

# Making a galaxy with Python: Merits and pitfalls in probabilistic programing

Vital Fernández



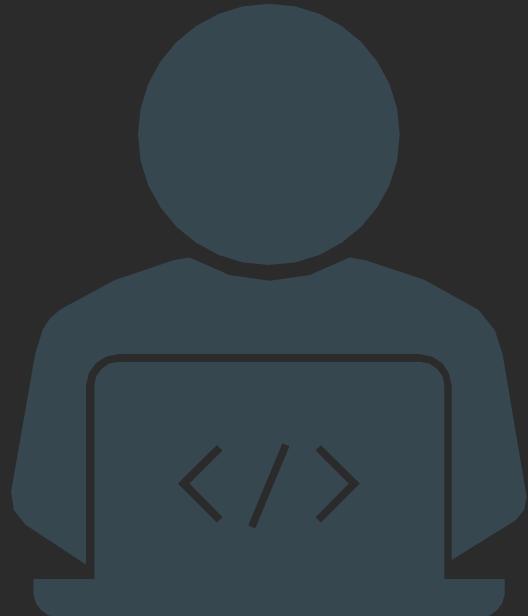
So...  
what is this about?

~~Programmer~~

~~Developer~~

~~Statistician~~

Lucky bastard for having Python



- To treat astronomical data
- To fit theoretical model
- To publish the results

# Talk Outline



Lewis Carroll (1865)

## Begin at the beginning (10 min)

- Galaxies: Light from stars and atoms
  - Spectra: Celestial histograms
- Atroinformatics: From the telescope to your model

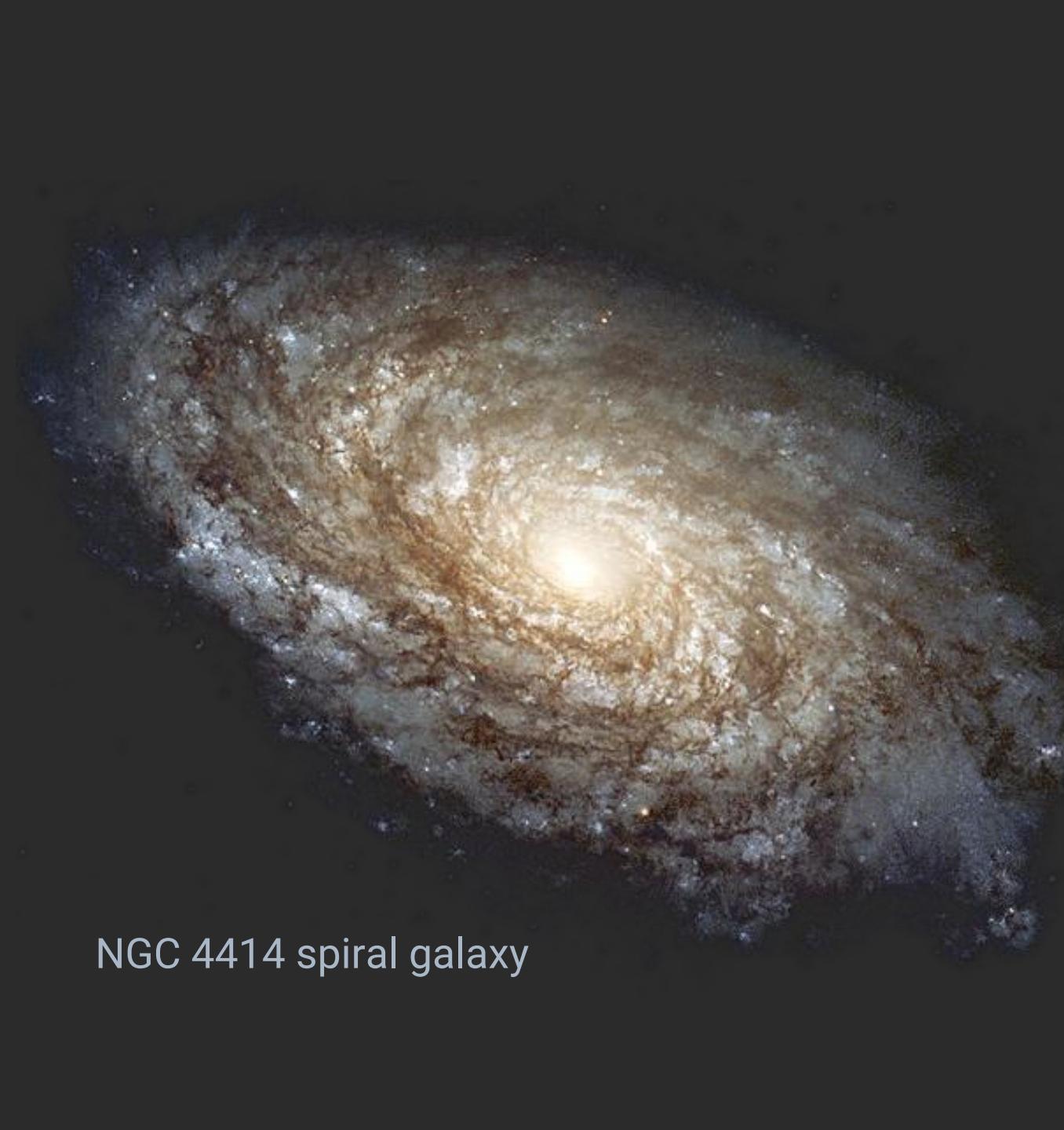
## and go on till you come to the end (10 min)

- Frequentist and Bayesian uncertainty
  - Monte Carlo samplers
  - PyMC3 Probabilistic programing

## then stop (10 min)

- Running models
- Printing results
- Diagnosing model convergence

What is a galaxy?



# What is a galaxy?

Quick answer:  
Bound system of gas, stars and  
dust

NGC 4414 spiral galaxy

Good answer:  
Light

What  
is light?

Photons we can see

What  
is darkness?  
Photons we can't see

# What is a photon ( $\gamma$ )?

It's an itsy bitsy teenie weenie  
thingy with a certain energy

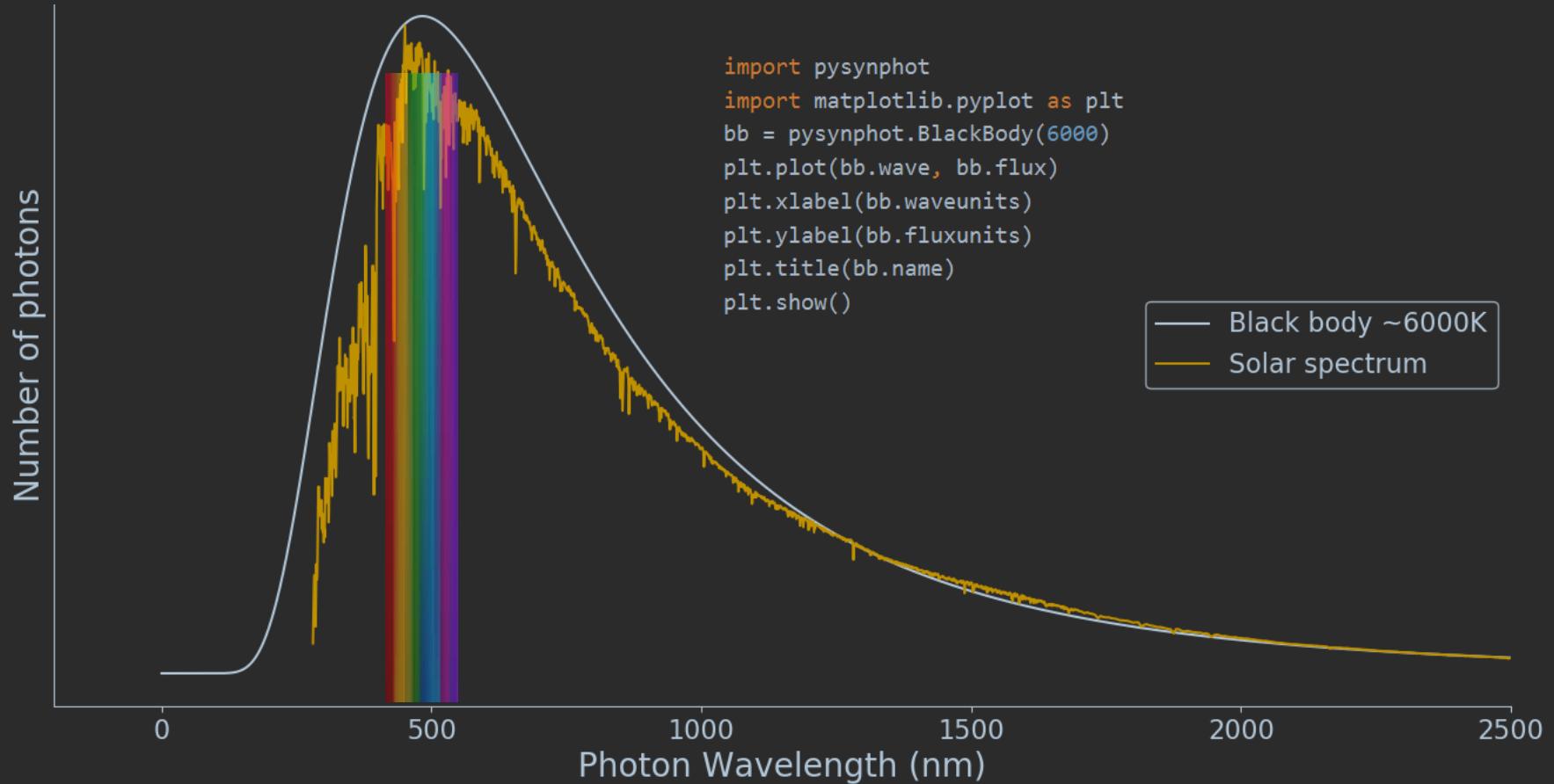
How to  
describe a bunch?  
A Histogram



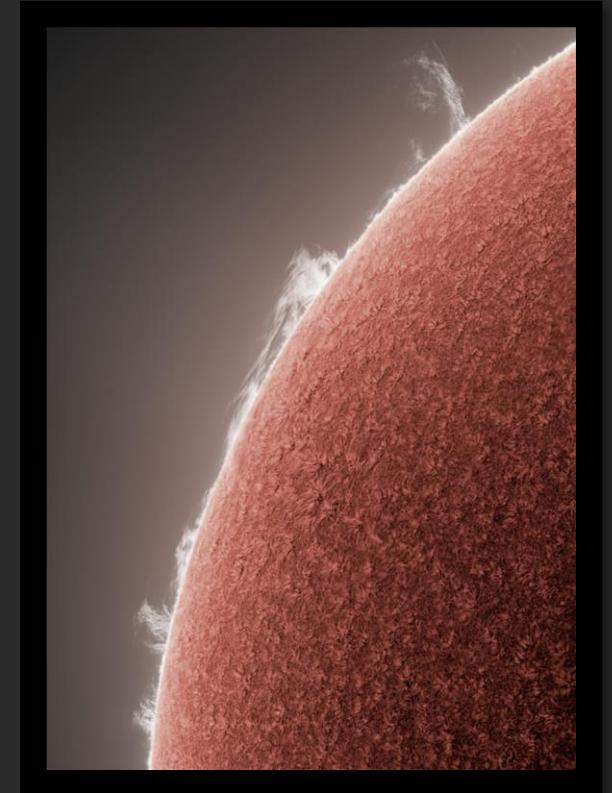
$$E = h\nu = \frac{hc}{\lambda}$$

Photon energy as a function of its frequency  
( $\nu$ ) and wavelength ( $\lambda$ ), where  $h$  is Planck's  
constant and  $c$  is the speed of light.

# A spectrum is a celestial histogram which disentangles the photons properties



Sun and black body spectra comparison at ~6000K. Most Earthlings vision has adapted to the atmospheric “window” at peak photons flux



Sun monochrome black and white camera picture courtesy Alan Friedman

# How to get spectra?



A) Download it!

# Astroquery package in The Astropy Project

Vamdc Queries (`astroquery.vamdc`)  
VizieR Queries (`astroquery.vizier`)  
VO Simple Cone Search (`astroquery.vo_conesearch`)  
VSA Queries (`astroquery.vsa`)  
xMatch Queries (`astroquery.xmatch`)  
ALFALFA Queries (`astroquery.alfalfa`)  
CosmoSim Queries (`astroquery.cosmosim`)  
Exoplanet Orbit Database (`astroquery.exoplanet_orbit_database`)  
Fermi Queries (`astroquery.fermi`)  
JPL Horizons Queries (`astroquery.jplhorizons/astroquery.solarsystem.jpl.horizons`)  
JPL SBDB Queries (`astroquery.jplsbdb/astroquery.solarsystem.jpl.sbdb`)  
LAMDA Queries (`astroquery.lamda`)  
NASA Exoplanet Archive (`astroquery.nasa_exoplanet_archive`)  
OAC API Queries (`astroquery.oac`)  
OGLE Queries (`astroquery.ogle`)  
Open Exoplanet Catalogue(`astroquery.open_exoplanet_catalogue`)  
SDSS Queries (`astroquery.sdss`)  
Spitzer Heritage Archive (`astroquery.sha`)

LMA Queries (`astroquery.alma`)  
Atomic Line List (`astroquery.atomic`)  
Besancon Queries (`astroquery.besancon`)  
Cadc (`astroquery.cadc`)  
CDS MOC Service (`astroquery.cds`)  
esa.hubble (`astroquery.esa.hubble`)  
ESASky Queries (`astroquery.esasky`)  
ESO Queries (`astroquery.eso`)  
Gaia TAP+ (`astroquery.gaia`)  
GAMA Queries (`astroquery.gama`)  
HEASARC Queries (`astroquery.heasarc`)  
HITRAN Queries (`astroquery.hitran`)  
IRSA Image Server program interface (IBE) Queries (`astroquery.ibe`)  
IRSA Queries (`astroquery.irsa`)  
IRSA Dust Extinction Service Queries (`astroquery.irsa_dust`)  
JPL Spectroscopy Queries (`astroquery.jplspec`)  
MAGPIS Queries (`astroquery.magpis`)  
MAST Queries (`astroquery.mast`)  
Minor Planet Center Queries (`astroquery.solarsystem.MPC`)  
NASA ADS Queries (`astroquery.nasa_ads`)  
NED Queries (`astroquery.ned`)  
NIST Queries (`astroquery.nist`)  
NRAO Queries (`astroquery.nrao`)  
NVAS Queries (`astroquery.nvas`)  
SIMBAD Queries (`astroquery.simbad`)  
Skyview Queries (`astroquery.skyview`)  
Splatatalogue Queries (`astroquery.splatalogue`)  
UKIDSS Queries (`astroquery.ukidss`)

# Finding objects by type and coordinates

```
from astroquery.vizier import Vizier
from astropy import coordinates
from astropy import units as u

v = Vizier(keywords=['stars:white_dwarf'])

c = coordinates.SkyCoord(0, 0, unit=('deg', 'deg'), frame='icrs')
result = v.query_region(c, radius=2*u.deg)

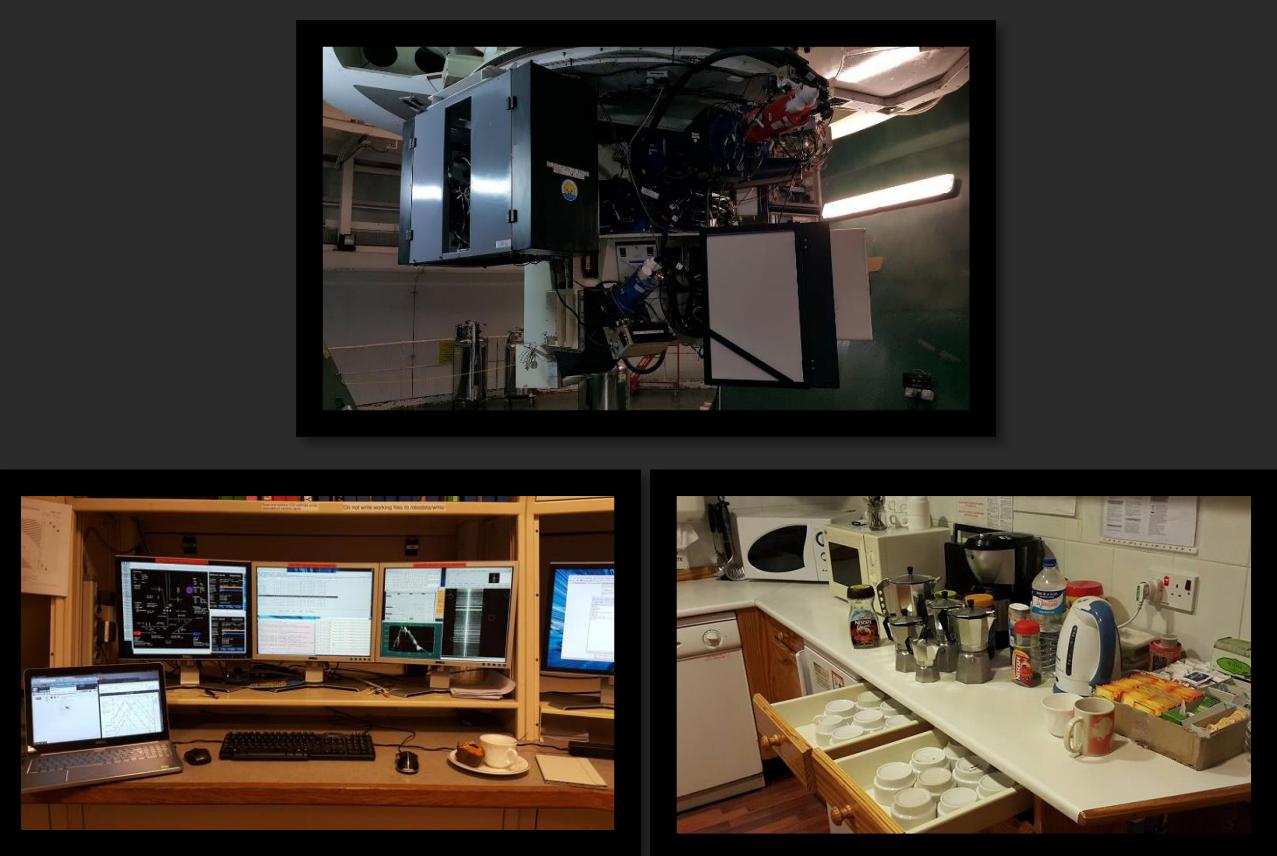
result[0].pprint()
```

LP	Rem	Name	RA1950	DE1950	...	pm	pmPA	_RA.icrs	_DE.icrs
			"h:m:s"	"d:m:s"	...	arcsec	/ yr	deg	"d:m:s"
-----	---	-----	-----	-----	...	-----	-----	-----	-----
584-0063			00 03 23	+00 01.8	...	0.219	93 00 05	56.8	+00 18 41
643-0083			23 50 40	+00 33.4	...	0.197	93 23 53	13.7	+00 50 15
584-0030			23 54 05	-01 32.3	...	0.199	193 23 56	38.8	-01 15 26

# B) Get your own

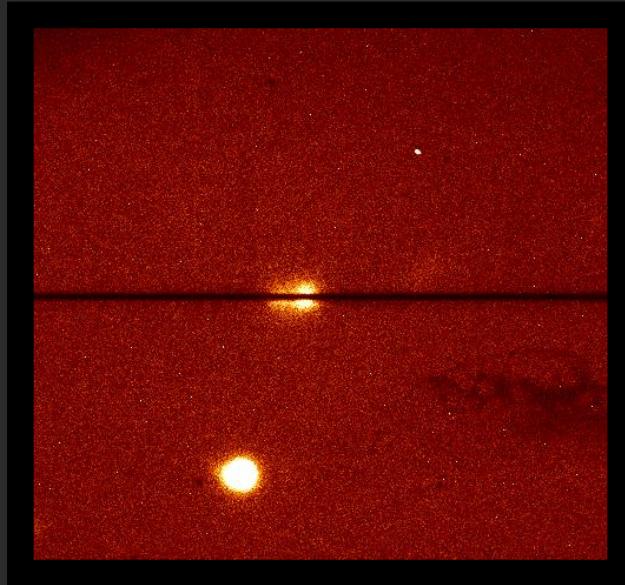


William Herschel Telescope at Roque de los  
Muchachos, isla La Palma, Canarias

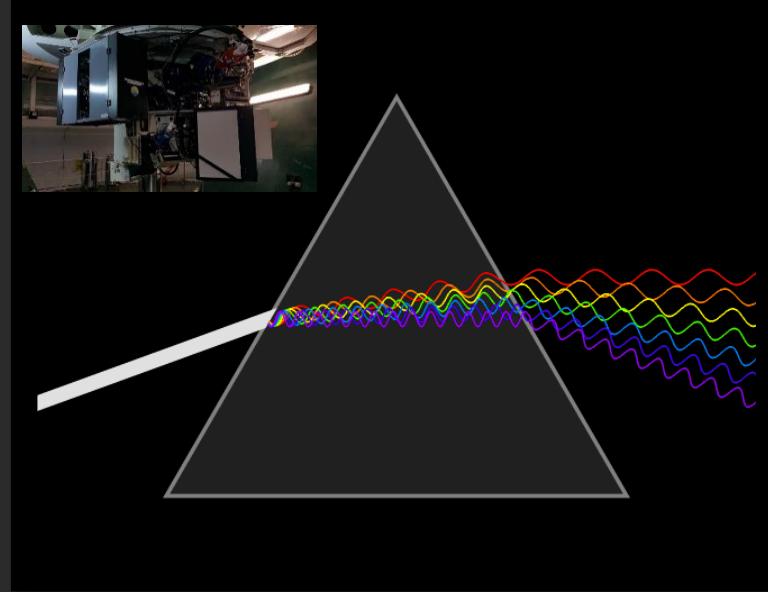
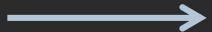


William Herschel Telescope insides

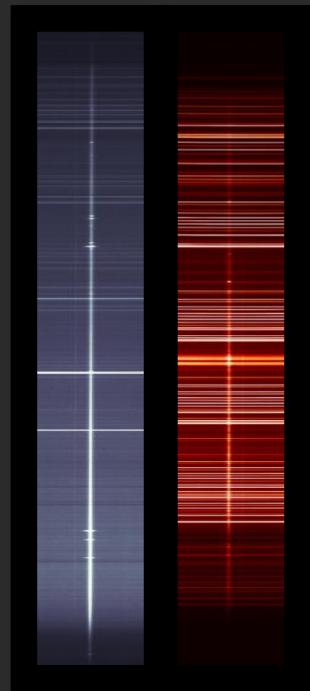
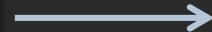
# So let's pick a galaxy



William Herschel Telescope  
instrument ISIS image  
acquisition of galaxy IZwicky18

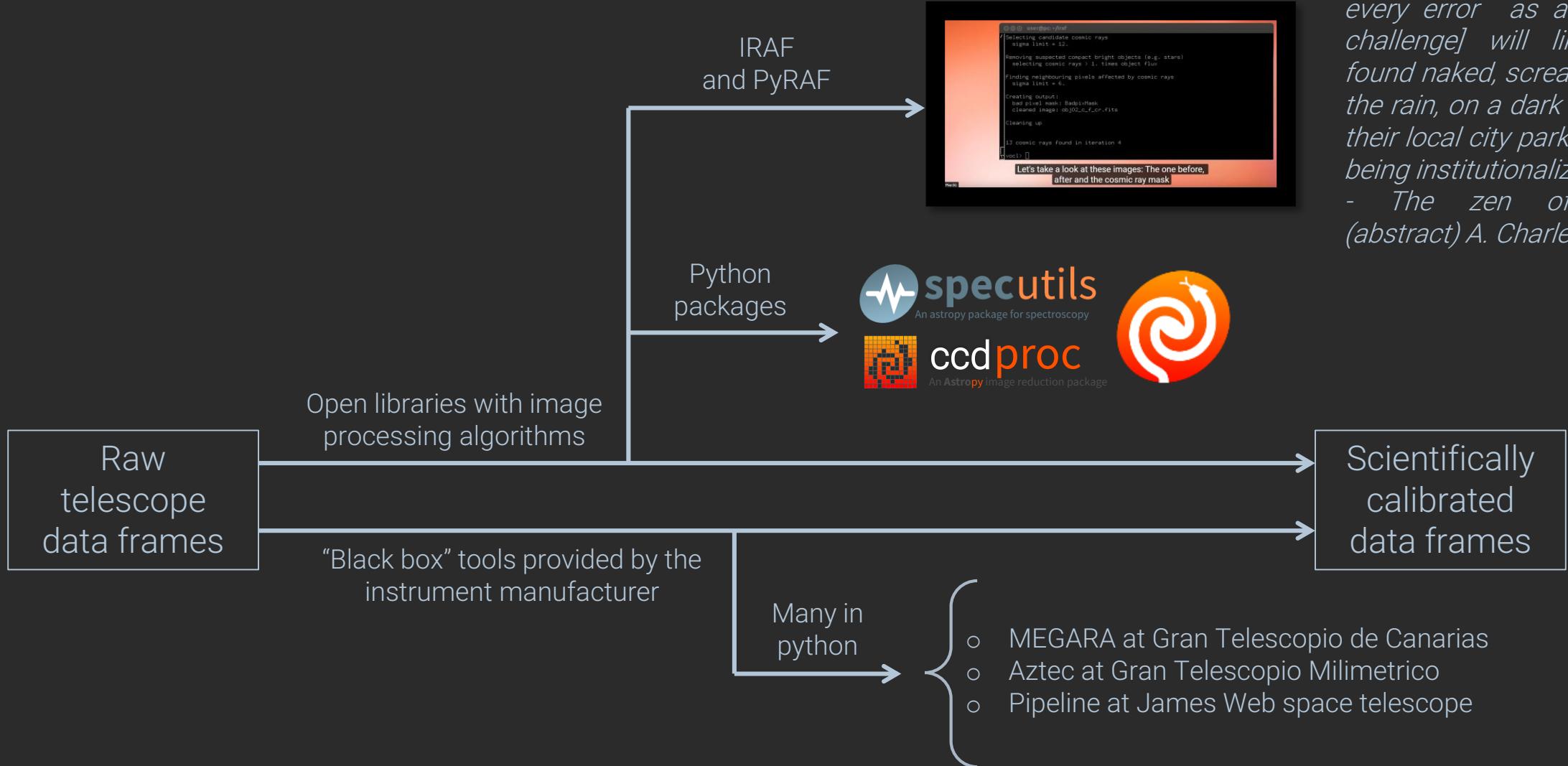


A spectrograph disperses the photons  
according to their wavelength



Output spectra 2D frames

# ... but you need to calibrate them



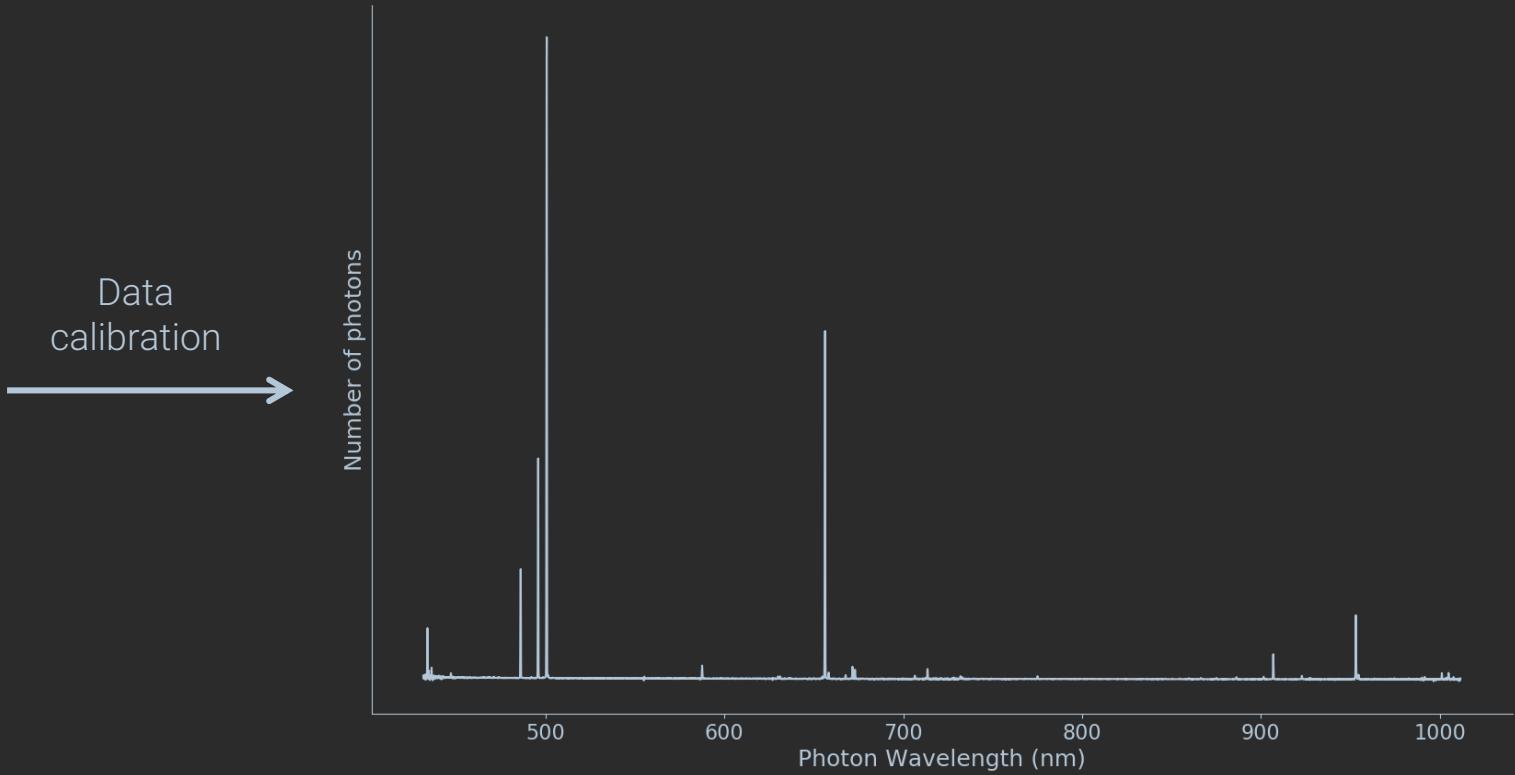
*The user who doesn't [see every error as a worthy challenge] will likely be found naked, screaming, in the rain, on a dark night, in their local city park prior to being institutionalized.*

- *The zen of IRAF (abstract)* A. Charles Pullen

# So let's take a look at this galaxy photons



Izwicky18 galaxy observation at the ~~Wubble~~  
space telescope

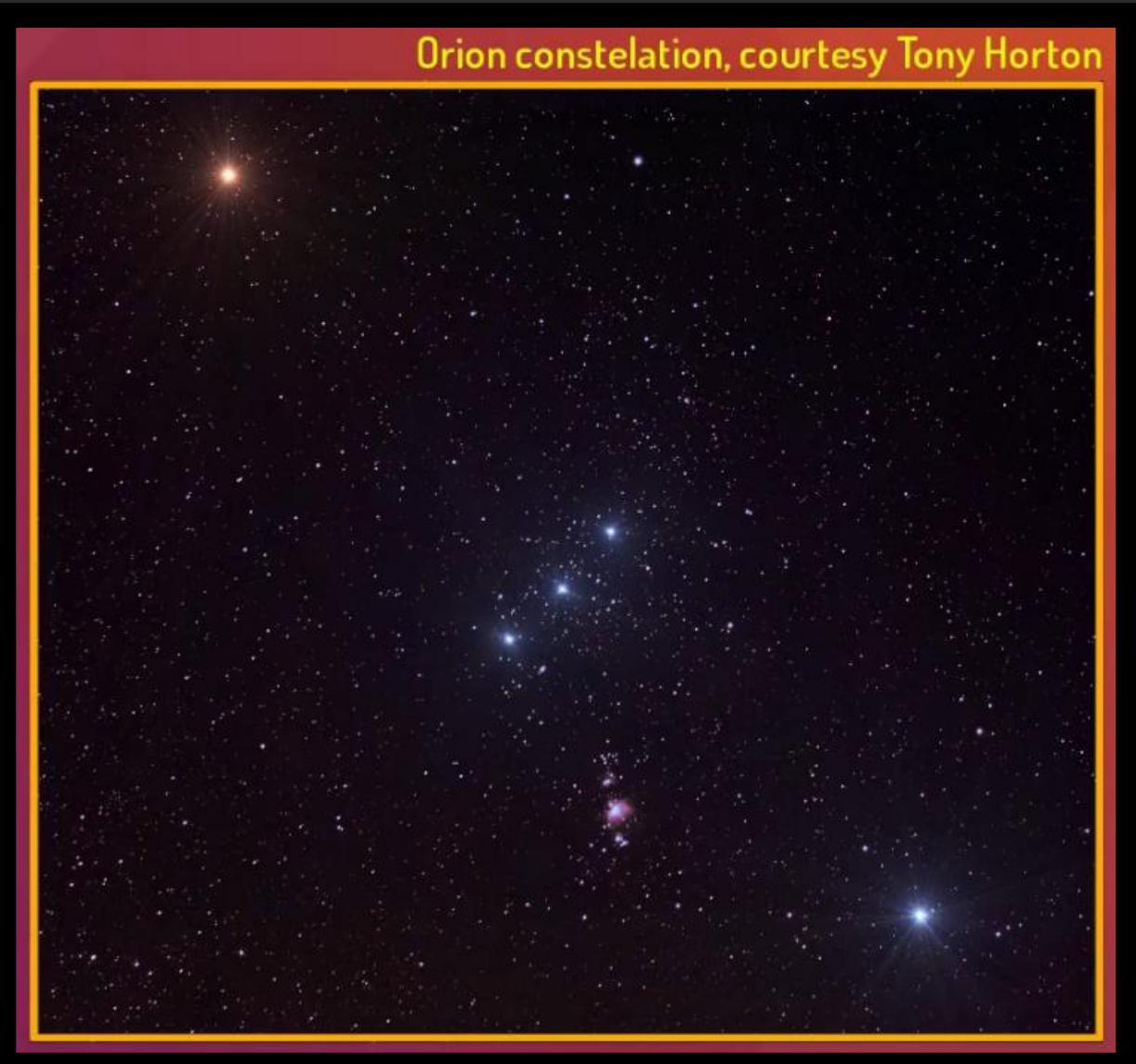


Izwycky18 spectrum from ISIS instrument at William Herschel telescope

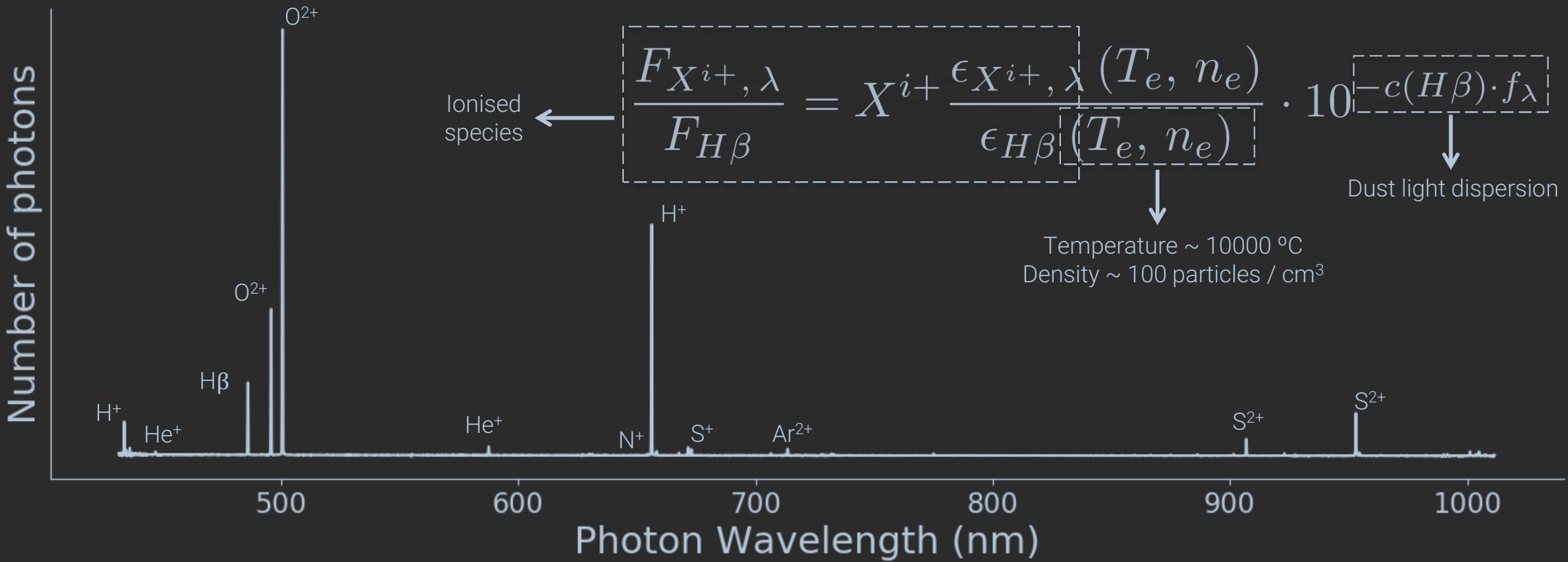
# Plasma ionisation process

Ionization process video tutorial in the orion Nebula  
using Cloudy (Ferland et al 2017) ([nublado.org](http://nublado.org))

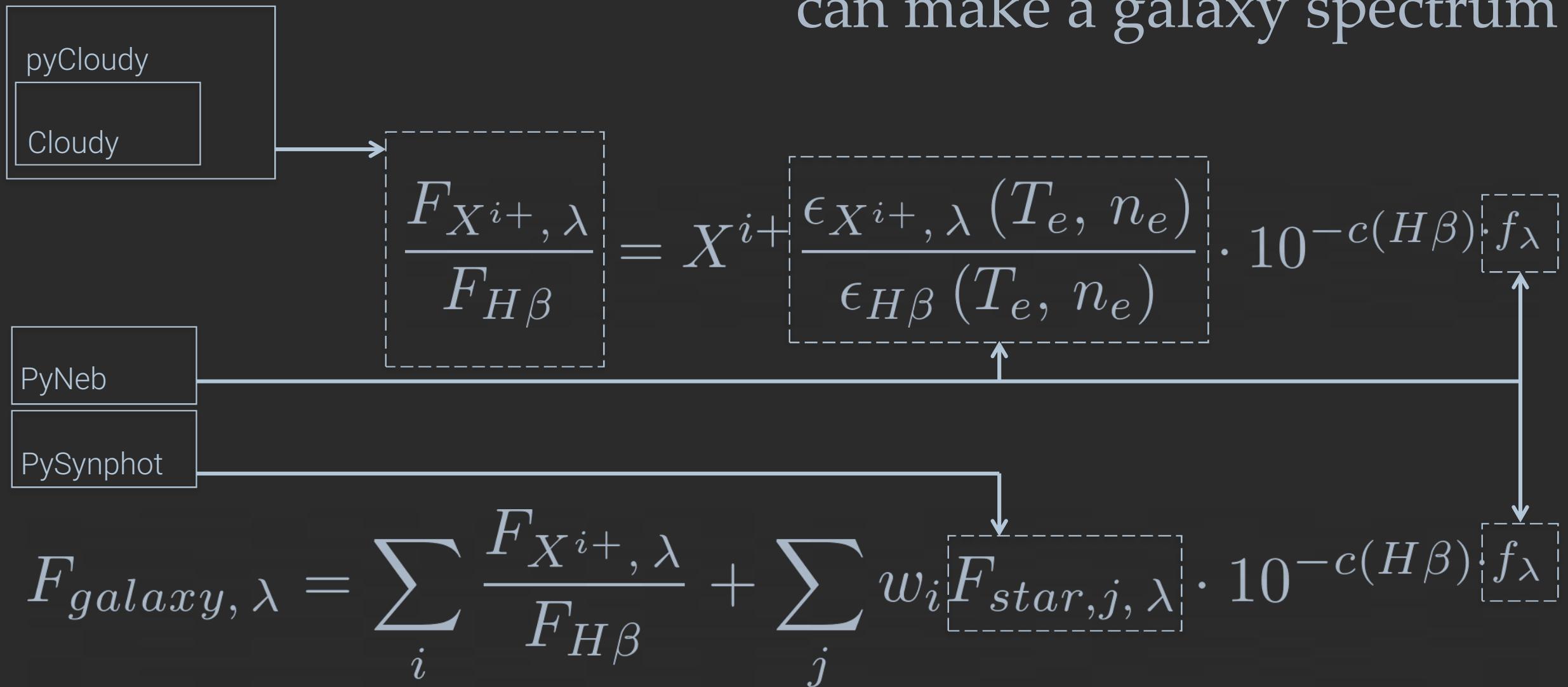
pyCloudy (Morisset et al 2016) can be used to lunch this  
program and extract its results efficiently



# The photon spikes provide us with the gas chemistry



With Python and a few equations you  
can make a galaxy spectrum



How to measure  
what a galaxy is made of?

# Solve system of equations:

$$\frac{F_\lambda}{F_{H\beta}} = He^{+\frac{\epsilon_{He^+, \lambda}(T_e, n_e)}{\epsilon_{H\beta}(T_e, n_e)}} \cdot 10^{-c(H\beta) \cdot f_\lambda}$$

$$\frac{F_\lambda}{F_{H\beta}} = He^{+\frac{\epsilon_{He^+, \lambda}(T_e, n_e)}{\epsilon_{H\beta}(T_e, n_e)}} \cdot 10^{-c(H\beta) \cdot f_\lambda}$$

$$\frac{F_\lambda}{F_{H\beta}} = He^{+\frac{\epsilon_{He^+, \lambda}(T_e, n_e)}{\epsilon_{H\beta}(T_e, n_e)}} \cdot 10^{-c(H\beta) \cdot f_\lambda}$$

$$\frac{F_\lambda}{F_{H\beta}} = He^{2+\frac{\epsilon_{He2+, \lambda}(T_e, n_e)}{\epsilon_{H\beta}(T_e, n_e)}} \cdot 10^{-c(H\beta) \cdot f_\lambda}$$

$$\frac{F_\lambda}{F_{H\beta}} = H^+ \frac{\epsilon_{H^+, \lambda}(T_e, n_e)}{\epsilon_{H\beta}(T_e, n_e)} \cdot 10^{-c(H\beta) \cdot f_\lambda}$$

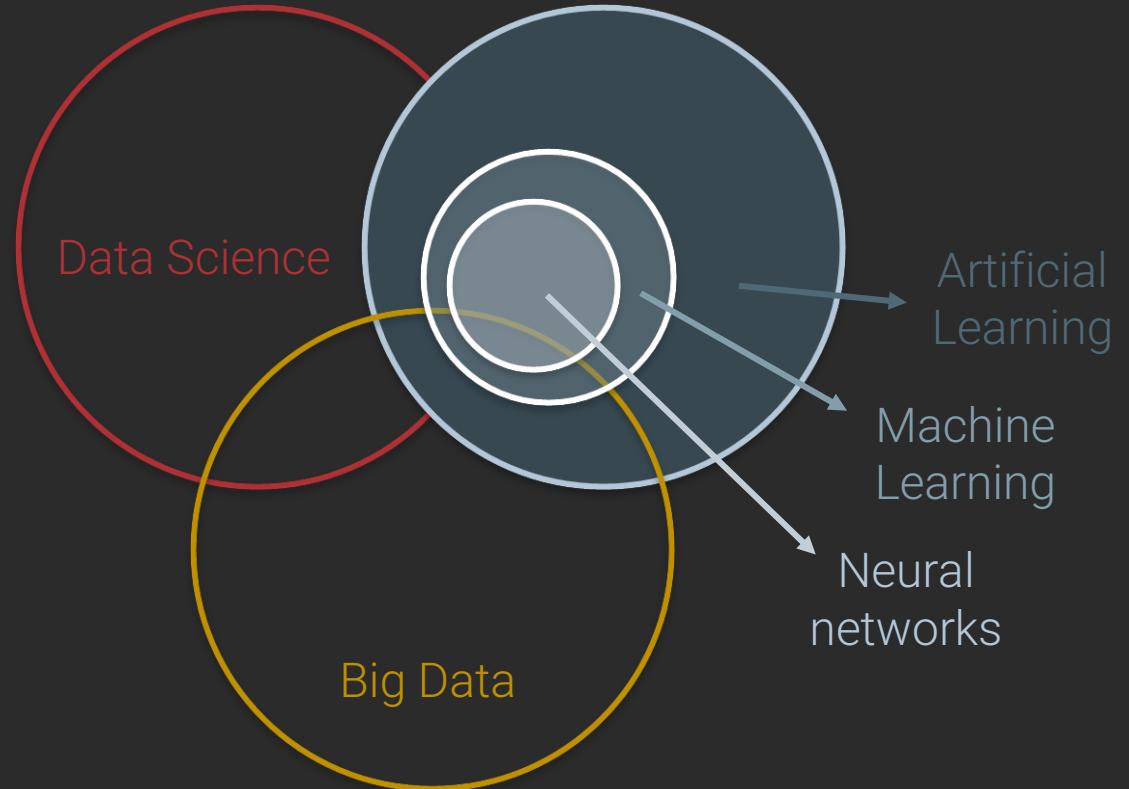
$$\frac{F_\lambda}{F_{H^+}} = H^+ \frac{\epsilon_{H^+, \lambda}(T_e, n_e)}{\epsilon_{H^+}(T_e, n_e)} \cdot 10^{-c(H\beta) \cdot f_\lambda}$$

$$\frac{F_\lambda}{F_{H\beta}} = O^+ \frac{\epsilon_{O^+, \lambda}(T_e, n_e)}{\epsilon_{H\beta}(T_e, n_e)} \cdot 10^{-c(H\beta) \cdot f_\lambda}$$

$$F_{H\beta}^{\lambda} = S^{2+\frac{\epsilon_{S^+,\lambda}(T_e,n_e)}{\epsilon_{H\beta}(T_e,n_e)}} \cdot 10^{-c(H\beta) \cdot f_\lambda}$$

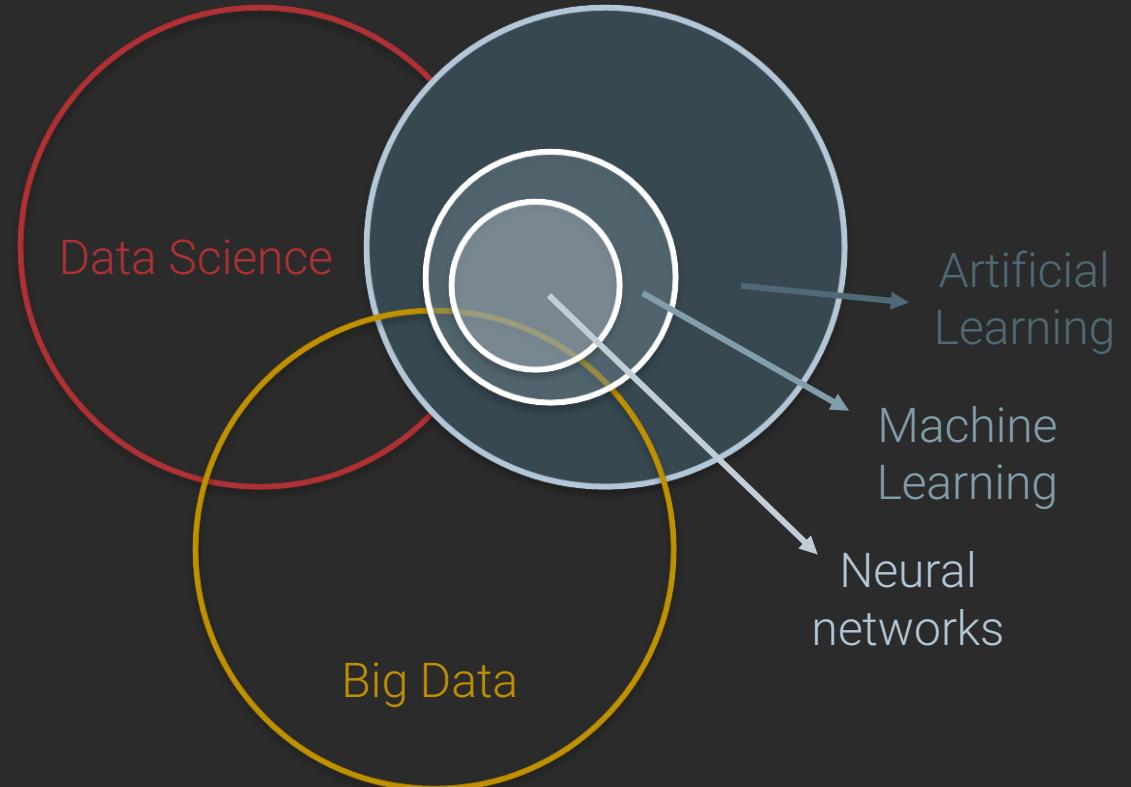
# We are still very far from Rosenblatt (1957) prediction:

Since the advent of electronic computers [...] an increasing amount of attention has been focused on the feasibility of constructing **a device possessing such human-like functions as perception, recognition, concept formation** and the ability to generalize from experience



We are still very far  
from Rosenblatt  
(1957) prediction:

a device  
capable of moving through very  
complex spaces



ESO (European Southern Observatory) Machine Learning workshop 2019  
(® Fraunhofer FOKUS)

Evaluate model against data

# Probabilistic programming library PyMC

PyMC2 implementing a  
Patil et al (2010)

PyMC3 implementing a  
Salvatier et al (2016)

PyMC4 implementing a

Programming  
language package

MCMC algorithm using a  
Markov Chain Monte Carlo

HMC algorithm using a  
Hamiltonian Monte Carlo

HMC algorithm using a  
Hamiltonian Monte Carlo

Mathematical  
principle

Adaptive metropolis sampler based on  
Haario et al (2001)

NUTs sampler based on  
Hoffman et al. (2011)

NUTs sampler based on  
Hoffman et al. (2011)

Numerical  
model

numpy arrays  
Oliphant (2006)

tensors  
Theano Development Team (2016)

tensors  
Tensorflow by Abadi et al  
(2016)

Memory  
unit

# Probabilistic programming library PyMC

PyMC2 implementing a MCMC algorithm using a Adaptive metropolis sampler based on numpy arrays

- Advantages: Easy to use, great compatibility with external libraries
- Disadvantages: Poor convergence and speed as the number of dimensions increases  $O(D^2)$

PyMC3 implementing a HMC algorithm using a NUTs sampler based on tensors

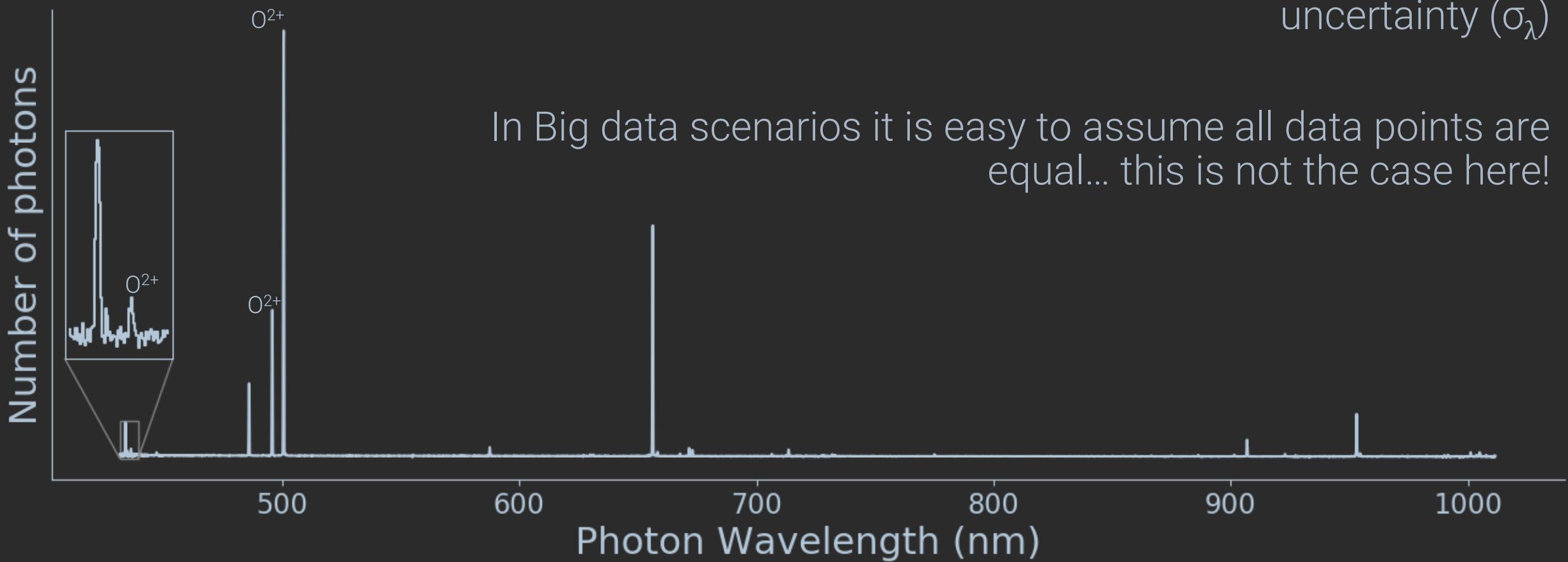
- Advantages: Great convergence and speed for complex models  $O(D^{5/4})$
- Disadvantages: Hard to code and incompatible with external functions

PyMC4 implementing a HMC algorithm using a NUTs sampler based on tensors

- Advantages: Larger Tensorflow community
- Disadvantages: In development

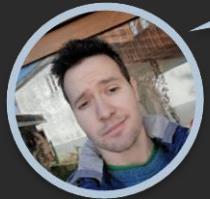
# We have two inputs:

Emission line photons flux ( $F_\lambda$ ) from every transition and its uncertainty ( $\sigma_\lambda$ )



Understanding measurement  
through its opposite: Uncertainty

# In a far away PyCon ...

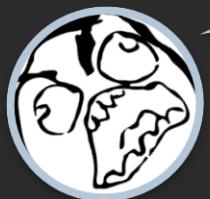


How would you handle data points which such different error magnitude?

Data does not have error



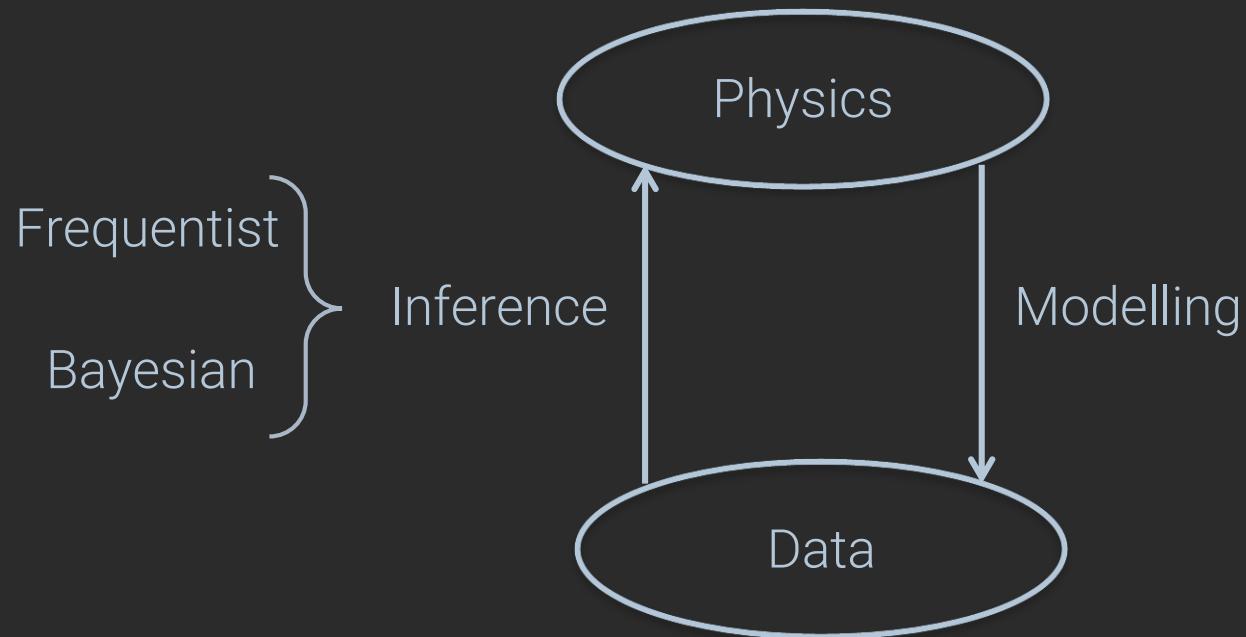
Chris Fonnesbeck  
core  
PyMC3 developer



FFFFFFFFFFFFFFUUUUUUUUUU

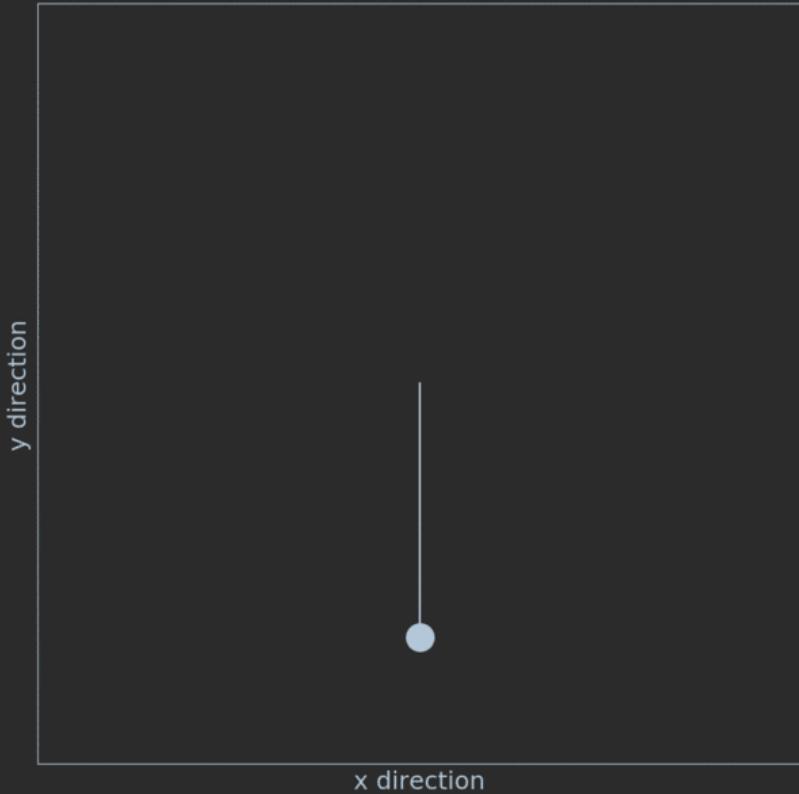
... Yet there is a lot of insight here

# Inference purpose



Uncertainty is the main disagreement between both inference paradigms

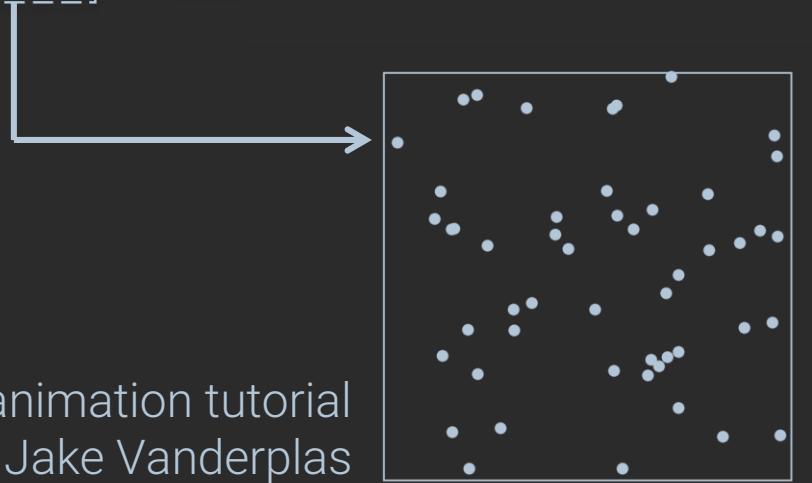
# Inference example: Pendulum period uncertainty



- **Frequentist interpretation:** The uncertainty is intrinsic to the measurement. As the sample size increases so does the accuracy and precision in your model parameters.
- **Bayesian interpretation:** The measurement is always true. Any intrinsic randomness is caused by the physical properties, which behave as a distribution. The more you sample this distribution the larger confidence you have in the physical properties.

# Another example: Electrons temperature in our model

$$\frac{F_{X^{i+}, \lambda}}{F_{H\beta}} = X^{i+} \frac{\epsilon_{X^{i+}, \lambda}(T_e, n_e)}{\epsilon_{H\beta}(T_e, n_e)} \cdot 10^{-c(H\beta) \cdot f_\lambda}$$



Matplotlib animation tutorial  
Jake Vanderplas

It can be proven that the plasma temperature behaves as a gaussian distribution because the electrons speed follows a gaussian Maxwellian distribution

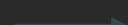
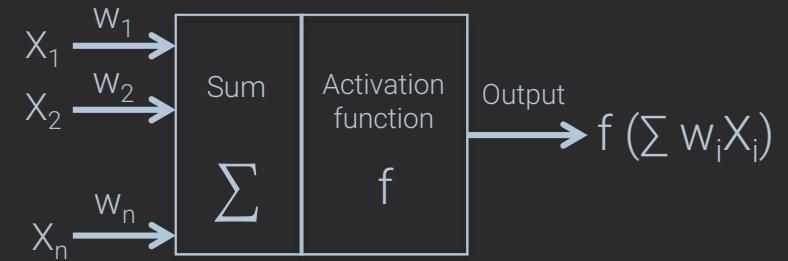
# Which inference paradigm to follow?

- Both frequentist and Bayesian schemes provide useful tools to fit a model to data
- Moreover, the numerical implementation can be very similar for both principles

# In practice, however, all Probabilistic programming libraries are intrinsically Bayesian

- A Bayesian model is easier to implement in high dimensional models
- A Bayesian model has a large affinity with neural networks

$$P(\theta|y) = \frac{P(y|\theta) P(\theta)}{P(y)}$$



# What does a probabilistic programming library do for you?

$$P(\theta|y) = \frac{P(y|\theta) P(\theta)}{P(y)}$$

- Sample: Draw values from probability distributions
- Condition: Use input data to update probabilities
- Infer: Measure something from the data given a model

$$P(\theta|y) = \frac{P(y|\theta) P(\theta)}{P(y)}$$

## Prior definition

$P(\theta)$  represents our knowledge on the model parameters before seeing any data

Un-informative priors are expected since they cover a wide parameter range and have small impact in the sampling

In contrast, formative priors are commonly criticised because they condition the sampling.

$$P(\theta|y) = \frac{P(y|\theta) P(\theta)}{P(y)}$$

Pymc3 prior definition

```
import pymc3

with pymc3.Model() as model:

    T_low = pymc3.Normal('Temperature_low', mu=15000.0, sd=5000.0)
    T_high = pymc3.Normal('Temperature_high', mu=15000.0, sd=5000.0)
    n_e = pymc3.Normal('density', mu=75.0, sd=25.0)
    cHbeta = pymc3.Lognormal('cHbeta', mu=0, sd=1)
    O2 = pymc3.Normal('O^+ abundance', mu=5.0, sd=5.0)
    O3 = pymc3.Normal('O^2+ abundance', mu=5.0, sd=5.0)
    S2 = pymc3.Normal('S^+ abundance', mu=5.0, sd=5.0)
    S3 = pymc3.Normal('S^2+ abundance', mu=5.0, sd=5.0)
    Ar3 = pymc3.Normal('Ar^2+ abundance', mu=5.0, sd=5.0)
    Ar4 = pymc3.Normal('Ar^3+ abundance', mu=5.0, sd=5.0)
    N2 = pymc3.Normal('N^+ abundance', mu=5.0, sd=5.0)
    He1 = pymc3.Lognormal('He^1+ abundance', mu=0, sd=1) * 0.01
    He2 = pymc3.Lognormal('He^2+ abundance', mu=0, sd=1) * 0.001
```

# Compute the theoretical model from these variables

$$\frac{F_{X^{i+}, \lambda}}{F_{H\beta}} = X^{i+} \frac{\epsilon_{X^{i+}, \lambda}(T_e, n_e)}{\epsilon_{H\beta}(T_e, n_e)} \cdot 10^{-c(H\beta) \cdot f_\lambda}$$

```
import theano.tensor as tt
from theano import function

def emisRatioFunction(temp, den, k1, k2, k3, k4):
    return k1 + k2 / (temp / 10000.0) + k3 * tt.log10(temp / 10000) + tt.log10(1 + k4 * den)

def fluxFunction(abund, emisRatio, flambda, cHbeta):
    return abund * emisRatio * tt.power(10, - cHbeta * flambda)

temp, den, k1, k2, k3, k4 = tt.dscalars('temp', 'den', 'k1', 'k2', 'k3', 'k4')
abund, emisRatio, flambda, cHbeta = tt.dscalars('abund', 'emisRatio', 'flambda', 'cHbeta')

emisRatio_tFunction = function(inputs=[temp, den, k1, k2, k3, k4],
                               outputs=emisRatioFunction(temp, den, k1, k2, k3, k4),
                               on_unused_input='ignore')

flux_tFunction = function(inputs=[abund, emisRatio, flambda, cHbeta],
                          outputs=fluxFunction(abund, emisRatio, flambda, cHbeta),
                          on_unused_input='ignore')
```

$$P(\theta|y) = \frac{P(y|\theta) P(\theta)}{P(y)}$$

Likelihood definition

$P(y | \theta)$  it provides an evaluation between the theory and the data



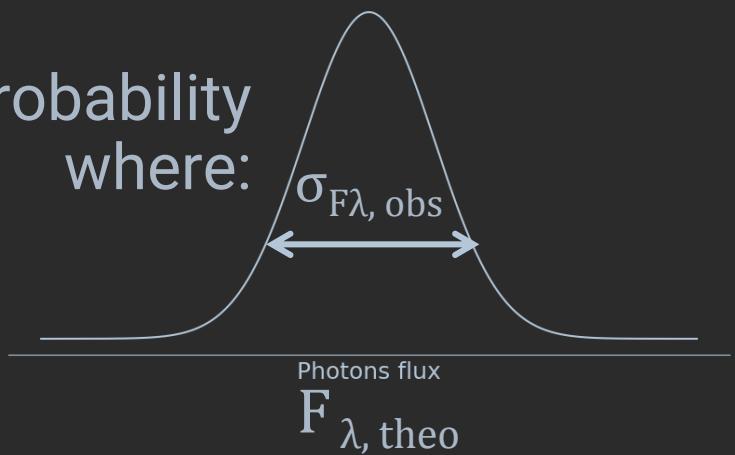
How would you handle data points which  
such different error magnitude?

... one way to do it

$$P(\theta|y) = \frac{P(y|\theta) P(\theta)}{P(y)}$$

Gaussian likelihood definition  
to account for data uncertainty

Define a normal likelihood probability  
where:



```
k1, k2, k3, k4 = coeffs_dict['O3']
emisRatio_i = emisRatio_tFunction(T_high, T_low, k1, k2, k3, k4)
theoFlux = flux_tFunction(O3, emisRatio_i, cHbeta, flamba_i)
likelihood_i = pymc3.Normal('likelihood_i', mu=theoFlux, sd=obsErr[i], observed=obsFlux[i])
```

$$\boxed{\frac{F_{X^{i+}, \lambda}}{F_{H\beta}} = X^{i+} \frac{\epsilon_{X^{i+}, \lambda}(T_e, n_e)}{\epsilon_{H\beta}(T_e, n_e)} \cdot 10^{-c(H\beta) \cdot f_\lambda}}$$

$$P(\theta|y) = \frac{P(y|\theta) P(\theta)}{P(y)}$$

Posterior definition

This is the result we want to compute. It provides us with the parameter credible region: "Given our observed data, there is a 95% probability that the true value lies in this distribution"

... but we are missing  $P(y)$ , the evidence. This is the probability the observational has been generated by the theoretical model.

$$P(y) = \int P(y|\theta) P(\theta) \leftarrow$$

# Posterior sampling



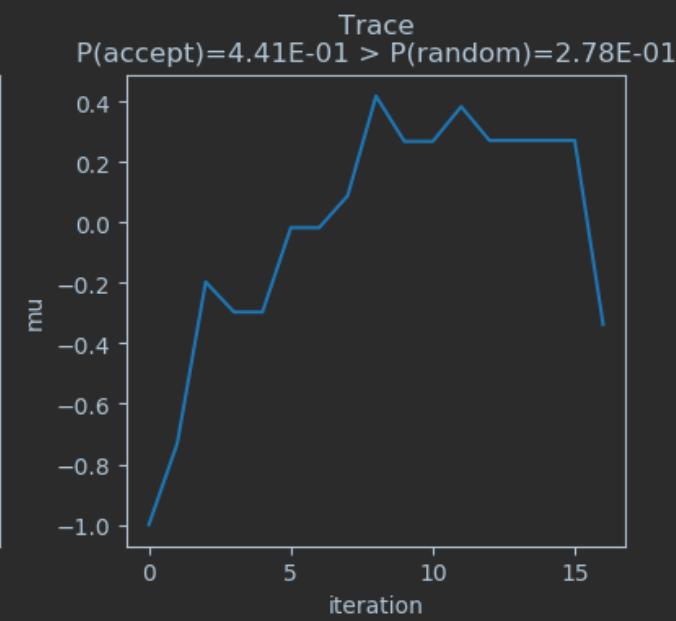
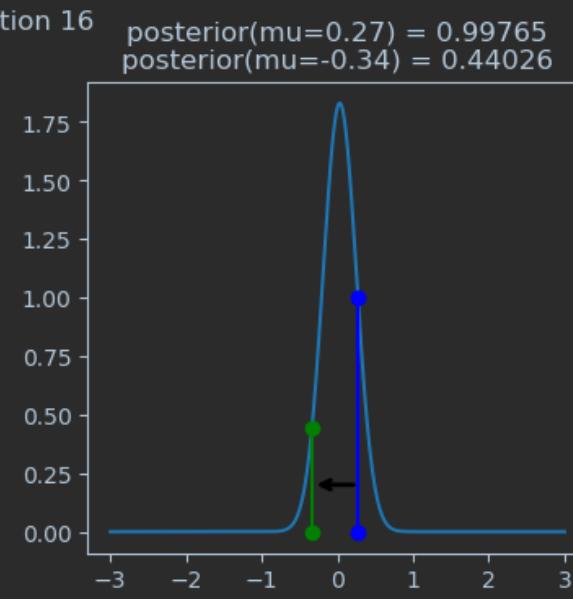
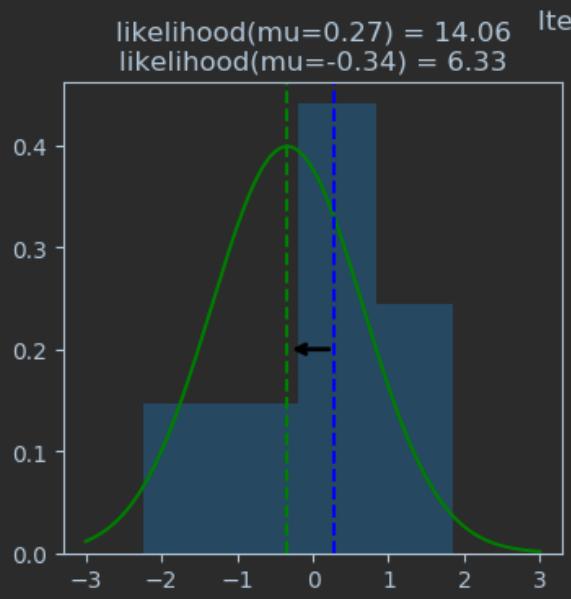
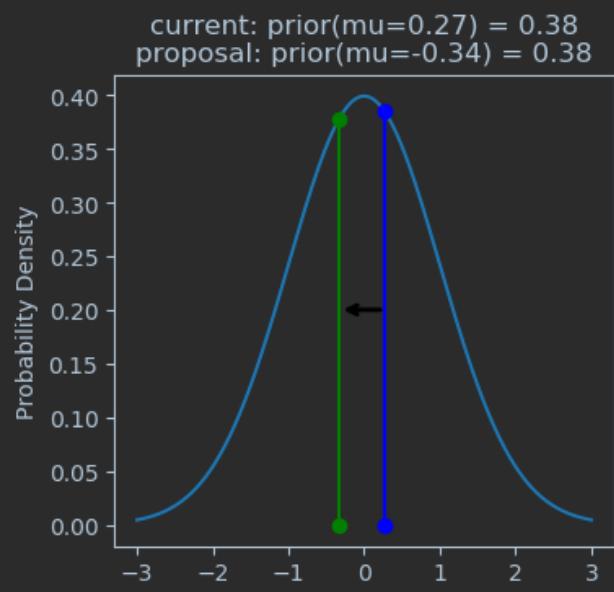
$$\frac{P(\theta|y)_{new}}{P(\theta|y)_{old}} = \frac{P(y|\theta)P(\theta)_{new}}{P(y|\theta)P(\theta)_{old}}$$

At each successful iteration, the sampler moves to a new coordinate and the posterior distribution gains a new value

A successful iteration does not always imply a coordinate with a higher probability

# Sampler philosophy

The Adaptive metropolis sampler believes that in your path you must fail as many times as you succeed



# Thomas Wiecki: MCMC sampling for dummies

# Sampler philosophy



The NUTs (No U Turns) sampler believes that if you have a **path guide**, you don't need to fail so many times.

The NUTS take advantage of the automatic gradient differentiation from the likelihood to reach the target coordinate.

It also avoids over sampling by avoiding U – Turns

# Finally you run it!

```
trace = pymc3.sample(draws=7000, tune=2000, chains=2, cores=2)
```

The diagram illustrates the parameters of the `pymc3.sample` function with the following annotations:

- Target simulation steps**: An annotation pointing to the `draws` parameter value `7000`.
- Number of simulations**: An annotation pointing to the `chains` parameter value `2`.
- Steps to adjust the simulation**: An annotation pointing to the `tune` parameter value `2000`.
- Number of CPUs for sampling**: An annotation pointing to the `cores` parameter value `2`.

How do we know  
the results are correct?

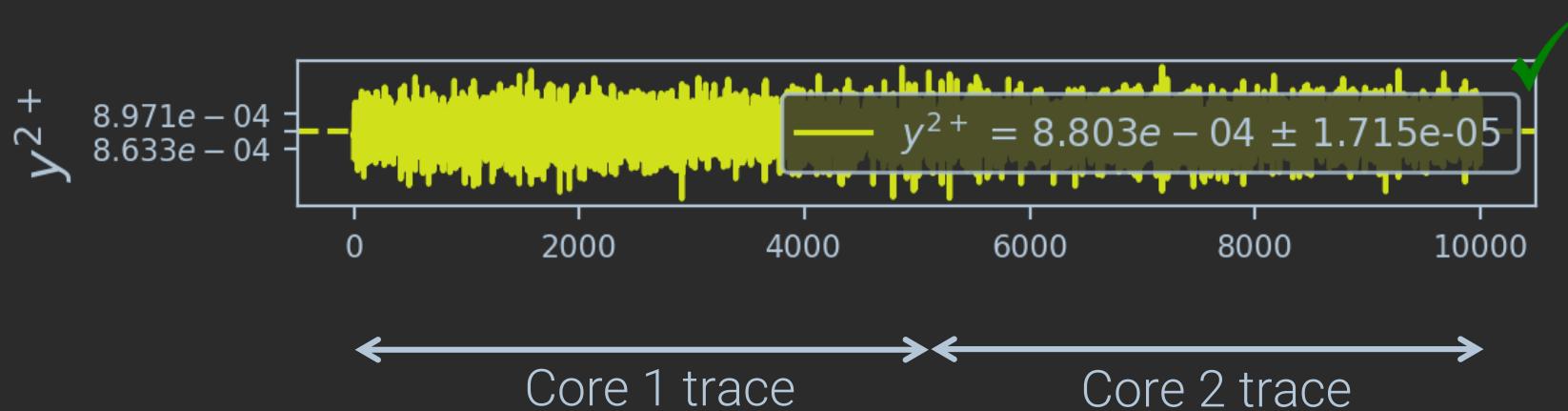
# Test fitting accuracy with synthetic data



$$\frac{F_{X^{i+}, \lambda}}{F_{H\beta}} = X^{i+} \frac{\epsilon_{X^{i+}, \lambda}(T_e, n_e)}{\epsilon_{H\beta}(T_e, n_e)} \cdot 10^{-c(H\beta) \cdot f_\lambda}$$

Parameter	True value
$T_{low}$	15590
$n_e$	500
$S^+$	5.48
$S^{2+}$	6.36
$O^+$	7.80
$O^{2+}$	8.05
$Ar^{2+}$	5.72
$Ar^{3+}$	5.06
$N^+$	5.84
$c(H\beta)$	0.100
$T_{high}$	16000
$y^+$	0.0850
$y^{2+}$	0.00088
$\tau$	1.0

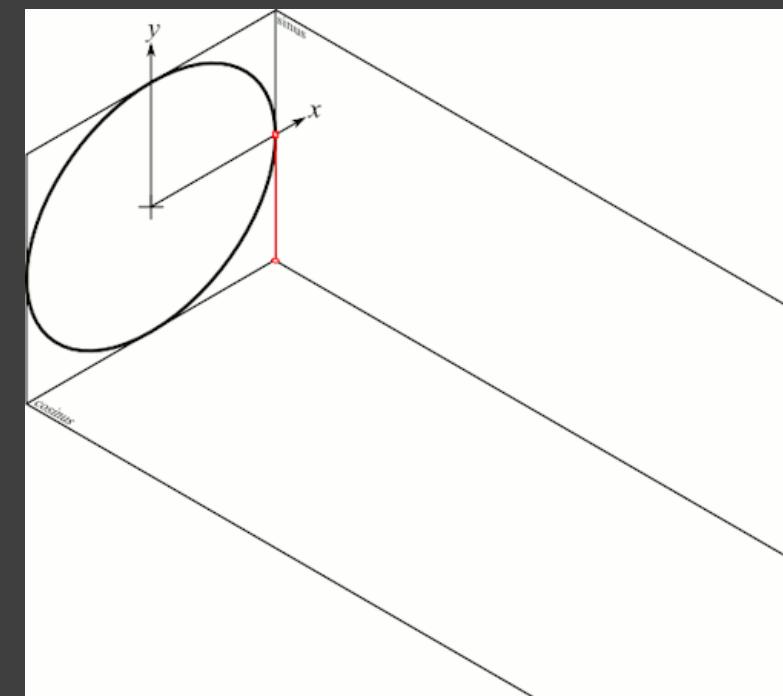
# Traces statistics



The traces represent each parameter coordinate during the simulation

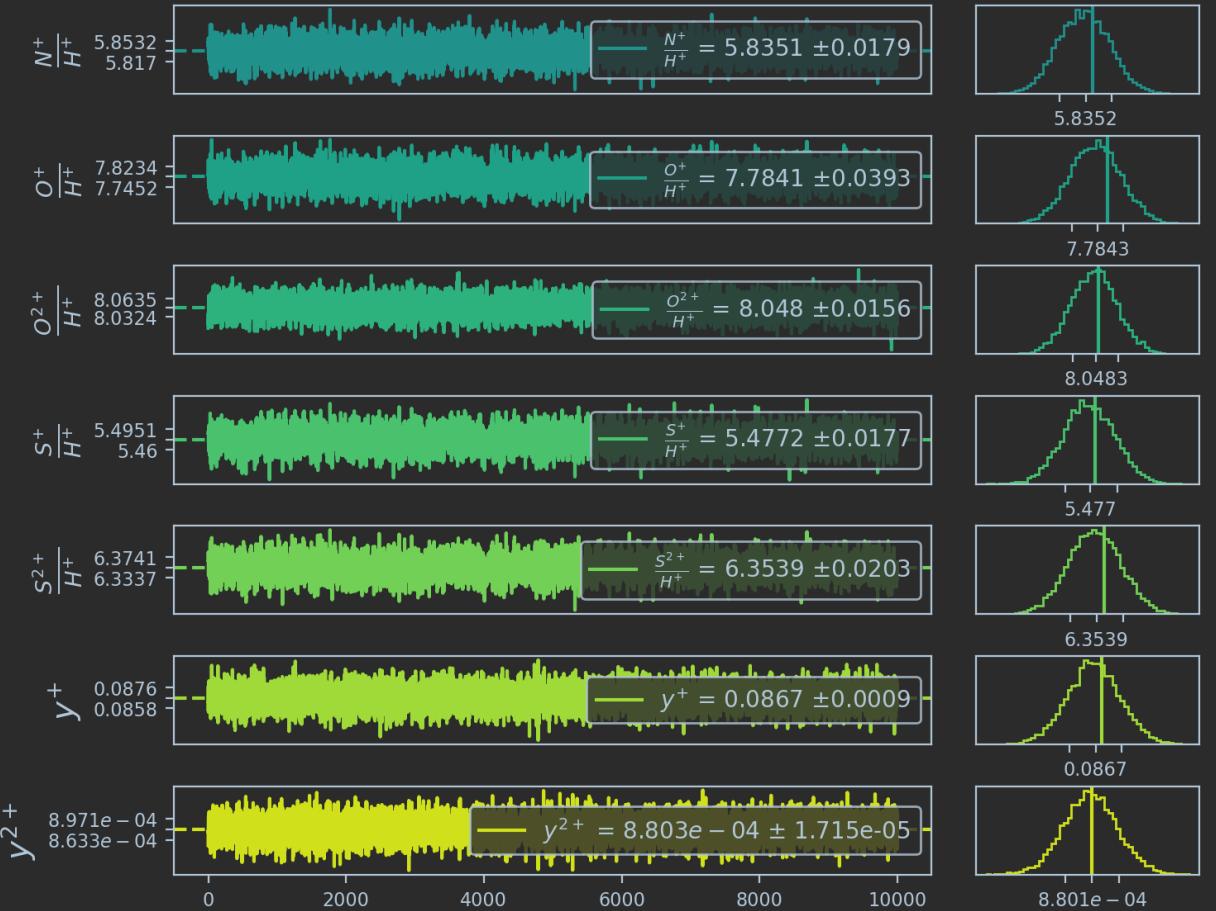
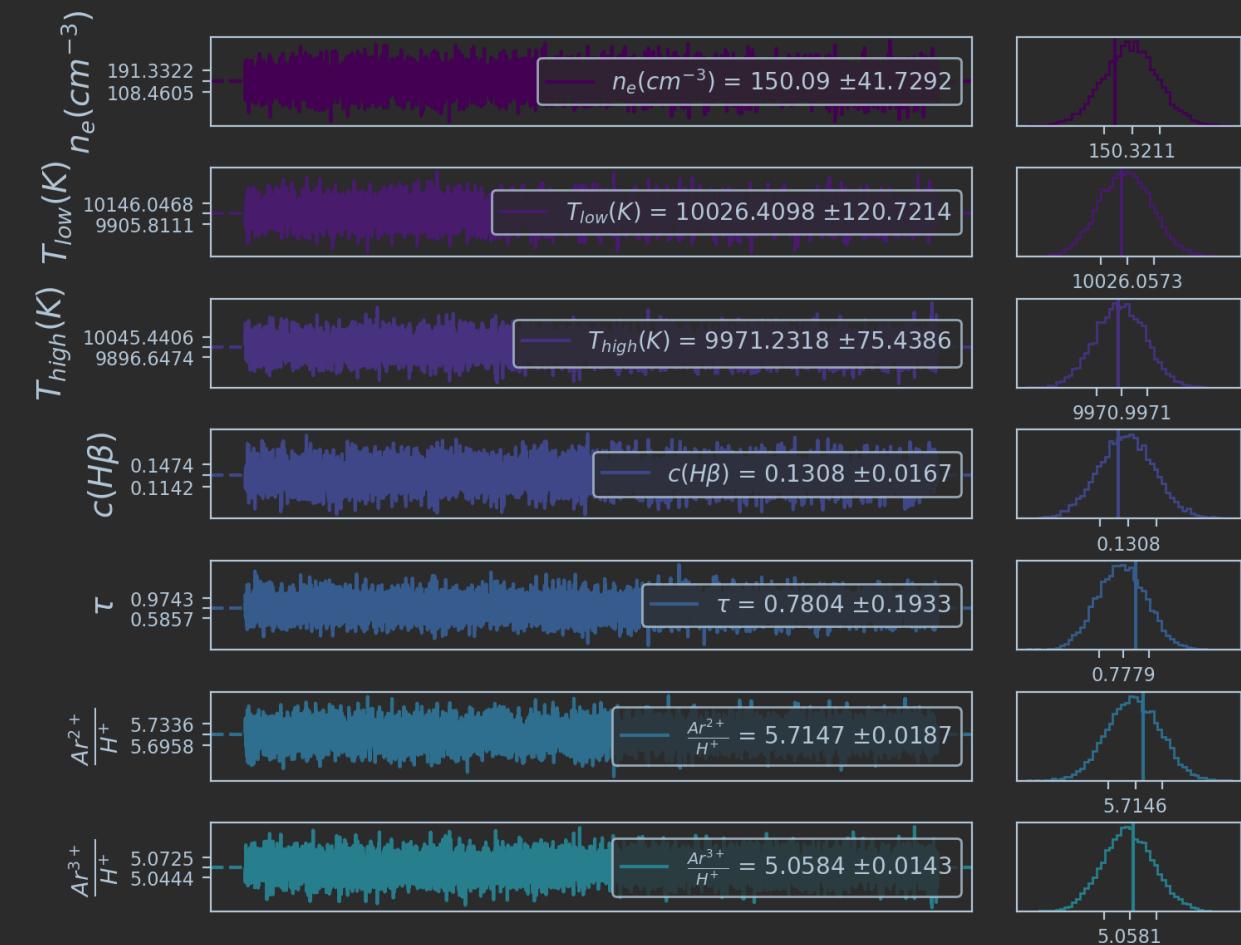
Graphical way to check for divergences in the chain but the probabilistic library should warn you

Several runs are necessary to confirm that the initial conditions are not affecting the results



Visualizing trigonometric waves from a circle.  
<https://gemmathematics.tumblr.com>

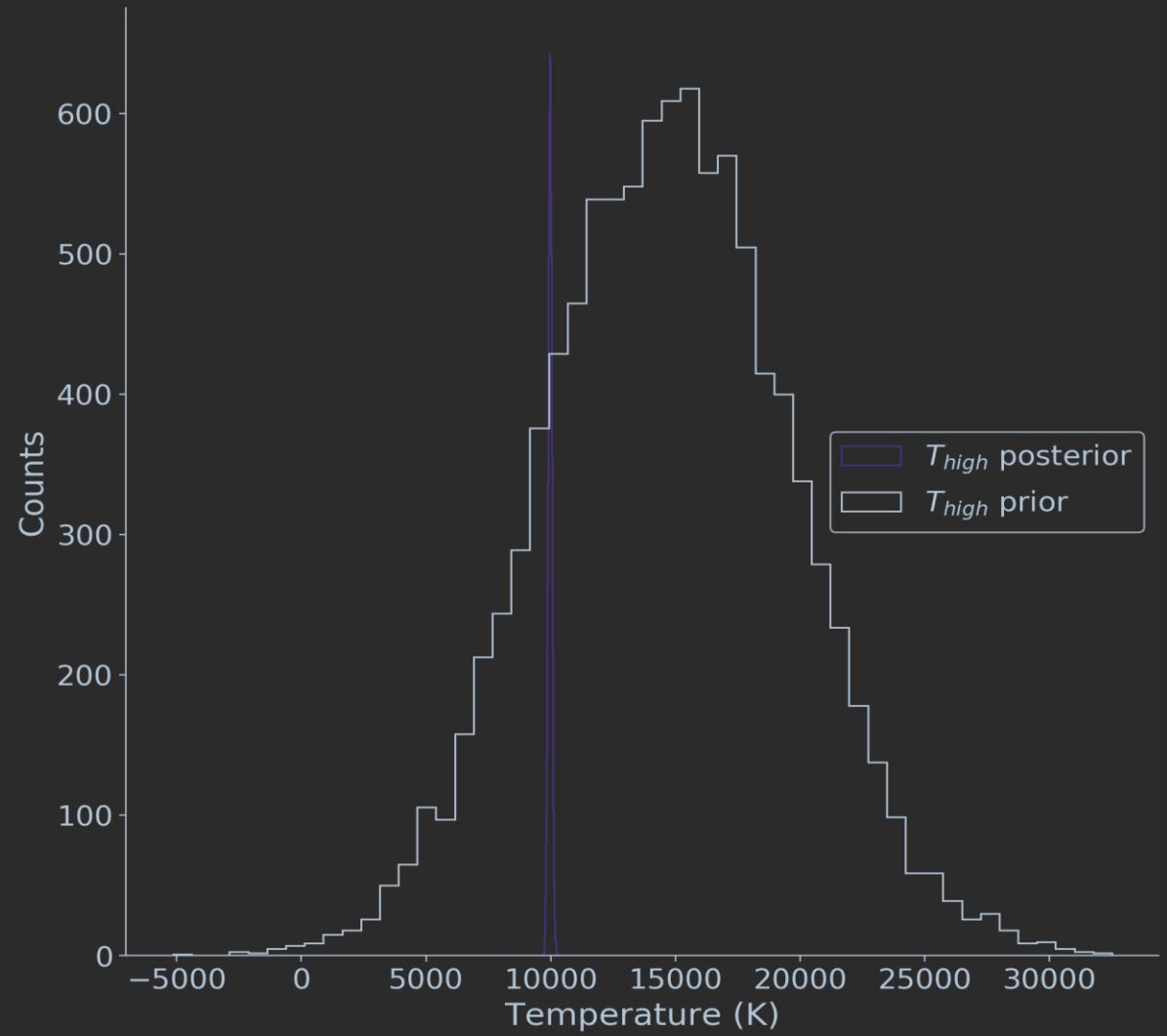
# Traces statistics



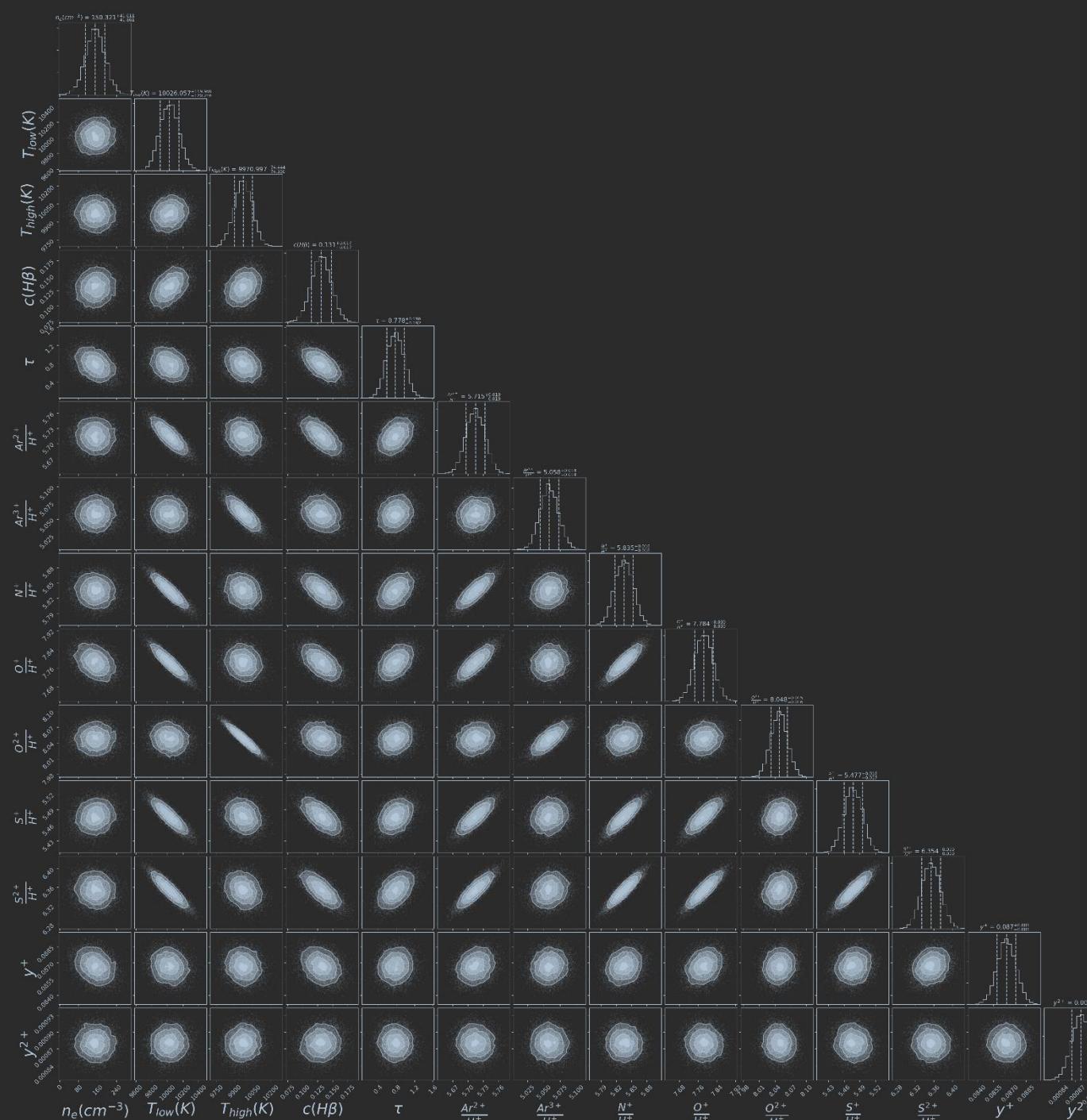
The trace histograms represent the posterior distributions

# Traces statistics

Prior – Posterior comparison

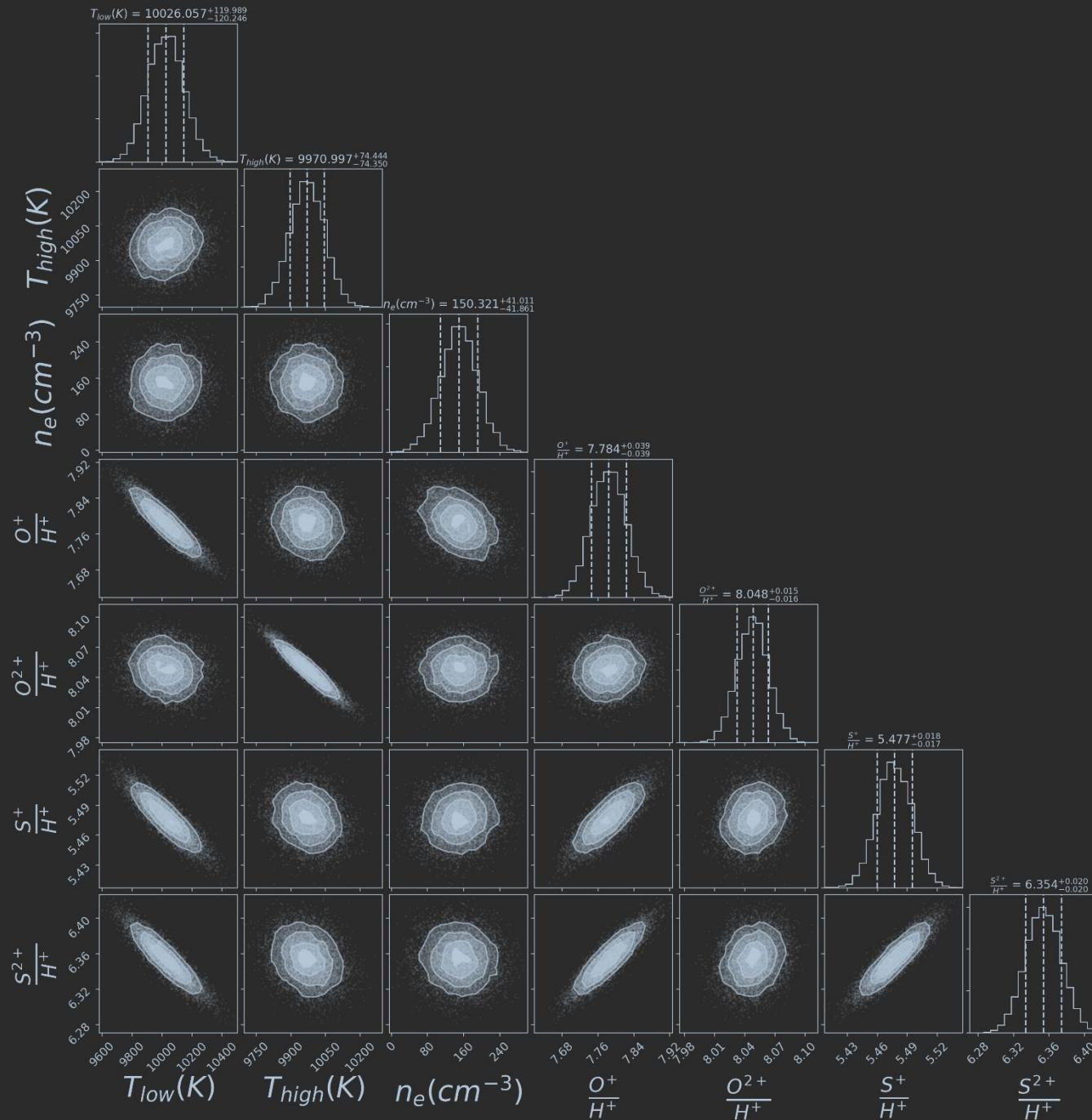


# Parameters correlation



Scatter plot matrix from  
corner.py by Foreman-Mackey

# Parameters correlation



Scatter plot matrix  
from corner.py by Foreman-Mackey

# Model reparameterization

$$\underbrace{X^{i+} = \sigma\theta + \mu}_{\frac{F_{X^{i+}, \lambda}}{F_{H\beta}} = X^{i+} \frac{\epsilon_{X^{i+}, \lambda}(T_e, n_e)}{\epsilon_{H\beta}(T_e, n_e)} \cdot 10^{-c(H\beta) \cdot f_\lambda}}$$

```
02_prior = pymc3.Normal('O^+ abundance', mu=0.0, sd=1.0)
02 = 5.0 * 02_prior + 5.0
```

- In this approach, we don't define the parameter space according to physical dimensions. Instead, we reshape it numerically model to make the parameter domains as even and linear as possible.
  - This makes the sampling faster and it can decrease the parameter correlation.

# Conclusions

- The Python community is responsible for remarkable break throughs in the astrophysics field
- Neural networks make possible the implementation of models with a size and complexity not seen before
- Probabilistic programing libraries, such as PyMC3, make the fitting of Bayesian models easy.  
However, it is necessary to be mindful of the results

# Some resources

For those interested in Probability theory:

- Michael Betancourt: Probability Theory (For Scientists and Engineers)  
[https://betanalpha.github.io/assets/case\\_studies/probability\\_theory.html](https://betanalpha.github.io/assets/case_studies/probability_theory.html)
- David S. Rosenberg: Foundations of Machine Learning  
<https://bloomberg.github.io/foml/#home>

## For those interested in PyMC3:

- Luciano Paz Blog

<https://lucianopaz.github.io/>

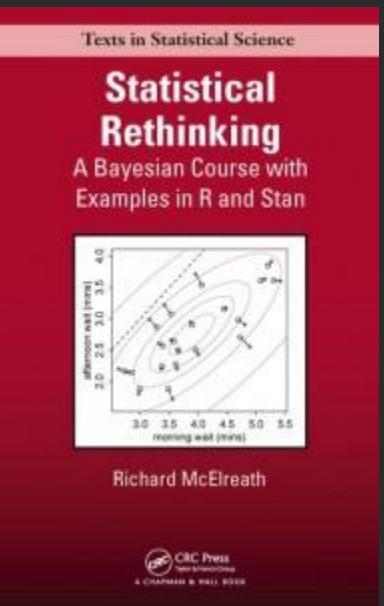
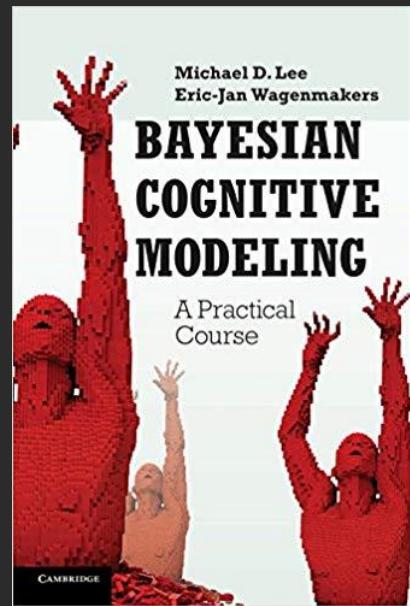
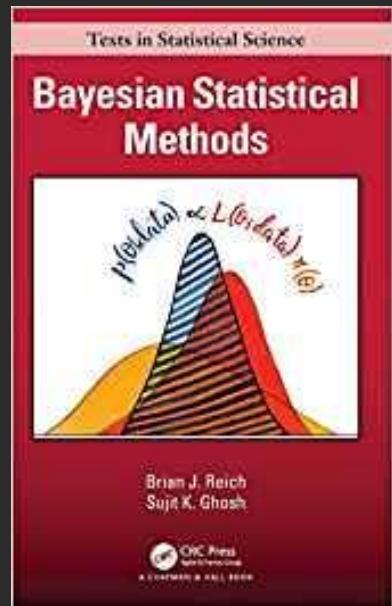
- Dan Foreman-Mackey

<https://dfm.io>

- Thomas Wiecki Blog

<https://twiecki.io/>

# For those interested in Bayesian statistics:



<https://github.com/pymc-devs/resources>

## Physical model

- Peimbert et al: Nebular Spectroscopy: A Guide on H ii Regions and Planetary Nebulae  
<https://doi.org/10.1088/1538-3873/aa72c3>
- Pérez Montero: Ionized gaseous nebulae chemical abundance determination using the direct method  
<https://doi.org/10.1088/1538-3873/aa5abb>
- Fernández et al (2018): Primordial helium abundance determination using sulfur as metallicity tracer  
<https://doi.org/10.1093/mnras/sty1206>
- Fernández et al (2019): A Bayesian direct method implementation to fit emission line spectra: Application to the primordial He abundance determination  
<https://doi.org/10.1093/mnras/stz1433>

Thank you very much!

Go NUTs !!!

