

Trinity College Dublin Coláiste na Tríonóide, Baile Átha Cliath The University of Dublin



Introduction to Bioinformatics and Computation Biology

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Pierpaolo Maisano Delser

mail: maisanop@tcd.ie ; pm604@cam.ac.uk

Outline:

- What is Bioinformatics and Computational Biology?
- Why do we need a bioinformatician?
- From personal computer to High Performance Computing facilities
- Daily examples where bioinformatics can be useful

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Biology + informatics (computer science)

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Main concept is the same ----- minor differences

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Application of techniques from computer science to problems from biology

A computational approach to solve biological problems

Development and application of analytical and theoretical methods, mathematical modelling and computational simulation techniques to the study of biological, behavioural and social data Application of information technology and computer science to the field of molecule biology

Application of computational tools on molecular data including the means to acquire, analyse or visualise such data

The branch of science concerned with information and information flow in biological systems, the use of computational methods in genetics and genomics

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There is not standard definition!!!

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Bioinformatics is different from Computational Biology ?



Bioinformatics is different from Computational Biology ?



Bioinformatics -----> genetics and genomics

Computational Biology -----> complex system, proteins, pathways

Biologists collect molecular data: DNA & Protein sequences, gene expression, etc.

> **Bioinformaticians** Study biological questions by analyzing molecular data

Computer scientists

(+Mathematicians, Statisticians, etc.) Develop tools, softwares, algorithms to store and analyze the data.

Who is a bioinformatician or a computation biologists?







Am I a bioinformatician/computational biologists???

Am I a bioinformatician/computational biologists???

- Master in bioinformatics;
- Course in bioinformatics/ programming for biologists;
- Courses at the universities;
- Integration between computer science and biology;
- Problem-driven knowledge;

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- Situations where a bioinformation can be useful;
- Which skills make a person a bioinformatician?





Master Degree, 240 samples, HVI mtDNA, 2009

- Alignment by hand (forward and reverse sequence);
- Comparing less than 1kb of DNA;
- Many samples but the amount of data was not much;
- Determine haplotypes by hand (simple software);
- Genetic statistics computed with a calculator;

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- Determine haplotypes by hand (simple software);
- Genetic statistics computed with a calculator;

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- Many samples but the amount of data was not much;
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- Genetic statistics computed with a calculator; I prefer to use the calculator in my

computer to save intermediate results



From ~600bp in 240 samples to 50kb in 250 samples (2010)

• New alignment with different raw files;

• Comparing ~50kb in 250 samples;

• Lots of data....analysis and storage?;

• Haplotypes?;

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• Lots of data....analysis and storage?;

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- Bash commands
- New software (i.e. bwa...)
- New file format (i.e. fastq)

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- New file format (i.e. fastq)
- Bash commands
- New software (i.e. samtools)
- New file format (i.e. vcf)
- Filtering and validation (scripting + new software i.e. vcftools)
- Perl;

• Haplotypes?;

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- Bash commands
- From personal computer to HPC facilities
- Time....

From ~600bp in 240 samples to 50kb in 250 samples (2010)



From ~600bp in 240 samples to 50kb in 250 samples (2010)



- How did we end up needing (possibly) a bioinformatician?
 - Situations are mainly dictated by the exponential increase of the amount of data:
 - Time;
 - Efficiency;
 - Accuracy;
 - Customisation (analyses);

- How did we end up needing (possibly) a bioinformatician?
- Situations where a bioinformation can be useful;
- Which skills make a person a bioinformatician?

• Situations where a bioinformation can be useful;

When analyses cannot be done by "hand" anymore When analyses could be done by "hand" but they would take too long (time factor)
• Situations where a bioinformation can be useful;

When analyses cannot be done by "hand" anymore

- Alignment;
- Variant calling;
- Indel-calling;
- Protein interactions;
- Pathway analyses;

When analyses could be done by "hand" but they would take longer (time factor)

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- Alignment;
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- Protein interactions;
- Pathway analyses;

When analyses could be done by "hand" but they would take longer (time factor)

- Allele frequency calculations;
- Database query;
- Literature review;
- Pairwise differences;

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There is no standard set of skills;

Depends on the task/project;

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Skills:

- Scripting (different languages);
- Statistics;
- Terminal(shell) friendly;
- Away from double-click!

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Depends on the task/project;

Skills:

- Scripting (different languages);
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Attitudes:

- Willing to learn and improve his knowledge;
- Facing daily new challenges;
- Always consider the final aim...

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Microsoft word in 13 floppy disk 3.5 inch



Processor (8-12 cores)

Memory (8-12 Gb RAM)



Disk Space (500 Gb SSD/ 1 Tb)



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Disk Space (500 Gb SSD/ 1 Tb)

Is it enough??





Processor (8-12 cores) Memory (8-12 Gb RAM) Disk Space (500 Gb SSD/ 1 Tb)

Is it enough??

Alignment (bwa) modern genome, 15-20x coverage, 32 cores with 8gb of RAM each, 2-3 days

GATK variant caller can require ~20GB of RAM

Merging dataset requires lots of memory

XXX.fastq.gz (~90Gb) -> trimmed (80Gb) -> bam.gz (70Gb) -> rmdup_bam.gz (55Gb) = 295 Gb

Processor (8-12 cores) Memory (8-12 Gb RAM) Disk Space (500 Gb SSD/ 1 Tb)

Is it enough??

Alignment (bwa) modern genome, 15-20x coverage, 32 cores with 8gb of RAM each, 2-3 days

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It is NOT enough!!

Merging dataset requires lots of memory

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HPC: High performance computing facilities

TOP 500 Supercomputer:



- 1) Summit (Department of Energy, Oak Ridge National Laboratory):
 - 2,282,544 cores;
 - 2,801,664 GB memory;
 - 122.3 petaflop (122.3 x 10^15 operations per second);

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101) Peta4 (University of Cambridge):

- 46,464 cores;
- 184,392 GB memory;
- 1.696 petaflop;















Additional storage:

- Personal or group based;
- Long term storage (cold storage);
- Backup hard drives;
- Multiple copies;

Suggestions:

- Multiple copies but with rationale...
- Published dataset
- Keep what it is essentials....we cannot keep everything anymore!

HPC: High performance computing facilities

Load module:

- Several software are already pre-installed in the clusters as modules;
- Bash is the shell on the cluster;
- Working on clusters is similar to the linux terminal;

HPC: High performance computing facilities

Different kind of "jobs":

Serial Jobs



Parallel Jobs





Job scheduler



Key factor: wall time...use it smartly!!!

HPC: High performance computing facilities

Conclusions:

- Analysing big dataset is no more feasible on personal computer;
- HPC facilities can help us;
- Manage your storage and archive your data;

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New articles from highly accessed journals

Adv Exp Med Biol (16)

Br J Sports Med (3)

Cancer (2)

Crit Care (3)

| S NCBI Resources | How To 🕑 | | | | | <u>pmd85</u> | <u>My NCBI</u> | <u>Sign Out</u> |
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| PubMed Tutorials | | | Clinical Queries | | <u>E-Utilities (API)</u> | | | |
| New and Noteworthy | | | Topic-Specific Queries | | LinkOut | | | |
| Latest Literature | | | Trending Articles | | | | | |

PubMed records with recent increases in activity

tumorigenesis.

improves health

Nature. 2018.

N-4----

Nuclear cGAS suppresses DNA repair and promotes

De novo NAD⁺ synthesis enhances mitochondrial function and

• Download data;

Use of key words;

۲

Literature review

Data mining

Scripts for specific queries;







Hallast P et al, 2015, MBE

Daily examples where bioinformatics can be useful

protein-protein interaction



Deoxyhemoglobin Rothschild

Daily examples where bioinformatics can be useful



TATGGTGCGGAGGCCCTGGAGAGGATGTTCCTGTCCTTCCCCACCACCACGACCTACTTCCCGCACTTCGACCTGAGCCACGGCTCTGCCCAGGTTAAGGGCCACGGCA CAACTTCAAGCTCCTAAGCCACTGCCTGCTGGTGACCCTGGCCGCCCACCTCCCCGCCGAGTTCACCCCTGCGGTGCACGCCTCCCTGGACAAGTTCCTGGCTTCTGTGGTGGTCTTTGAATAAAGTCTGAGTGGGCGGCACTCTTCTGGTCCCCACAGACTCAGAGAGAACCCACCATGGTGCTGTCTCCTGCCGACAAGACCAACGTCAAGGCCGC CTGGGGTAAGGTCGGCGCGCGCGCGCGCGGGGGGGTATGGTGCGGAGGGCCCTGGAGGGGGGTGTTCCTGTCCTCCCCACCACCACGACCTACTTCCCCGCACTTCGACCTGAGCCACGGCTCTGCCCAGGTTAAGGGCCACGGCAAGAAGGTGGCCGACGCGCTGACCAACGCCGTGGCGCACGTGGACGACATGCCCAACGCGCTGTCCGCCCTGAGCGACCCCGCCTCCCTGGACAAGTTCCTGGCTTCTGTGAGCACCGTGCTGACCTCCAAATACCGTTAAGCTGGAGCCTCGGTGGCCATGCTTCTTGCCCCCTTGGGCCTCCCCCCAGCCCCTCCTCCCCCTTCCTGCACCCGTACCCCCGTGGTCTTTGAATAAGTCTGAGTGGGCGGCACTCTTCTGGTCCCCACAGACTCAGAGAGAACCCCACCATGGTGCTGTACCTCCCCGCCGAGTTCACCCCTGCGGTGCACGCCTCCCTGGACAAGTTCCTGGCTTCTGTGAGCACCGTGCTGACCTCCAAATACCGTTAAGCTGGAGCCTCGGTGGCCGCCCACCTCCCCGCCGAGTTCACCCCTGCGGTGCACGCCTCCCTGGACAAGTTCCTGGCTTCTGTGAGCACCGTGCTGACCTCCAAATACCGTTAAGCTGGAGCCTCGGTGGCCATGCTTCTTGCCCCCTTGGGCCTCCCCCCAGCCCCTCCTCCCCCTGCACCCGTACCCCCGTGGTCTTTGAATAAAGTCTGAGTGGGCGGCACTCTTCTGGT GGCCCTGGAGAGGATGTTCCTGTCCTTCCCCACCACCAAGACCTACTTCCCGCACTTCGACCTGAGCCACGGCTCTGCCCAGGTTAAGGGCCACGGCAAGAAGGTGGCC

Daily examples where bioinformatics can be useful

a) Model SINGLE_MT Model MULTIPLE_MT Nanc3 Tlevant Nanc2 Tsplit Nanc2 Nanc1w Nanc1e Nanc1l 11,000 YA 🕂 Nanc1 10,500 YA 🕂 Nbotw Nbote Nbotl Nbotl Nbotw Nbote g1l g1w g1e g1l g1w g1e 8,000 YA **L** 3W 3E 3L 3W 3E 3L Nneol Nneow Nneoe Nneol Nneoe Nneow

Coalescent simulations

Daily examples where bioinformatics can be useful

Climatic and vegetation modelling


Conclusions:

- Bioinformatics/Computational Biology is a relatively recent discipline "which applies tools from computer sciences to biological problems"
- Skills can vary depending on the problem;

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