Coursework

Your own computational biology project

Coursework structure

- You are asked to write Python code that reads in some input, does some processing, then output some results.
- This should take the form of a complete project:
 - separate data files
 - An executable python script
 - Generation of an output
 - Commented and tested
 - With version control used

Coursework

- I will provide "real-life" examples, or as close to it as possible
- (Optional) Write me a paragraph about a topic you find interesting, related to bioinformatics / computing.
 - Or if you have a project in mind, write about that too!

Projects

Projects

- Classify cryo-EM particles (images)
- Identify a dog breed

Cryo-EM particle picker

Context: you are building a pipeline for cryo-EM reconstruction

• Identify whether the picked(selected) particle are similar enough to manually

selected ones.

Input: images (adapted from <u>EMPIAR</u>)

- Output: a decision per image
- Stretch goal 1: image clusterings
- Stretch goal 2: clustering visualisation

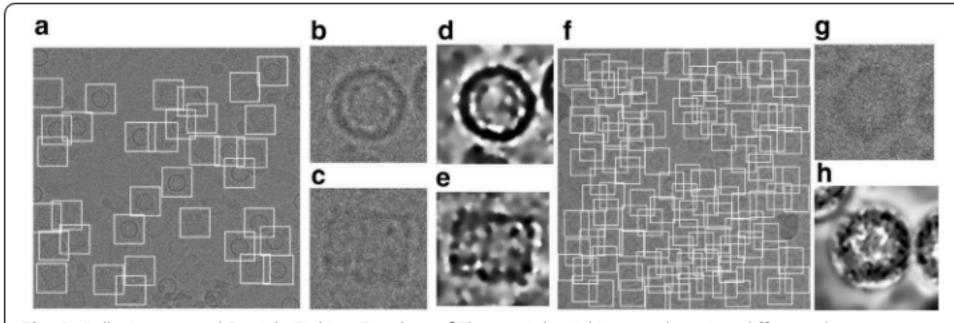


Fig. 2 Fully Automated Particle Picking Results. **a**, **f** The particle picking results using different datasets (Apoferritin [11] and KLH [12]). **b**, **c** The original KLH particle picking results. **d**, **e** The preprocessed KLH particle picking results. **g** The original Apoferritin particle picking results. **h** The Apoferritin preprocessed particle picking results

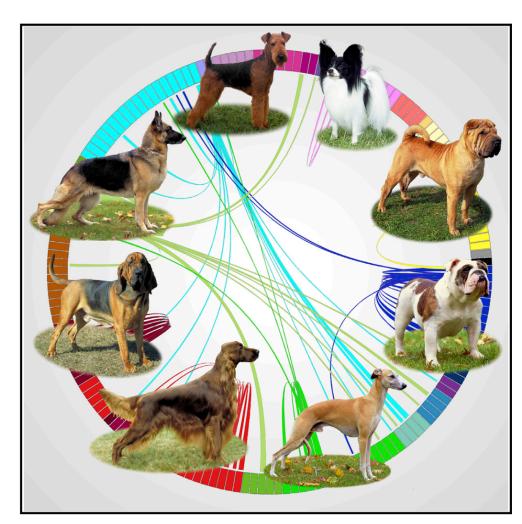
https://doi.org/10.1186/s12859-020-03885-9

• N.B.: I will provide the decision routine

Identify the most similar sequence

- Context: you want to develop a DNA identification service
- Identify the closest sequence in the database to the provided sequence
- Input: sequence database (adapted from <u>GEO</u>), test sequence
- Output: the closest sequence, and the difference
- Stretch goal 1: Probabilities across database, p-value
- Stretch goal 2: reconstructed phylogeny





Projects

- Both are real-life problems (although limited in scope here)
- Both make use of modern techniques (machine learning, NGS data)
- Both are about as hard as the other
- Choose one, stick with it!
- We will see how to structure projects
- It doesn't have to be perfect, just good enough

Evaluation

Elements of evaluation

- Project organisation and quality:
 - Is the project organised in folders / subfolders
 - Is there documentation?
 - Are you using a VCS to manage changes?
- Correctness
 - Does the code run?
 - Is the output correct?

Elements of evaluation

- Code quality
 - Is the code clear and consistent?
 - Are the variable/class/module names meaningful?
 - Is the code organised in function, class, modules?
 - N.B.: Do not use class if you can't see the point of it!
 - Are there tests?
 - Unit, integration tests?

Example marks

 Pass: the code just about runs and give a correct/reasonable output (maybe with *very* minor changes)

 Merit: the above, and project is well documented, tested, and organised, with one stretch goal

• Distinction: all of the above, extensive docs and tests, both stretch goals