FAIR_bioinfo : Open Science and FAIR principles in a bioinformatics project

How to make a bioinformatics project more reproducible

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June 2021

Literate programming

Introduction

What is literate programming ?
Let us change our traditional attitude to the construction of programs: Instead of imagining that our main task is to instruct a computer what to do, let us concentrate rather on explaining to humans what we want the computer to do.
— Donald E. Knuth, Literate Programming, 1984

Introduction

What is literate programming ?

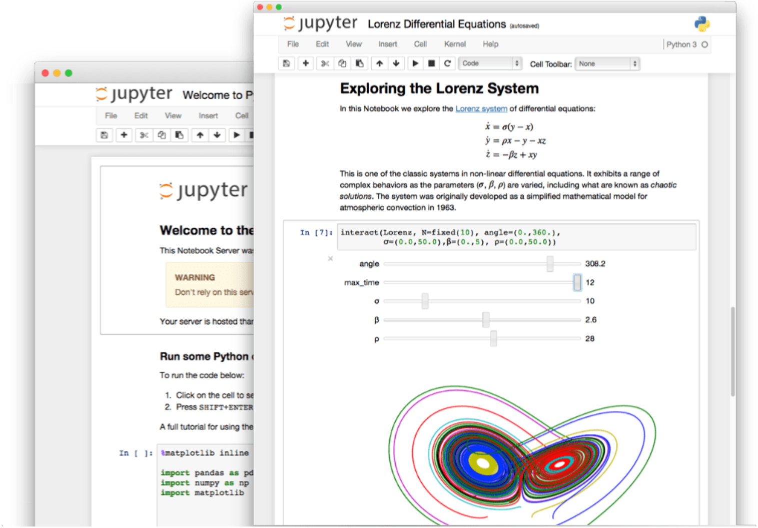
Definition

"Literate programming is a **programming paradigm** introduced by Donald Knuth in which a computer program is given an explanation of its logic in a **natural language**, such as English, **interspersed with snippets of macros and traditional source code**, from which compilable source code can be generated." Donald Knuth, 1984.

Wikipedia, 18/08/2020
`https://en.wikipedia.org/wiki/Literate_programming#Workflow`

Introduction

What does it look like ?



jupyter

Welcome to the

This Notebook Server wa

WARNING

Don't rely on this serv

Your server is hosted tha

Run some Python

To run the code below:

1. Click on the cell to se
2. Press SHIFT+ENTER

A full tutorial for using the

```
In [ ]: %matplotlib inline

        import pandas as pd
        import numpy as np
        import matplotlib
```

Exploring the Lorenz System

In this Notebook we explore the Lorenz system of differential equations:

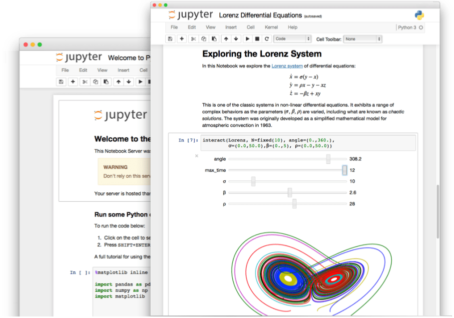
$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = \rho x - y - xz$$
$$\dot{z} = -\beta z + xy$$

This is one of the classic systems in non-linear differential equations. It exhibits a range of complex behaviors as the parameters (σ, β, ρ) are varied, including what are known as *chaotic solutions*. The system was originally developed as a simplified mathematical model for atmospheric convection in 1963.

```
In [7]: interact(Lorenz, N=fixed(10), angle=(0.,360.),
                 σ=(0.0,50.0),β=(0.,5), ρ=(0.0,50.0))
```

angle 308.2
max_time 12
σ 10
β 2.6
ρ 28

Introduction



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```
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                 σ=(0.0,50.0),β=(0.,5), ρ=(0.0,50.0))
```

Interactive programming interface allowing to combine both natural and computer languages.

In one file:

- Explanations
- Code
- Results
- Graphs and plots

Introduction

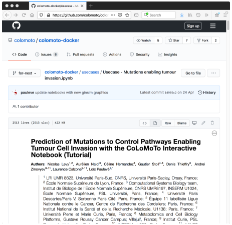
Why using literate programming frameworks ?

Use cases:

- Day to day analyses
- Analysis reports
- Writing scientific articles

Example of an article entirely written using a notebook

File (on a repository)



colomoto / colomoto-docker

colomoto-docker / usecases / Usecase - Mutations enabling tumour invasion.ipynb

pauleve update notebooks with new ginsim graphics Latest commit 14985c2 on 24 Apr

1 contributor

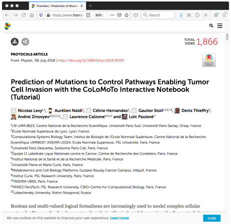
2513 lines (2513 sloc) | 422 KB

Prediction of Mutations to Control Pathways Enabling Tumour Cell Invasion with the CoLoMoTo Interactive Notebook (Tutorial)

Authors: Nicolas Levy[1,2], Aurélien Naldi[3], Céline Hernandez[3], Gautier Stoll[4-8], Denis Thieffry[3], Andrei Zinovyev[9-11], Laurence Calzone[9-11], Loïc Paulevé[1,*]

> [1] LRI UMR 8623, Université Paris-Sud, CNRS, Université Paris-Saclay, Orsay, France; [2] École Normale Supérieure de Lyon, France; [3] Computational Systems Biology team, Institut de Biologie de l'Ecole Normale Supérieure, CNRS UMR8197, INSERM U1024, École Normale Supérieure, PSL Université, Paris, France; [4] Université Paris Descartes/Paris V, Sorbonne Paris Cité, Paris, France; [5] Équipe 11 labellisée Ligue Nationale contre le Cancer, Centre de Recherche des Cordeliers; Paris, France; [6] Institut National de la Santé et de la Recherche Médicale, U1138; Paris, France; [7] Université Pierre et Marie Curie, Paris, France; [8] Metabolomics and Cell Biology Platforms, Gustave Roussy Cancer Campus; Villejuif, France; [9] Institut Curie, PSL

Published article



TOTAL VIEWS 1,866

PROTOCOLS ARTICLE

Front. Physiol., 06 July 2018 | https://doi.org/10.3389/fphys.2018.00787

Prediction of Mutations to Control Pathways Enabling Tumor Cell Invasion with the CoLoMoTo Interactive Notebook (Tutorial)

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[2] École Normale Supérieure de Lyon, Lyon, France
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[11] MINES ParisTech, PSL Research University, CBIO-Centre for Computational Biology, Paris, France
[12] Lobachevsky University, Nizhni Novgorod, Russia

Boolean and multi-valued logical formalisms are increasingly used to model complex cellular

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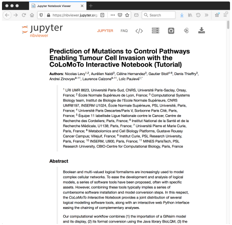
Executable file



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Abstract

> Boolean and multi-valued logical formalisms are increasingly used to model complex cellular networks. To ease the development and analysis of logical models, a series of software tools have been proposed, often with specific assets. However, combining these tools typically implies a series of cumbersome software installation and model conversion steps. In this respect, the *CoLoMoTo Interactive Notebook* provides a joint distribution of several logical modelling software tools, along with an interactive web Python interface easing the chaining of complementary analyses.
>
> Our computational workflow combines (1) the importation of a GINsim model and its display, (2) its format conversion using the Java library BioLQM, (3) the

Literate programming

This session :

- Markdown
- Rmarkdown / RStudio
- Jupyter

Markup and markdown

Definition

A markup language uses tags to define elements within a document.

Three different types and usage :

- Presentational (used by traditional word-processing systems)
  - Markup is invisible
- Procedural, provides instructions to process the text (e.g. TeX, PostScript)
  - Markup is visible and can be directly manipulated by the author.
- Descriptive, to label documents parts (e.g. LaTeX, HTML, XML...)
  - Emphasizes the document structure.

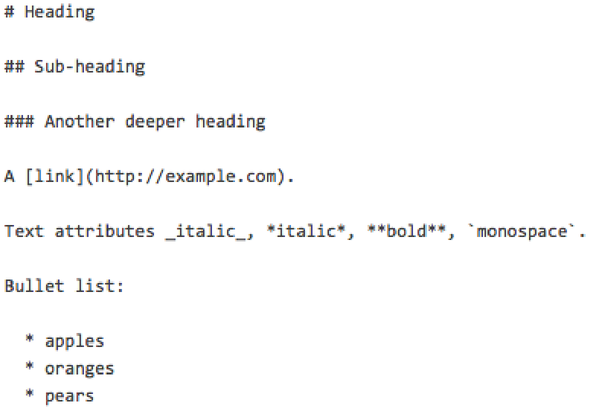
Markdown language

Markdown is a Lightweight markup language.
Designed to be :

- easy to **write** using any generic text editor (plain-text-formatting syntax)
- easy to **read** in its raw form

Markdown language

You've probably see it already on GitHub (README), Wikipedia...



```
# Heading

## Sub-heading

### Another deeper heading

A [link](http://example.com).

Text attributes _italic_, *italic*, **bold**, `monospace`.

Bullet list:

  * apples
  * oranges
  * pears
```

Github guide :
urlhttps://guides.github.com/features/mastering-markdown/

Literate programming

But how is this useful for literate programming?

When you want to weave both code (to be interpreted) and formatting information, you precisely need a lightweight language for the formatting part.

The challengers

No need to hide, there are currently two main frameworks used in bioinformatics:
RMarkdown and Jupyter

RMarkdown

RMarkdown

RMarkdown

At the beginning, there was nothing.

RMarkdown

At the beginning, there was nothing.

Then came Sweave.
Leisch, Friedrich (2002). "Sweave, Part I: Mixing R and LaTeX: A short introduction to the Sweave file format and corresponding R functions"

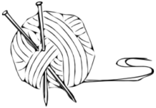
RMarkdown

At the beginning, there was nothing.

Then came Sweave.
Leisch, Friedrich (2002). "Sweave, Part I: Mixing R and LaTeX: A short introduction to the Sweave file format and corresponding R functions"
And people saw that the path would be long...

RMarkdown

knitR (2011)



"The knitr package was designed to be a transparent engine for dynamic report generation with R, solve some long-standing problems in Sweave, and combine features in other add-on packages into one package"
`https://yihui.org/knitr/`

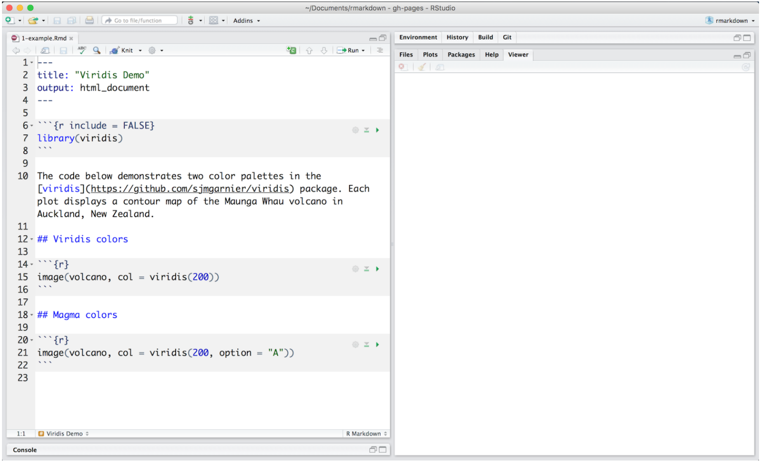
RMarkdown

RMarkdown

"When you run render, R Markdown feeds the .Rmd file to knitr, which executes all of the code chunks and creates a new markdown (.md) document which includes the code and its output.
The markdown file generated by knitr is then processed by pandoc which is responsible for creating the finished format."
`https://rmarkdown.rstudio.com`

RMarkdown

RMarkdown

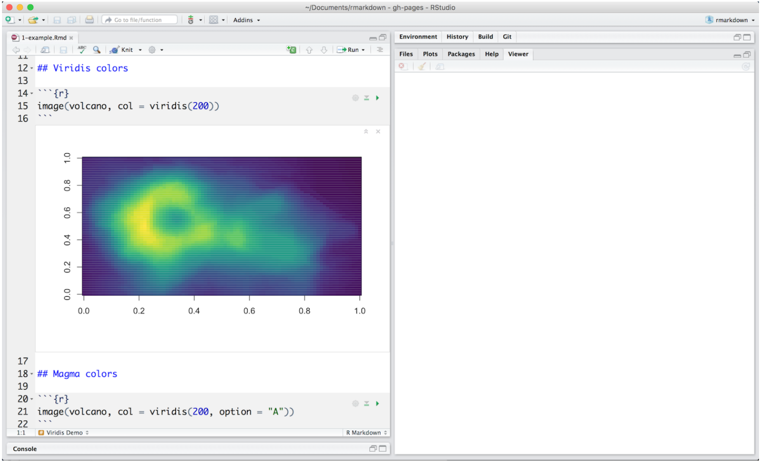


~~~
---
title: "Viridis Demo"
output: html_document
---

```{r include = FALSE}
library(viridis)
```

The code below demonstrates two color palettes in the
[viridis](https://github.com/sjmgarnier/viridis) package. Each
plot displays a contour map of the Maunga Whau volcano in
Auckland, New Zealand.

## Viridis colors

```{r}
image(volcano, col = viridis(200))
```

## Magma colors

```{r}
image(volcano, col = viridis(200, option = "A"))
```
~~~

Integrated into RStudio, IDE for R.

RMarkdown

R Notebooks



~~~
## Viridis colors

```{r}
image(volcano, col = viridis(200))
```

## Magma colors

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image(volcano, col = viridis(200, option = "A"))
```
~~~
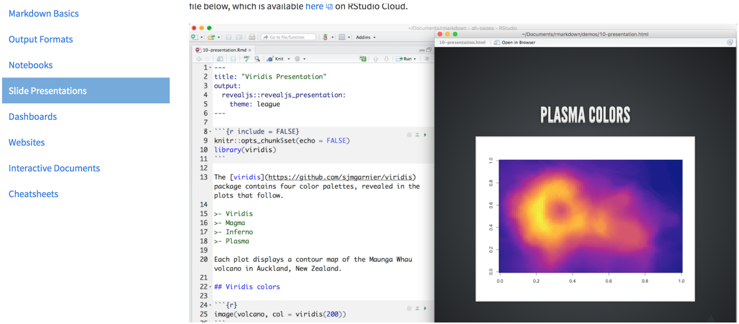

RMarkdown

R Notebooks and more...



file below, which is available here on RStudio Cloud.

~~~
---
title: "Viridis Presentation"
output:
  revealjs::revealjs_presentation:
    theme: league
---

```{r include = FALSE}
knitr::opts_chunk$set(echo = FALSE)
library(viridis)
```


The [viridis](https://github.com/sjmgarnier/viridis) package contains four color palettes, revealed in the plots that follow.

>- Viridis
>- Magma
>- Inferno
>- Plasma

Each plot displays a contour map of the Maunga Whau volcano in Auckland, New Zealand.

## Viridis colors

```{r}
image(volcano, col = viridis(200))
~~~

Jupyter

Jupyter

Jupyter

A bit of history...

- 2011 : IPython (interactive Python shell) with notebook functionalities
- 2014 : Spin-off project called Project Jupyter
- a non-profit, open-source project maintained by a strong Community
- "Jupyter will always be 100% open-source software, free for all to use and released under the liberal terms of the modified BSD license"
- A reference to the three core programming languages supported by Jupyter (Julia, Python and R)

`https://jupyter.org/`

Jupyter

What can it do?

Jupyter

What can it do?
Everything (excepted coffee)

Jupyter

But what is it exactly ?

Jupyter

But what is it exactly ?
Web-based interactive computational environment.

Jupyter

But what is it exactly ?
Web-based interactive computational environment.

- Web-based : client/server

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- Interactive : notebook system

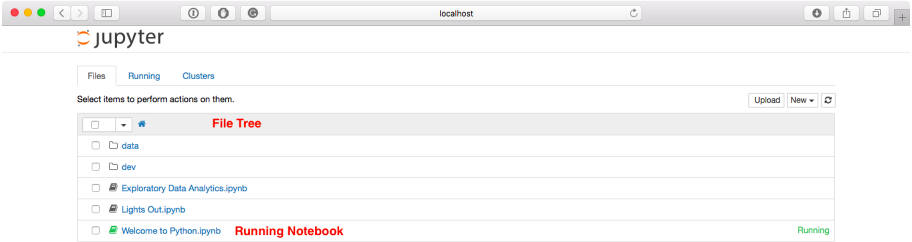
Jupyter

But what is it exactly ?
Web-based interactive computational environment.

- Web-based : client/server
- Interactive : notebook system
- Computational environment : console, many kernels available...

Jupyter

Dashboard



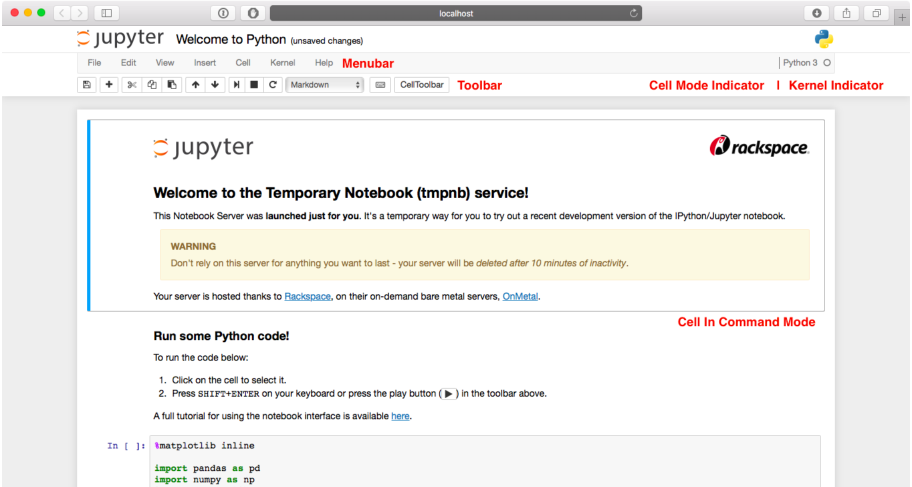
Select items to perform actions on them.

File Tree

- ☐ data
- ☐ dev
- ☐ Exploratory Data Analytics.ipynb
- ☐ Lights Out.ipynb
- ☐ Welcome to Python.ipynb **Running Notebook** Running

Jupyter

Notebook editor



jupyter

Welcome to the Temporary Notebook (tmpnb) service!

This Notebook Server was **launched just for you**. It's a temporary way for you to try out a recent development version of the IPython/Jupyter notebook.

WARNING

Don't rely on this server for anything you want to last - your server will be *deleted after 10 minutes of inactivity*.

Your server is hosted thanks to Rackspace, on their on-demand bare metal servers, OnMetal.

Run some Python code!

To run the code below:

1. Click on the cell to select it.
2. Press `SHIFT+ENTER` on your keyboard or press the play button (▶) in the toolbar above.

A full tutorial for using the notebook interface is available here.

```
In [ ]: %matplotlib inline

        import pandas as pd
        import numpy as np
        import matplotlib
```

Jupyter

Project Jupyter

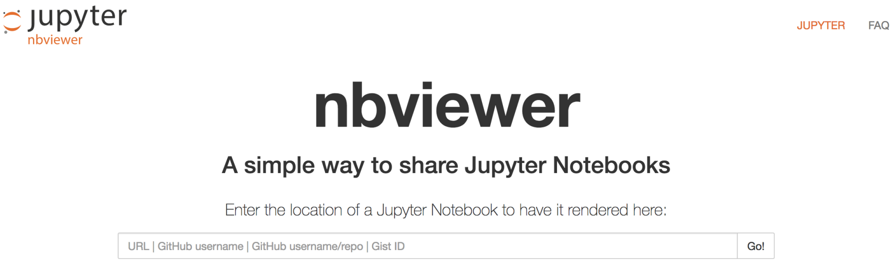
- A non-profit, open-source project maintained by a **strong** Community
- Adopted by the biggest in the Cloud industry (Google, Microsoft, Amazon...)
- And financed by the biggest (Google, Microsoft, EU Horizon 2020 program, Alfred P. Sloan Foundation...)

Inside the Python community (snakemake, conda...)

Integration with GitHub since 2015 (renderer)

Jupyter

Nbviewer : a static renderer for Jupyter notebooks



jupyter nbviewer

JUPYTER FAQ

nbviewer

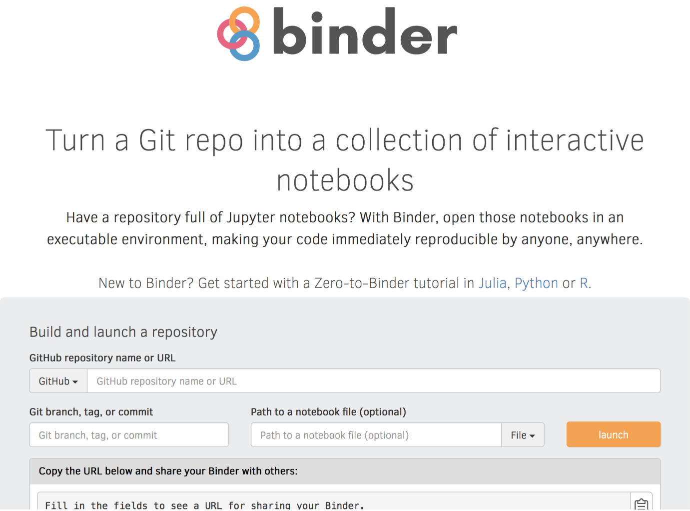
A simple way to share Jupyter Notebooks

Enter the location of a Jupyter Notebook to have it rendered here:

`https://nbviewer.jupyter.org/`

Jupyter

Jupyter + Docker = binder



binder

Turn a Git repo into a collection of interactive notebooks

Have a repository full of Jupyter notebooks? With Binder, open those notebooks in an executable environment, making your code immediately reproducible by anyone, anywhere.

New to Binder? Get started with a Zero-to-Binder tutorial in Julia, Python or R.

Build and launch a repository

GitHub repository name or URL

GitHub ▾ | GitHub repository name or URL

Git branch, tag, or commit

Git branch, tag, or commit

Path to a notebook file (optional)

Path to a notebook file (optional) | File ▾

launch

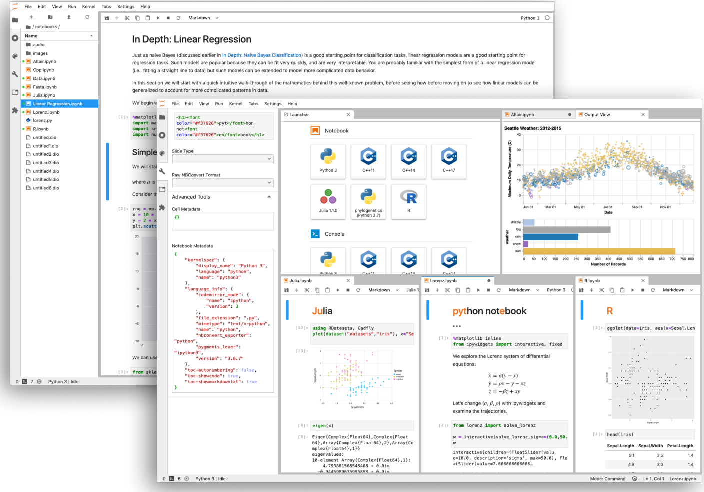
Copy the URL below and share your Binder with others:

```
Fill in the fields to see a URL for sharing your Binder.
```

`https://mybinder.org/`

Jupyter

Since June 2019 : Jupyter Lab v1.0 (now v3.0.16)



In Depth: Linear Regression

Just as naive Bayes (discussed earlier in In Depth: Naive Bayes Classification) is a good starting point for classification tasks, linear regression models are a good starting point for regression tasks. Such models are popular because they can be fit very quickly, and are very interpretable. You are probably familiar with the simplest form of a linear regression model (i.e., fitting a straight line to data) but such models can be extended to model more complicated data behavior.

In this section we will start with a quick intuitive walk-through of the mathematics behind this well-known problem, before seeing how before moving on to see how linear models can be generalized to account for more complicated patterns in data.

```
<h1><font
color="#f37626">pyt</font>hon
not<font
color="#f37626">e</font>book</h1>
```

Slide Type

Raw NBConvert Format

Advanced Tools

Cell Metadata

```
{}
```

Notebook Metadata

```
{
    "kernelspec": {
        "display_name": "Python 3",
        "language": "python",
        "name": "python3"
    },
    "language_info": {
        "codemirror_mode": {
            "name": "ipython",
            "version": 3
        },
        "file_extension": ".py",
        "mimetype": "text/x-python",
        "name": "python",
        "nbconvert_exporter":
"python",
        "pygments_lexer":
"ipython3",
        "version": "3.6.7"
    },
    "toc-autonumbering": false,
    "toc-showcode": true,
    "toc-showmarkdowntxt": true
}
```

Julia

```
[10]: using RDatasets, Gadfly
      plot(dataset("datasets","iris"), x="Se
```

```
[8]: eigen(x)
```

```
[8]: Eigen{Complex{Float64},Complex{Float
     64},Array{Complex{Float64},2},Array{Co
     mplex{Float64},1}}
     eigenvalues:
     10-element Array{Complex{Float64},1}:
         4.793881566545466 + 0.0im
       -0.9445989635995898 + 0.0im
```

python notebook

```
[1]: %matplotlib inline
     from ipywidgets import interactive, fixed
```

We explore the Lorenz system of differential equations:

$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = \rho x - y - xz$$
$$\dot{z} = -\beta z + xy$$

Let's change (σ, β, ρ) with ipywidgets and examine the trajectories.

```
[2]: from lorenz import solve_lorenz

     w = interactive(solve_lorenz,sigma=(0.0,50.
     w

     interactive(children=(FloatSlider(valu
     e=10.0, description='sigma', max=50.0), Flo
     atSlider(value=2.666666666666…
```

R

```
[3]: ggplot(data=iris, aes(x=Sepal.Len
```

```
[1]: head(iris)
```

Sepal.Length	Sepal.Width	Petal.Length
5.1	3.5	1.4
4.9	3.0	1.4

Conclusion ?

Who’s the best?

Conclusion ?

Who's the best?

It depends...

Conclusion ?

Who's the best?

It depends...

- R analyses? Go for RMarkdown/RStudio
- R analyses for a publication ? Consider Jupyter with an R kernel

Conclusion ?

Who's the best?

It depends...

- R analyses? Go for RMarkdown/RStudio
- R analyses for a publication ? Consider Jupyter with an R kernel
- Python analyses ? Why do you even ask...

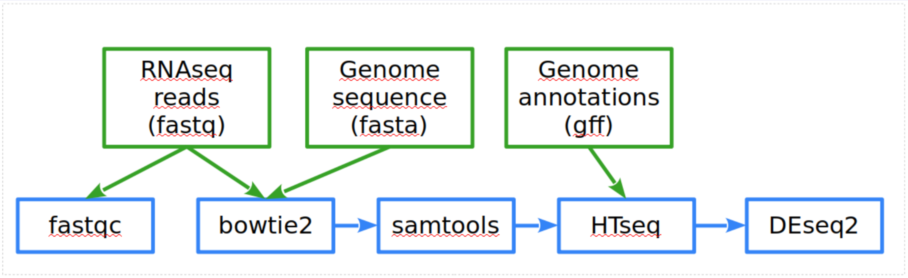
Practical session

Savoir FAIRe

- Markdown
- Learn the structure of an Rmd file
- Turn a script into a notebook
- Extend the notebook with new functionalities
- This afternoon: Jupyter with the IFB cluster

Analysis workflow

Analysis workflow



green=input, blue=tool

fastqc	control quality of the input reads
bowtie2	reads mapping on the genome sequence
samtools	mapped reads selection & formatting
HTseq	count table of mapped reads on genes (annotations)
DESeq2	statistical analysis: genes list having differential expression