Stefano Allesina. “Ten Simple (Empirical) Rules for Writing Science.” PLoS Computational Biology 11, no. 4 (2015): 11–13.

Lortie, Christopher J. “Ten Simple Rules for Writing Statistical Book Reviews.” PLoS Computational Biology 15, no. 1 (2019): 1–5.

Frassl, Marieke A., David P. Hamilton, et al. “Ten Simple Rules for Collaboratively Writing a Multi-Authored Paper.” PLoS Computational Biology 14, no. 11 (2018): 6–13.

Erren, T, P Cullen, M Erren, and P Bourne. “Ten Simple Rules for Doing Your Best Research, According to Hamming.” PLoS Computational Biology 3, no. 10 (January 1, 2007): e213.

Final comments

Take care of yourself

- Drink a lot of water
    - Especially when you drink alcohol
- Get enough sleep
    - Don’t fry your brain, you only have one
- Try to make a routine. Minimize trivial decisions
    - Save your energy for important things
- Go for a walk every day

Become a writer

- Write every day. No exceptions.
  - Start with 150 or 200 daily words
  - Ideal is 750 daily words
- Once you see yourself as “someone who writes every day”, it will be easy to write papers, projects, thesis, etc.
- Get addicted to write, as you are addicted to social media
- Try the *Pomodoro technique*

References

Allen, David. 2011. *Getting Things Done*. Little, Brown Book Group.

Annesley, Thomas M. 2010a. “Bars and pies make better desserts than figures.” *Clinical Chemistry* 56 (9): 1394–1400. https://doi.org/10.1373/clinchem.2010.152298.

———. 2010b. “Bring your best to the table.” *Clinical Chemistry* 56 (10): 1528–34. https://doi.org/10.1373/clinchem.2010.153502.

———. 2010c. “"It was a cold and rainy night": Set the scene with a good introduction.” *Clinical Chemistry* 56 (5): 708–13. https://doi.org/10.1373/clinchem.2010.143628.

———. 2010d. “Put your best figure forward: Line graphs and scattergrams.” *Clinical Chemistry* 56 (8): 1229–33. https://doi.org/10.1373/clinchem.2010.150060.

———. 2010e. “Show your cards: The results section and the poker game.” *Clinical Chemistry* 56 (7): 1066–70. https://doi.org/10.1373/clinchem.2010.148148.

———. 2010f. “The abstract and the elevator talk: a tale of two summaries.” *Clinical Chemistry* 56 (4): 521–24. https://doi.org/10.1373/clinchem.2009.142026.

———. 2010g. “The discussion section: Your closing argument.” *Clinical Chemistry* 56 (11): 1671–74. https://doi.org/10.1373/clinchem.2010.155358.