Topics on Methods and Modelling in Astrophysics

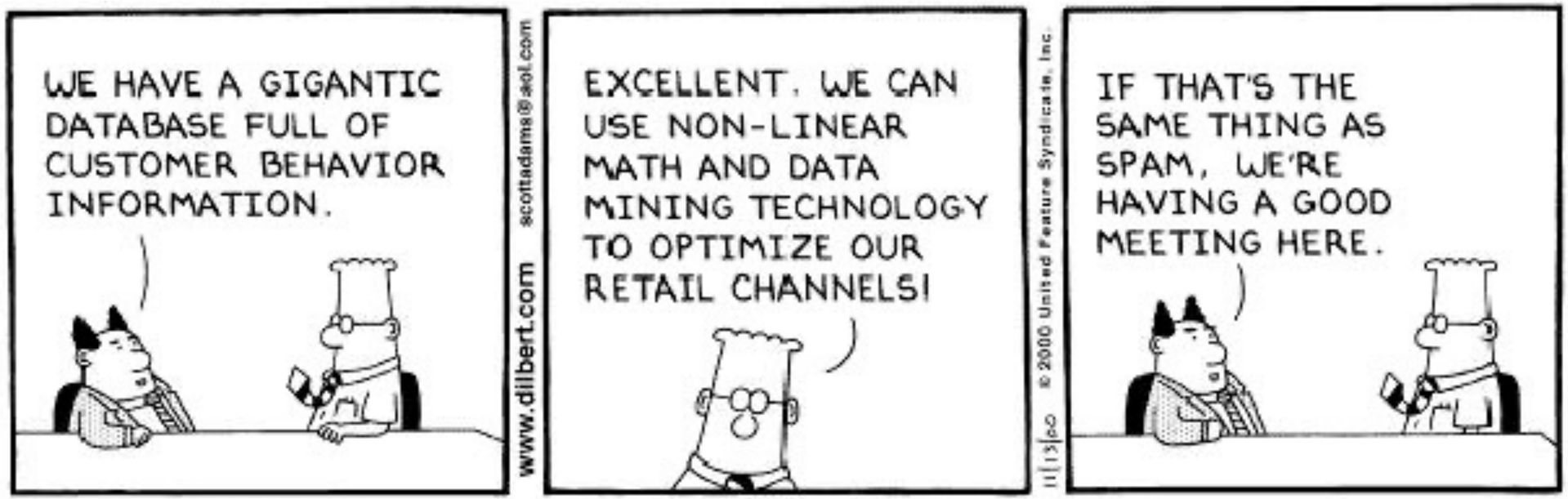
Machine Learning and Databases in Astronomy

https://github.com/jbrinchmann/MLD2025

Introduction

Why are you here?

The old view:



Why are you here?

https://imgs.xkcd.com/comics/machine_learning.png

Why are you here?

What is machine learning (in this course)?

https://imgs.xkcd.com/comics/machine_learning.png

What is machine learning (in this course)?

My definition:

Techniques to extract patterns/information/structure from data

What is machine learning (in this course)?

My definition:

Techniques to extract patterns/information/structure from data

There are many other definitions around, the Wikipedia one is fairly broad:

> *Machine learning (ML) is the scientific study of algorithms and statistical models that computer systems use to effectively perform a specific task without using explicit instructions, relying on patterns and inference instead. It is seen as a subset of artificial intelligence.* https://en.wikipedia.org/wiki/Machine_learning

What is machine learning (in this course)?

My definition:

Techniques to extract patterns/information/structure from data

There are many other definitions around, the Wikipedia one is fairly broad:

> *Machine learning (ML) is the scientific study of algorithms and statistical models that computer systems use to effectively perform a specific task without using explicit instructions, relying on patterns and inference instead. It is seen as a subset of artificial intelligence.* https://en.wikipedia.org/wiki/Machine_learning

This, from From “Deep Learning”, Goodfellow, Bengio, Courville, is also good:

> “Machine learning is essentially a form of applied statistics with increased emphasis on the use of computers to statistically estimated complicated functions and a decreased emphasis on prov[id]ing confidence intervals around these functions”

Examples outside of astronomy:

Amazon recommends .....

Use the buying patterns of all customers to create characteristic directions (books) in a multi-dimensional space. Apply this to individual customers to predict their preferences.

https://giphy.com/gifs/shopping-fAhOtxIzrTxyE

Examples outside of astronomy:

Organisation of merchandise in a supermarket

Find clusters of products that are bought together. Ensure you don’t discount both at the same time.

https://giphy.com/gifs/shopping-fAhOtxIzrTxyE

Examples outside of astronomy:

Organisation of merchandise in a supermarket

Find clusters of products that are bought together. Ensure you don't discount both at the same time.

https://giphy.com/gifs/shopping-fAhOtxlzrTxyE

Examples outside of astronomy:

Amazon recommends .....

Use the buying patterns of all customers to create characteristic directions (books) in a multi-dimensional space. Apply this to individual customers to predict their preferences.

Determine the structure of proteins

Predict 3D structure from chains of amino acids using deep learning

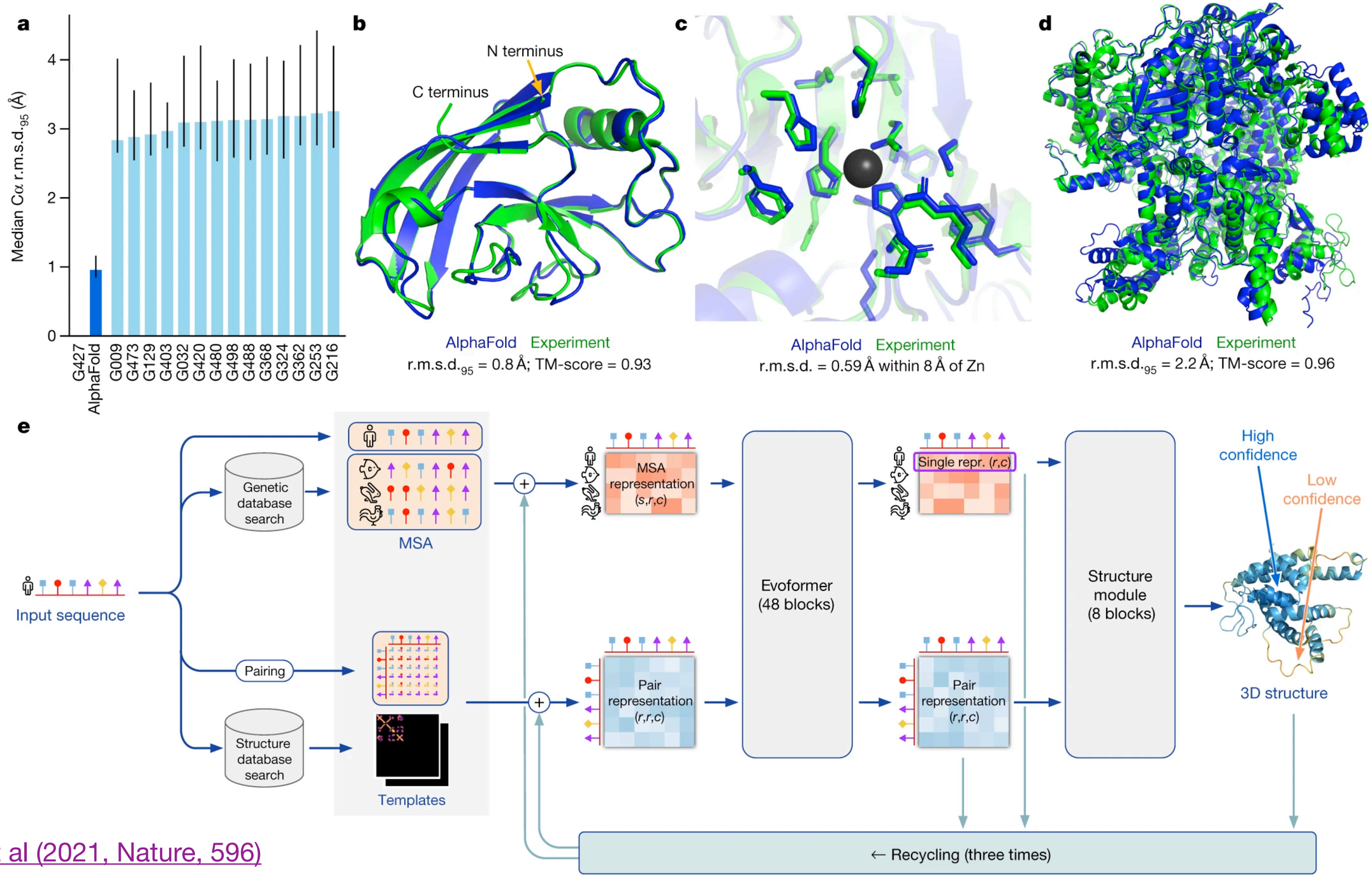
Examples outside of astronomy:

Organisation of merchandise in a supermarket

Find clusters of products that are bought together. Ensure you don’t discount both at the same time.

Determine the structure of proteins

Predict 3D structure from chains of amino acids using deep learning



Jumper et al (2021, Nature, 596)

The how and why questions

AlphaFold has been spectacularly successful in predicting *how* a protein will fold based on its sequence of amino acids - essentially all biologically important proteins now have this knowledge

This tackles the **how** question. But in some cases it might be that **why** is the important question. This is particularly true when enormous databases of proteins and their matches are made - even a tiny fraction of false positives in, say,10^{12} configurations can lead you massively astray.

We will return to this later - you should choose your tools according to the question you need to answer.

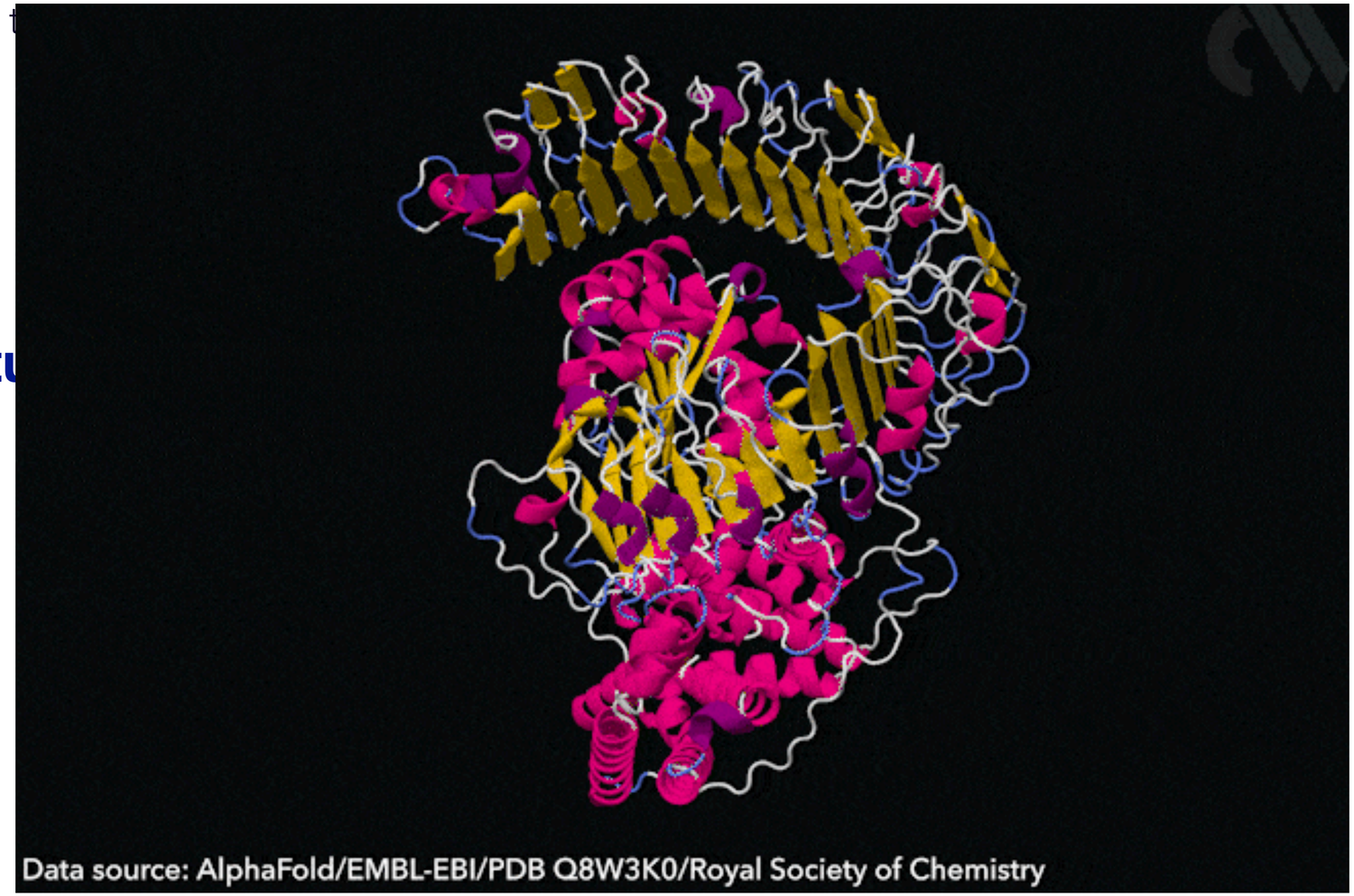
See e.g.: *Nature* **622**, 15-17 (2023)

Examples outside of astronomy:

Amazon recommends .....

Use the buying patterns of all customers to create characteristic directions (books) in a multi-dimensional space. Apply this t

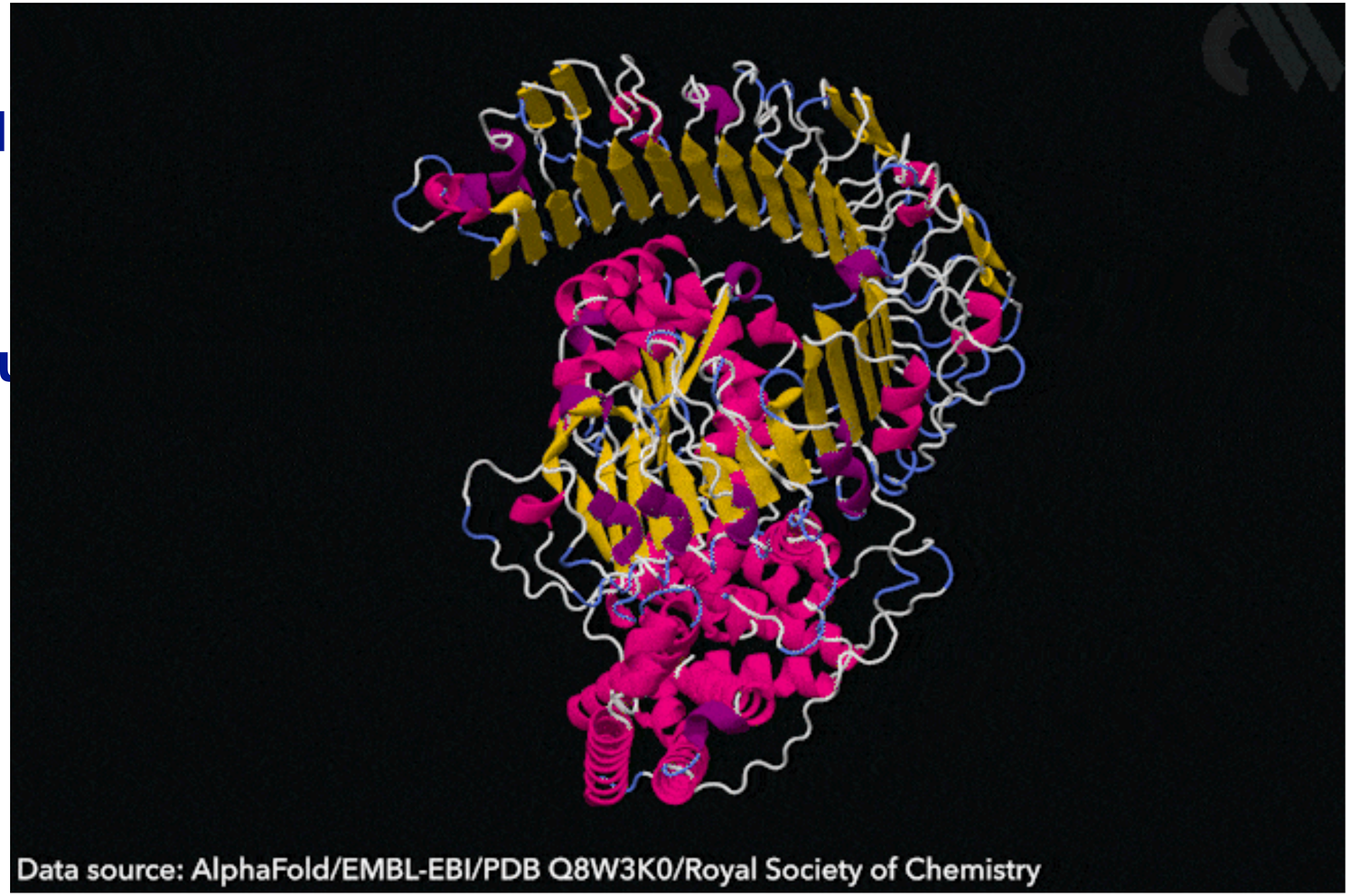
Determine the structu



Examples outside of astronomy:

Organisation of merchand

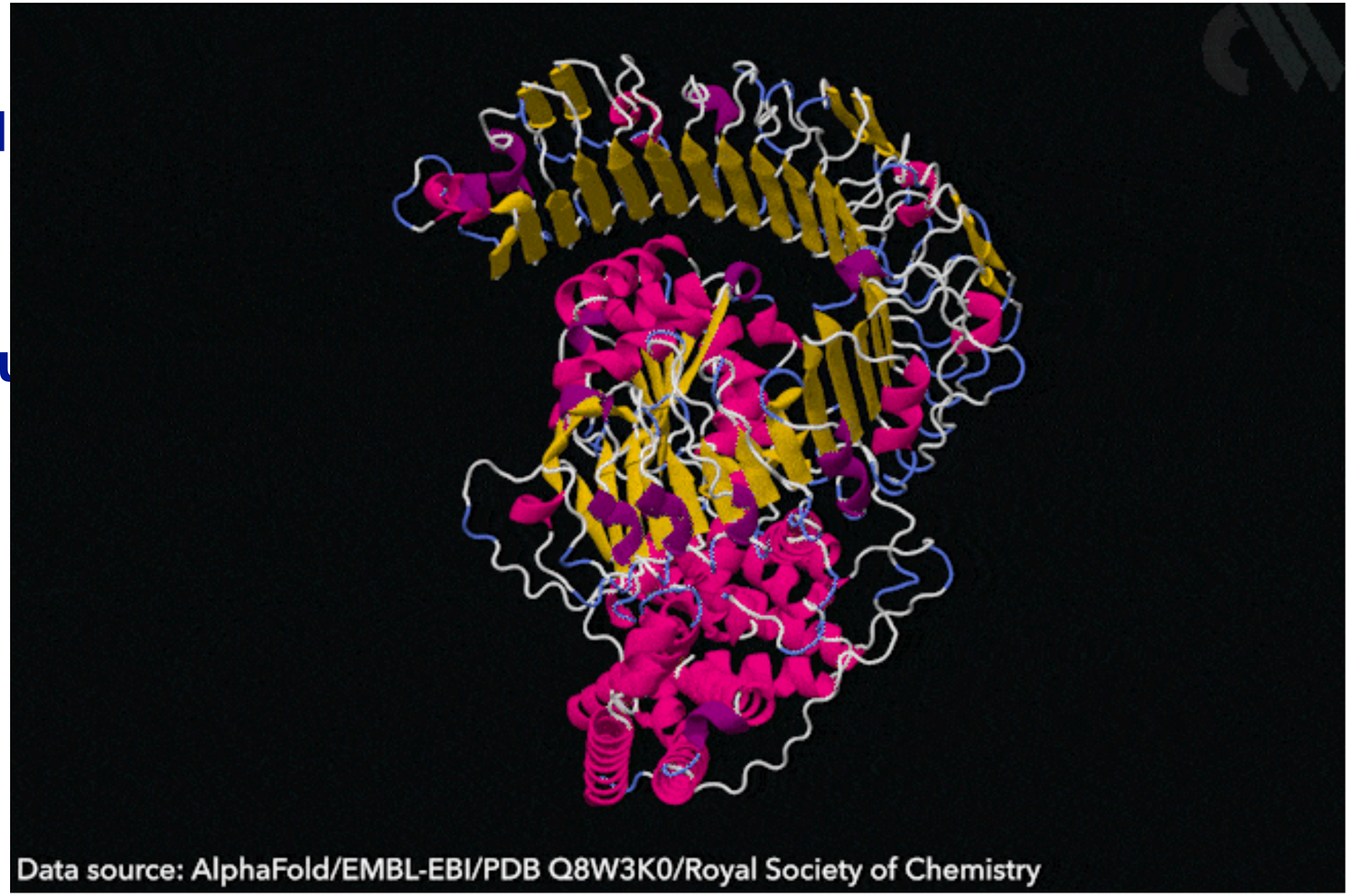
Determine the structu



Examples outside of astronomy:

Organisation of merchand

Determine the structu



Examples outside of astronomy:

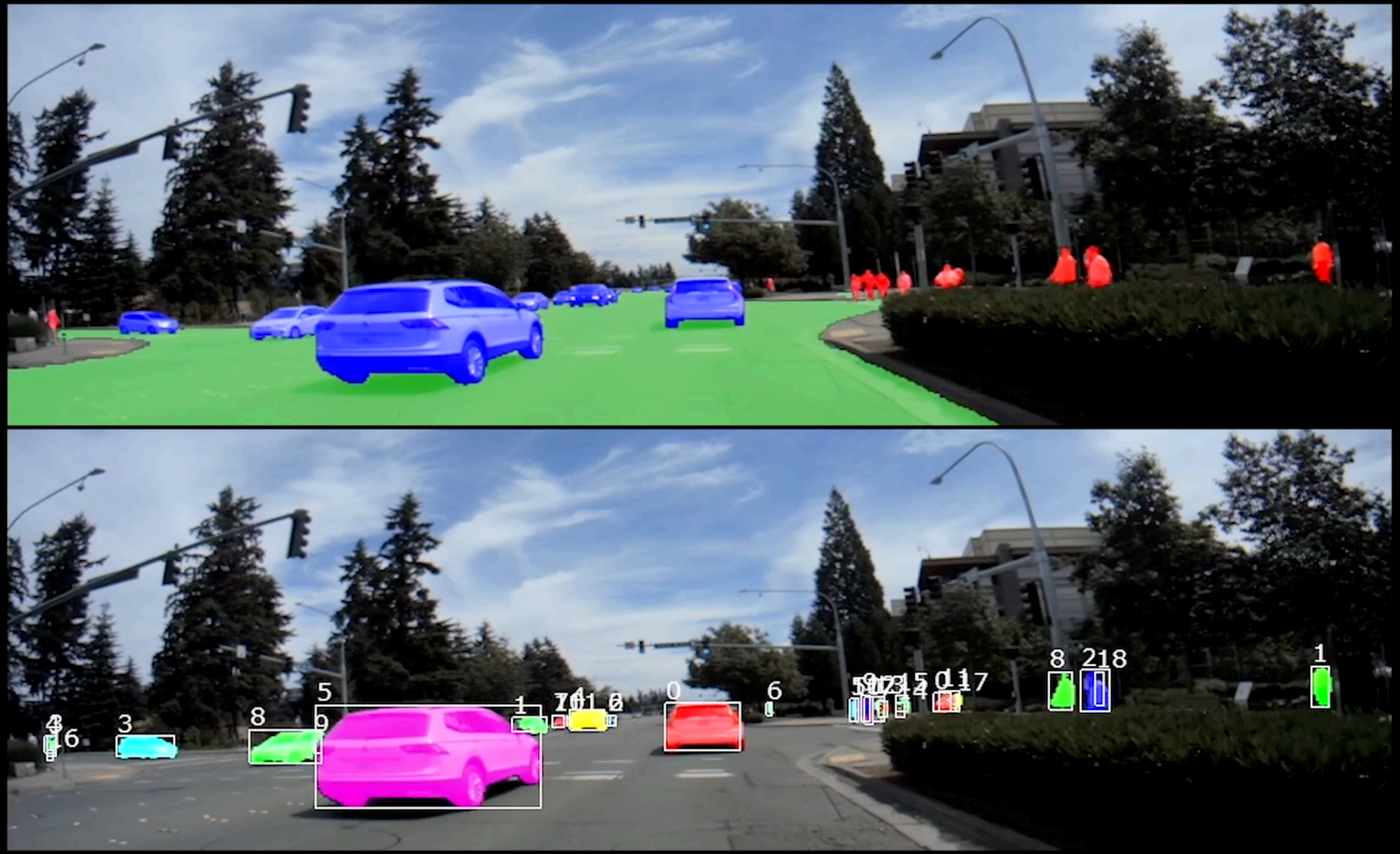
Identifying plant diseases

Train machines using the strategy of human experts - maybe they will outperform their teachers in the end (it happened for soy plants).

Examples outside of astronomy:

Self-driving cars

Deep learning used for visual identification


3
8
5
1
0
6
8
2
18
1

Examples inside astronomy:

Regression: Hubble's law, Tully-Fisher relation ++++

Clustering: Identifying asteroid classes from SDSS photometry

Hierarchical trees: Galaxy morphology classification, photometric redshifts

MCMC & friends: Most fields.

Density estimators: Most fields.

Support Vector Machines: Stellar classification

Gaussian process regression: Time-series, galaxy formation

Random trees: Photometric redshifts for galaxies

Principal Component Analysis: PSF estimation, post-starbursts, data reduction improvements +++

Self-organising maps: Photometric redshifts, Υ-ray source classification.

Neural nets: Photometric redshifts, stellar classification, galaxy morphology

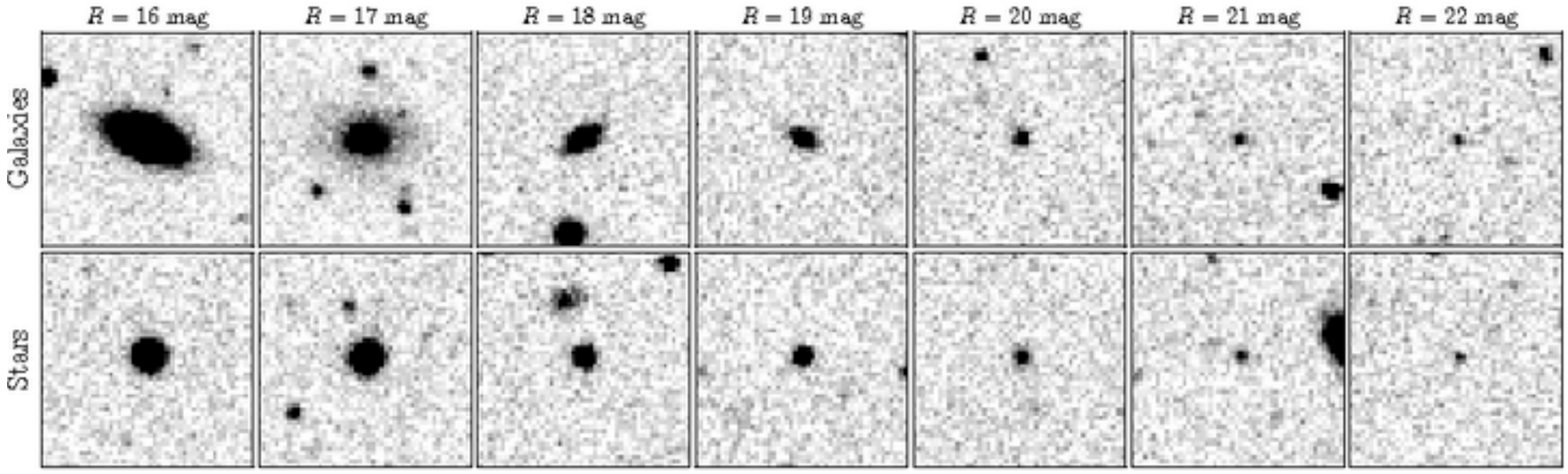
Deep neural nets: galaxy morphology, image generation, gravitational lens finders, classification of light-curves, ++

What is Machine learning?

What is machine learning (in this course)?

Thus machine learning can be a useful **tool** for astronomy and allows us to ask questions like:

- Is this blob of photons a galaxy or a star?

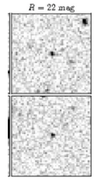


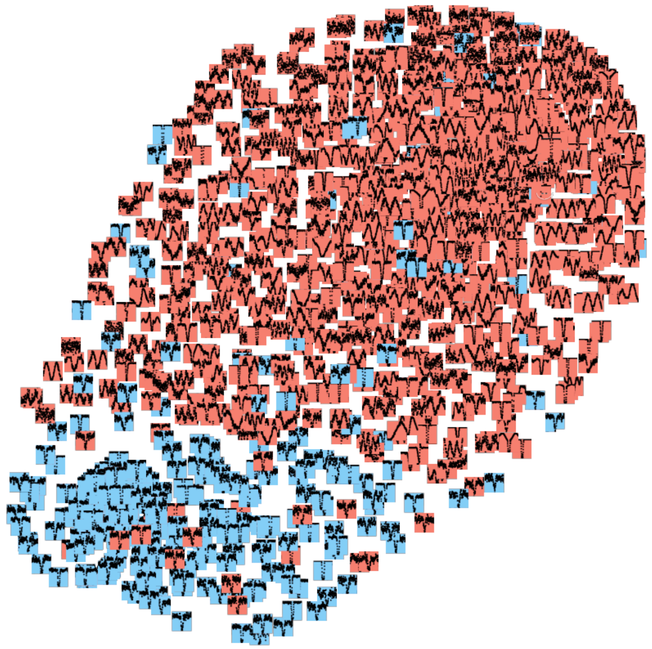
Miller et al (2017, arXiv:1703.07356)

What is machine learning (in this course)?

Thus machine learning can be a useful **tool** for astronomy and allows us to ask questions like:

- Is this blob of photons a galaxy or a star?
- Classify light curves from Kepler

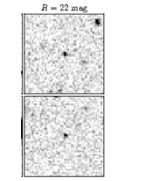


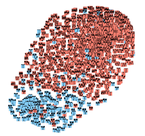


Shallue & Vanderburg (2018, AJ, 155)

What is machine learning (in this course)?

Thus machine learning can be a useful **tool** for astronomy and allows us to ask questions like:





- Is this blob of photons a galaxy or a star?
- Identify possible transiting exo-planets in Kepler light-curves
- What is the relationship between rotation velocity and luminosity in galaxies?
- How many classes of asteroids are there?
- etc etc.

What does it involve?

Data preparation

e.g.: Extract measurements from data
Check for quality/accuracy

What does it involve?

Data preparation

e.g.: Extract measurements from data
Check for quality/accuracy

Inject data into a database

Create the database structure.
Read data using X and insert into database using SQL.

Get data from database

What does it involve?

Data preparation

e.g.: Extract measurements from data
Check for quality/accuracy

Inject data into a database

Create the database structure.
Read data using X and insert into database using SQL.

Sometimes optional

Get data from database

What does it involve?

Data preparation

e.g.: Extract measurements from data
Check for quality/accuracy

Inject data into a database

Sometimes optional

Create the database structure.
Read data using X and insert into database using SQL.

Get data from database

Apply a machine learning technique

The main methods

- Classification
  - Given a set of images, say, that we know the morphology of, we want to be able to classify a large set of other objects. Other examples: Classification of stellar spectra with GAIA, classification of transient sources, variable source detection etc.
- Estimation/prediction
- Grouping/clustering
- Dimension reduction

The main methods

- Classification
- Estimation/prediction
  - You have X, Y, Z, ... and you want to predict a value A. An example would be if you are given a set of emission lines and you want to estimate the metal abundance in the gas. Most fitting methods fall into this category. Another area of interest is to estimate distributions from a few observations - the aim of kernel estimation techniques.
- Grouping/clustering
- Dimension reduction

The main methods

- Classification
- Estimation/prediction
- Grouping/clustering
  - This is used to find groups objects with similar properties. One example is to find different asteroid families from orbital information. Another might be to find galaxy clusters, or simply to find outliers/weirdoes.
- Dimension reduction

The main methods

- Classification
- Estimation/prediction
- Grouping/clustering
- Dimension reduction
  - It is much easier to handle & visualise low-dimensional data. Dimension reduction techniques allow you to go from multi-dimensional data, with 1000s of dimensions, to a manageable set of variables. This can be used for model fitting (e.g. principal components analysis) and for exploratory data visualisation.

The nomenclature of machine learning

Supervised vs unsupervised learning

In supervised learning significant information is provided with each training example.

The nomenclature of machine learning

Supervised vs unsupervised learning

In supervised learning significant information is provided with each training example.

Active versus Passive learning

An active learner interacts with the environment during training - we won’t use these.

The nomenclature of machine learning

Supervised vs unsupervised learning

In supervised learning significant information is provided with each training example.

Active versus Passive learning

An active learner interacts with the environment during training - we won't use these.

Normal, statistical and adversarial trainer/teacher

A normal "teacher" tries to provide helpful training samples. A statistical trainer uses what comes in (typical in astronomy), and an adversarial trainer tries to break the machine learning algorithm.

The nomenclature of machine learning

Supervised vs unsupervised learning

In supervised learning significant information is provided with each training example.

Active versus Passive learning

An active learner interacts with the environment during training - we won't use these.

Normal, statistical and adversarial trainer/teacher

A normal "teacher" tries to provide helpful training samples. A statistical trainer uses what comes in (typical in astronomy), and an adversarial trainer tries to break the machine learning algorithm.

Online and batch learning

An online learner will respond immediately when it starts receiving data, a batch learner will only respond after having a sufficient number of training examples.

The nomenclature of machine learning - a more formal approach

Input:

Domain set: a set, $\mathcal{X}$, of objects we might want to label. Each domain point will be represented by a vector of **features**. The domain points are also known as **instances** and the domain set as **instance space**.

Label set: a set, $\mathcal{Y}$, of possible labels for our sample, also called **predictors**.

Training data: A finite sequence of pairs in $\mathcal{X} \times \mathcal{Y}$:$S = \big((x_1, y_1) \ldots (x_m, y_m)\big)$

Output:

The learning algorithm is a map $h : \mathcal{X} \to \mathcal{Y}$, called a **predictor** or **classifier**. We may assume that there is true map $f(x)$ that h approximates.

Based on Shalev-Shwartz & Ben-David, “Understanding Machine Learning”

The nomenclature of machine learning - a more formal approach

Input:

The origin: training samples are drawn from some distribution, $\mathscr{D}$, which is *not known to the learning algorithm*. It is normally assumed that the training samples are fair samples from $\mathscr{D}$ - that may not be the case!

Error: the error of h relative to the true function f is known as the **true error** or sometimes the **generalisation error**. In real life we do not know f so we are usually focused on the **training error**, also known as the **empirical error**.

These are the foundations for a careful mathematical analysis of learning algorithms - we will not follow that here but the terms are still very relevant and frequently seen. If you want a more mathematical approach, “Understanding Machine Learning “ by Shalev-Shwarz & Ben-David is good.

Shalev-Shwartz & Ben-David, “Understanding Machine Learning”

Big data in astronomy

Why is this important?

Big surveys HENCE DATABASES

The last decades has seen a trend towards big surveys and massive theoretical calculations.
This will continue to produce vast amounts of data.

Large amounts of data HENCE STATISTICS

Large amounts of data offers a lot of potential but can be hard to work with/explore.
This means that we will need other tools to make optimal use of the new data.

Sharing of data and resources HENCE VO/GRID/CLOUD..

It is now essential to share your data to get the most out of them and to have the highest impact, and many surveys already plan how to do this. But distributed computing is also a thing - e.g. using Amazon's services for calculations.

This is all true for observational, experimental and theoretical data!

Some specific examples

- Data rates are increasing - astronomers today produce data at about ~few Tb/night integrated over all (optical) telescopes. But LSST expect produce ~15 Tb *per night*! [3 sq deg each 10-15 seconds]. How do you store/organise the data?

  Pre-processing & data bases!

- These large surveys produce large number of objects. (SDSS & 2MASS all contain > 100 million objects with perhaps 1000 attributes each, Gaia has ~2×10^9 sources). How do you check that all data are ok?

  Robust analysis, system engineering

- How do you analyse these kinds of data? To find the closest match using naïve search on 10^8 objects requires 10^{16} operations so correlation functions can be hard to calculate - and how do you find new relationships & events?

  Data mining/statistical methods/ clever algorithms

	# sources in Gaia DR3
Total number of sources	**1,811,709,771**
	Gaia Early Data Release 3
Number of sources with full astrometry	1,467,744,818
Number of 5-parameter sources	585,416,709
Number of 6-parameter sources	882,328,109
Number of 2-parameter sources	343,964,953
Gaia-CRF sources	1,614,173
Sources with mean G magnitude	1,806,254,432
Sources with mean G_{BP}-band photometry	1,542,033,472
Sources with mean G_{RP}-band photometry	1,554,997,939
	New in Gaia Data Release 3
Sources with radial velocities	33,812,183
Sources with mean G_{RVS}-band magnitudes	32,232,187
Sources with rotational velocities	3,524,677
Mean BP/RP spectra	219,197,643
Mean RVS spectra	999,645
Variable-source analysis	10,509,536
Variability types (supervised machine learning)	24
Supervised machine-learning classification for variables	9,976,881
Specific Object Studies – Cepheids	15,021
Specific Object Studies – Compact companions	6,306
Specific Object Studies – Eclipsing binaries	2,184,477
Specific Object Studies – Long-period variables	1,720,588
Specific Object Studies – Microlensing events	363
Specific Object Studies – Planetary transits	214
Specific Object Studies – RR Lyrae stars	271,779
Specific Object Studies – Short-timescale variables	471,679
Specific Object Studies – Solar-like rotational modulation variables	474,026

Specific Object Studies – Eclipsing binaries	2,184,477
Specific Object Studies – Long-period variables	1,720,588
Specific Object Studies – Microlensing events	363
Specific Object Studies – Planetary transits	214
Specific Object Studies – RR Lyrae stars	271,779
Specific Object Studies – Short-timescale variables	471,679
Specific Object Studies – Solar-like rotational modulation variables	474,026
Specific Object Studies – Upper-main-sequence oscillators	54,476
Specific Object Studies – Active galactic nuclei	872,228
Photometrically-variable sources with radial-velocity time series	1,898
Sources with object classifications	1,590,760,469
Stars with emission-line classifications	57,511
Sources with astrophysical parameters from BP/RP spectra	470,759,263
Sources with astrophysical parameters assuming an unresolved binary	348,711,151
Sources with spectral types	217,982,837
Sources with evolutionary parameters (mass and age)	128,611,111
Hot stars with spectroscopic parameters	2,382,015
Ultra-cool stars	94,158
Cool stars with activity index	1,349,499
Sources with H-alpha emission measurements	235,384,119
Sources with astrophysical parameters from RVS spectra	5,591,594
Sources with chemical abundances from RVS spectra (up to 13 species)	2,513,593
Sources with a diffuse interstellar band (DIB) in their RVS spectrum	472,584
Non-single stars (astrometric, spectroscopic, eclipsing, orbits, trends)	813,687
Non-single stars - orbital astrometric solutions	169,227
Non-single stars - orbital spectroscopic solutions (SB1 / SB2)	186,905
Non-single stars - eclipsing binaries	87,073
QSO candidates	6,649,162
QSO candidates - redshifts	6,375,063
QSO candidates - host galaxy detected	64,498
QSO candidates - host galaxy surface brightness profiles	15,867

Some numbers...

#Galaxies: 10^5 galaxies per square degree when going to m_I=25.5
(for every two magnitudes deeper you detect an order of magnitude more objects)

#Galaxies: 20,000 deg^2 "extragalactic sky" ⇒ ~10^9 sources

#Stars: $10^{5\text{-}6}$ stars per square degree per magnitude at low galactic latitudes

#Imaging data:

$$N_{\rm pix} = 1.44 \times 10^8 \left(\frac{\theta}{0.3"}\right)^2 \left(\frac{A}{1{\rm deg}^2}\right) \ {\rm pixels}$$

CFHT MegaCam: 36 CCDs with 2048 x 4612 pixels (340 megapixels)
~720 Mb per file for ~ 18000 pixels on the side (expanding to 1.4 Gb when converted to float...)

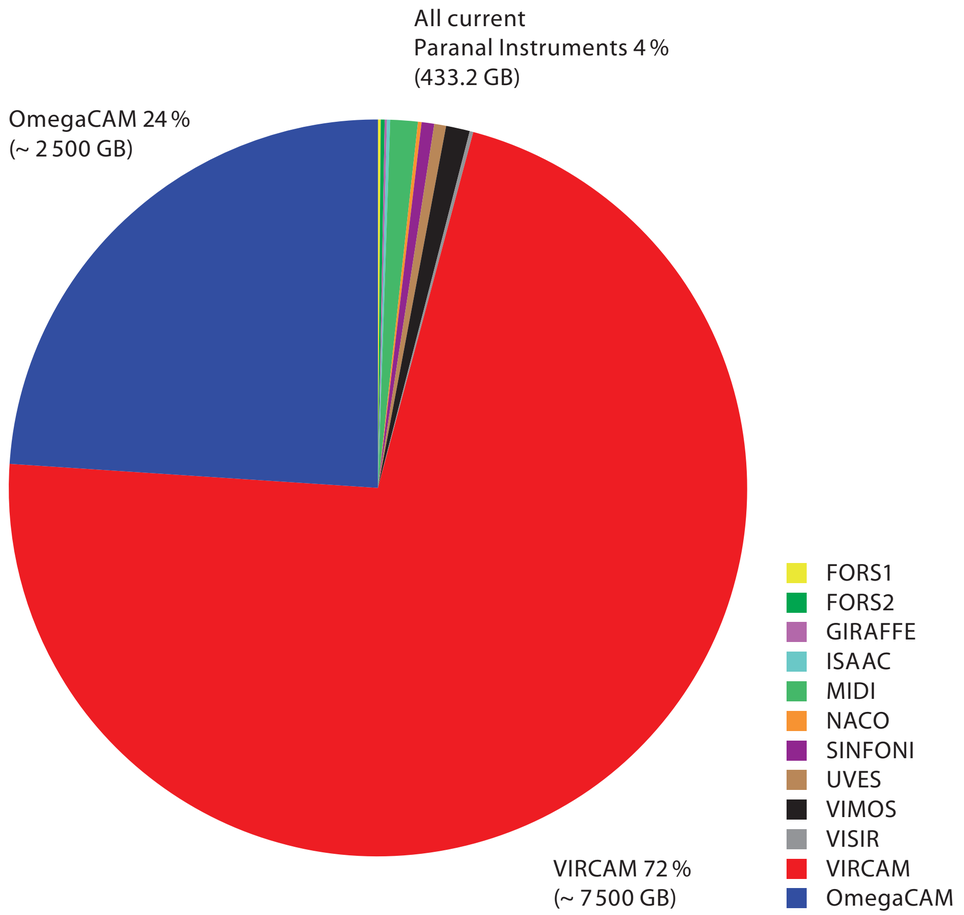
That is for one filter and one exposure - we normally need 4-5 filters and multiple exposures.

#Gaia: ~10^{21}-10^{22} Flops needed, future missions even more

Recall:
#seconds per year ~ 3x10^7
(top computers ~ 10^{15} Flops)

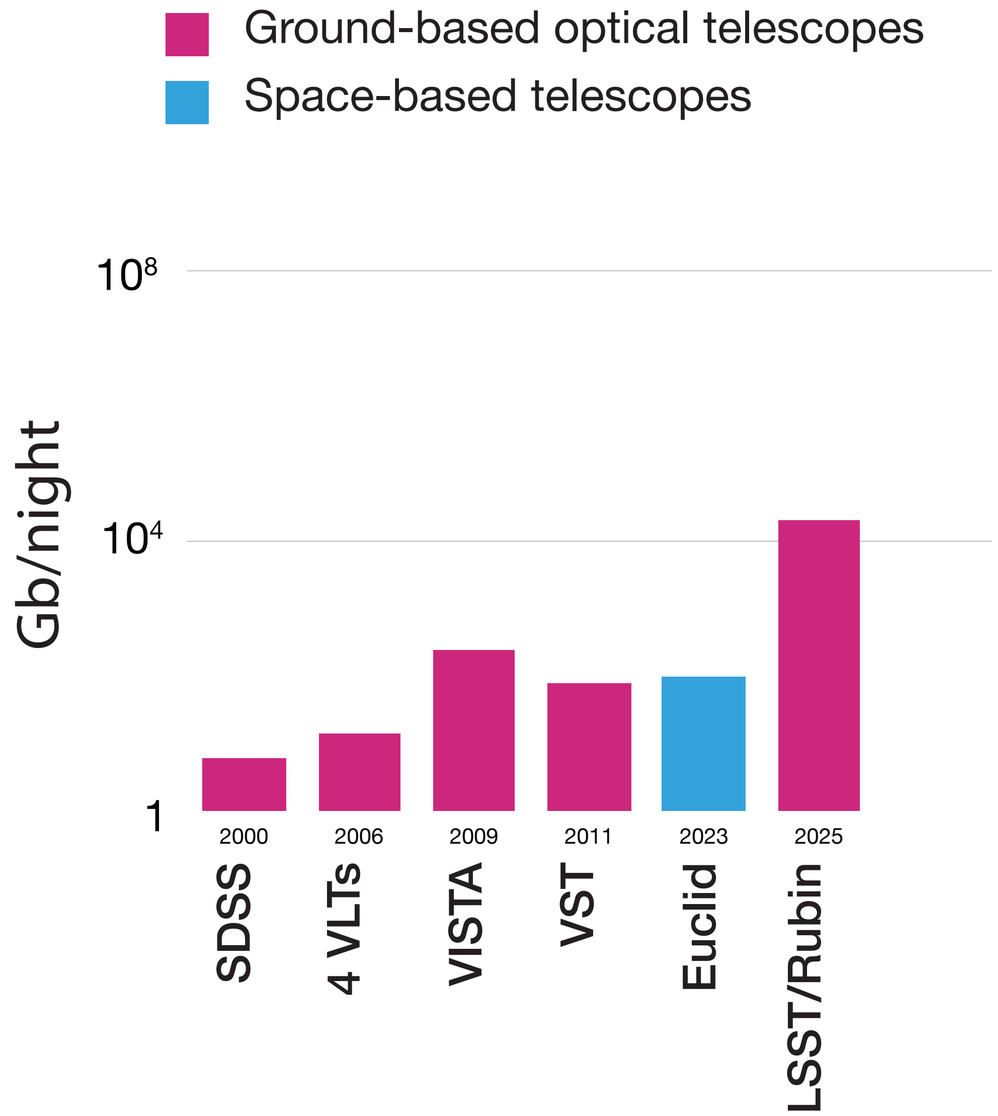
The ESO pie - or the changing world

The way the science changed over the last decade - and will continue to do so in the foreseeable future.



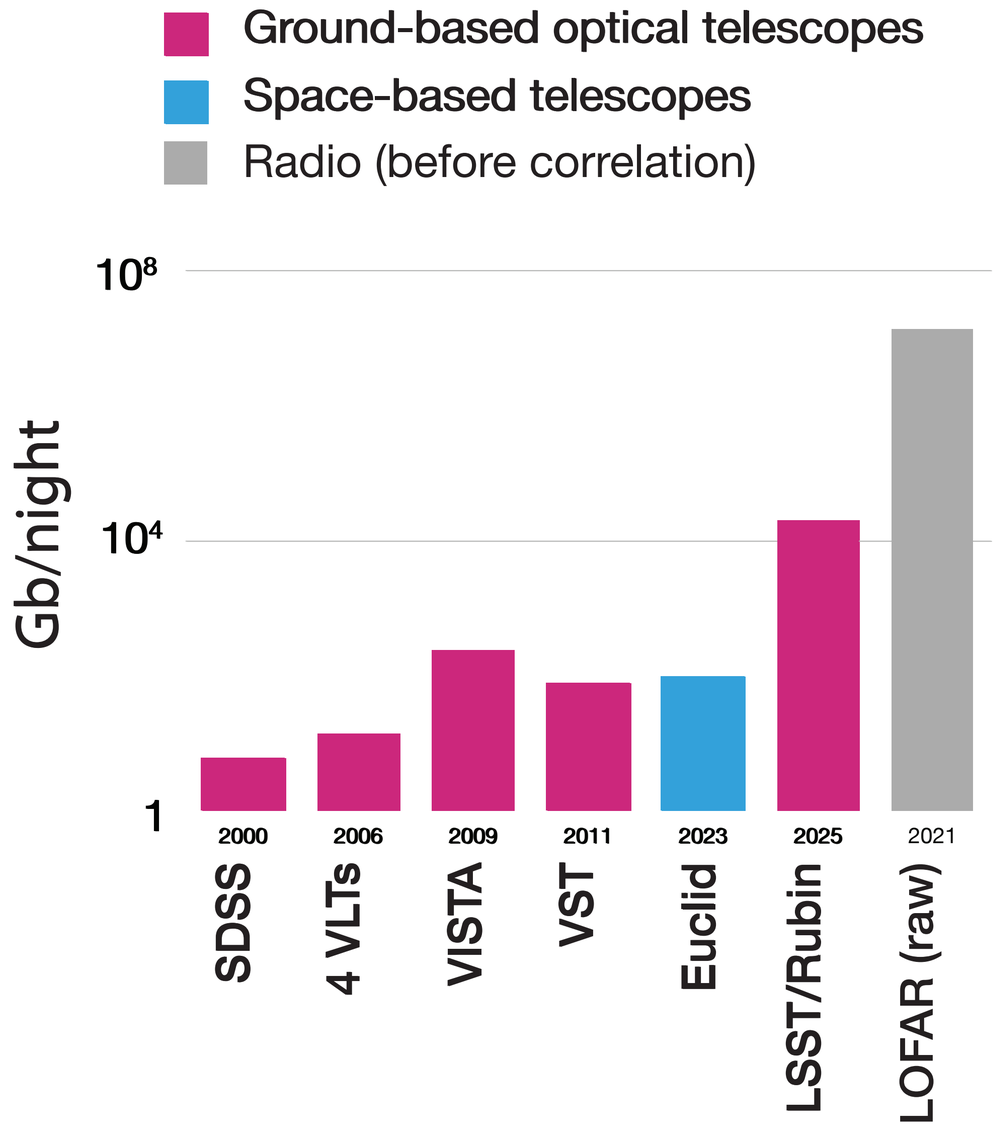
Arnaboldi et al (2007)

Data rates per night



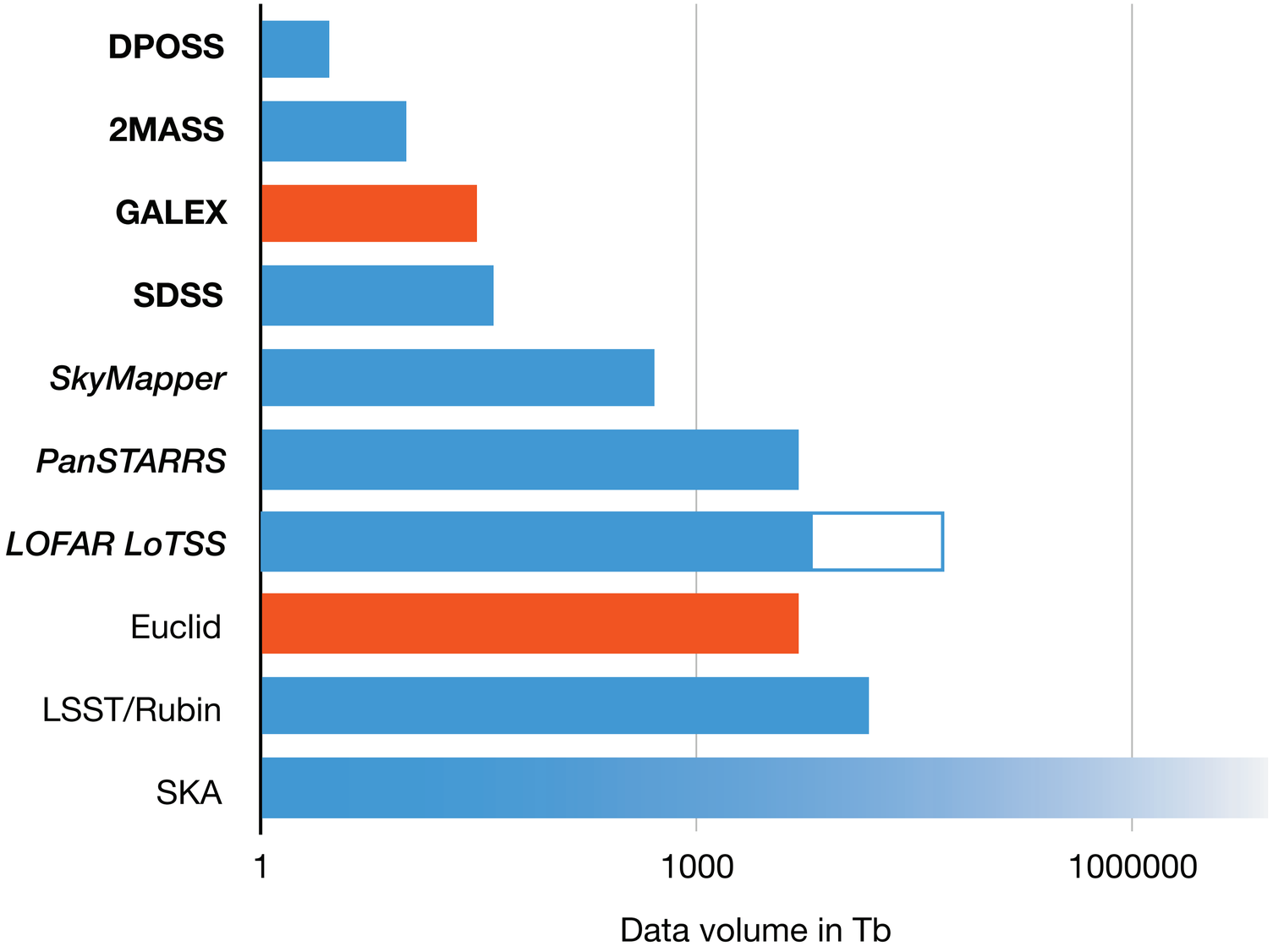
Data rates in future optical/ near-IR telescopes can easily reach 10s of Tbs per day - radio telescopes much more.

Data rates per night



Data rates in future optical/ near-IR telescopes can easily reach 10s of Tbs per day - radio telescopes much more.

Astronomy as big data



Astronomy has long been a big data science. It is not expected to change - but remember that “small data” can lead to big science!

Note the logarithmic scale!

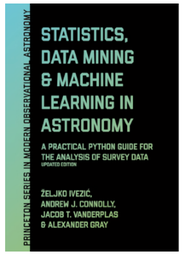
Various sources, including Zhang & Zhao (2015, Data Science Journal, 14, p11)

Plan for the course

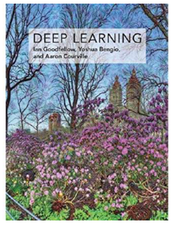
- 1. Managing data, simple regression and model choice
  - Covering git and SQL
  - Introducing machine learning through regression techniques.
  - Cross-validation
- 2. Visualisation and inference methods
  - Visualisation of data, do's and don't's
  - Classical inference
  - Bayesian inference
  - MCMC
- 3. Density estimation and classification
  - Estimating densities, parametric & non-parametric
  - Bias-variance trade-off
  - Classification
- 4. Dimensional reduction
  - Standardising data.
  - Principal Component Analysis
  - Manifold learning
- 5. Ensemble methods, neural networks, deep learning
  - Local regression methods
  - Random forests and other boosting methods
  - Neural networks & deep learning

Literature

No obligatory book, but I will roughly follow:

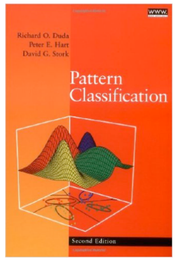


Statistics, Data Mining, and Machine Learning in Astronomy - *Ivezic, Connolly, VanderPlas & Gray*

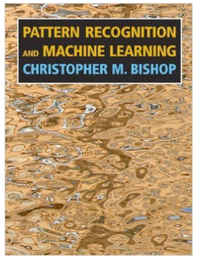


with some inspiration from:
Deep Learning - *Goodfellow, Bengio & Courville*

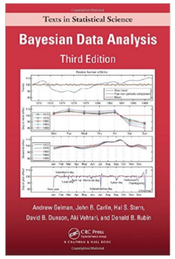
Other useful books among many others:



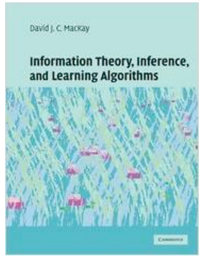
Pattern Classification - *Duda, Hart & Stork*



Pattern Recognition and Machine Learning - *Bishop*

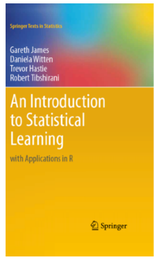


Bayesian Data Analysis - *Gelman*



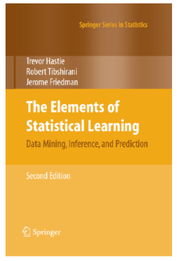
Information Theory, Inference and Learning Algorithms - *MacKay*

Online



Introduction to Statistical Learning - *James et al*

Online



Elements of Statistical Learning - *Hastie et al*

Online

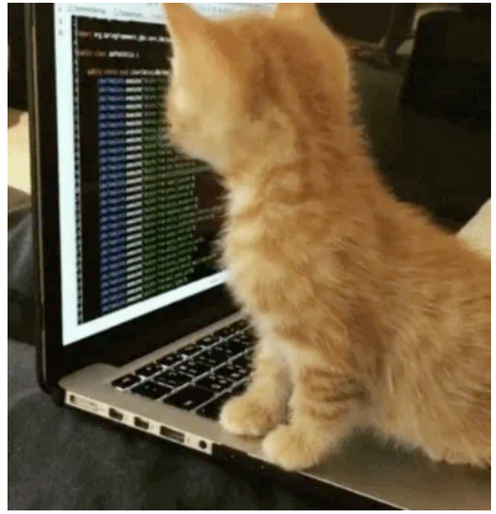
Language choice

In this course we will use **Python** and in particular the scikit-learn (sklearn) toolkit for machine learning. (and **SQL**)

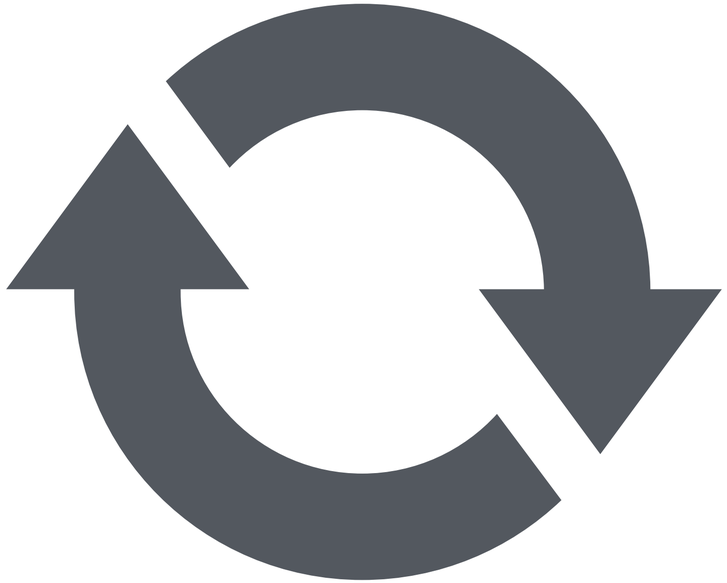
Other languages are widely used in machine learning and you could easily come across:

- **R**. The statistical computing language is very widely used and many new algorithms are implemented in R first. Well worth learning.
- **C/C++**. Often required for speed. Many frameworks are written in these languages (e.g. Torch, TensorFlow)
- **Java**. Influential deep learning frameworks like Deeplearning4j are coded in Java and it is a popular deployment platform.
- **Matlab**. A traditional choice for algorithm development thus you might come across Matlab code that does exactly what you want.
- **Julia**. A scientific programming language, ~as fast as C but simple like Python. At the moment a niche language but might expand.

Practical functioning:

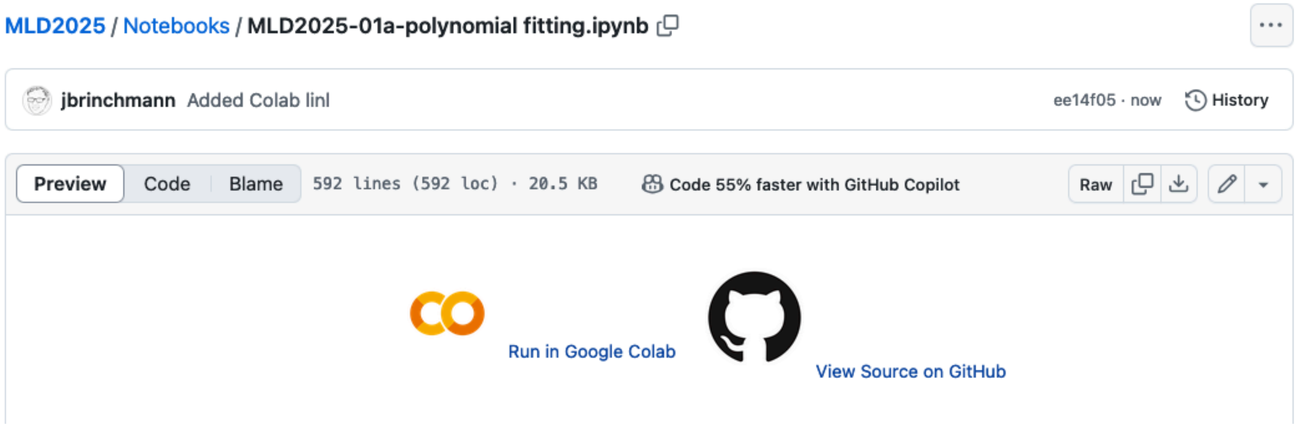


Lecture introducing a concept



Move to Google Colab to explore

Google Colab?



Google Colaboratory is a convenient way to run python notebooks without having to install packages on your computer. To use it you need a Google account and then go to the notebook in Github, and click on the 'Run in Google Colab' icon on the top to run in Colab (this also works if you have downloaded the notebook).

If you do not have a Google account or do not want to use Google Colab, you can also follow the instructions in the README for the course and clone the Github repository and run the notebook locally - that works just as well!

Practicalities- working in data science

An excellent start:

“How to set up your first machine learning project in astronomy”

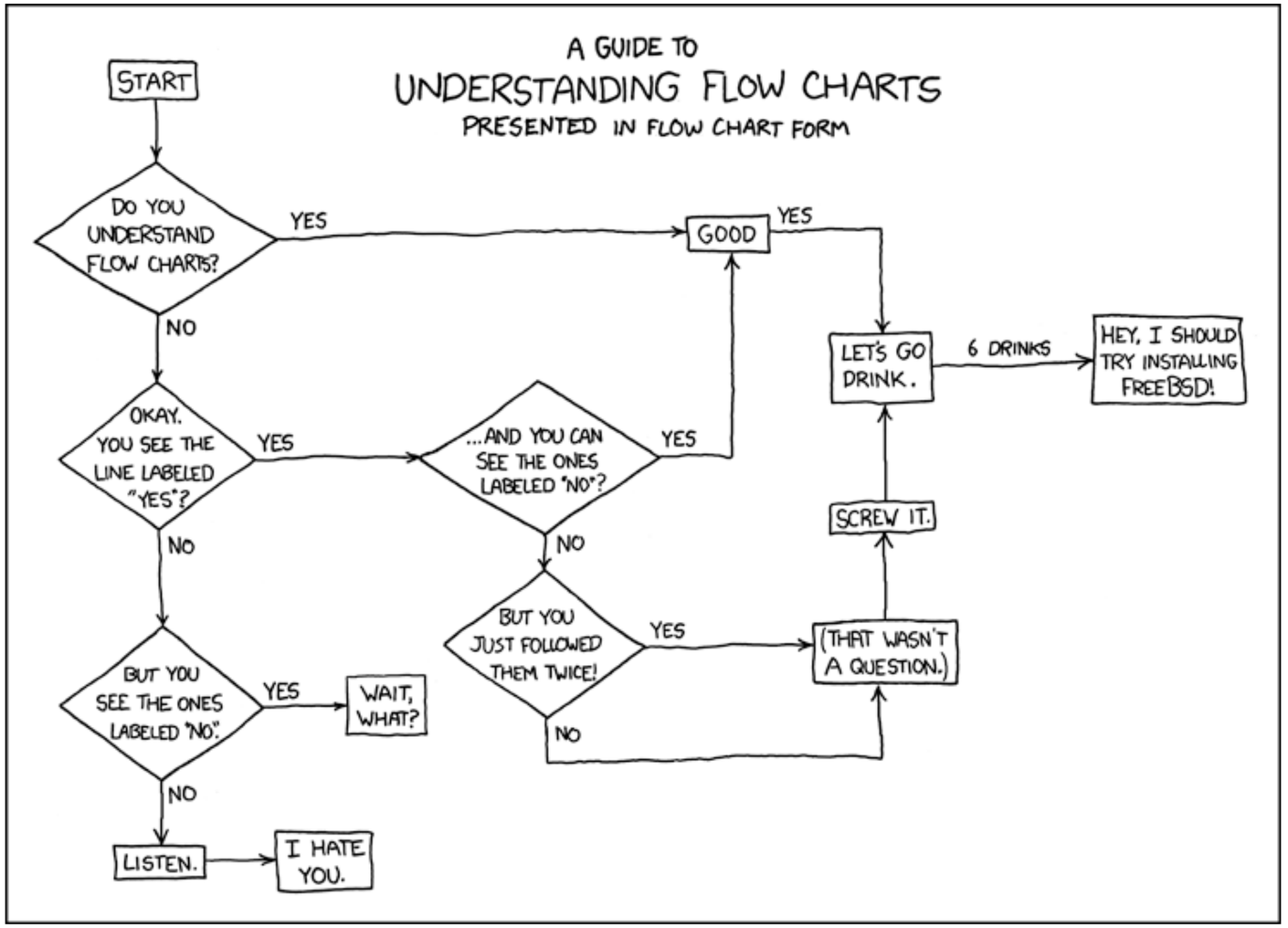
Buchner & Fotopoulou, Nature Reviews Physics
volume 6, pages 535–545 (2024)

Online access:

https://tinyurl.com/4tem2dpx

Good enough practices in scientific computing

Wilson et al (2017) - https://doi.org/10.1371/journal.pcbi.1005510



https://xkcd.com/518/

Good enough practices in scientific computing

The topics of their paper:

Wilson et al (2017) - https://doi.org/10.1371/journal.pcbi.1005510

Good enough practices in scientific computing

The topics of their paper:

- Data management: saving both raw and intermediate forms, documenting all steps, creating tidy data amenable to analysis.

Wilson et al (2017) - https://doi.org/10.1371/journal.pcbi.1005510

Good enough practices in scientific computing

The topics of their paper:

- Data management: saving both raw and intermediate forms, documenting all steps, creating tidy data amenable to analysis.
- Software: writing, organizing, and sharing scripts and programs used in an analysis.

Wilson et al (2017) - https://doi.org/10.1371/journal.pcbi.1005510

Good enough practices in scientific computing

The topics of their paper:

- Data management: saving both raw and intermediate forms, documenting all steps, creating tidy data amenable to analysis.
- Software: writing, organizing, and sharing scripts and programs used in an analysis.
- Collaboration: making it easy for existing and new collaborators to understand and contribute to a project.

Wilson et al (2017) - https://doi.org/10.1371/journal.pcbi.1005510

Good enough practices in scientific computing

The topics of their paper:

- Data management: saving both raw and intermediate forms, documenting all steps, creating tidy data amenable to analysis.
- Software: writing, organizing, and sharing scripts and programs used in an analysis.
- Collaboration: making it easy for existing and new collaborators to understand and contribute to a project.
- Project organization: organizing the digital artifacts of a project to ease discovery and understanding.

Wilson et al (2017) - https://doi.org/10.1371/journal.pcbi.1005510

Good enough practices in scientific computing

The topics of their paper:

- Data management: saving both raw and intermediate forms, documenting all steps, creating tidy data amenable to analysis.
- Software: writing, organizing, and sharing scripts and programs used in an analysis.
- Collaboration: making it easy for existing and new collaborators to understand and contribute to a project.
- Project organization: organizing the digital artifacts of a project to ease discovery and understanding.
- Tracking changes: recording how various components of your project change over time.

Wilson et al (2017) - https://doi.org/10.1371/journal.pcbi.1005510

Good enough practices in scientific computing

The topics of their paper:

- Data management: saving both raw and intermediate forms, documenting all steps, creating tidy data amenable to analysis.
- Software: writing, organizing, and sharing scripts and programs used in an analysis.
- Collaboration: making it easy for existing and new collaborators to understand and contribute to a project.
- Project organization: organizing the digital artifacts of a project to ease discovery and understanding.
- Tracking changes: recording how various components of your project change over time.
- Manuscripts: writing manuscripts in a way that leaves an audit trail and minimizes manual merging of conflicts

Wilson et al (2017) - https://doi.org/10.1371/journal.pcbi.1005510

Data management

- ✓Save the raw data.
- ✓Ensure that raw data are backed up in more than one location.
- ✓Create the data you wish to see in the world.
- ✓Create analysis-friendly data.
- ✓Record all the steps used to process data.
- ✓Anticipate the need to use multiple tables, and use a unique identifier for every record.
- ✓Submit data to a reputable DOI-issuing repository so that others can access and cite it.

Wilson et al (2017) - https://doi.org/10.1371/journal.pcbi.1005510

Data management

- ✓Save the raw data.
- ✓Ensure that raw data are backed up in more than one location.
- ✓Create the data you wish to see in the world.
- ✓Create analysis-friendly data.
- ✓Record all the steps used to process data.
- ✓Anticipate the need to use multiple tables, and use a unique identifier for every record.
- ✓Submit data to a reputable DOI-issuing repository so that others can access and cite it.

Backup & storage

Wilson et al (2017) - https://doi.org/10.1371/journal.pcbi.1005510

Data management

- ✓Save the raw data.
- ✓Ensure that raw data are backed up in more than one location.
- ✓Create the data you wish to see in the world.
- ✓Create analysis-friendly data.
- ✓Record all the steps used to process data.
- ✓Anticipate the need to use multiple tables, and use a unique identifier for every record.
- ✓Submit data to a reputable DOI-issuing repository so that others can access and cite it.

Backup & storage

Data reduction,
Data organisation

Wilson et al (2017) - https://doi.org/10.1371/journal.pcbi.1005510

Data management

- ✓Save the raw data.
- ✓Ensure that raw data are backed up in more than one location.
- ✓Create the data you wish to see in the world.
- ✓Create analysis-friendly data.
- ✓Record all the steps used to process data.
- ✓Anticipate the need to use multiple tables, and use a unique identifier for every record.
- ✓Submit data to a reputable DOI-issuing repository so that others can access and cite it.

Backup & storage

Data reduction,
Data organisation

Think about your data in advance and plan for sharing with the world.

Wilson et al (2017) - https://doi.org/10.1371/journal.pcbi.1005510

Project organisation

- ✓Put each project in its own directory, which is named after the project.
- ✓Put text documents associated with the project in the doc directory.
- ✓Put raw data and metadata in a data directory and files generated during cleanup and analysis in a results directory.
- ✓Put project source code in the src directory.
- ✓Put external scripts or compiled programs in the bin directory.
- ✓Name all files to reflect their content or function.

Probably the most “personal” of recommendations - a good idea to follow but not the only way to do it!

Wilson et al (2017) - https://doi.org/10.1371/journal.pcbi.1005510

Keeping track of changes

- ✓Back up (almost) everything created by a human being as soon as it is created.
- ✓Keep changes small.
- ✓Share changes frequently.
- ✓Create, maintain, and use a checklist for saving and sharing changes to the project.
- ✓Store each project in a folder that is mirrored off the researcher's working machine.
- ✓Add a file called CHANGELOG.txt to the project's docs subfolder.
- ✓Copy the entire project whenever a significant change has been made.
- ✓Use a version control system.

Prone to errors

← Use this!

Wilson et al (2017) - https://doi.org/10.1371/journal.pcbi.1005510

Version control using git

Managing your work - version control

When you carry out a complex task, you are advised to use a version control (VC) system. We will use **git**.

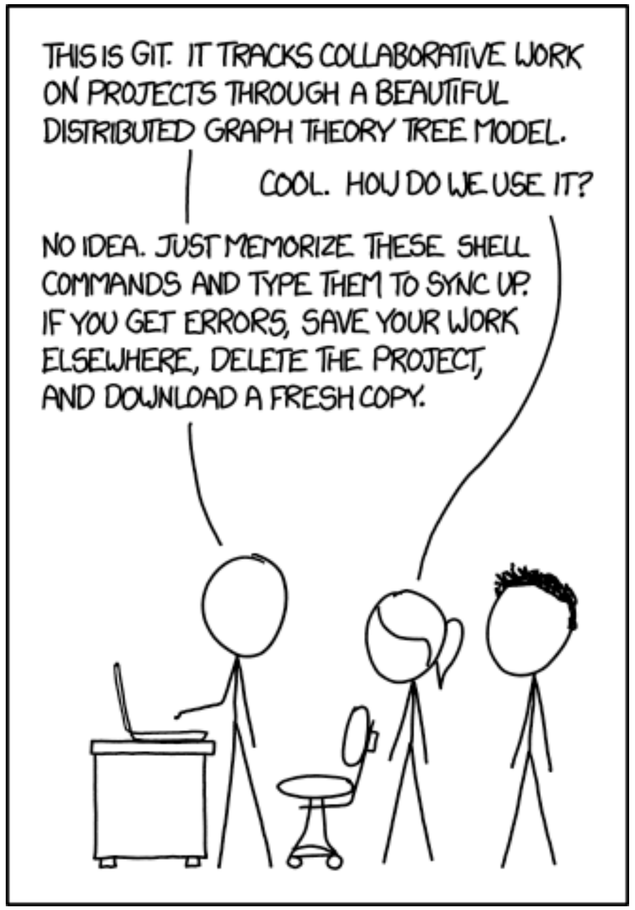
A VC helps keep track of changes made to your documents/code/ whatever and allows you to branch out to try something new.

There are multiple possible ways to use git - local repositories and online repositories. Here we will use an online repository: github [github.com]

(there are many others, e.g. bitbucket.org)

Added benefit: important inside & outside academia!

But really - why should I bother?



- ✓Keeps track of your work.
- ✓The history allows you to check what you changed x days ago.
- ✓Adds structure to your work.
- ✓Simplifies collaboration on code.
- ✓Simplifies sharing of code with the world.
- ✓Keeps a backup of your code!
- ✓Allows you to implement new features while not breaking a released code (‘branching’)

A bird's eye view of how we use VCs

I need to implement a new function in my code

1. Check if there have been updates to the code (if I work with someone else) — `git status` `git pull`

2. Implement all or parts of the new functionality. Save.

3. Add the changed file to a list of changes (git keeps track of what you changed) — `git add`

4. Commit the modification with a small note to say what you have done — `git commit`

5. Send it all away — `git push`

Making a local repository

Create a working directory where your project will live, and go into it

```
> mkdir Project

> cd Project
```

Initialise a git repository:

```
> git init
```

Put a file in the repository - this is the simplest way

```
> touch README
```

And check the status

```
> git status
```

Making a local repository - still!

```
> git status
On branch master

Initial commit

Untracked files:
  (use "git add <file>..." to include in what will be committed)

   README

nothing added to commit but untracked files present (use "git add" to
track)
```

Making a local repository - still!

Add the files

```
> git add README
```

Commit the changes

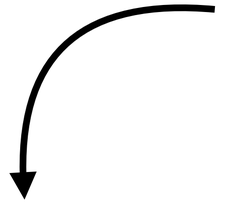
```
> git commit -m “First commit”
```

Making a local repository - still!

Add the files

```
> git add README
```

Comments! Important!



Commit the changes

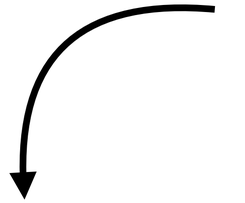
```
> git commit -m “First commit”
```

Making a local repository - still!

Add the files

```
> git add README
```

Comments! Important!



Commit the changes

```
> git commit -m “First commit”
```

---

moving files

```
> git mv <oldfile> <newfile>
```

Oops, get the old version of the file

```
> git checkout --  filename
```

More: https://www.codementor.io/citizen428/git-tutorial-10-common-git-problems-and-how-to-fix-them-aajv0katd

Using git - checking out a project

You need to know the address of the project:

```
https://github.com/jbrinchmann/MyRepo1.git
```

Then you check it out:

```
git clone https://github.com/jbrinchmann/MyRepo1.git
```

You now have this repository in the MyRepo1 directory

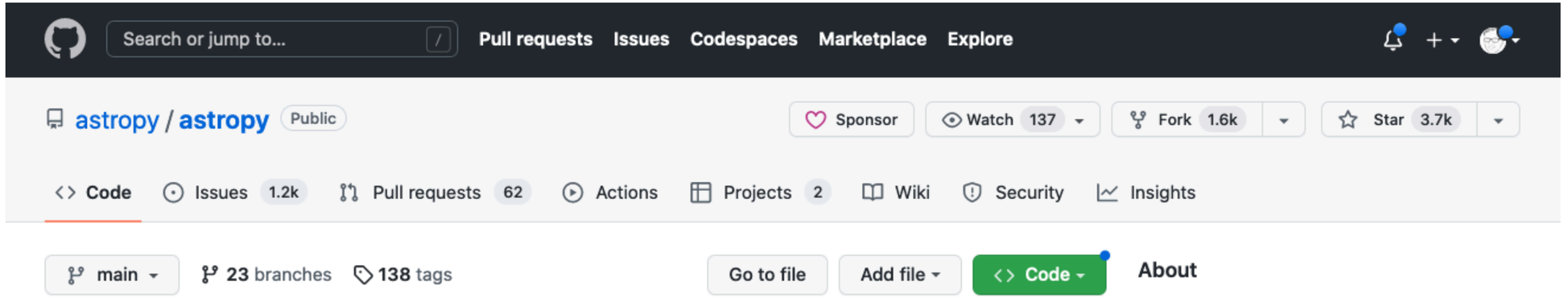
To get a new version (if someone has changed something) - go into the MyRepo1 directory and type:

```
git pull
```

Using git - forking a project

Sometimes you want to modify a project owned by someone else

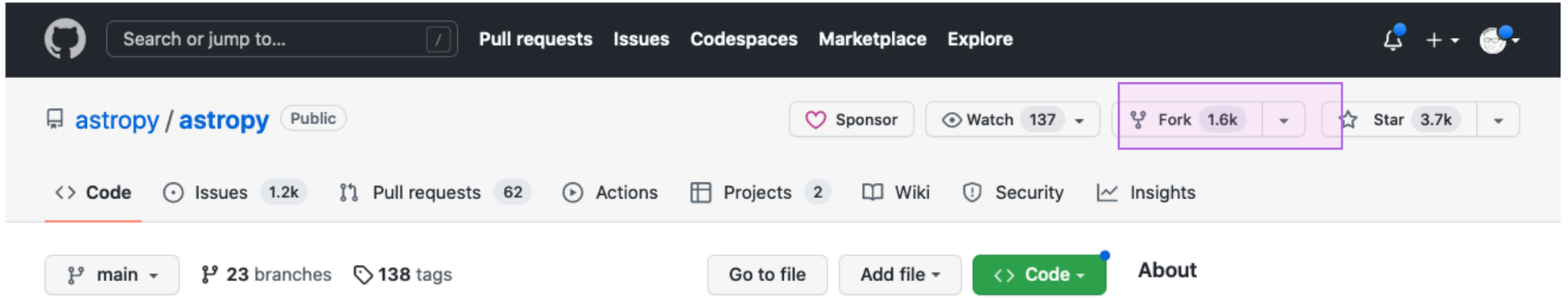
For that you want to **fork** a project - we do this usually in the Github or Bitbucket interface.



Using git - forking a project

Sometimes you want to modify a project owned by someone else

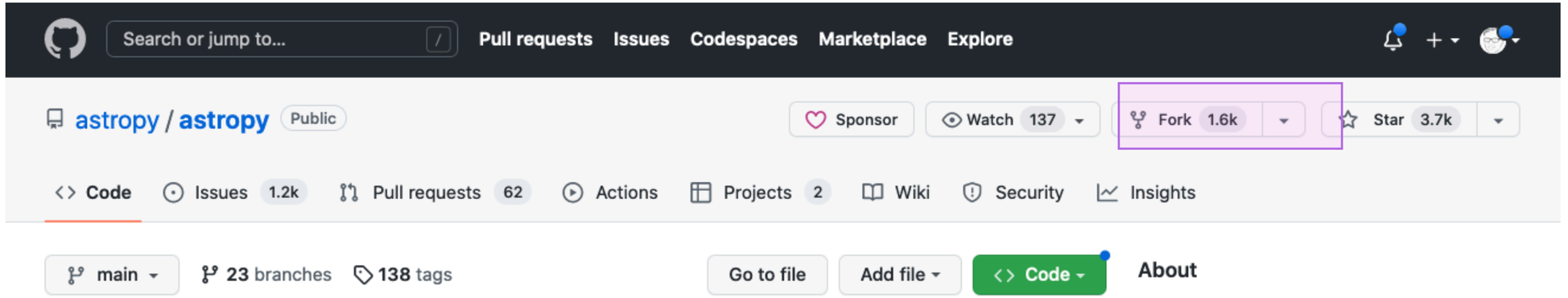
For that you want to **fork** a project - we do this usually in the Github or Bitbucket interface.



Using git - forking a project

Sometimes you want to modify a project owned by someone else

For that you want to **fork** a project - we do this usually in the Github or Bitbucket interface.



This is also usually what we do when we want to **contribute to a project** that we are not involved - we fork it, make modifications, and send **a pull request** to the original project.

We do not need that here in this course.

git - workflow with GitHub

Make GitHub repository	`https://github.com/<your username>`
Check it out	`git clone <address>`
Edit a file on your computer	`git add square.py` add the file if new
Commit your changes	`git commit -m “Fixed exponent bug”`
Push the changes to the repository	`git push`

Another reason for using it:

You need it for the course, **well, kinda**

For you to do:

Check the repository at
https://github.com/jbrinchmann/MLD2025

Here you will find a small document with math/statistics reminders which I expect you to have read!

I will also place some problems that we will work with in the practical session, on this site.

Ingredients of machine learning

Key ingredients of machine learning

Examples:

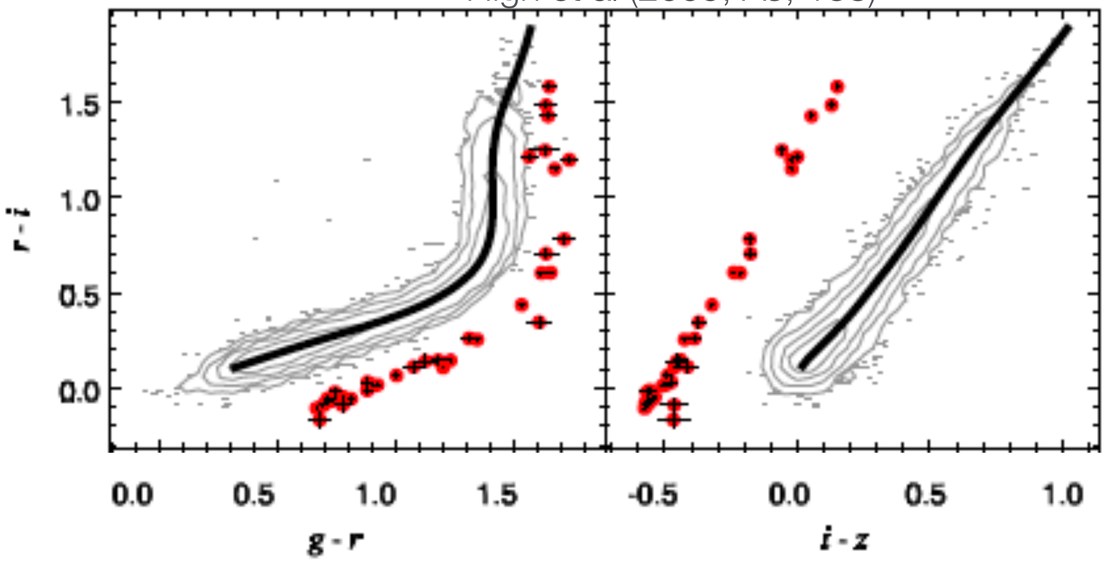
A machine learning method cannot “learn” unless it is provided with examples. These are composed of **features**.

Key ingredients of machine learning

Examples:

A machine learning method cannot “learn” unless it is provided with examples. These are composed of **features**.

High et al (2009, AJ, 138)

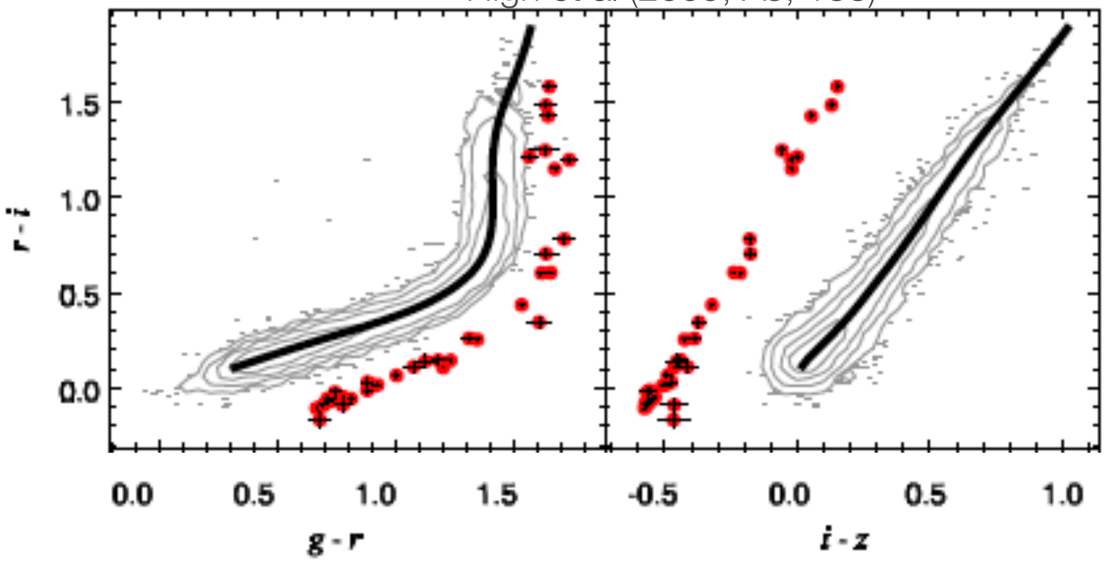


Key ingredients of machine learning

Examples:

A machine learning method cannot “learn” unless it is provided with examples. These are composed of **features**.

High et al (2009, AJ, 138)



Features: g-r, r-i, i-z
Example: [g-r, r-i, i-z]

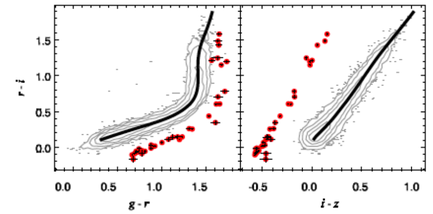
Key ingredients of machine learning

amples:

A machine learning method cannot “learn” unless it is provided with examples. These are composed of **features**.

High et al (2009, AJ, 138)

Features: g-r, r-i, i-z
Example: [g-r, r-i, i-z]



Often summarised in a **design matrix**. Here each example makes up one row - e.g. for 4 points:

$$\begin{pmatrix} g_1 - r_1 & r_1 - i_1 & i_1 - z_1 \\ g_2 - r_2 & r_2 - i_2 & i_2 - z_2 \\ g_3 - r_3 & r_3 - i_3 & i_3 - z_3 \\ g_4 - r_4 & r_4 - i_4 & i_4 - z_4 \end{pmatrix}$$

Key ingredients of machine learning

Accuracy/error-rate

How well is our algorithm doing? A common measure - the mean squared error:

$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y - y_{\mathrm{pred}})^2$$

Key ingredients of machine learning

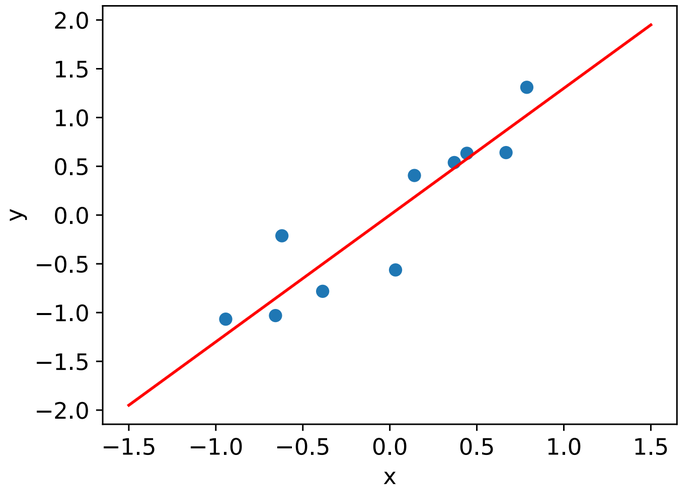
Accuracy/error-rate

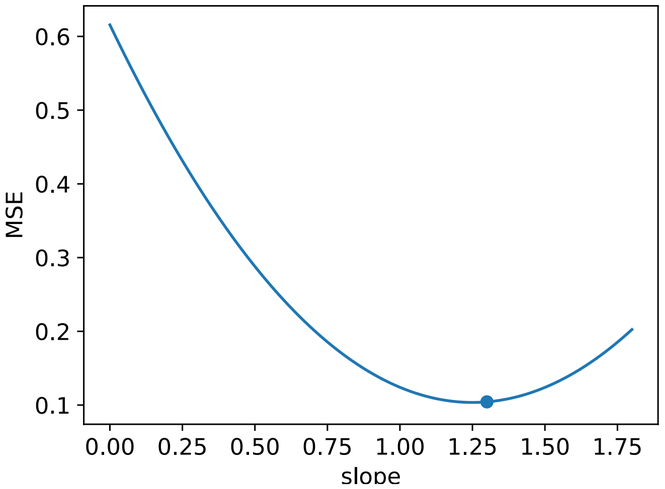
How well is our algorithm doing? A common measure - the mean squared error:

$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y - y_{\mathrm{pred}})^2$$

Try this on linear regression

$$y = \mathrm{slope} \times x$$





Let’s switch to Colab!

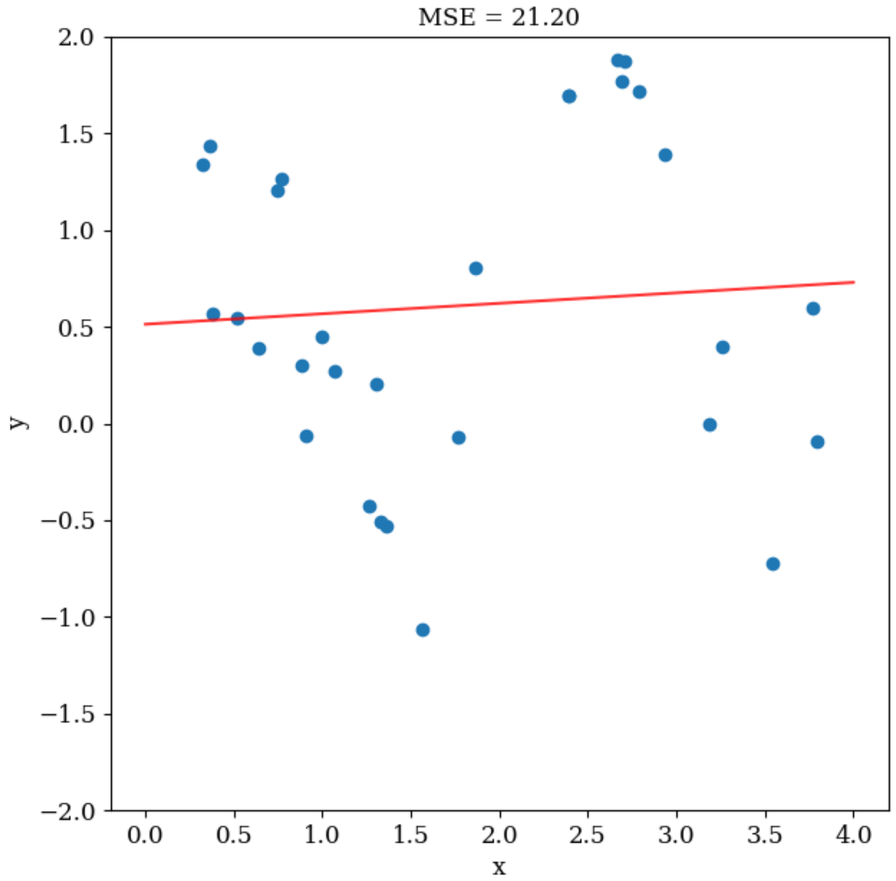
Notebook: MLD2025-01a-polynomial fitting

Direct link

A simple example - fitting a polynomial

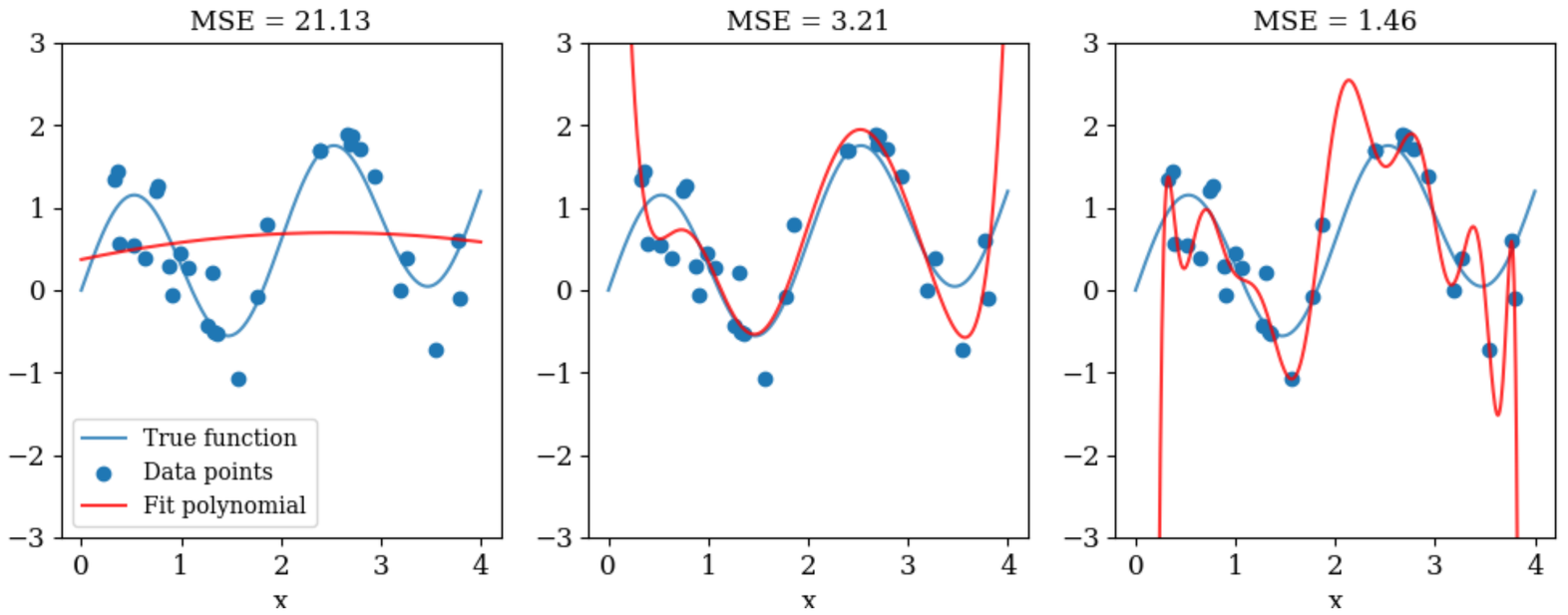
Overfitting, underfitting

We want our method to **generalise** well



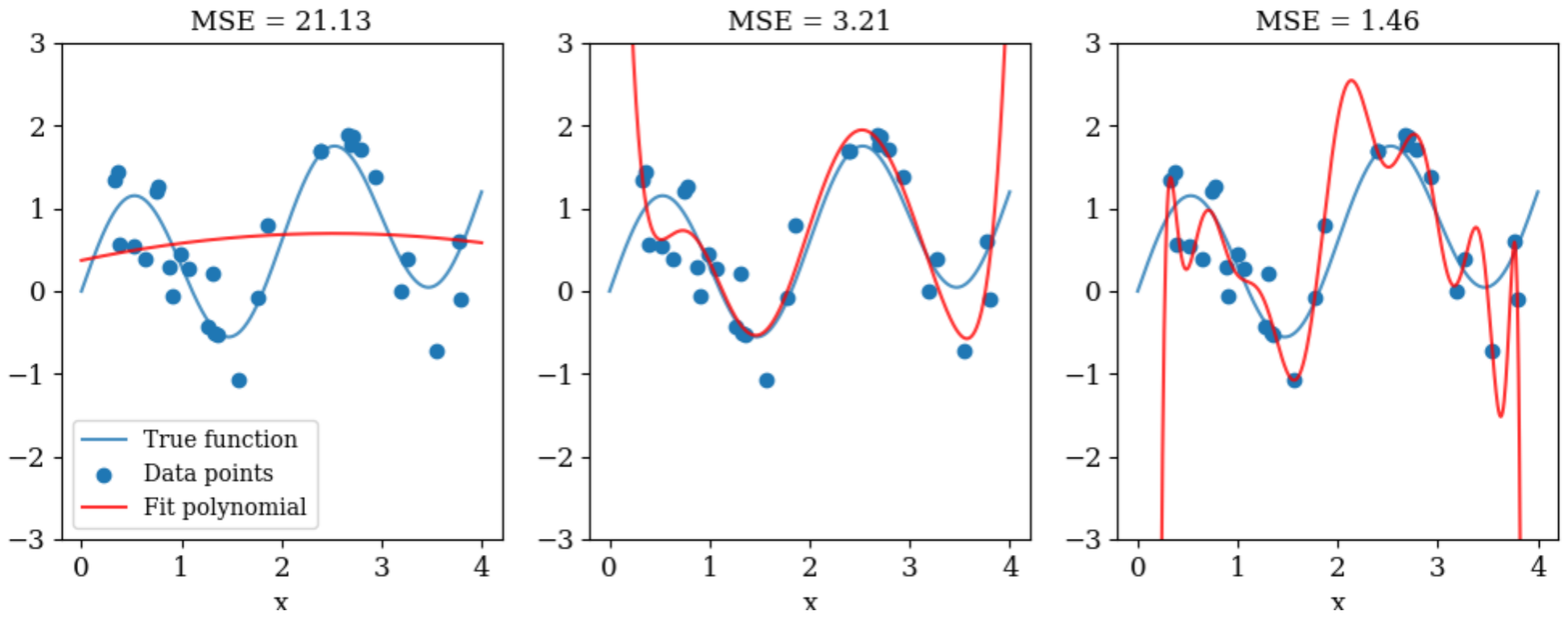
High bias!

Increasing the flexibility:



$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y - y_{\mathrm{pred}})^2$$

Increasing the flexibility:



Underfitting

Overfitting

$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y - y_{\mathrm{pred}})^2$$

Key ingredients of machine learning

Parameters, hyper-parameters

Consider a polynomial: $$y = \sum_{i=0}^{M} a_i x^i$$

Here a_i are the **parameters** of the model and what our machine learning algorithm will give us.

But M - the maximum polynomial power is *also* a parameter. It is a different kind of parameter and we call this a **hyperparameter**.

There might be situations where you have a physical justification for a particular value of M, but in general you need to determine the best value for M. This is hyperparameter optimisation.

How do you decide

We will return to this but we should think of dividing our data in three:

The training set

This is what we use to find the best-fitting parameters and we minimise the **training error** (e.g. MSE) on this.

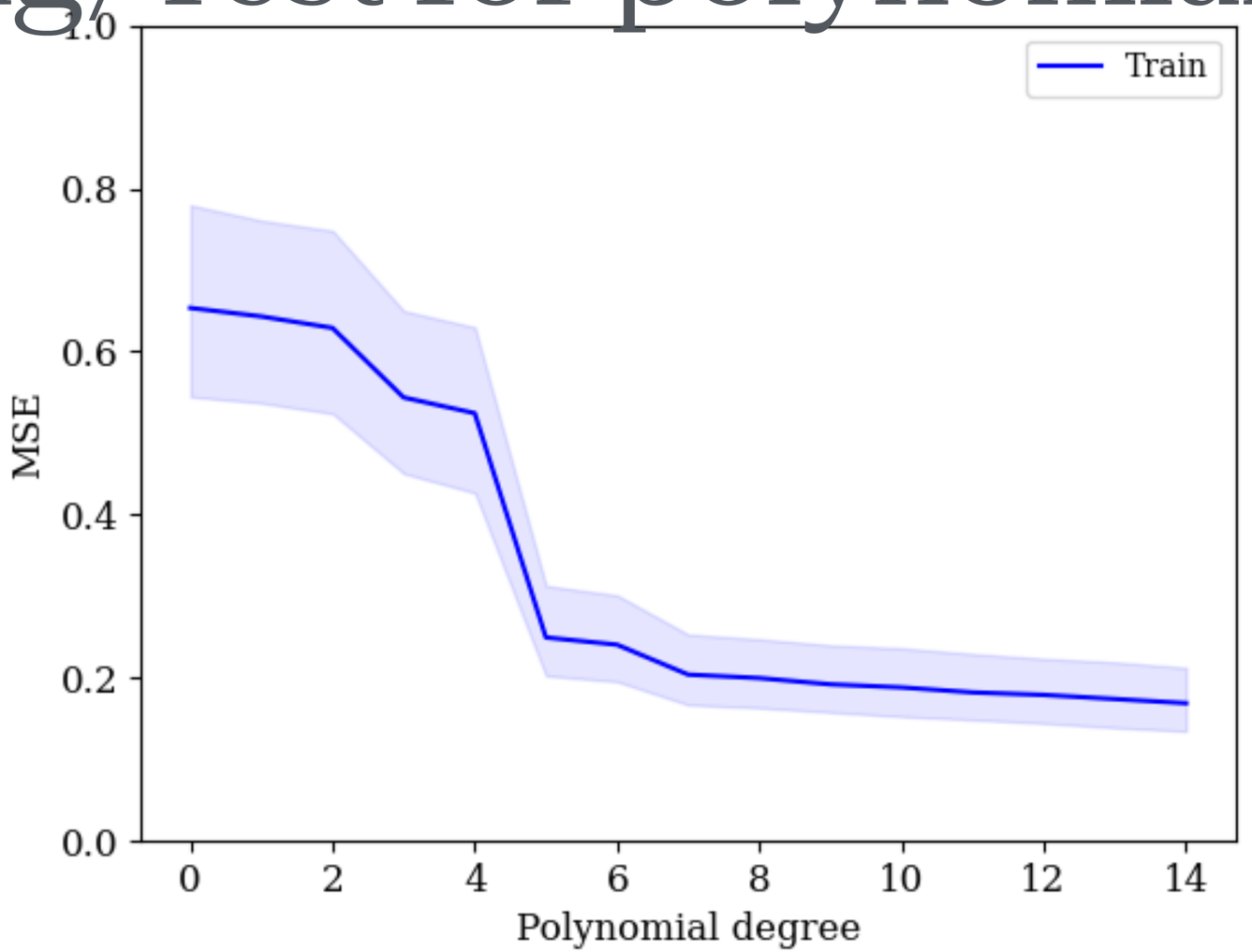
The validation set

We use this to determine the optimal settings of the hyper-parameters.

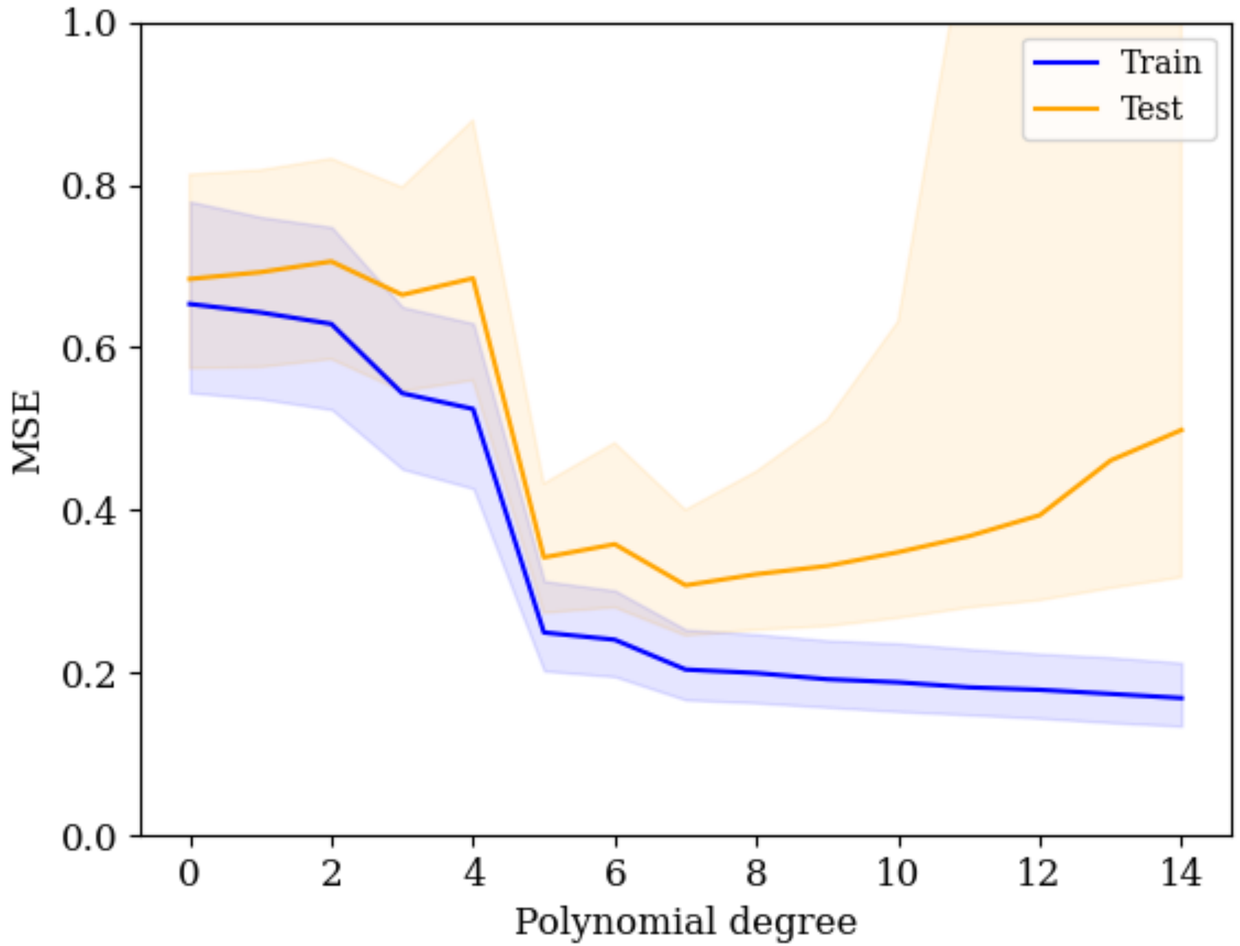
The test set

We evaluate the generalisation error of our algorithm on this sample. These data are *not* used for the fitting. We refer to the error achieved on this set as the **test error**.

Training/Test for polynomial fit



Training/Test for polynomial fit



What we see here is not specific to this example, but is rather a general illustration of what is called the bias-variance trade-off which we will get back to later.

When is good, good enough?

Model choice/complexity decision

Key ingredients of machine learning

Reminder

Accuracy/error-rate

How well is our algorithm doing? A common measure - the mean squared error:

$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{N}\left(y - y_{\mathrm{pred}}\right)^2$$

Key ingredients of machine learning

Reminder

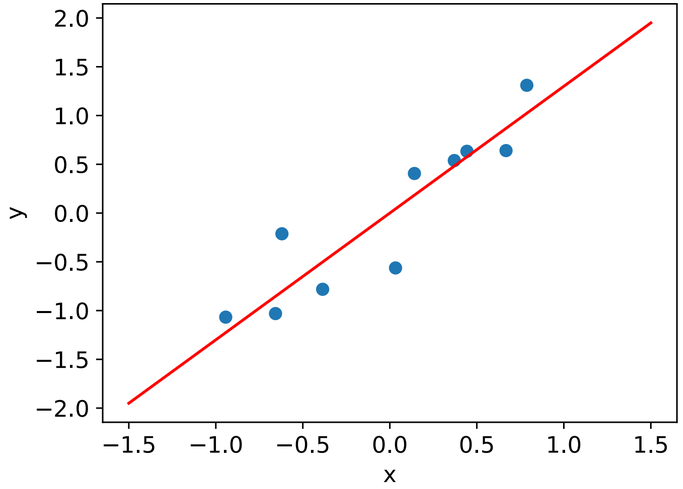
Accuracy/error-rate

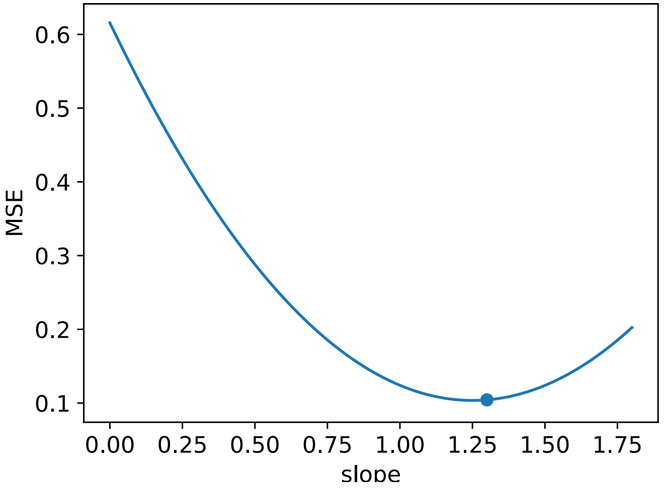
How well is our algorithm doing? A common measure - the mean squared error:

$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y - y_{\mathrm{pred}})^2$$

Try this on linear regression

$$y = \mathrm{slope} \times x$$



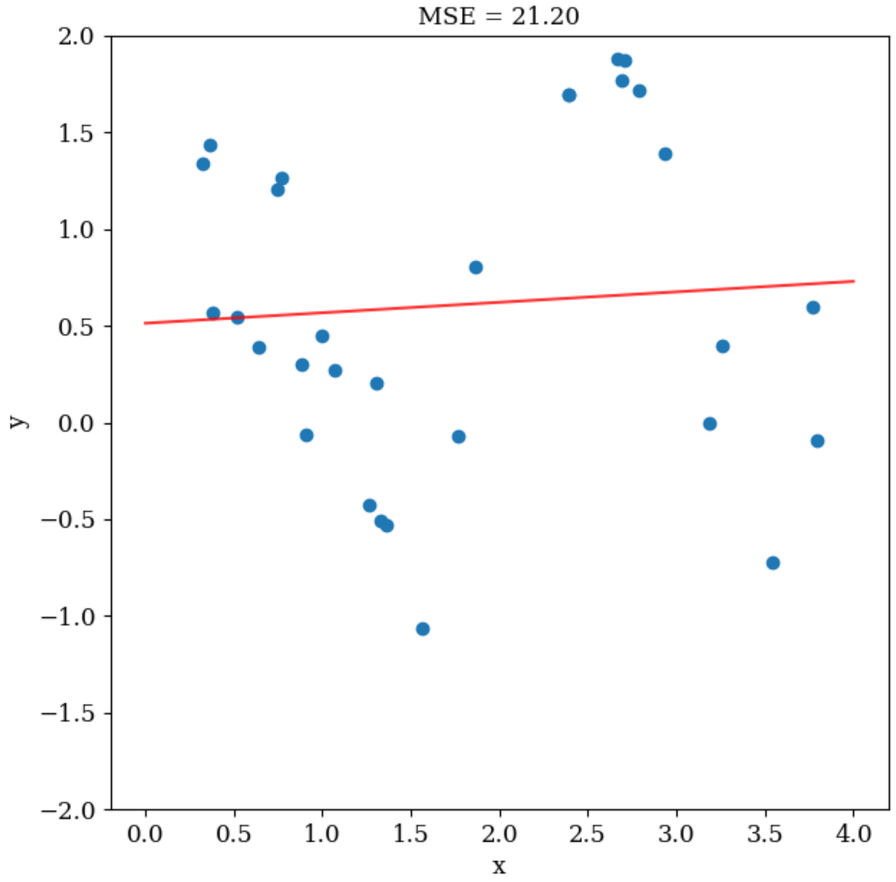


A simple example - fitting a polynomial

Reminder

Overfitting, underfitting

We want our method to **generalise** well



High bias!

A simple example - fitting a polynomial

Reminder

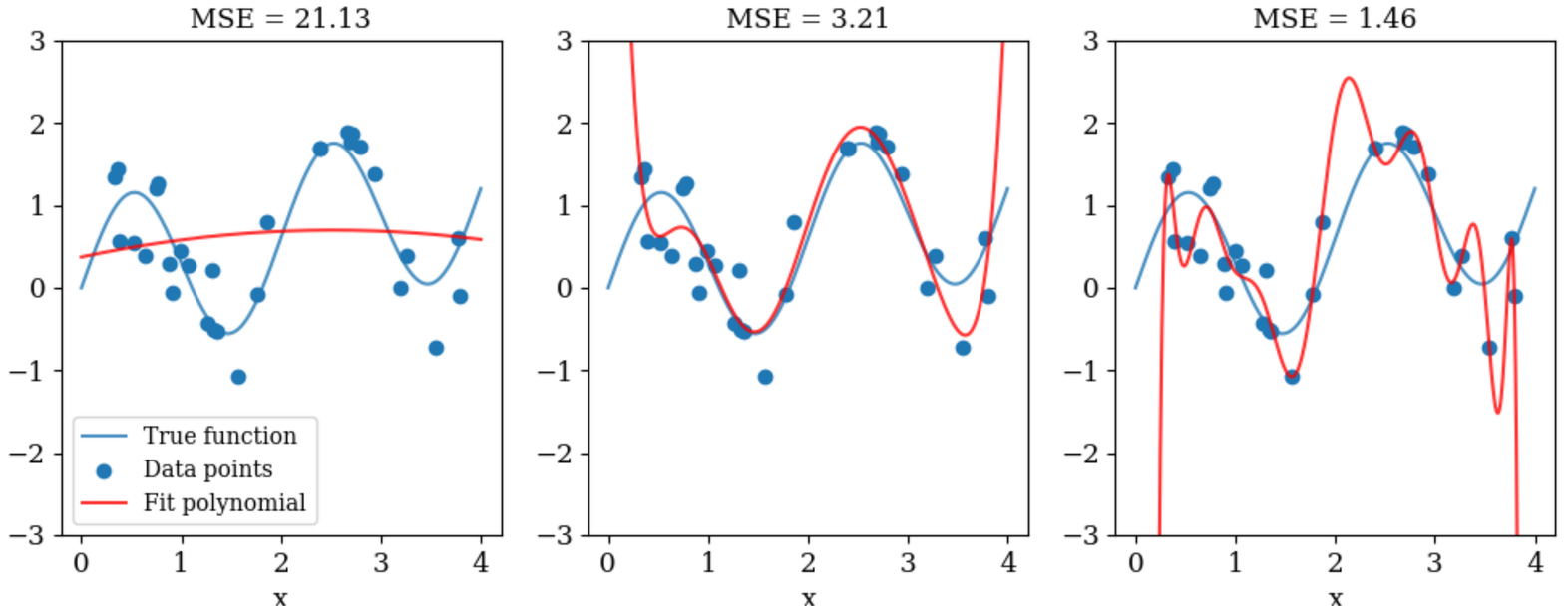
```
import numpy as np
from numpy.polynomial import Polynomial

<… Get data x & y …>

p = Polynomial.fit(x, y, degree)
y_pred = p(x)
```

And we can also easily calculate the MSE:

```
mse = np.sum((y_pred-y)**2)
```

Increasing the flexibility:

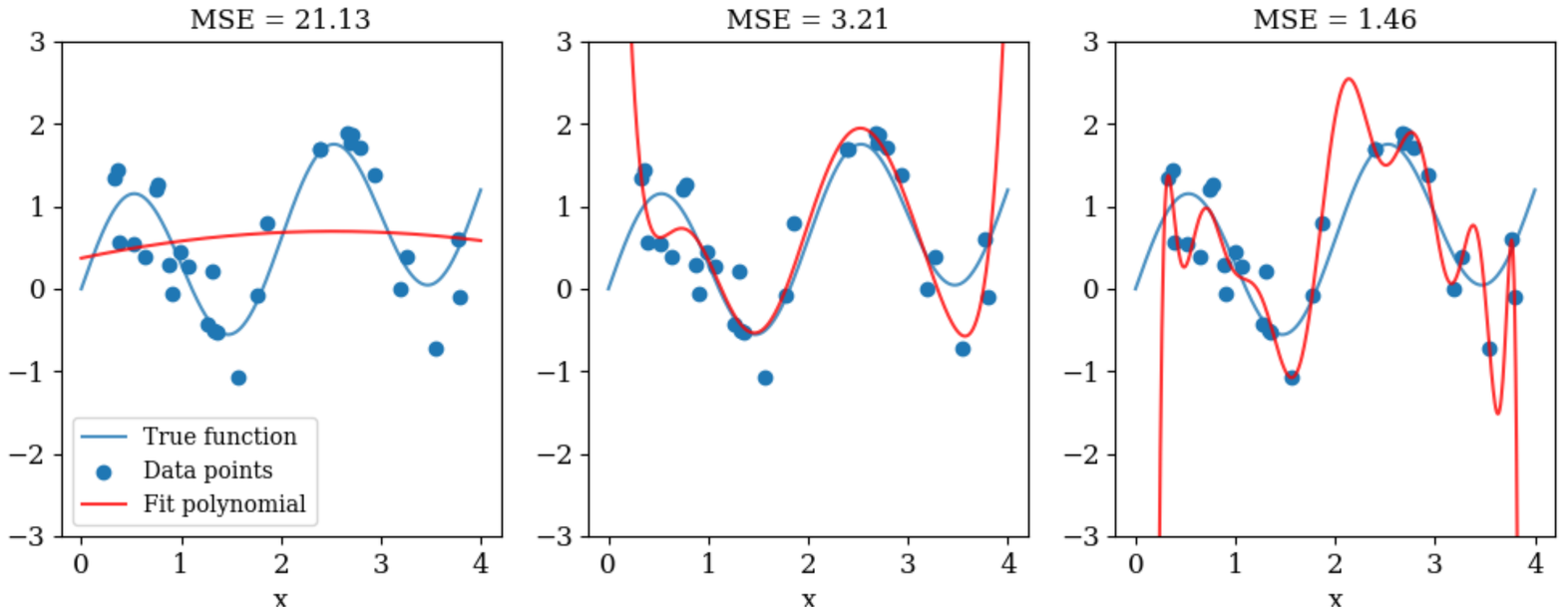
Reminder



$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y - y_{\mathrm{pred}})^2$$

Increasing the flexibility:

Reminder



Underfitting

Overfitting

$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y - y_{\mathrm{pred}})^2$$

Key ingredients of machine learning

Reminder

Parameters, hyper-parameters

Consider a polynomial: $$y = \sum_{i=0}^{M} a_i x^i$$

Here a_i are the parameters of the model and what our machine learning algorithm will give us.

But M - the maximum polynomial power is *also* a parameter. It is a different kind of parameter and we call this a **hyperparameter**.

How do you decide

Reminder

We will return to this but we should think of dividing our data in three:

The training set

This is what we use to find the best-fitting parameters and we minimise the **training error** (e.g. MSE) on this.

The validation set

We use this to determine the optimal settings of the hyper-parameters.

The test set

We evaluate the generalisation error of our algorithm on this sample. These data are *not* used for the fitting. We refer to the error achieved on this set as the **test error**.

Taking this for our polynomial example

1. For each polynomial order M, fit a polynomial to the test data.
2. Use this fitted polynomial on the validation set and calculate an MSE for this.
3. Repeat for the next M
4. Choose the M that gives the smallest MSE on the validation set.
5. Calculate the MSE on the test set to get a quantitative estimate of how well the calculation did go.

Evaluating the generalisation error

What we want:

How well does a fitted function or trained Machine Learning method work on new data?

Generalisation error

We can’t quite have that - but this is where we use the test set/validation set.

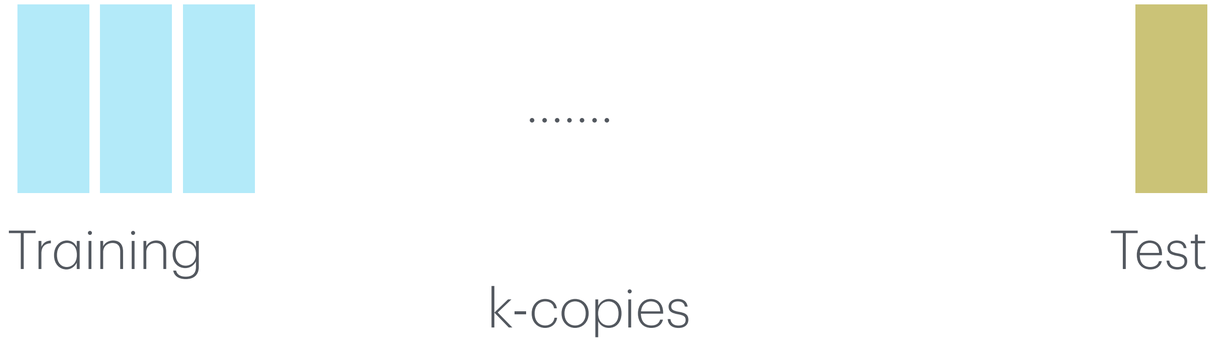
One (not very good) possibility

This is fine if we have 100,000s of data (usually), but can leave too few points to train on.

Cross-validation to the rescue

One possibility

k-fold CV



Do this splitting k times.

It is generally recommended to use 5- or 10- fold cross-validation.

Practical steps

You can do CV completely manually - but I recommend using the **`sklearn.cross_validation`** package:

```
from sklearn.cross_validation import KFold



# Create folds for N data points in n_folds:

kf = KFold(N, n_folds=n_folds)



for train, test in kf:
```

Short-cutting CV - BIC & AIC

A full CV evaluation can be very costly time-wise - in that case you might want a cheaper way to assess quality of fit.

Enter the information criteria:

The Bayesian and the Akaike: BIC & AIC

$$\mathrm{BIC} = -2\ln L_{\max} + k\ln N$$

$$\mathrm{AIC} = -2\ln L_{\max} + 2k + \frac{2k(k+1)}{N-k-1}$$

k: number of parameters

N: number of data points

$L_{\max}$: max likelihood

Let’s switch to Colab!

Notebook: MLD2025-01b-Deciding when good is good enough

Direct link

Why does it matter - the bias-variance trade-off

Complexity versus simplicity - the bias variance trade-off

Assume that the true relation between x & y is

$$y = f(x) + \epsilon \qquad \epsilon \sim N(0, \sigma_\epsilon)$$

And write the predicted value of y at x_0 $\hat{y}$

Let us ask what the expected mean square error in our prediction at $x{=}x_0$ is:

$$\mathrm{E}\left[(f(x_0) - \hat{y})^2\right]$$

Small versus big bins - the bias variance trade-off

Expected mean square error at $x=x_0$:

$$\mathrm{E}\left[(f(x_0) - \hat{y})^2\right]$$

$$y = f(x) + \epsilon$$

$$\epsilon \sim N(0, \sigma_\epsilon)$$

We can expand this and add and subtract $(\mathrm{E}\left[\hat{y}\right])^2$

to get:

$$\mathrm{Err}(x_0) = \sigma_\epsilon^2 + (E\left[\hat{y}\right] - f(x_0))^2 + \mathrm{E}\left[(\hat{y} - \mathrm{E}[\hat{y}])^2\right]$$

Small versus big bins - the bias variance trade-off

Expected mean square error at $x=x_0$:

$$\mathrm{E}\left[(f(x_0)-\hat{y})^2\right]$$

$$y = f(x) + \epsilon$$

$$\epsilon \sim N(0, \sigma_\epsilon)$$

We can expand this and add and subtract $(\mathrm{E}[\hat{y}])^2$

to get:

$$\mathrm{Err}(x_0) = \sigma_\epsilon^2 + (E[\hat{y}] - f(x_0))^2 + \mathrm{E}\left[(\hat{y} - \mathrm{E}[\hat{y}])^2\right]$$

Bias^2

Small versus big bins - the bias variance trade-off

Expected mean square error at $x=x_0$:

$$\mathrm{E}\left[(f(x_0)-\hat{y})^2\right]$$

$$y = f(x) + \epsilon$$

$$\epsilon \sim N(0, \sigma_\epsilon)$$

We can expand this and add and subtract $(\mathrm{E}[\hat{y}])^2$

to get:

$$\mathrm{Err}(x_0) = \sigma_\epsilon^2 + (E[\hat{y}] - f(x_0))^2 + \mathrm{E}\left[(\hat{y} - \mathrm{E}[\hat{y}])^2\right]$$

Bias^2 Variance

Small versus big bins - the bias variance trade-off

Expected mean square error at $x=x_0$:

$$\mathrm{E}\left[(f(x_0) - \hat{y})^2\right]$$

$$y = f(x) + \epsilon$$

$$\epsilon \sim N(0, \sigma_\epsilon)$$

We can expand this and add and subtract $(\mathrm{E}\left[\hat{y}\right])^2$

to get:

$$\mathrm{Err}(x_0) = \underbrace{\sigma_\epsilon^2}_{\text{Irreducible}} + \underbrace{(E\left[\hat{y}\right] - f(x_0))^2}_{\text{Bias}^2} + \underbrace{\mathrm{E}\left[(\hat{y} - \mathrm{E}[\hat{y}\right)^2]}_{\text{Variance}}$$

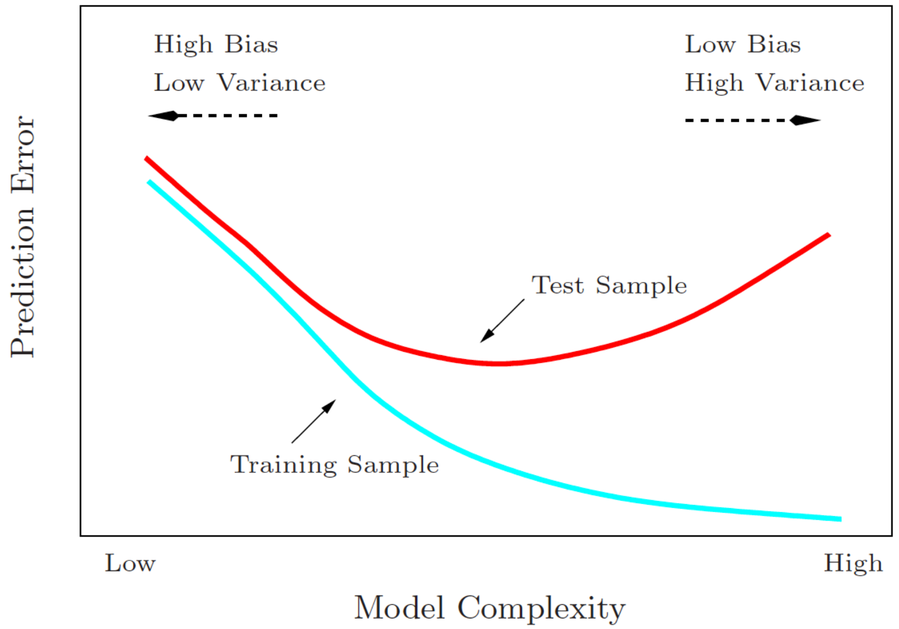
Error

The bias variance trade-off

$$\mathrm{Err}(x_0) = (E\,[\hat{y}] - f(x_0))^2 + \mathrm{E}\left[(\hat{y} - \mathrm{E}[\hat{y})^2\right]$$

Bias^2 Variance

This decomposition into two positive terms is a general result and usually we have to choose our method to have low bias *or* low variance but not both.



From "The Elements of Statistical Learning - Data Mining, Inference, and Prediction", Hastie, Tibshirani & Friedmann, second edition, Figure 2.11

Databases & archives - some examples

Sloan Digital Sky Survey - the reference database in astronomy

Millennium, EAGLE, Illustris, IlustrisTNG, FIRE - cosmological simulations

Kepler, TESS, GAIA - stellar treasure troves

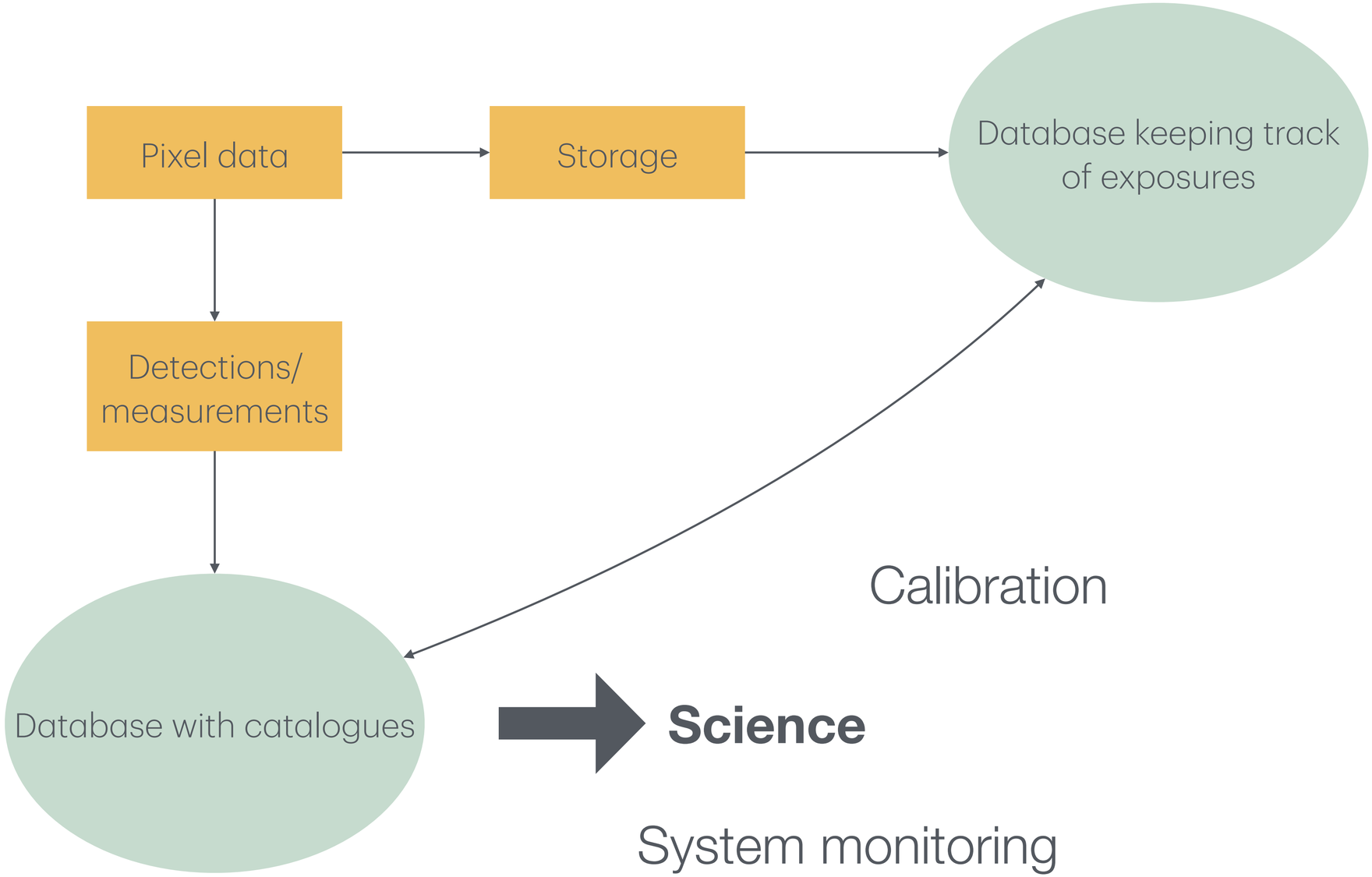
GALEX, 2MASS, etc etc.

ESO archive - observational data from ESO telescopes

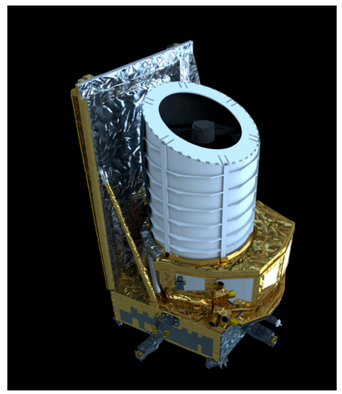
MAST archive - observational data from space telescopes

Euclid survey - the next reference database in astronomy? - the link is to the early release observations

The role of databases - a modern view



Euclid as an example



DPS

Data releases

SAS

General users

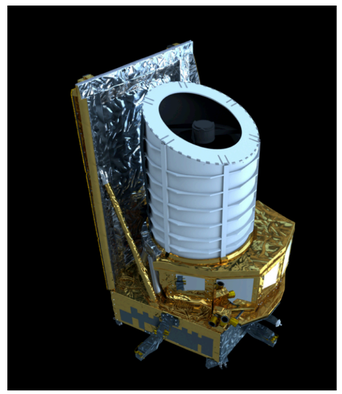
Calibration
Quality control

SDC

Data reduction
Analysis

Euclid consortium users

Euclid as an example



DPS

Data releases

Total amount:
300 Tb Raw data
~100 Pb total

SAS

General users

Calibration
Quality control

SDC

Data reduction
Analysis

Euclid consortium users

SQL - Structured Query Language

The standard way to interact with databases.

Used for instance for Gaia, Euclid, SDSS, Galex,

(although astronomical databases typically use a dialect called ADQL)

What we are doing next - and where it fits in

- The aim is always the data - today we will look a bit at how we can use a database to handle data.
- We will see how we can
  - Find data in a table
  - Combine tables
  - Possible exercise: Create tables in a data-base
- There will be some technical detail - this needs to be learned, but you should always keep in mind what your goal is: To do science with the data.

An example problem: keeping track of observations

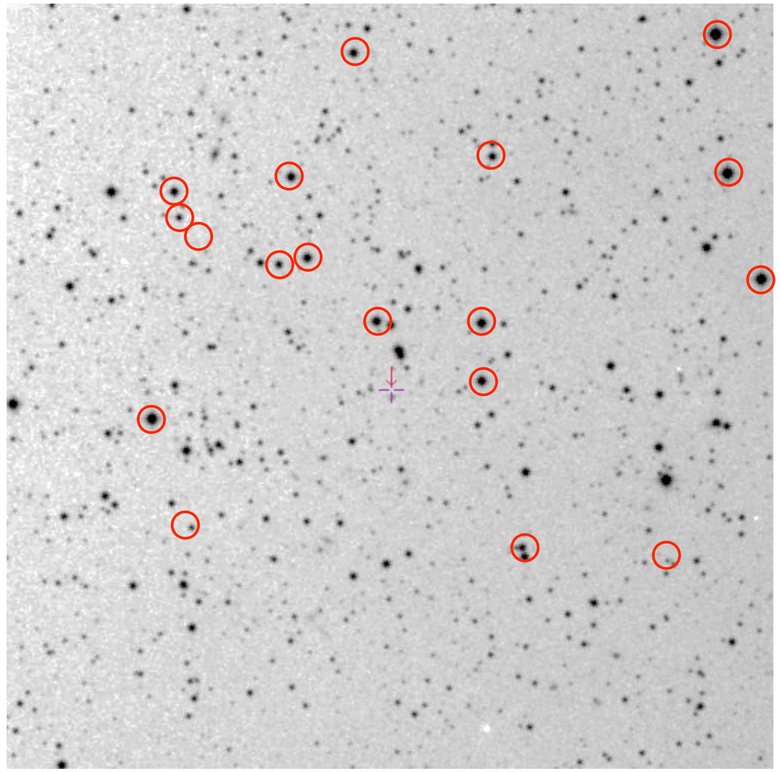
Observations:

```
         # Field      Date          Exptime   Quality   WhereStored
StF-043  92.9885764     23.2         1         /disks/yaeps-1/StF-043.fits
StF-044  97.3323764     30.2         1         /disks/yaeps-1/StF-044.fits
StF-045  93.5532134     29.5         0.5       /disks/yaeps-1/StF-045.fits
```

An example problem: keeping track of observations

Observations:

#	Field	Date	Exptime	Quality	WhereStored
StF-043	92.9885764	23.2	1		/disks/yaeps-1/StF-043.fits
StF-044	97.3323764	30.2	1		/disks/yaeps-1/StF-044.fits
StF-045	93.5532134	29.5	0.5		/disks/yaeps-1/StF-045.fits



Within each field we will detect a number of stars.

An example problem: keeping track of observations

Observations:

```
# Field      Date          Exptime   Quality   WhereStored
StF-043  92.9885764     23.2       1         /disks/yaeps-1/StF-043.fits
StF-044  97.3323764     30.2       1         /disks/yaeps-1/StF-044.fits
StF-045  93.5532134     29.5       0.5       /disks/yaeps-1/StF-045.fits
```

Stars:

```
# Star     Ra         Dec         g      r
 S1  198.8475000 10.5034722 14.5   15.2
 S2  198.5654167 11.0231944 15.3   15.4
 S5  198.9370833  9.9168889 16.4   15.8
 S7  199.2516667 10.3486944 14.6   14.1
```

If, for each star I keep information about the observations, I can waste a LOT of space. => Relational databases.

Relational databases:

Table A - lastnames

1 Smith

2 Kovacs

3 Tanahaka

.....

Table B - course grades

1 2.3 5.4 6.2 7.8

3 8.5 7.4 9.2 8.8

7 2.2 7.0 8.2 7.5

9 8.0 7.0 8.0 7.5

Relational databases:

Table A - lastnames

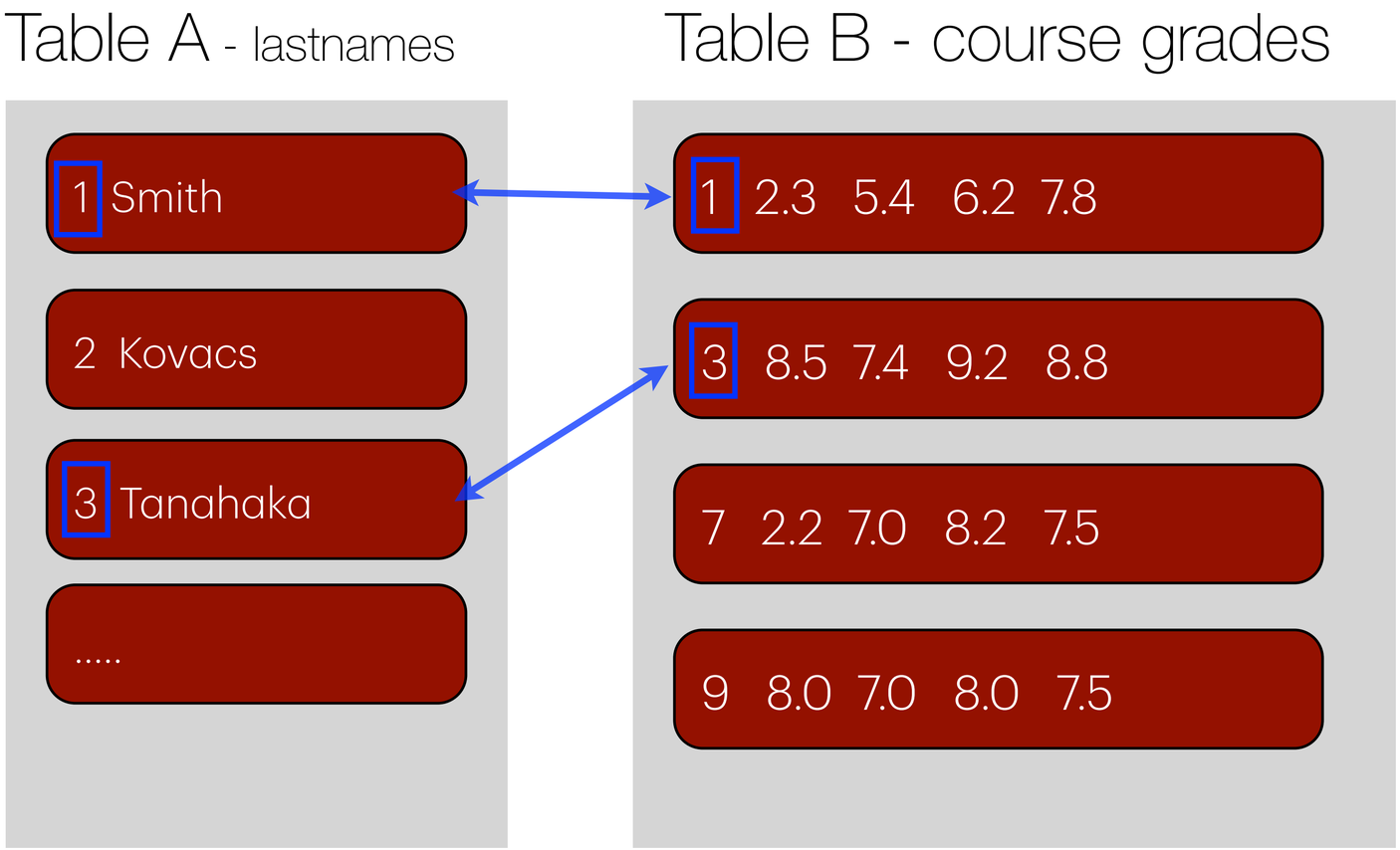
1 Smith
2 Kovacs
3 Tanahaka
.....

Table B - course grades

1	2.3	5.4	6.2	7.8
3	8.5	7.4	9.2	8.8
7	2.2	7.0	8.2	7.5
9	8.0	7.0	8.0	7.5

While a relational database is formally defined with no reference to tables, it is useful to think of it as a collection of tables where (some) rows can be related.

Relational databases:



While a relational database is formally defined with no reference to tables, it is useful to think of it as a collection of tables where (some) rows can be related.

Relational databases - the observing example

Observations:

```
# Field      Date          Exptime   Quality   WhereStored
StF-043  92.9885764     23.2       1         /disks/yaeps-1/StF-043.fits
StF-044  97.3323764     30.2       1         /disks/yaeps-1/StF-044.fits
StF-045  93.5532134     29.5       0.5       /disks/yaeps-1/StF-045.fits
```

Stars:

```
# Star     Ra         Dec        g      r
 S1  198.8475000 10.5034722 14.5   15.2
 S2  198.5654167 11.0231944 15.3   15.4
 S5  198.9370833  9.9168889 16.4   15.8
 S7  199.2516667 10.3486944 14.6   14.1
```

How should we link these?

One possibility: Create an ID column

Relational databases - the observing example

Table: Observations

#	ID	Field	Date	Exptime	Quality	WhereStored
1	StF-043	92.9885764	23.2	1		/disks/yaeps-1/StF-043.fits
2	StF-044	97.3323764	30.2	1		/disks/yaeps-1/StF-044.fits
3	StF-045	93.5532134	29.5	0.5		/disks/yaeps-1/StF-045.fits

Table: Stars

#	FieldID	StarID	Star	Ra	Dec	g	r
	1	1	S1	198.8475000	10.5034722	14.5	15.2
	1	2	S2	198.5654167	11.0231944	15.3	15.4
	3	3	S5	198.9370833	9.9168889	16.4	15.8
	2	4	S7	199.2516667	10.3486944	14.6	14.1

Relational databases - the observing example

Table: Observations

#	ID	Field	Date	Exptime	Quality	WhereStored
1	StF-043	92.9885764	23.2	1		/disks/yaeps-1/StF-043.fits
2	StF-044	97.3323764	30.2	1		/disks/yaeps-1/StF-044.fits
3	StF-045	93.5532134	29.5	0.5		/disks/yaeps-1/StF-045.fits

Table: Stars

#	FieldID	StarID	Star	Ra	Dec	g	r
	1	1	S1	198.8475000	10.5034722	14.5	15.2
	1	2	S2	198.5654167	11.0231944	15.3	15.4
	3	3	S5	198.9370833	9.9168889	16.4	15.8
	2	4	S7	199.2516667	10.3486944	14.6	14.1

Note that there are two IDs in the Stars table:

The ID of each star (StarID) **Primary key**

The ID of the field it was observed id (FieldID) **Foreign key**

Relational databases - the observing example

# ID	Field	Date	Exptime	Quality	WhereStored
1	StF-043	92.9885764	23.2	1	/disks/yaeps-1/StF-043.fits
2	StF-044	97.3323764	30.2	1	/disks/yaeps-1/StF-044.fits
3	StF-045	93.5532134	29.5	0.5	/disks/yaeps-1/StF-045.fits

Table Observations

# FieldID	StarID	Star	Ra	Dec	g	r
1	1	S1	198.8475000	10.5034722	14.5	15.2
1	2	S2	198.5654167	11.0231944	15.3	15.4
3	3	S5	198.9370833	9.9168889	16.4	15.8
2	4	S7	199.2516667	10.3486944	14.6	14.1

Table Stars

We would like to ask questions like:

1. Give me all stars brighter than r=14.5
2. How many stars have 0.1 < g-r < 0.4?
3. When did we observe S2?
4. Where is the FITS image for star S5 stored?
5. Give me a list of all stars observed on the same FieldID

Choice of database solution

For concreteness I will use **sqlite** as my database as well as CasJobs

Lightweight & convenient

Advantages of sqlite: Light-weight, no need for complex setup, supports most of SQL. Easy to use for local work. Very widely used (e.g. Firefox, Chrome) and bindings for many languages.

Disadvantages: Not a client-server solution. Not all of SQL is supported and some features (e.g. ALTER TABLE) are only partially available.

Alternatives: MySQL, Oracle, PostgreSQL, Microsoft SQL Server.

Outline of creation of databases

- Determine the format for each table in your database - its *schema*. Insert this to create your table.

```
CREATE TABLE IF NOT EXISTS Stars (<schema>);
```

- Import data into each table.

```
.separator ,
.import YAEPS.stars-table-sqlite.dat Stars
```

The devil is in the details!

1. Go to the Github site for the course

2. Go to the ProblemSets/MakeTable directory and download the MLD2025.db file

3. Open this file using:
   sqlite3 MLD2025.db

4. Check which tables are available using
   sqlite> .tables
   Observations Stars

5. Follow what I do!

Querying databases - SQL

1. Give me all stars brighter than r=14.5

# FieldID	StarID	Star	Ra	Dec	g	r
1	1	S1	198.8475000	10.5034722	14.5	15.2
1	2	S2	198.5654167	11.0231944	15.3	15.4
3	3	S5	198.9370833	9.9168889	16.4	15.8
2	4	S7	199.2516667	10.3486944	14.6	14.1

In SQL we do:

```
SELECT *
FROM Stars
WHERE r < 14.5
```

In sqlite:

```
sqlite> SELECT * FROM Stars WHERE r < 14.5;
4,2,S7,199.2516667,10.3486944,14.6,14.1
```

not the prettiest formatting (mysql is nicer) but good enough.

Breaking down the SELECT query:

1. Give me all stars brighter than r=14.5

Breaking down the SELECT query:

1. Give me all stars brighter than r=14.5

```
SELECT *
```

Return all columns for all the rows that matches the constraints. We can also specify specific columns.

Breaking down the SELECT query:

1. Give me all stars brighter than r=14.5

```
SELECT *
```

Return all columns for all the rows that matches the constraints. We can also specify specific columns.

```
FROM Stars
```

Use the table named Stars for this query.

Breaking down the SELECT query:

1. Give me all stars brighter than r=14.5

```
SELECT *
```

Return all columns for all the rows that matches the constraints. We can also specify specific columns.

```
FROM Stars
```

Use the table named Stars for this query.

```
WHERE r < 14.5
```

Only return those **rows** that satisfy the criteri(on/a) that we specify.

Choosing columns to output

FieldID	StarID	Star	Ra	Decl	g	r
1	1	S1	198.8475	10.5034722	14.5	15.2
1	2	S2	198.5654167	11.0231944	15.3	15.4
3	3	S5	198.9370833	9.9168889	16.4	15.8
2	4	S7	199.2516667	10.3486944	14.6	14.1

```
SELECT Star, g, r
    FROM Stars
```

Choosing columns to output

FieldID	StarID	Star	Ra	Decl	g	r
1	1	S1	198.8475	10.5034722	14.5	15.2
1	2	S2	198.5654167	11.0231944	15.3	15.4
3	3	S5	198.9370833	9.9168889	16.4	15.8
2	4	S7	199.2516667	10.3486944	14.6	14.1

```
SELECT Star, g, r
    FROM Stars
```

```
sqlite> SELECT Star, g, r FROM Stars;
S1,14.5,15.2
S2,15.3,15.4
S5,16.4,15.8
S7,14.6,14.1
```

Choosing columns to output

FieldID	StarID	Star	Ra	Decl	g	r
1	1	S1	198.8475	10.5034722	14.5	15.2
1	2	S2	198.5654167	11.0231944	15.3	15.4
3	3	S5	198.9370833	9.9168889	16.4	15.8
2	4	S7	199.2516667	10.3486944	14.6	14.1

```
SELECT Star, g, r
FROM Stars
WHERE r < 14.5
```

But what if I want some combination of columns?

Choosing columns to output

FieldID	StarID	Star	Ra	Decl	g	r	g-r
1	1	S1	198.8475	10.5034722	14.5	15.2	-0.7
1	2	S2	198.5654167	11.0231944	15.3	15.4	-0.1
3	3	S5	198.9370833	9.9168889	16.4	15.8	0.6
2	4	S7	199.2516667	10.3486944	14.6	14.1	0.5

```
SELECT Star, g, r, g-r as gr
FROM Stars
WHERE FieldID = 1
```

Choosing columns to output

FieldID	StarID	Star	Ra	Decl	g	r	g-r
1	1	S1	198.8475	10.5034722	14.5	15.2	-0.7
1	2	S2	198.5654167	11.0231944	15.3	15.4	-0.1
3	3	S5	198.9370833	9.9168889	16.4	15.8	0.6
2	4	S7	199.2516667	10.3486944	14.6	14.1	0.5

```
SELECT Star, g, r, g-r as gr
FROM Stars
WHERE FieldID = 1
```

```
sqlite> SELECT Star, g, r, g-r as gr FROM Stars WHERE FieldID
= 1;
S1,14.5,15.2,-0.699999999999999
S2,15.3,15.4,-0.0999999999999996
```

Getting a few values - SQL flavours...

When you have very large tables, you often want to try out statements or just get few examples back. This is easy but depends on the SQL flavour you use:

Microsoft SQL (used in SDSS):

```
SELECT TOP 2 r FROM STARS
```

MySQL and sqlite:

```
SELECT r FROM STARS LIMIT 2
```

Oracle (used in AstroWISE):

```
SELECT r FROM STARS WHERE ROWNUM < 2
```

Recall:

Table Observations

#	ID	Field	Date	Exptime	Quality	WhereStored
1	StF-043	92.9885764	23.2	1		/disks/yaeps-1/StF-043.fits
2	StF-044	97.3323764	30.2	1		/disks/yaeps-1/StF-044.fits
3	StF-045	93.5532134	29.5	0.5		/disks/yaeps-1/StF-045.fits

Table Stars

#	FieldID	StarID	Star	Ra	Dec	g	r
	1	1	S1	198.8475000	10.5034722	14.5	15.2
	1	2	S2	198.5654167	11.0231944	15.3	15.4
	3	3	S5	198.9370833	9.9168889	16.4	15.8
	2	4	S7	199.2516667	10.3486944	14.6	14.1

Now let us go back to our questions:

3. When did we observe S2?
4. Where is the FITS image stored for star S5?
5. Give me a list of all stars observed on the same FieldID

#	ID	Field	Date	Exptime	Quality	WhereStored
1	StF-043	92.9885764	23.2	1		/disks/yaeps-1/StF-043.fits
2	StF-044	97.3323764	30.2	1		/disks/yaeps-1/StF-044.fits
3	StF-045	93.5532134	29.5	0.5		/disks/yaeps-1/StF-045.fits

#	FieldID	StarID	Star	Ra	Dec	g	r
	1	1	S1	198.8475000	10.5034722	14.5	15.2
	1	2	S2	198.5654167	11.0231944	15.3	15.4
	3	3	S5	198.9370833	9.9168889	16.4	15.8
	2	4	S7	199.2516667	10.3486944	14.6	14.1

In these cases we need to be able to link information between two tables. In SQL we do this using JOINs

First a theoretical view:

Two sets of values: $\{x_i\}$ $\{y_j\}$ (the elements can be vectors/matrices etc)

Possible ways to combine:

Union: $\{x_i, y_j | i=1, n; j=1, m\}$ elements must be the same

Cross-join: $\{(x_i, y_j) | i=1, n; j=1, m\}$ ie. all possible pairs

Left Outer join: $\{(x_i, y_i)$ if y_i exists, $(x_i$, NULL) otherwise$\}$

Right Outer join: $\{(x_i, y_i)$ if x_i exists, (NULL, y_i) otherwise$\}$

Inner join: $\{(x_i, y_i)$ if y_i exists$\}$

All these are supported in SQL.

How do you combine?

ID	u
1	19.3
2	17.5
3	20.5

ID	EW
1	75Å
3	0.5Å

JOIN

ID	u	EW
1	19.3	75Å
3	20.5	0.5Å

How do you combine?

ID	u
1	19.3
2	17.5
3	20.5

ID	EW
1	75Å
3	0.5Å

JOIN

ID	u	EW
1	19.3	75Å
3	20.5	0.5Å

```
SELECT P.u, S.EW
FROM Photo as P
   JOIN  Spectro as S
ON P.ID=S.ID
```

How do you combine?

ID	u
1	19.3
2	17.5
3	20.5

ID	EW
1	75Å
3	0.5Å

JOIN

ID	u	EW
1	19.3	75Å
3	20.5	0.5Å

```
SELECT P.u, S.EW
FROM Photo as P
   JOIN  Spectro as S
ON P.ID=S.ID
```

OR

```
SELECT P.u, S.EW
FROM Photo as P,
Spectro as S
WHERE P.ID=S.ID
```

How do you combine?

ID	u
1	19.3
2	17.5
3	20.5

ID	EW
1	75Å
3	0.5Å

JOIN

ID	u	EW
1	19.3	75Å
3	20.5	0.5Å

```
SELECT P.u, S.EW
FROM Photo as P
   JOIN  Spectro as S
ON P.ID=S.ID
```

Explicit INNER JOIN

OR

```
SELECT P.u, S.EW
FROM Photo as P,
Spectro as S
WHERE P.ID=S.ID
```

Implicit INNER JOIN

(or *old-style* INNER JOIN)

Explicit vs implicit JOINs

JOIN ... ON a=b

or

WHERE a = b

Mostly up to you - there should be no significant difference between the two.

The main disadvantage of an implicit JOIN is that you have less control of the order things are done if you have more than two tables.

I personally prefer explicit JOINs because they show more clearly what your intention is and if you have a problem because your query runs too slowly, you can more easily figure out the execution order.

UNION

It must make sense to glue the tables together!

```
Select TOP 10
ra, dec
FROM SpecPhoto
WHERE ra > 120
AND DEC < 0

UNION

Select TOP 10
ra, dec
From SpecPhoto
WHERE ra < 10
AND DEC > 0
```

Table 1

Table 2

Try it in SDSS!

UNION

It must make sense to glue the tables together!

```
Select TOP 10
ra, dec
FROM SpecPhoto
WHERE ra > 120
AND DEC < 0

UNION

Select TOP 10
ra, dec
From SpecPhoto
WHERE ra < 10
AND DEC > 0
```

Table 1

Table 2

Ra	Dec

Try it in SDSS!

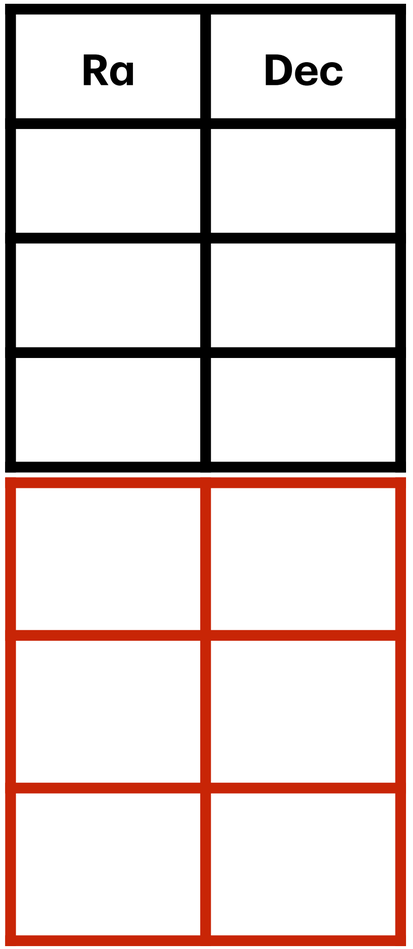
UNION

It must make sense to glue the tables together!

```
Select TOP 10
ra, dec
FROM SpecPhoto
WHERE ra > 120
AND DEC < 0

UNION

Select TOP 10
ra, dec
From SpecPhoto
WHERE ra < 10
AND DEC > 0
```

Table 1

Table 2



Try it in SDSS!

But if we want to keep **all** possible pairs we need an **OUTER JOIN**

```
SELECT P.u, S.z
FROM Photo as P
LEFT OUTER JOIN  Spectro as S
ON P.ID=S.ID
```

But if we want to keep **all** possible pairs we need an **OUTER JOIN**

```
SELECT P.u, S.z
FROM Photo as P
LEFT OUTER JOIN  Spectro as S
ON P.ID=S.ID
```

ID	u
1	19.3
2	17.5
3	20.5

ID	EW
1	75Å
3	0.5Å

ID	u	EW(Ha)
1	19.3	75Å
2	17.5	NULL
3	20.5	0.5Å

Returning to our questions:

3. When did we observe S2?

#	ID	Field	Date	Exptime	Quality	WhereStored
1	StF-043	92.9885764	23.2	1		/disks/yaeps-1/StF-043.fits
2	StF-044	97.3323764	30.2	1		/disks/yaeps-1/StF-044.fits
3	StF-045	93.5532134	29.5	0.5		/disks/yaeps-1/StF-045.fits

#	FieldID	StarID	Star	Ra	Dec	g	r
	1	1	S1	198.8475000	10.5034722	14.5	15.2
	1	2	S2	198.5654167	11.0231944	15.3	15.4
	3	3	S5	198.9370833	9.9168889	16.4	15.8
	2	4	S7	199.2516667	10.3486944	14.6	14.1

Our link is FieldID in Stars to ID in Observations

Returning to our questions:

3. When did we observe S2?

#	ID Field	Date	Exptime	Quality	WhereStored
1	StF-043	92.9885764	23.2	1	/disks/yaeps-1/StF-043.fits
2	StF-044	97.3323764	30.2	1	/disks/yaeps-1/StF-044.fits
3	StF-045	93.5532134	29.5	0.5	/disks/yaeps-1/StF-045.fits

#	FieldID	StarID	Star	Ra	Dec	g	r
	1	1	S1	198.8475000	10.5034722	14.5	15.2
	1	2	S2	198.5654167	11.0231944	15.3	15.4
	3	3	S5	198.9370833	9.9168889	16.4	15.8
	2	4	S7	199.2516667	10.3486944	14.6	14.1

Our link is FieldID in Stars to ID in Observations

```
select s.Star, o.Field, o.Date
from
   stars as s
   JOIN Observations as o
   ON s.fieldID = o.ID
Where s.Star = ‘S2’
```

Returning to our questions:

3. When did we observe S2?

```
select s.Star, o.Field, o.Date
from
  stars as s
  JOIN Observations as o
  ON s.fieldID = o.ID
Where Star = ‘S2’
```

We must specify what table to get a quantity from.

JOIN the tables explicitly

Choose our star

Useful: We can do **multiple** stars by changing the WHERE statement to:

Returning to our questions:

3. When did we observe S2?

```
select s.Star, o.Field, o.Date
from
  stars as s
  JOIN Observations as o
  ON s.fieldID = o.ID
Where Star = ‘S2’
```

We must specify what table to get a quantity from.

JOIN the tables explicitly

Choose our star

Useful: We can do **multiple** stars by changing the WHERE statement to:

```
Where Star IN (‘S2’, ‘S1’)
```

Returning to our questions:

3. When did we observe S2?

```
select s.Star, o.Field, o.Date
from
  stars as s
  JOIN Observations as o
  ON s.fieldID = o.ID
Where Star = ‘S2’
```

We must specify what table to get a quantity from.

JOIN the tables explicitly

Choose our star

Useful: We can do **multiple** stars by changing the WHERE statement to:

```
Where Star IN (‘S2’, ‘S1’)
```

That’s it for now - more advanced topics for SQL are included at the end of the slides for self-study

Let’s switch to Colab!

Notebook: MLD2025-01c-Python and SQL

Direct link

Creation of databases & using them from Python

Creating a sqlite database

Let us set up a simple database to start with:

```
> sqlite3 MLD2025.db
SQLite version 3.8.10.2 2015-05-20 18:17:19
Enter ".help" for usage hints.
sqlite> .tables
sqlite> .exit
```

This should give you nothing because there are no tables.
We need to make one.

Step 2 - inserting a table

Get: YAEPS.stars-table-sqlite.dat and sqlite3-make-stars-table.sql from the GitHub site (ProblemSet/MakeTables). Edit the latter to reflect the location of YAEPS.stars-table-sqlite.dat

When that is done:

```
> sqlite3 MLD2025.db
SQLite version 3.8.10.2 2015-05-20 18:17:19
Enter ".help" for usage hints.
sqlite> .read sqlite3-make-stars-table.sql
sqlite> .tables
Stars
```

Magic?

First we need to create a schema

To do this we need to understand our data:

```
# StarID FieldID  Star     Ra          Dec         g      r
   1         1      S1   198.8475000 10.5034722 14.5    15.2
   2         1      S2   198.5654167 11.0231944 15.3    15.4
   3         3      S5   198.9370833  9.9168889 16.4    15.8
   4         2      S7   199.2516667 10.3486944 14.6    14.1
```

Column	Type	SQL type	Other
StarID	Integer	INT	PrimaryKey,
FieldID	Integer	INT	ForeignKey
Star	String	varchar(10)	Length < 10
Ra	Real number	DOUBLE	
Dec	Real number	DOUBLE	
g	Real number	DOUBLE	
r	Real number	DOUBLE	

Schema

Creating databases and tables

Our star table is created with:

```
CREATE TABLE IF NOT EXISTS Stars (
   StarID INT,
   FieldID INT,
   Star varchar(10),
   ra DOUBLE,
   decl DOUBLE,
   g FLOAT,
   r FLOAT,
   UNIQUE(StarID),
   PRIMARY KEY(StarID),
   FOREIGN KEY(FieldID) REFERENCES
   Observations(ID)
   );
```

You can type this on the command line, but it is easier to store it in a file!

Creating databases and tables

Our star table is created with:

```
CREATE TABLE IF NOT EXISTS Stars (
   StarID INT,
   FieldID INT,
   Star varchar(10),
   ra DOUBLE,
   decl DOUBLE,
   g FLOAT,
   r FLOAT,
   UNIQUE(StarID),
   PRIMARY KEY(StarID),
   FOREIGN KEY(FieldID) REFERENCES
   Observations(ID)
   );
```

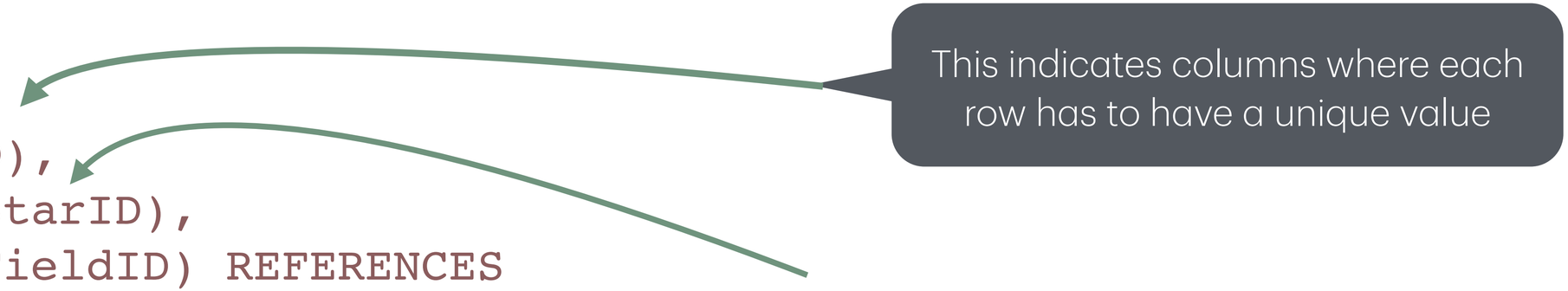
Notice the definition of strings

You can type this on the command line, but it is easier to store it in a file!

Creating databases and tables

Our star table is created with:

```
CREATE TABLE IF NOT EXISTS Stars (
   StarID INT,
   FieldID INT,
   Star varchar(10),
   ra DOUBLE,
   decl DOUBLE,
   g FLOAT,
   r FLOAT,
   UNIQUE(StarID),
   PRIMARY KEY(StarID),
   FOREIGN KEY(FieldID) REFERENCES
   Observations(ID)
   );
```



You can type this on the command line, but it is easier to store it in a file!

Creating databases and tables

Our star table is created with:

```
CREATE TABLE IF NOT EXISTS Stars (
   StarID INT,
   FieldID INT,
   Star varchar(10),
   ra DOUBLE,
   decl DOUBLE,
   g FLOAT,
   r FLOAT,
   UNIQUE(StarID),
   PRIMARY KEY(StarID),
   FOREIGN KEY(FieldID) REFERENCES
   Observations(ID)
   );
```

This can optionally be used to indicate the primary key in this database

You can type this on the command line, but it is easier to store it in a file!

Creating databases and tables

Our star table is created with:

```
CREATE TABLE IF NOT EXISTS Stars (
   StarID INT,
   FieldID INT,
   Star varchar(10),
   ra DOUBLE,
   decl DOUBLE,
   g FLOAT,
   r FLOAT,
   UNIQUE(StarID),
   PRIMARY KEY(StarID),
   FOREIGN KEY(FieldID) REFERENCES
   Observations(ID)
   );
```

Optional: Use this to indicate foreign keys in the table. This can be useful for clarity at least.

You can type this on the command line, but it is easier to store it in a file!

Creating databases and tables

well, we need some more (this is database specific:)

```
.separator ,
.import YAEPS.stars-table-sqlite.dat Stars
```

These quick import routines are not part of SQL so vary from database to database (but they are handy!)

Creating databases and tables

well, we need some more (this is database specific:)

```
.separator ,
.import YAEPS.stars-table-sqlite.dat Stars
```

These quick import routines are not part of SQL so vary from database to database (but they are handy!)

In MySQL for instance it would be:

```
LOAD DATA INFILE 'YAEPS.stars-table-sqlite.dat' INTO TABLE Stars
  FIELDS TERMINATED BY ‘,’;
```

here I can also add IGNORE 1 LINES at the end if I want to skip a header line.

Getting rid of a table & altering it

Everyone makes mistakes. Sometimes the best is to just get rid of a table. It is easy:

```
DROP TABLE Galaxy;
```

It is also possible to modify (alter) a table - but note that this does not fully work in sqlite!

```
ALTER TABLE Galaxy ADD rmag  FLOAT
```

Adding column

```
ALTER TABLE Galaxy DROP COLUMN rmag
```

Deleting column

```
ALTER TABLE Galaxy ALTER rmag DOUBLE
```

Changing the type of a column

Putting data into the database - row by row

Adding data one row at a time is done using INSERT:

```
INSERT INTO Galaxy VALUES (1,
12.334, 14.433);
```

GalaxyID	ra	decl

GalaxyID	**ra**	**decl**
1	12.334	14.433

You can also insert only some values but then you have to say what columns they are for:

```
INSERT INTO Galaxy (GalaxyID,
decl) VALUES (2, 17.5);
```

GalaxyID	**ra**	**decl**
1	12.334	14.433
2	NULL	17.5

Note: You can also insert multiple rows if you copy from one table to another.

Putting data into the database - in one go

INSERT is quite slow, in part because the database is reorganised after each insert. This is fine for small jobs but not for 100,000s of entries. For this case we use LOAD DATA.

```
LOAD DATA INFILE <filename> INTO TABLE
Stars
  FIELDS TERMINATED BY ',' IGNORE 1 LINES;
```

(optional)

will load from a file where each column is separated by a comma (the default is TAB), and rows by newline but it will skip the first line. The column types must match the Table definition - so in this case a file that can be loaded would be:

```
# StarID FieldID Star Ra Dec    g    r
1,1,S1,198.8475000,10.5034722,14.5,15.2
2,1,S2,198.5654167,11.0231944,15.3,15.4
```

This is fine for those situations where your data are already known - for instance if you downloaded a catalogue.

Updating data

Most astronomical data can change (calibration files can be updated, measurement techniques improved etc.)

We often then want to create a new table, but sometimes you want to update a row instead. This is done in SQL using the UPDATE command.

```
UPDATE Galaxy SET ra=11.3 WHERE decl=17.5
```

This is ok, in particular where information is acquired after most of the table is assembled.

Next: A more fancy criterion

2. How many stars have 0.1 < g-r < 0.4?

```
SELECT *
FROM Stars
WHERE g-r BETWEEN 0.1 AND 0.4
```

or

```
SELECT *
FROM Stars
WHERE g-r > 0.1
  AND g-r < 0.4
```

Try this now for your newly created table - remember to put a ; at the end of each line!

Reminder:

```
# StarID FieldID  Star     Ra          Dec         g      r
   1         1      S1   198.8475000 10.5034722 14.5   15.2
   2         1      S2   198.5654167 11.0231944 15.3   15.4
   3         3      S5   198.9370833  9.9168889 16.4   15.8
   4         2      S7   199.2516667 10.3486944 14.6   14.1
```

Column	Type	SQL type	Other
StarID	Integer	INT	PrimaryKey,
FieldID	Integer	INT	ForeignKey
Star	String	varchar(10)	Length < 10
Ra	Real number	DOUBLE	
Dec	Real number	DOUBLE	
g	Real number	DOUBLE	
r	Real number	DOUBLE	

Create a new table - now for the Observations

```
# FieldID  Field      Date       Exptime   Quality          WhereStored
   1       StF-043  92.9885764    23.2       1        /disks/yaeps-1/StF-043.fits
   2       StF-044  97.3323764    30.2       1        /disks/yaeps-1/StF-044.fits
   3       StF-045  93.5532134    29.5       0.5      /disks/yaeps-1/StF-045.fits
```

Column	Type	SQL type	Other
FieldID			
Field			
Date			
Exptime			
Quality			
WhereStored			

In practice:

Get YAEPS.observations-table-sqlite.dat and sqlite3-make-observations-table.sql from Github. Edit the latter to reflect the location of YAEPS.observations-table-sqlite.dat

```
> sqlite3 MLD2025.db
SQLite version 3.8.10.2 2015-05-20 18:17:19
Enter ".help" for usage hints.
sqlite> .read sqlite3-make-observations-table.sql
sqlite> .tables
Observations  Stars
```

sqlite from Python
or - what you really want to know

sqlite3 in python - an example

```
import sqlite3 as lite;
```

Load what is necessary

The database must be created first!

```
con = lite.connect(database)
```

Connect to database

```
with con:
```

Use **with** to gracefully handle exceptions

```
   # Get a cursor.
   cur = con.cursor()

   # Execute commands
   cur.execute(command)
```

cursors are used to navigate relational databases and are often needed in programatic access

Building the table in python:

```
# Next, we create a connection to the database.
con = lite.connect(database)
with con:

    table = ‘Stars’
    # Create the command to create the table. I use a
    # multiline string to ease readability here.
    command = """CREATE TABLE IF NOT EXISTS {0} (StarID INT,
              FieldID INT, Star varchar(10), ra DOUBLE,
              decl DOUBLE, g FLOAT, r FLOAT,
              UNIQUE(StarID), PRIMARY KEY(StarID),
              FOREIGN KEY(FieldID) REFERENCES Observations(ID))""".format(table)

    # Next, actually execute this command.
    con.execute(command)

    # Now that this is working, let us loop over the table entries
    # and insert these into the table.
    for row in cat:
        command = "INSERT INTO Stars VALUES({0},{1},'{2}',{3},{4},{5},{6})".format(row[0], row[1],
row[2], row[3], row[4], row[5], row[6])
        print command
        con.execute(command)
```

See the GitHub site for the script - now build one for the observations. It is much easier to do this with Pandas!

Using python to query the database:

```
In [1]: import sqlite3 as lite;

In [2]: con = lite.connect('MLD19-python.db')

In [3]: rows = con.execute('SELECT ra, decl FROM Stars')

In [4]: for row in rows:
   ...:     print "Ra={0}  Dec={1}".format(row[0], row[1])
   ...:
Ra=198.8475  Dec=10.5034722
Ra=198.5654167  Dec=11.0231944
Ra=198.9370833  Dec=9.9168889
Ra=199.2516667  Dec=10.3486944
```

As should be clear: The execute statements executes SQL statements in the database and returns a list of results.