Good Practices in (Statistical) Software Development

Alex Sánchez-Pla and Pol Castellano-Escuder

Genetics, Microbiology and Statistic Department. UB
Statistics and Bioinformatics Unit. VHIR
Grup de Recerca en Bioestadística i Bioinformatica (GRBio)

Jan 26, 2019 - BIOSTATNET Meeting

Readme

- License: Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International License http://creativecommons.org/licenses/by-nc-sa/4.0/
- You are free to:
  - **Share** : copy and redistribute the material
  - **Adapt** : rebuild and transform the material
- Under the following conditions:
  - **Attribution** : You must give appropriate credit, provide a link to the license, and indicate if changes were made.
  - **NonCommercial** : You may not use this work for commercial purposes.
  - **Share Alike** : If you remix, transform, or build upon this work, you must distribute your contributions under the same license to this one.

Outline

- Introduction to the session.
- Statistics and Programming
  - The role of coding in statistical work
  - Teaching programming to statisticians and data scientists
- Can we build better software (software better?)
  - When do we call a piece of software "good"?
  - Which aspects should we account for
- Good practices for statistical software development

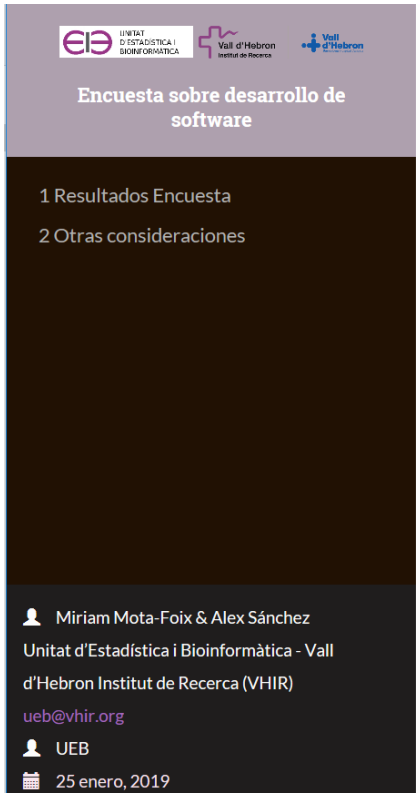
Introduction

- Presenter: Alex Sánchez Pla
- Job 1: Associate Professor. Statistics department, UB. "Traditional approach"
  - Teach statistics (SI, ED), make research (GRBio)
  - Mostly programmed for myself. Some R packages.
- Job 2: Head of Statistics and Bioinformatics Unit. "Real world"
  - Coordinate (more than do) applied biostatistics and bioinformatics.
  - Lots of data, lots of programming
  - Discovered new concepts: Validation, Regulation, SOPs, Best Practices, ...

What is software development

- *Software development is a process by which standalone or individual software is created using a specific programming language. It involves writing a series of interrelated programming code, which provides the functionality of the developed software*
- Simple, yet functional. It embraces most programming activities we may be involved in,
  - From writing simple scripts, automating functions, running simulations.
  - Creating web programs, mobile apps, etc.
  - But also writing code for performing any type of statisytical analyses.

How do we do software development?



https://servirredcap.vhir.org/redcap/surveys/?s=J3RW8YPFXF

How important is programming in a mathematician's training?

1r Curs - Fase Inicial			
Càlcul en una variable	Àlgebra lineal	Informàtica	Fonaments de la matemàtica
Càlcul diferencial	Geometria afí i euclidiana	Àlgebra lineal numèrica	Matemàtica discreta
2n Curs			
Càlcul integral	Àlgebra multilineal i geometria	Algorísmia	Programació matemàtica
Funcions de variable complexa	Topologia	Física	Anàlisi real
3r Curs			
Equacions diferencials ordinàries	Estructures algebraiques	Càlcul numèric	Teoria de la probabilitat
Equacions en derivades parcials	Geometria diferencial	Models matemàtics de la física	Estadística
4t Curs			
Models matemàtics de la tecnologia	Optativa 1	Optativa 2	Optativa 3
Treball de fi de grau	Optativa 4	Optativa 4	Optativa 6

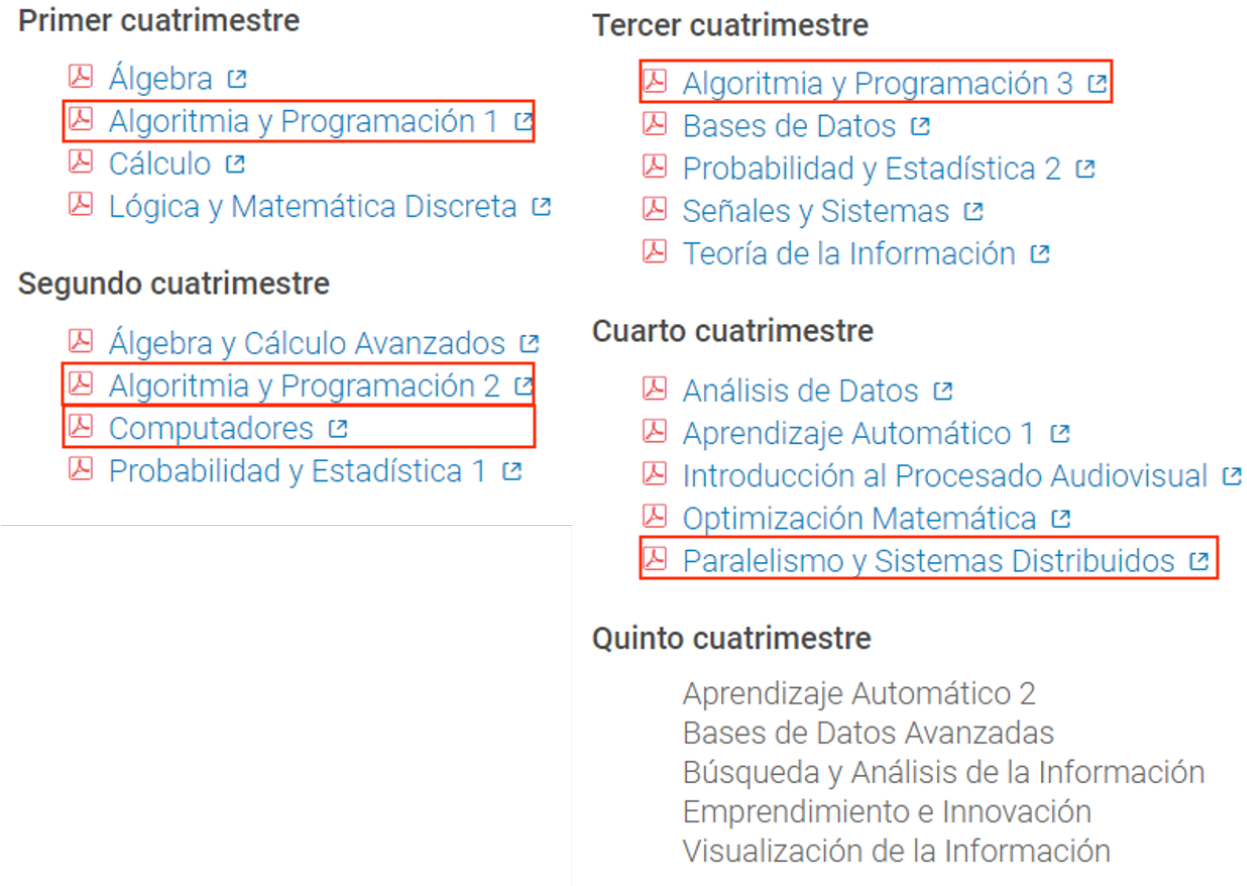
Figure 1: Compulsory courses. Mathematics degree. UPC. (One course)

How important is programming in a statistician's training?

1r curs (UAB)	2n curs (UAB)
- Càlcul	- Distribucions Multidimensionals
- Estadística Descriptiva (1) (4)	- Optimització i Processos Estocàstics
- Mètodes Algebraics per a l'Estadística	- Bases de Dades (2) (3)
- Introducció a la Programació (2)	- Inferència Estadística I
- Eines Informàtiques per a l'Estadística (1) (6)	- Estadística Oficial i Disseny d'Enquestes
- Càlcul de Probabilitats	- Disseny d'Experiments
- Estructures de Dades i Algorismes (2)	- Models Lineals
- Programació Lineal	- Mostreig Estadístic
- Modelització Matemàtica	- Inferència Estadística II
- Temes de Biociència i Ciència (anual) (1) (3) (4) (5) (6)	- Anàlisi de la Supervivència i Fiabilitat
3r curs (UAB)	**4t curs (UAB)**
- Anàlisi de Dades Categòriques	- Treball de Final de Grau
- Anàlisi Multivariant	
- Sèries Temporals i Predicció	
- Aplicacions de l'Estadística a la Bioinformàtica	
- Aplicacions de l'Estadística a les Ciències de la Salut	
- Mineria de Dades	
- Modelització Avançada	
- Simulació, Remostreig i Aplicacions	
- Introducció a l'Econometria	
- Control de Qualitat i Estadística Industrial	

Figure 2: Compulsory courses. Applied Statistics degree at UAB. (Three courses)

How important is programming in a data scientist's training?



Primer cuatrimestre

- Álgebra
- Algoritmia y Programación 1
- Cálculo
- Lógica y Matemática Discreta

Segundo cuatrimestre

- Álgebra y Cálculo Avanzados
- Algoritmia y Programación 2
- Computadores
- Probabilidad y Estadística 1

Tercer cuatrimestre

- Algoritmia y Programación 3
- Bases de Datos
- Probabilidad y Estadística 2
- Señales y Sistemas
- Teoría de la Información

Cuarto cuatrimestre

- Análisis de Datos
- Aprendizaje Automático 1
- Introducción al Procesado Audiovisual
- Optimización Matemática
- Paralelismo y Sistemas Distribuidos

Quinto cuatrimestre

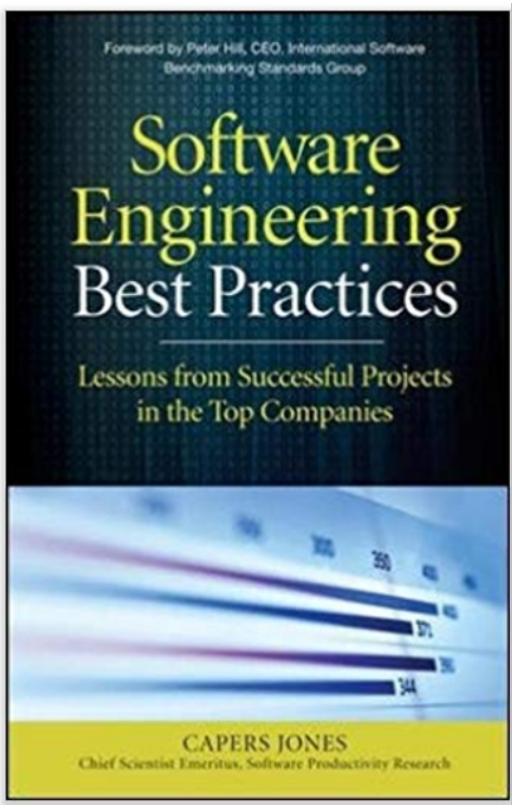
Aprendizaje Automático 2
Bases de Datos Avanzadas
Búsqueda y Análisis de la Información
Emprendimiento e Innovación
Visualización de la Información

Figure 3: Compulsory courses. Data Engineering degree. UPC. (Five courses)

Good practices in (statistical) software development

- *A good practice is not only a practice that is good, but a practice that has been proven to work well and produce good results, and is therefore recommended as a model*.
- There is no universally accepted list of “good practices” for software development but we can easily agree (can we?) on some practices that (maybe) can help our programs to be better.
- When we talk about software, we must bear in mind that there are many different types of software and that, sometimes, "good practices" can be different between software types. Some types of software could be: CLI (Command Line Interface), GUI (Graphical User Interface), Scripts, Packages or Web Apps.

Best practices in Software Engineering

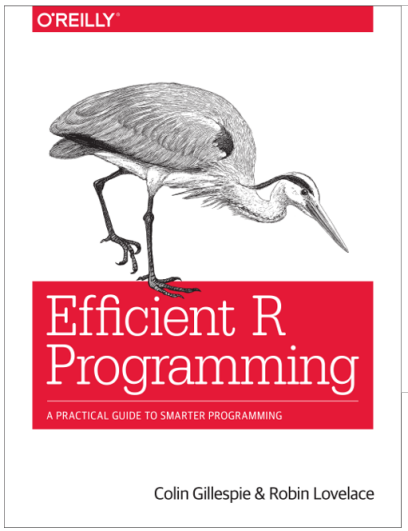


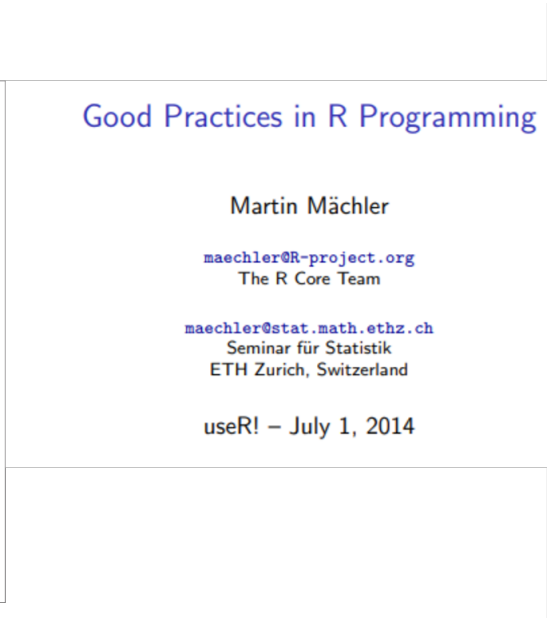
Contents at a Glance

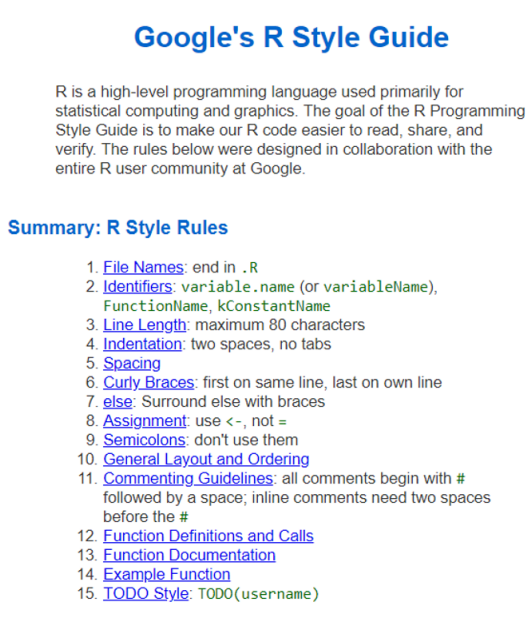
- We don't discuss this!

Good practices in Statistical Software Development

- Instead I have browsed through some materials which focus on statistical software development







GP: Document your code

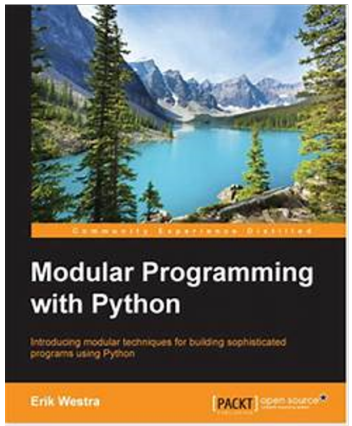
- **Comment** as much as you can.
- Write **help** for your programs.
- Create **user manuals** and **user guides**.
- Use tools to facilitate documentation building.

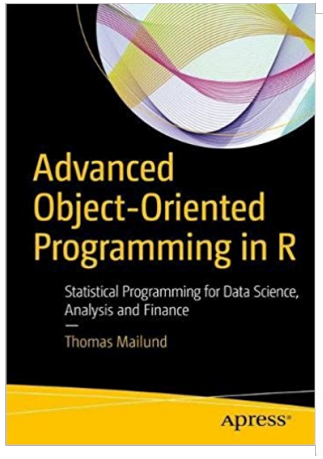
```r
#' Add together two numbers
#'
#' @param x A number
#' @param y A number
#' @return The sum of \code{x} and \code{y}
#' @examples
#' add(1, 1)
#' add(10, 1)
add <- function(x, y) {
  x + y
}
```

GP: Modularize

"Modular programming consists in separate the functionality of a program into independent and interchangeable modules."

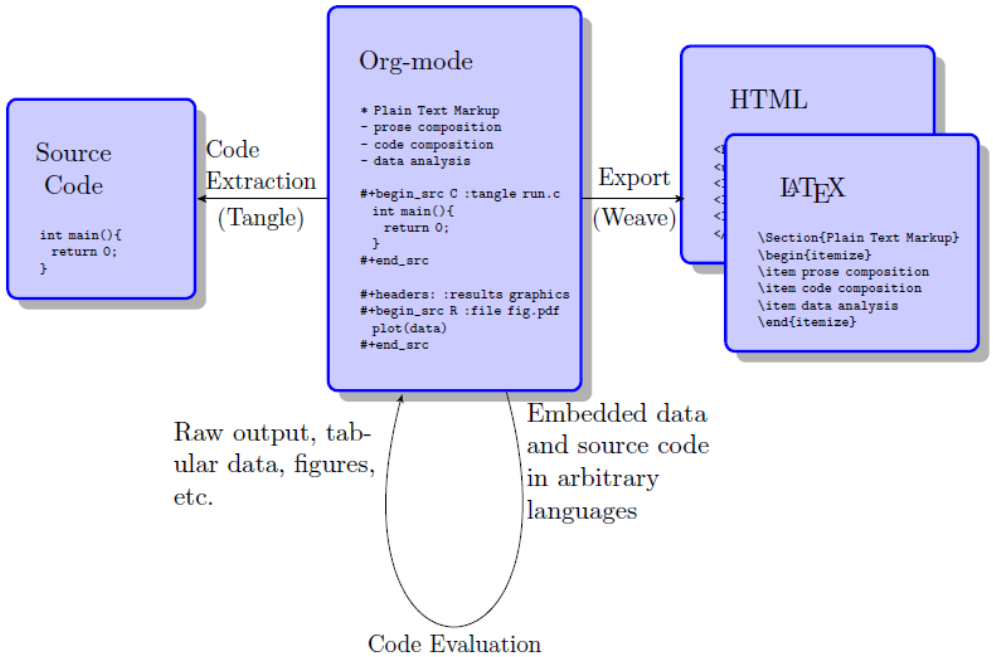
- If a piece of code has to be used repeteadly or it is too long to affect code legibility it is recommended to encapsulate it into some type of *module*
- Modularization can happen at distinct levels.
  - *functions*
  - *classes and methods* (OOP)
  - *libraries* or *packages*





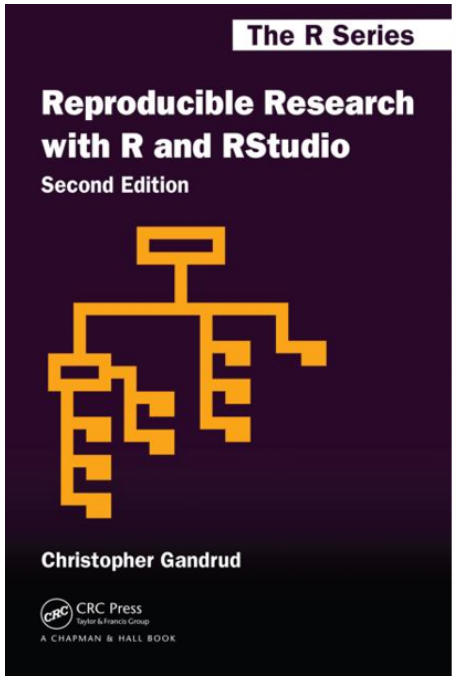
GP: Literate programming enhances reproducibility

- **Literate programming**: Enhances traditional software development by embedding code in explanatory essays and encourages *treating the act of development as one of communication*.
- **Reproducible research**: Embeds executable code in research reports and publications, with the aim of *allowing readers to re-run the analyses described*.

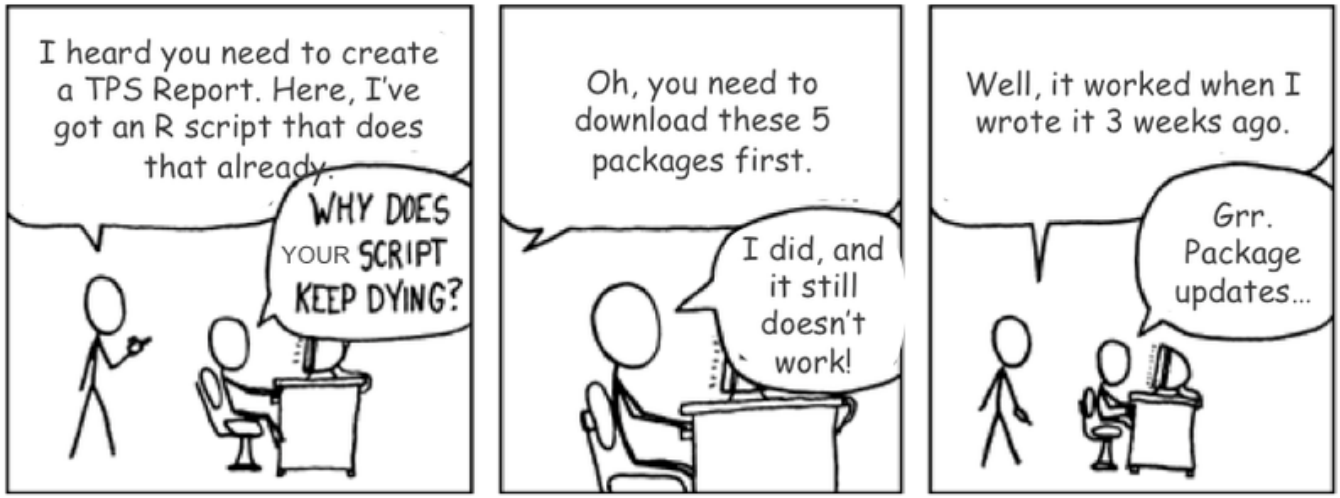


Reproducible research with R and Rstudio

- Using literate programing for reproducible research is a change of paradigm.
- Coding, Analyzing and Reporting become a unique piece of work.

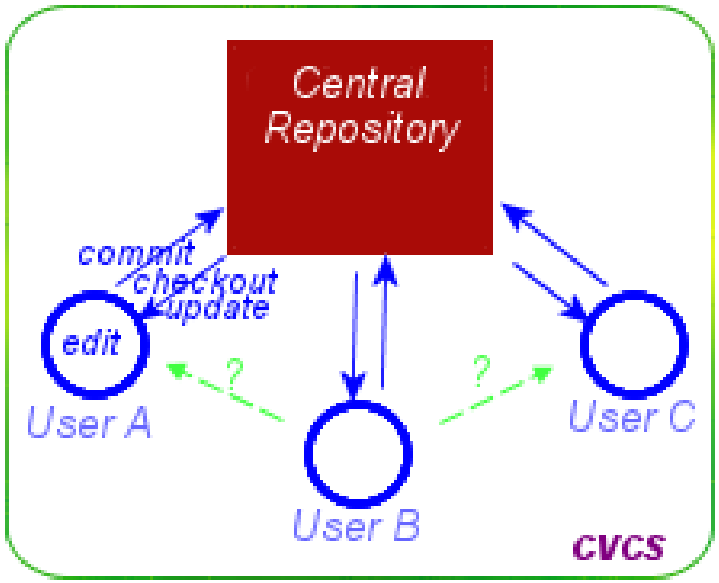


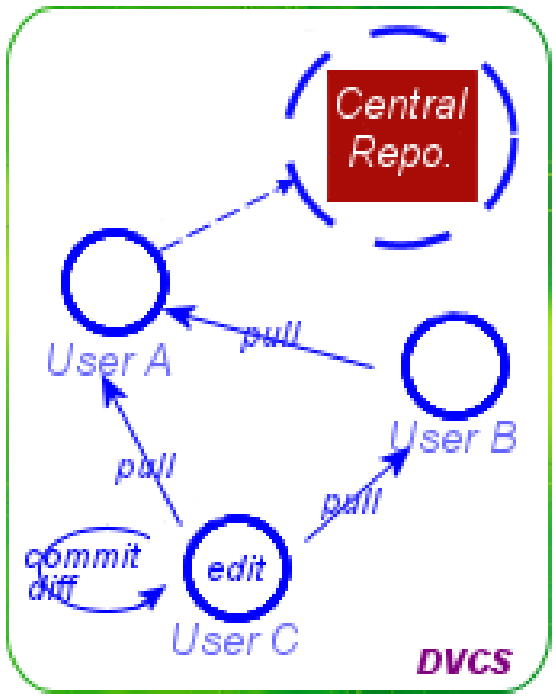
GP: Use Control Version Systems (CVS)



- **Version control systems** are a category of software tools that help a software developper/team manage changes to source code over time.
- **Version control software** keeps track of every modification to the code in a special kind of database.
  - If a mistake is made, developers can turn back the clock and compare earlier versions of the code to help fix the mistake while minimizing disruption to all team members.

Type of Control version systems





Git and Github: a standard *de facto*

- `GitHub` is a hosting service for `Git` repositories.
- `GitHub` offers all the `Git` functionality adding a series of own characteristics.
  - Web and Desktop-based graphical interface.
  - *Access control*, *bug tracking*, *task management*, *wikis* ...
- *GitHub brings together the worlds largest community of developers to **discover**, **share**, and **build** better software*

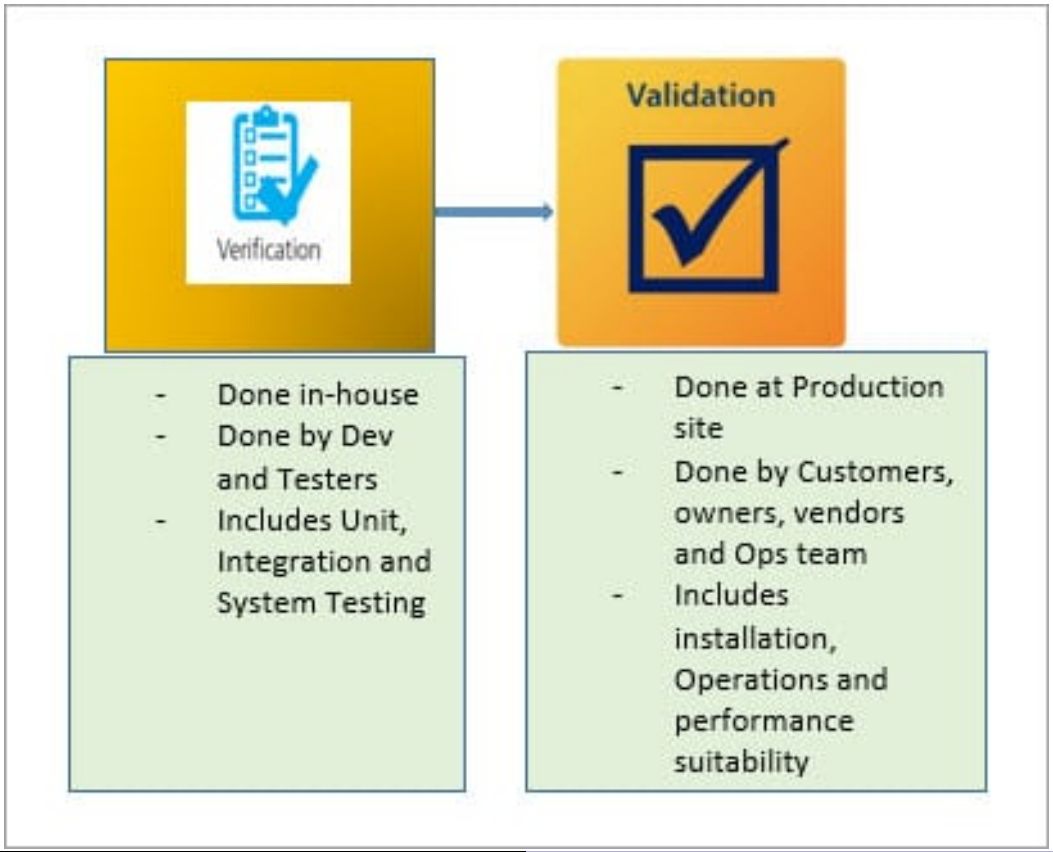
)

GP: Share your programs

- Sharing software is one great way to improve it.
  - Developers take care of details so that users will be staisfied with the program.
  - Users can provide feedback and can help improve the program.
- Sharing can be done in many different ways
  - Put a library in a repository
  - Create a web page
  - Sell the program
- Many scientist's work is better known by their software tools than by their papers

GP: Verify and Validate your software

- How do we know that the code does what it is intended to do?
  - Prepare a battery of tests, apply them. Document it.
- How do we know that our code contains no mistakes?
  - Make someone else review your work. Document it.
- How do we know if the code can be installed and set to work?
  - Make someone else install and run the programs. Document it.



GP: Optimize efficiently

- Optimization may improve a program's performance *if it doesn't consume more time than the time it saves*.
  - Before you start to optimise your code, ensure you know where the bottleneck lies; use a code profiler.
  - Use the appropriate data structures (e.g. matrices instead of data frames) and
  - Use the right functions to work with them (Use specialised row and column functions whenever possible)
- Learn to use techniques that can improve speed orders of magnitude. Apply if needed.
  - Parallelization can be great if many processes will be executed "in parallel" (e.g. Monte Carlo SImulations)
  - Learn to combine languages. Consider re-writing key parts of your code in C++.

GP: Manage error control and detection proactively

- Testing and reviewing can detect some errors
  - Some of these (e.g. programmers' errors) can be removed.
  - Others (e.g. wrong input) cannot be avoided.
- Learn **how to debug** your code
- **Plan reaction to errors** according to their severity.
- Learn how to do **Exception handling** tho help avoid program crashes.

GP: Plan the process

Think, plan, code it! And NOT in another order!
This will not take much time but, however, will save us a significant amount of time.

- Software development is a **process**
- There exist a myriad of methodologies and tools for planning and executing. Use the one you prefer.

- What we want? How are we going to do it? How do we want the output/s?

GP: Design

- Design or aesthetics may not seem so important, but nevertheless they are, especially in web applications.
- Sometimes, a very good software with a design that does not attract the user may not give the maximum performance that is expected of it. However, if the software is friendly and is accompanied by a good design, we can obtain better results.
- To achieve this goal, we suggest the use of html, css, markdown, rmarkdown, javascript, latex...

GP: Other good practices

It is easy to find lists of good or best practices in software development. **Just go through them and select thos that fit best you or your project!**

Conclusions

- Software development may be a "secondary" activity or may be our main source of work.
- The more we know about software development the better we can do the job.
- Applying a few good practices can considerably improve our performance.
- Remember that:

"You shouldn't feel ashamed about your code -if it solves the problem, it's perfect the way it is. But also, it could always be better"

-Hadley Wickam

Good Practices Summary

- Documentation
- Modularize
- Literate programming
- Version Control
- Share our programs
- Verify and Validate
- Optimize efficiently
- Error Control
- Planification
- Design