

Scientific Programming

Practical 1

Introduction

Luca Bianco - Academic Year 2018-19
luca.bianco@fmach.it

Outline

- ❖ Personal introduction
- ❖ Introduction to the practical
- ❖ Hands-on practical

About me

Computer Science

Ph.D. at the University of Verona, Italy, with thesis on Simulation of Biological Systems

Research Fellow at Cranfield University - UK

Three years at Cranfield University working at proteomics projects (GAPP, MRMaid, X-Tracker...)

Module manager and lecturer in several courses of the MSc in Bioinformatics

Bioinformatician at IASMA – FEM

Currently bioinformatician in the Computational Biology Group at Istituto Agrario di San Michele all'Adige – Fondazione Edmund Mach, Trento, Italy

Collaborator uniTN - CiBio

I run the Scientific Programming Lab A last year

Fondazione Edmund Mach

FEM – San Michele, Trento - Italy



Agricultural Institute

Research and Innovation Centre

Genomics, metabolomics wet labs on
fruits (apple, grape, small fruits,...)

Bioinformatics and computational biology

Bioinformatics @FEM (UBC)

❖ Genomics

- Assembly and annotation of complex genomes (plants, insects, etc.)
- Development of SNP Chips for genetic screening
- Resequencing of genomes

❖ Metagenomics

- Targeted metagenomic data
- *Feature selection* algorithms
- Algorithms for strain-level identification from un-targeted metagenomics

❖ Transcriptomics

- RNA-seq data analysis, gene and pathway enrichment
- Data integration and compilation of expression atlases

❖ Metabolomics

- Data analysis pipelines for targeted and untargeted data
- Methods for MS imaging

❖ Statistical data analysis

- Integration of -omic data and analysis of correlation networks



Bix @FEM - Examples

Genome assembly

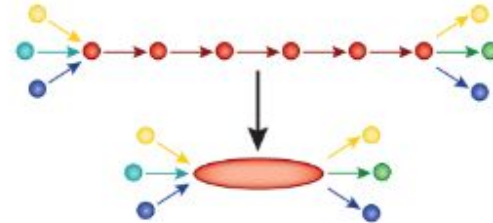
1. Fragment DNA and sequence



2. Find overlaps between reads

...AGCCTAGACCTACA**GGATGCGCGACACGT**
GGATGCGCGACACGTCGCATATCCGGT

3. Assemble overlaps into contigs



4. Assemble contigs into scaffolds



[from M. Baker, Nature Methods, 2014]

Bix @FEM - Examples

Genome assembly of DH of Pear and Apple

Input data:

Illumina ~60x – 100x PE information + (mate pairs for Apple)

Pacific Biosciences ~ 30x + 30x (35x only for Apple)

Bionano optical maps: ~ 600x (for both)

Genetic maps: integrated genetic map from 21 mapping populations (Apple only)

Output result (for Apple, Pear is in progress):

Chromosome scale assembly

Contigs: 2150 for a total of 625Mb

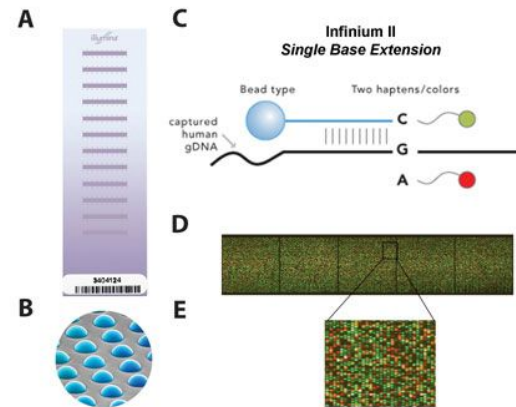
N50 Contigs (hybrid dbg2olc): ~ 620Kbps

280 Scaffolds, for an N50 5,6Mb

17 chromosomes + lg0 unanchored sequences



[Daccord et al, Nature Genetics, 49, 2017]

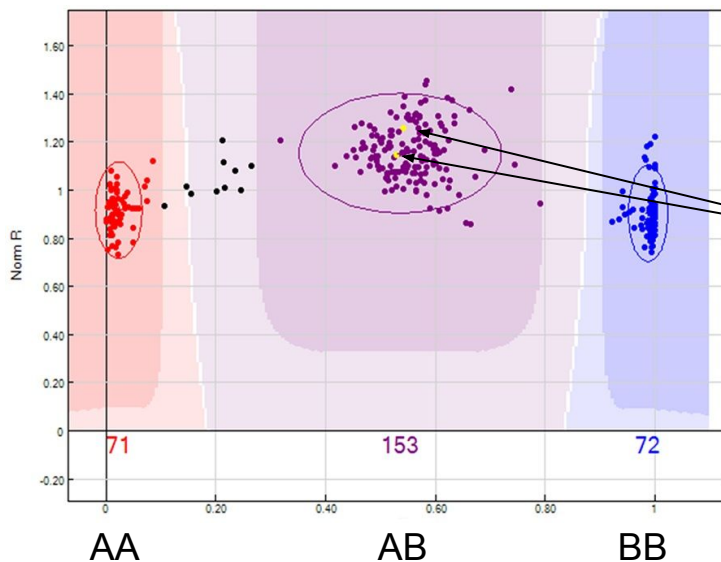


Bix @FEM - Examples

SNP-Chips development for GWAS

20K SNP Illumina Infinium II Array (reseq of 16 Apple cultivars, Illumina 30x)

487K SNP Affymetrix Axiom Array (reseq of 63 Apple cultivars, Illumina 20-30x)



Task:

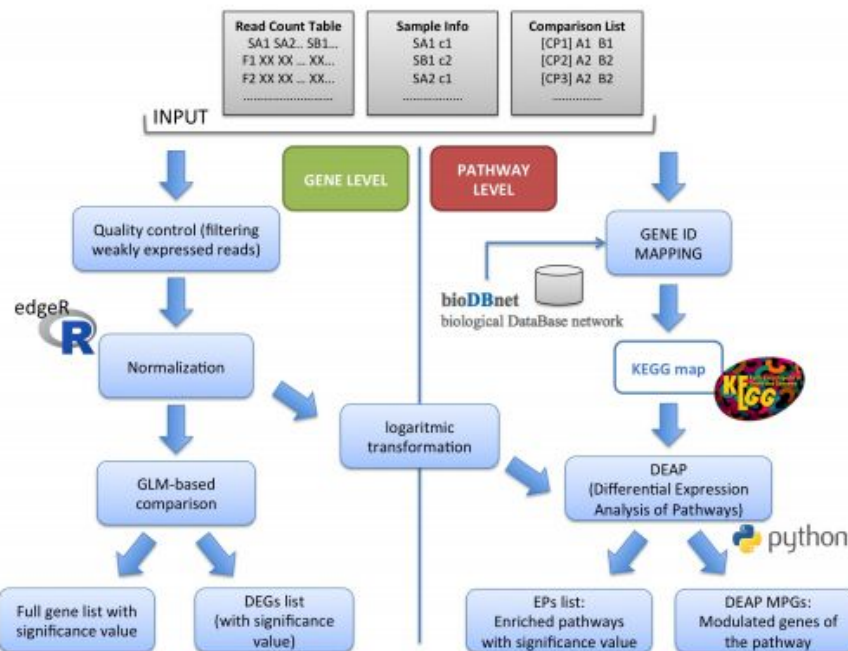
Analyze 500,000 of these...
(1 x SNP)

parents

genotypes

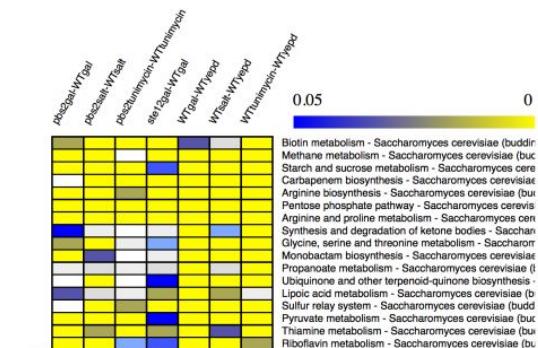
Bix @FEM - Examples

RNAseq data analysis with Pathway Inspector



Bix @FEM - Examples

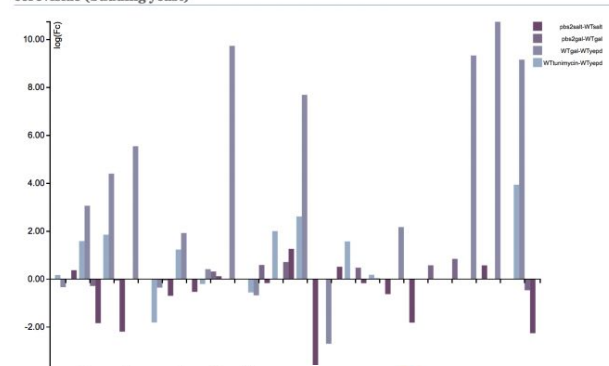
RNAseq data analysis with Pathway Inspector



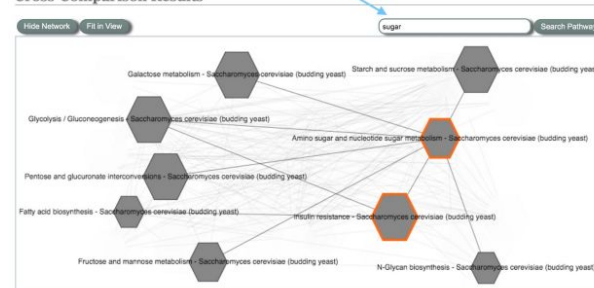
Intersection pbs2salt-WTsalt WTtunimycin-WTyeptd pbs2gal-WTgal WTgal-WTyeptd

Gene	Comparison	P-value	Fold Change	FDR
YOR04W	pbs2salt-WTsalt	0.02848082028946	0.2420311772254	0.0481361748189205
	WTtunimycin-WTyeptd	2.38460349315057e-07	0.524172138345184	4.474873128693e-07
	pbs2gal-WTgal	0.00087890548504028	-0.30105531814261	0.0207830810500887
	WTgal-WTyeptd	2.86788386434103e-15	0.83218803220708	7.1912488256014e-15
YIL140W	pbs2salt-WTsalt	3.85247940741733e-08	0.833589168058476	1.85448837803025e-07
	WTtunimycin-WTyeptd	1.58817878171733e-24	1.001649102893	5.8239103817754e-24
	pbs2gal-WTgal	1.87826251152733e-09	0.30764051192865	1.49862020134624e-08
	WTgal-WTyeptd	0.3034912942367044	0.276548277440217	0.0548210627660931
YLR130C	pbs2salt-WTsalt	0.301481019188815	0.31882150138888	0.0308287774872549
	WTtunimycin-WTyeptd	3.0140342877802e-06	-1.58765788614284	3.8332178378679e-05
	pbs2gal-WTgal	2.7870331888813e-09	0.488214138134541	2.3895374291845e-08
	WTgal-WTyeptd	8.8037203388888e-18	-0.8312188730247	1.8224549730366e-17
YOR011W	pbs2salt-WTsalt	1.00574728111917e-16	0.72183031688741	8.2817487473501e-16
	WTtunimycin-WTyeptd	0.010862387803186	0.21641810221331	0.014715787255527

Comparative analysis for Amino sugar and nucleotide sugar metabolism - Saccharomyces cerevisiae (budding yeast)



Cross-Comparison Results



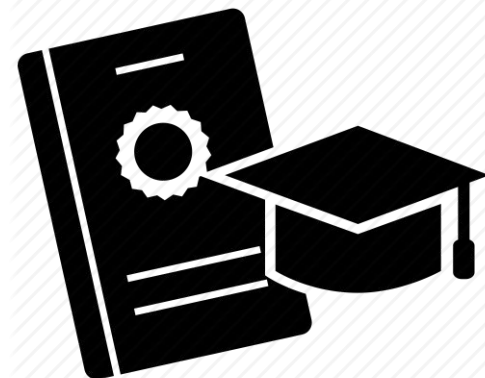
Opportunities @FEM

MSc External thesis

Are you interested in a bioinformatics project in NGS data analysis, RNA Seq, data integration?

Come and talk to me or email me at:

luca.bianco@fmach.it



Scientific Programming Practical

Back to business now!



Scientific Programming Practical

In this practical you will

1. Install Python 3.x (and pip)
2. Install Visual Studio Code
3. Get familiar with the Python console
4. Start using Visual Studio Code and advanced features (like debugging)
5. End the session with some exercises

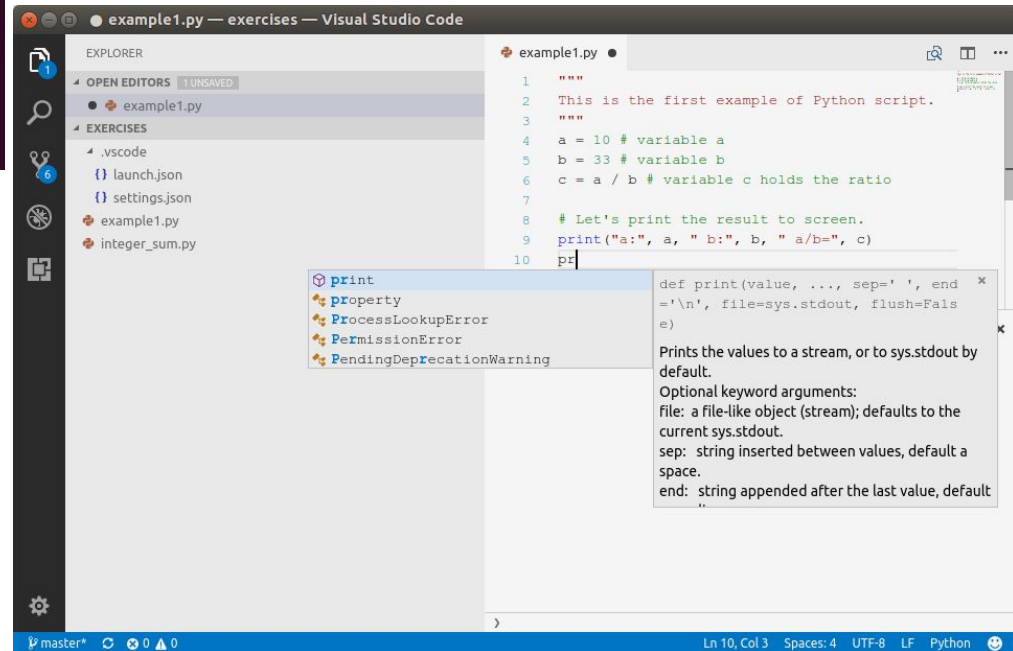


Scientific Programming Practical

Console VS. Integrated Development Environment (IDE)

```
biancol@bluhp:~$ python3
Python 3.5.2 (default, Aug 18 2017, 17:48:00)
[GCC 5.4.0 20160609] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> 
```

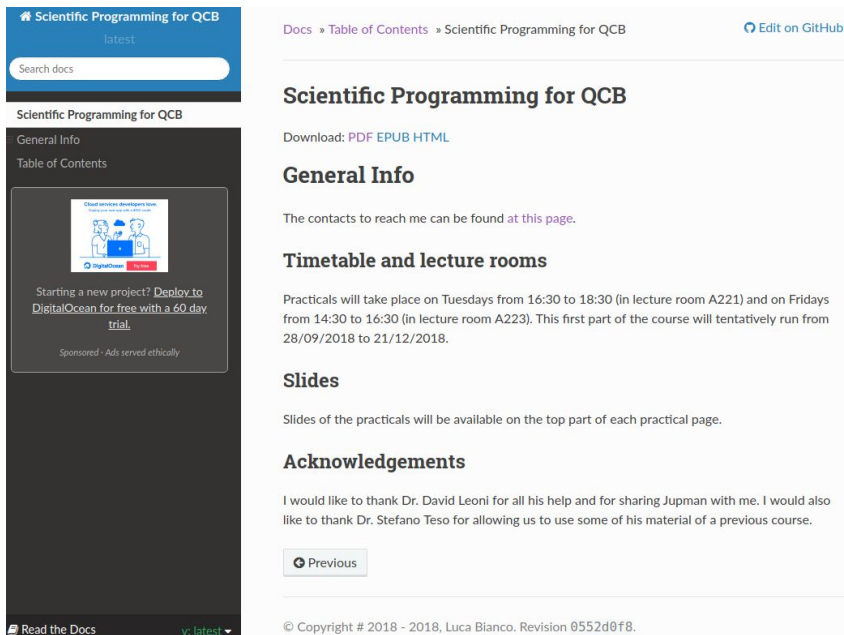
```
>>> print("Hi there")
Hi there
>>> print("{} + {} = {}".format(10,20, 10+20))
10 + 20 = 30
>>> 
```



Resources

All material regarding practicals will be found here:

<http://qcbsciprolab.readthedocs.io>



The screenshot shows the Read the Docs interface for the 'Scientific Programming for QCB' project. The left sidebar contains a search bar, the project name, and navigation links for 'General Info' and 'Table of Contents'. The main content area has a breadcrumb trail 'Docs » Table of Contents » Scientific Programming for QCB' and an 'Edit on GitHub' link. Below this is the title 'Scientific Programming for QCB' and download links for 'PDF', 'EPUB', and 'HTML'. The 'General Info' section includes a link to contact information. The 'Timetable and lecture rooms' section details the course schedule. The 'Slides' section mentions their availability. The 'Acknowledgements' section thanks Dr. David Leoni and Dr. Stefano Teso. At the bottom, there is a 'Previous' button and a copyright notice.

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General Info

The contacts to reach me can be found [at this page](#).

Timetable and lecture rooms

Practicals will take place on Tuesdays from 16:30 to 18:30 (in lecture room A221) and on Fridays from 14:30 to 16:30 (in lecture room A223). This first part of the course will tentatively run from 28/09/2018 to 21/12/2018.

Slides

Slides of the practicals will be available on the top part of each practical page.

Acknowledgements

I would like to thank Dr. David Leoni for all his help and for sharing Jupman with me. I would also like to thank Dr. Stefano Teso for allowing us to use some of his material of a previous course.

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luca.bianco@fmach.it

Timetable

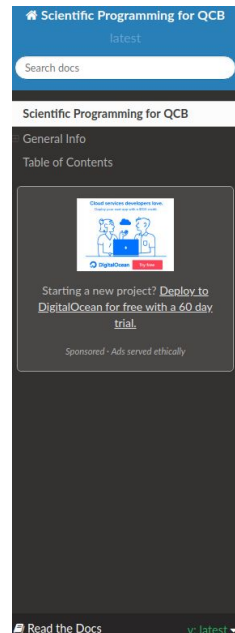
Tuesdays:

A221: 16,30 - 18,30

Fridays:

A223: 14,30 - 16,30

Most probably we will skip October 30th practical.



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Any questions?

If not, go to:

<https://qcbsciprolab.readthedocs.io/en/latest/introduction.html>

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Practical 1

In this practical we will set up a working Python3 development environment and will start familiarizing a bit with Python.

Slides

The slides shown in the introduction can be found here: [Intro](#)

Setting up the environment

We will need to install several pieces of software to get a working programming environment suitable for this practical. In this section we will install everything that we are going to need in the next few weeks.

Python3 is available for Windows, Linux and Mac.

Our toolbox

If you work on Windows or Mac, you can safely skip the following and go straight to the section "Windows/Mac installation". Note that, regardless your operating system, a useful source of information on how to install python can be found [here](#).

Linux installation

1. The Python interpreter. In this course we will use python version 3.x. A lot of information on python can be found on the [python web page](#). Open a terminal and try typing in:



luca.bianco@fmach.it