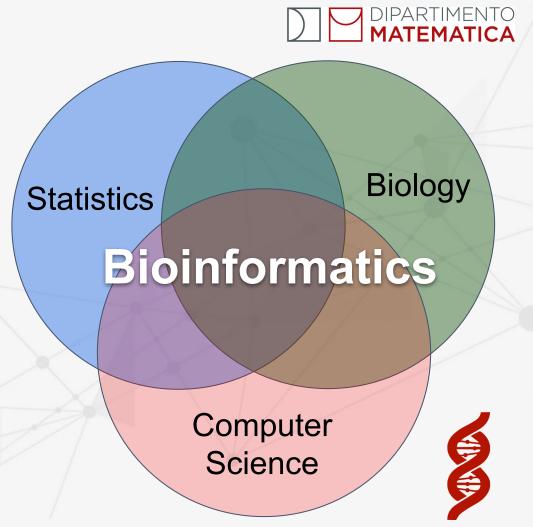# Bioinformatics

- Biological information can be studied with approaches typical of information theory

- Understanding biology requires statistical analyses
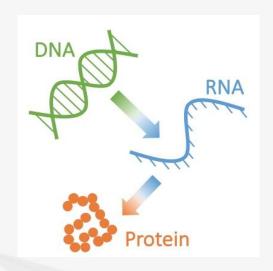
- Computer science as a tool for biological data management

Structural Bioinformatics
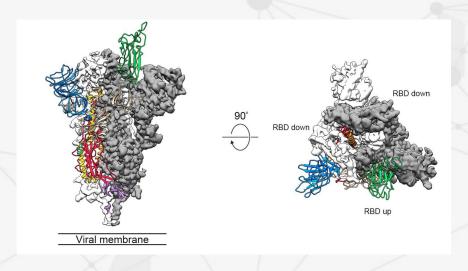
An example... **Coronavirus**
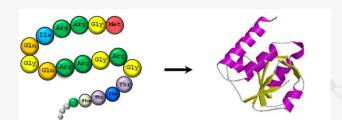
The Central Dogma of life

Cryo-EM structure of the 2019-nCoV spike in the prefusion conformation.
Wrapp D et al. **Science. *26 Feb 2020***
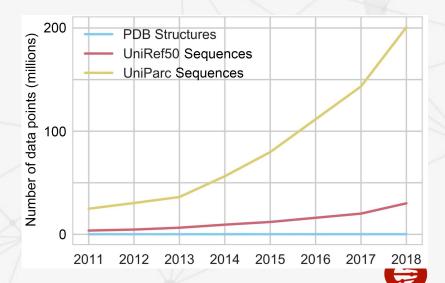
Why structure prediction?
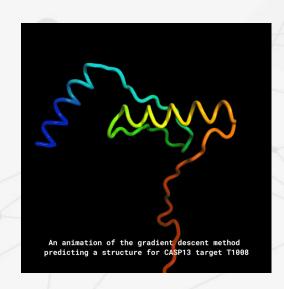
The sequence-structure gap

The protein folding problem

An example, the protein folding problem:

- **Molecular Dynamics** simulations take **years** of calculation

- **Deep learning** algorithms take **hours**

An animation of the gradient descent method predicting a structure for CASP13 target T1008

AlphaFold
Google DeepMind lab

Course information

Prof. Damiano Piovesan

- **Office hours**: Tuesday 5-6 PM

- **Office**: BioComputingUP lab - Vallisneri building, ground floor, near the library

- **Email:** damiano.piovesan@unipd.it

- **Twitter:** *@DamianoPiovesan*

Dott. Alexander Monzon (assistant)

- **Office**: BioComputingUP lab - Vallisneri building, ground floor, near the library

- **Email:** alexander.monzon@unipd.it

- **Twitter:** *@AlexanderMonzon*

Teaching

Theoretical lectures

- Introduction to biochemistry, molecular dynamics, homology modelling, ab initio prediction, structural analysis

Hands-on

- Personal laptop, no particular HW requirements, possibly a Linux like OS (Ubuntu, Mac)

- Python, BioPython, PyMol, command line executables

Prospective student's background

We welcome students with a **good background** in:

- Computer science, Computer Engineering, ICT

- Mathematics, Statistics, Physics

- Biology, Medicine and related (with math/statistics fundamentals)

Prospective students should:

- Have an attitude on both basic science (biology, biochemistry, physics) and computer science

BDA curriculum (for DS students)

BDA curriculum (for DS students)

- Two **optional** courses, two **electives**

- Optional: at least one from **group A** and one from **group B**

COMPUTER SCIENCE	MATHEMATICAL CELL BIOLOGY [B]	DEEP LEARNING [A]	BIG DATA COMPUTING [A]	NETWORK SCIENCE [A]

BIOLOGY, ECONOMICS, HUMAN & SOCIAL SCIENCE	SYSTEM BIOLOGY [B]	OMICS IN HUMAN DISEASE [B]

ELECTIVE	12 CFU

Success stories
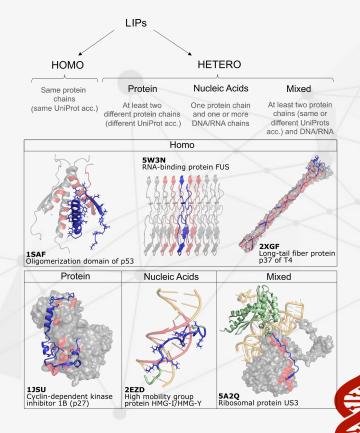
JMB - Impact Factor 4.76, 1st quartile considering "Biochemistry and Molecular Biology" category

Journal impact factor

$$IF_{2017} = \frac{Citations_{2017}}{Publications_{2016} + Publications_{2015}} = \frac{74090}{880 + 902} = 41.577$$

2019 journal impact factor

Impact factor (2 years)

Clarivate InCite Journal Citation Report (https://jcr.clarivate.com)

Journals by category
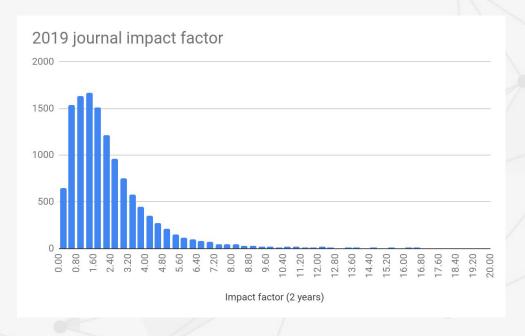
Rank	Category	# Journals	Total Cites	Median Impact Factor	Aggregate Impact Factor
1	ECONOMICS	373	1,116,324	1.411	2.219
2	MATHEMATICS	325	565,491	0.794	0.993
3	MATERIALS SCIENCE, MULTIDISCIPLINARY	314	5,001,499	2.528	5.274
4	**BIOCHEMISTRY & MOLECULAR BIOLOGY**	**297**	**3,962,918**	**3.167**	**4.696**
5	NEUROSCIENCES	272	2,548,868	3.052	4.041
6	PHARMACOLOGY & PHARMACY	271	1,769,982	2.681	3.442
7	ENGINEERING, ELECTRICAL & ELECTRONIC	266	2,097,197	2.204	3.361
8	ENVIRONMENTAL SCIENCES	265	2,622,685	2.4	4.313
9	EDUCATION & EDUCATIONAL RESEARCH	263	421,337	1.585	1.804
10	MATHEMATICS, APPLIED	261	631,053	1.162	1.568
11	ONCOLOGY	244	2,187,273	3.297	4.84
12	PLANT SCIENCES	234	1,292,836	1.576	3.005
13	MANAGEMENT	226	892,977	2.465	3.288
14	SURGERY	210	1,327,558	1.901	2.558
15	CLINICAL NEUROLOGY	204	1,438,476	2.611	3.513
16	GEOSCIENCES, MULTIDISCIPLINARY	200	1,166,162	2.207	3.062
17	CELL BIOLOGY	195	2,359,746	3.683	6.278
18	PUBLIC, ENVIRONMENTAL & OCCUPATIONAL HEALTH	193	1,050,617	2.104	2.915
19	LINGUISTICS	187	177,076	0.895	1.305
20	POLITICAL SCIENCE	181	270,661	1.366	1.699

DIPARTIMENTO MATEMATICA