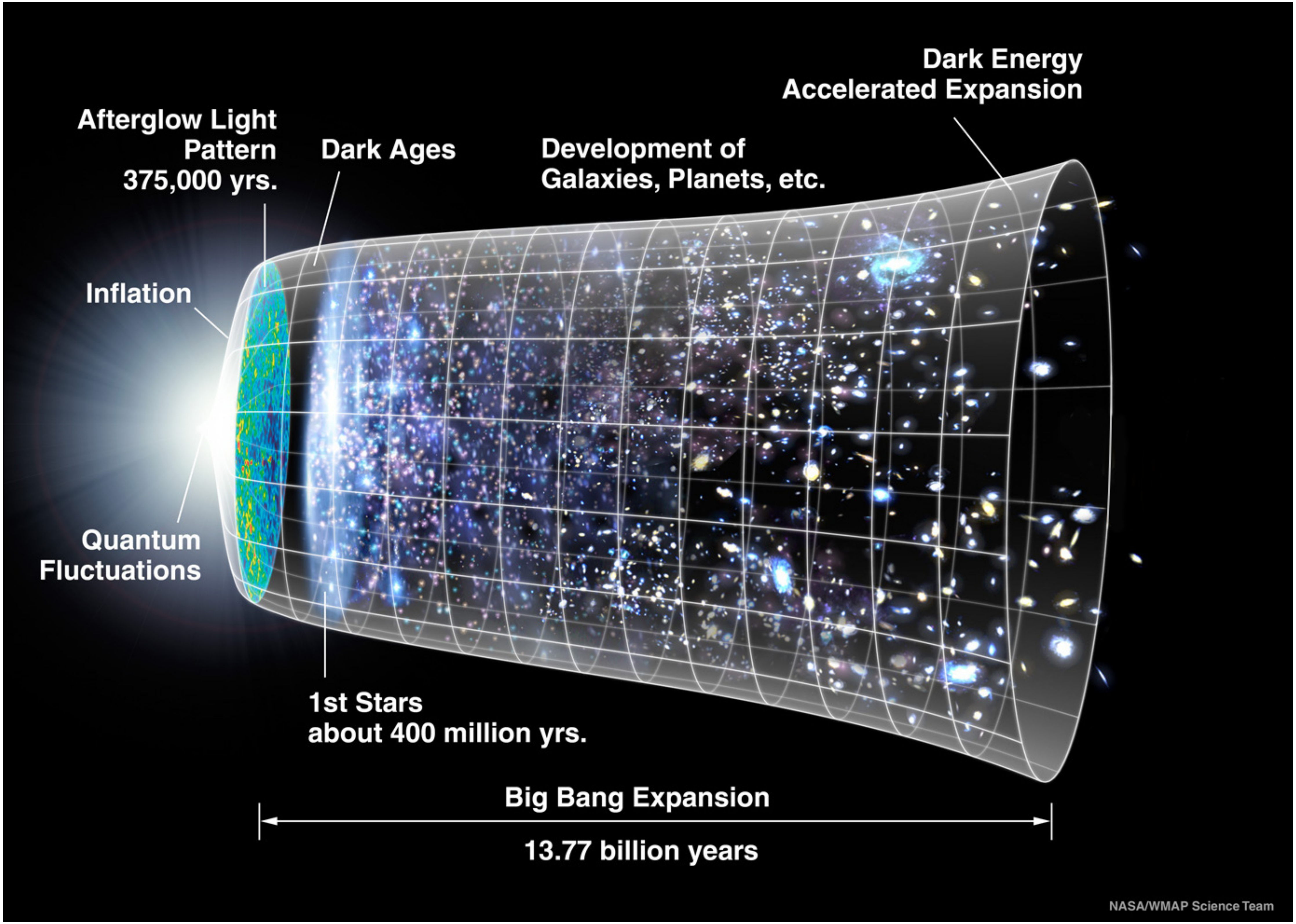
Machine learning classification and statistical analyses: challenges in supernova cosmology

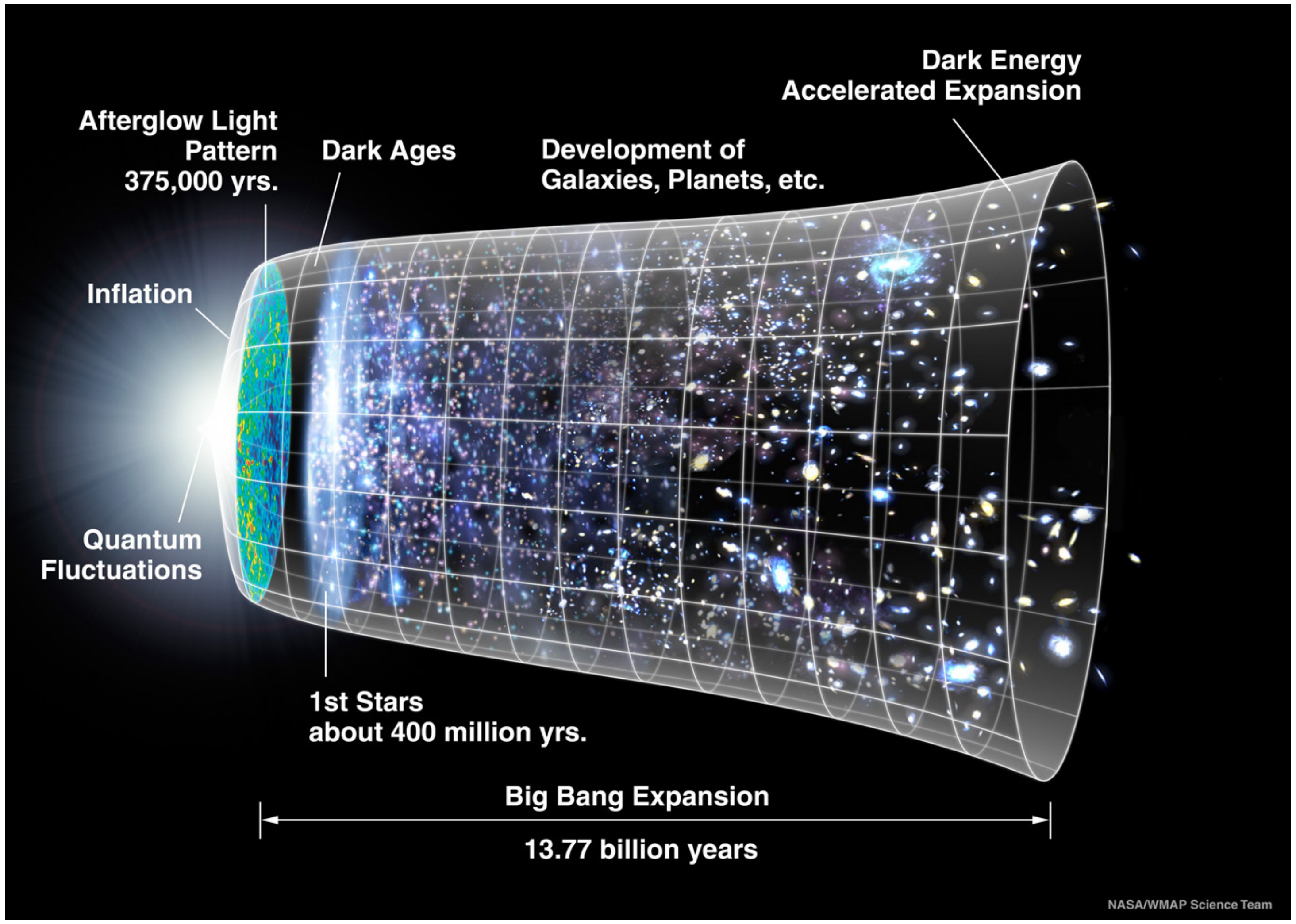
Anais Möller
CNRS / LPC Clermont

Advanced Pattern Recognition workshop
October 23rd, 2019

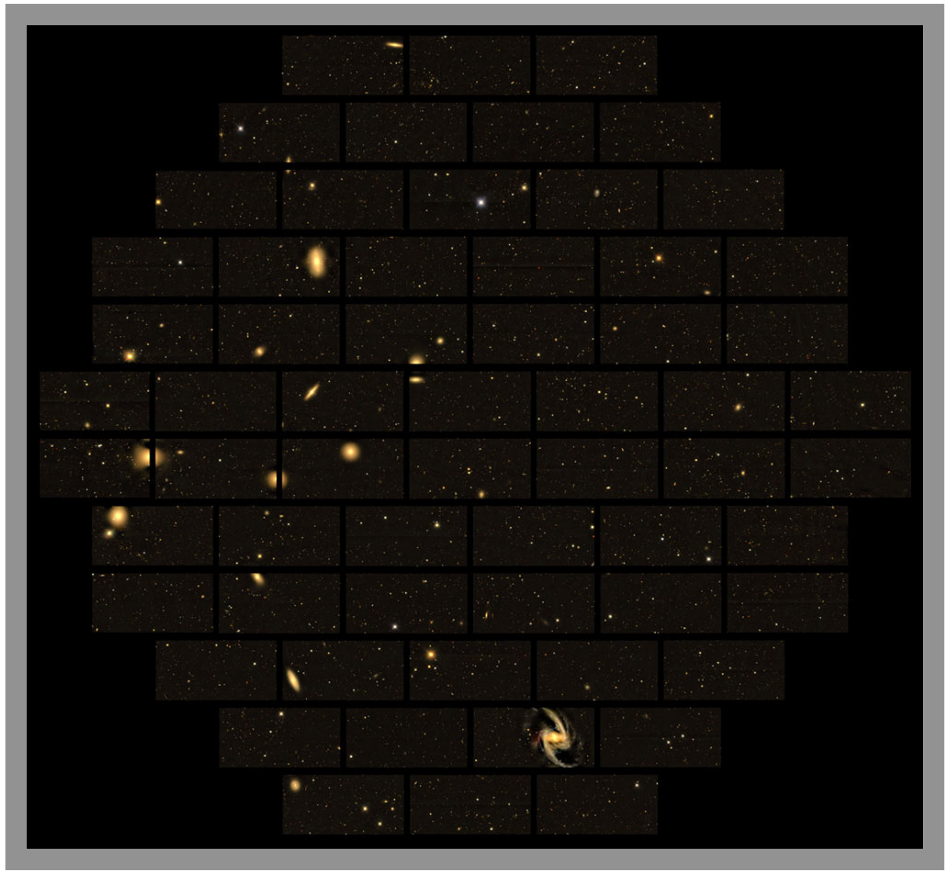
LambdaCDM universe



LambdaCDM universe

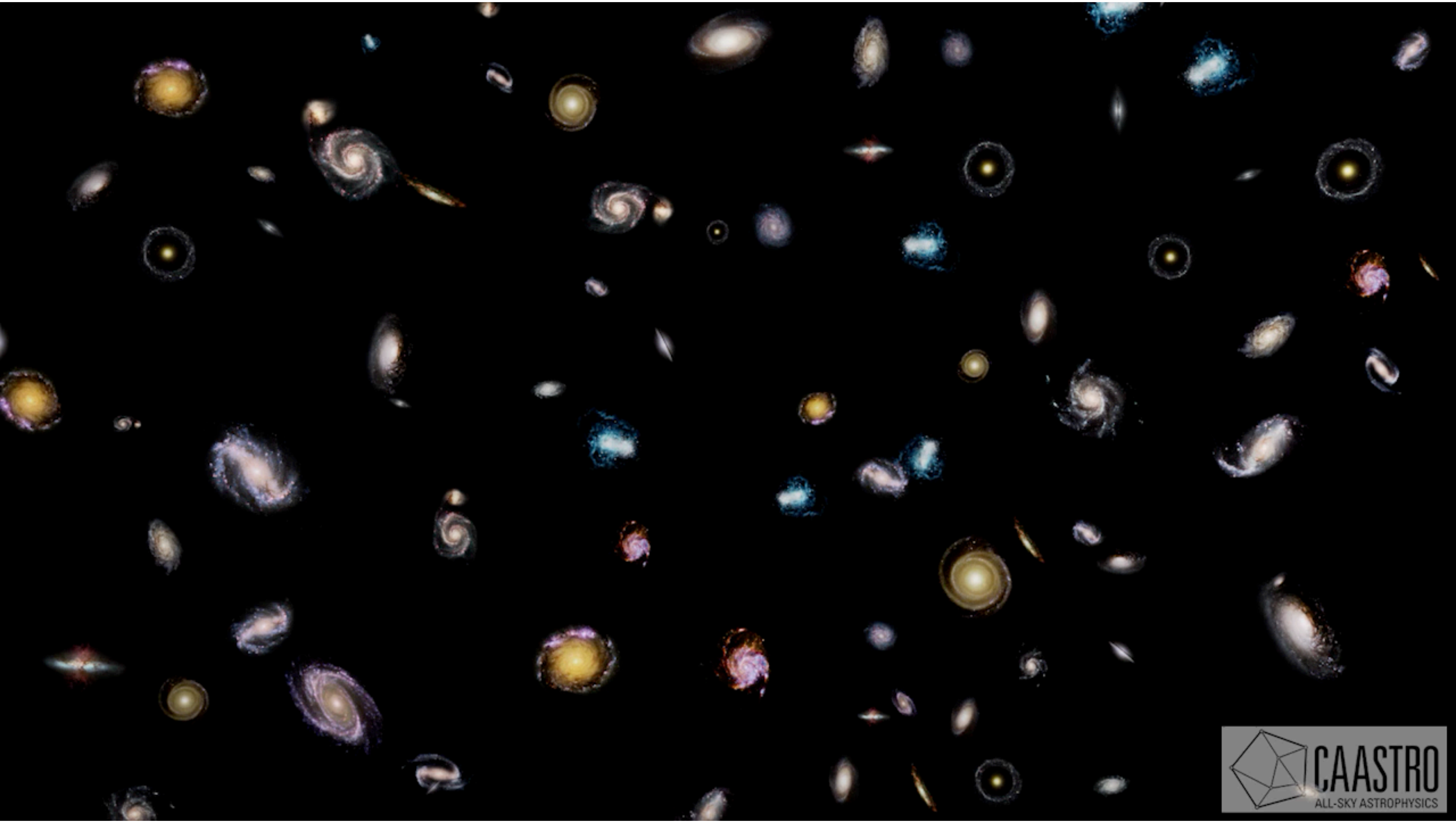


DECam @ Blanco telescope in Chile



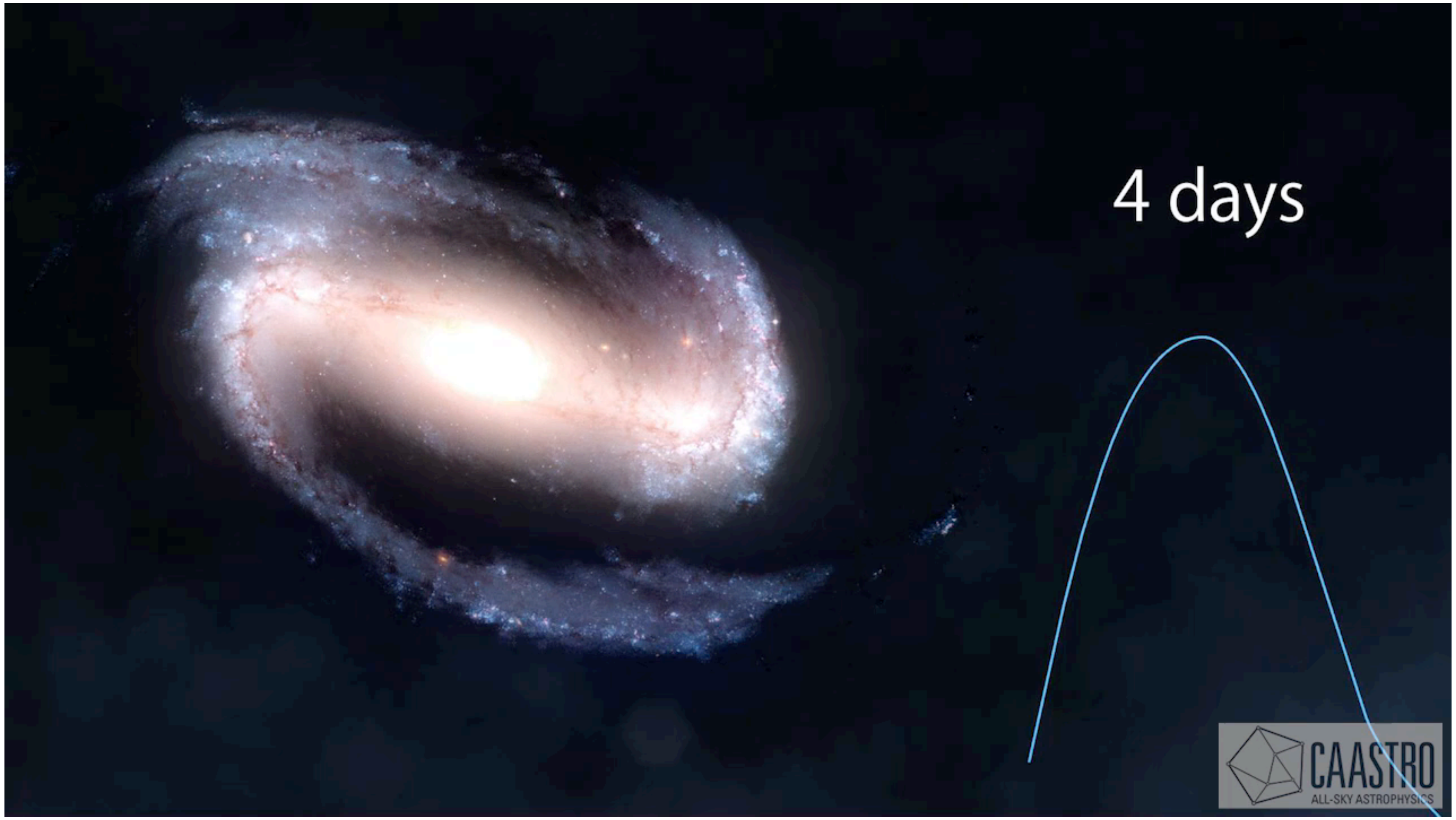
galaxy clusters, weak lensing, large scale structure, type Ia SNe, gravitational waves (kilonovae), …

Cosmic expansion

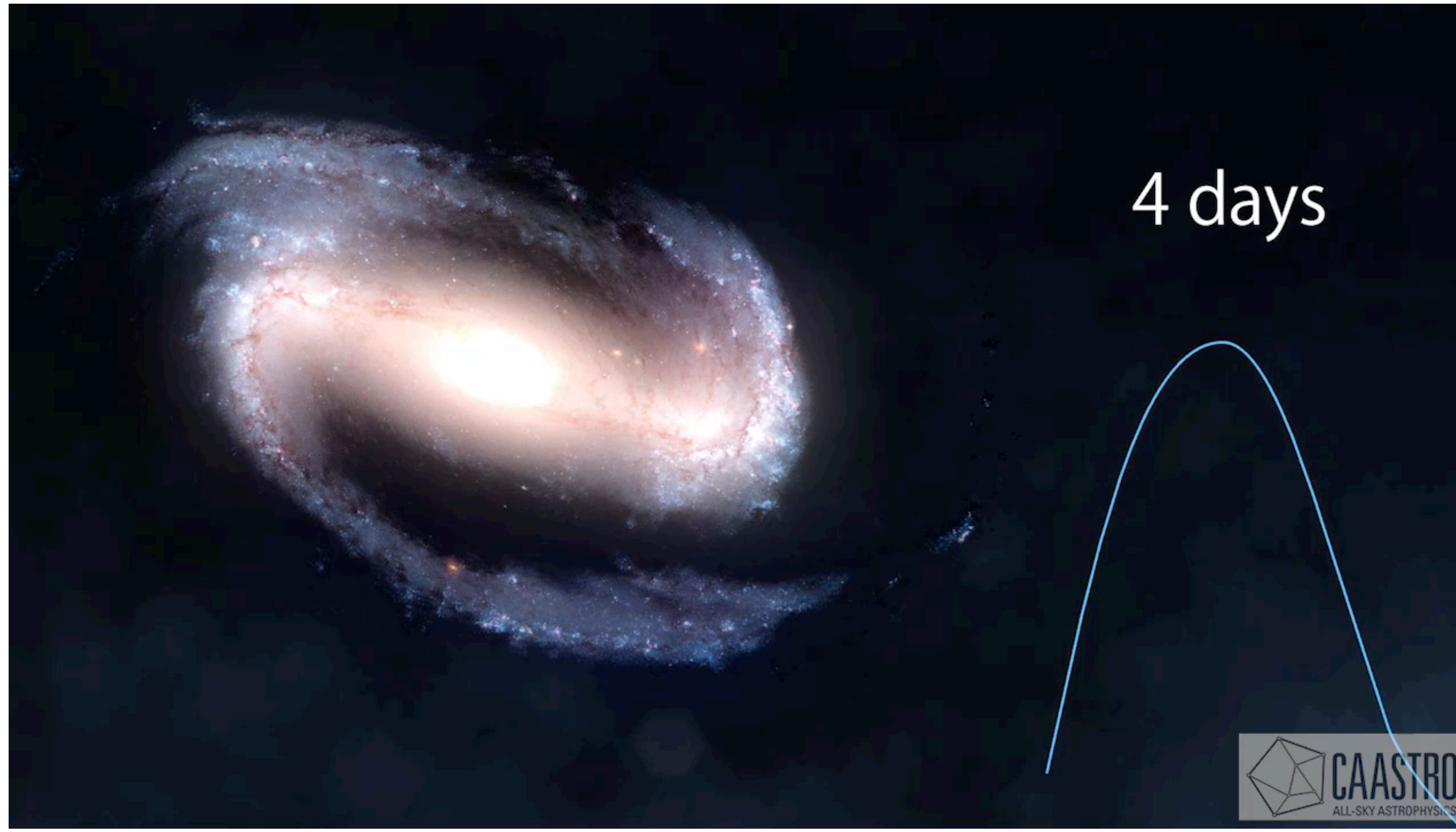


supernovae

- stellar explosions (transient events)



supernovae



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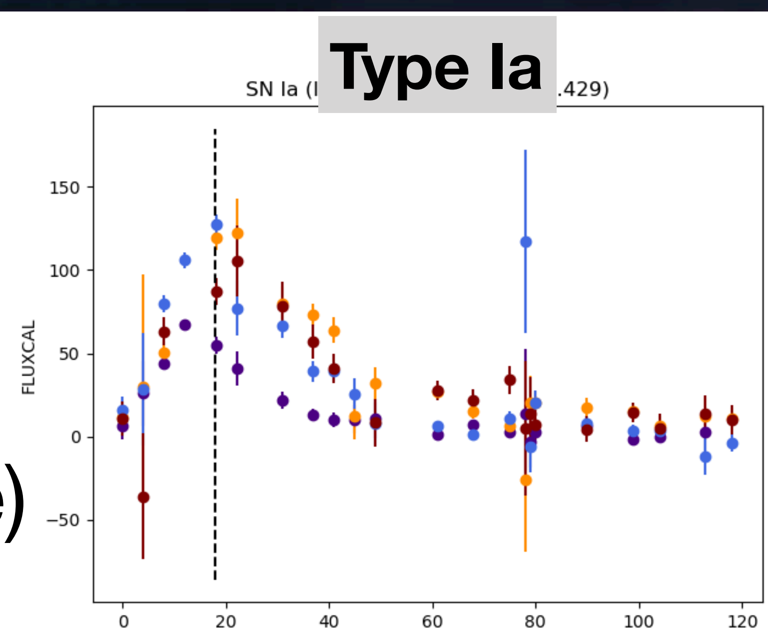
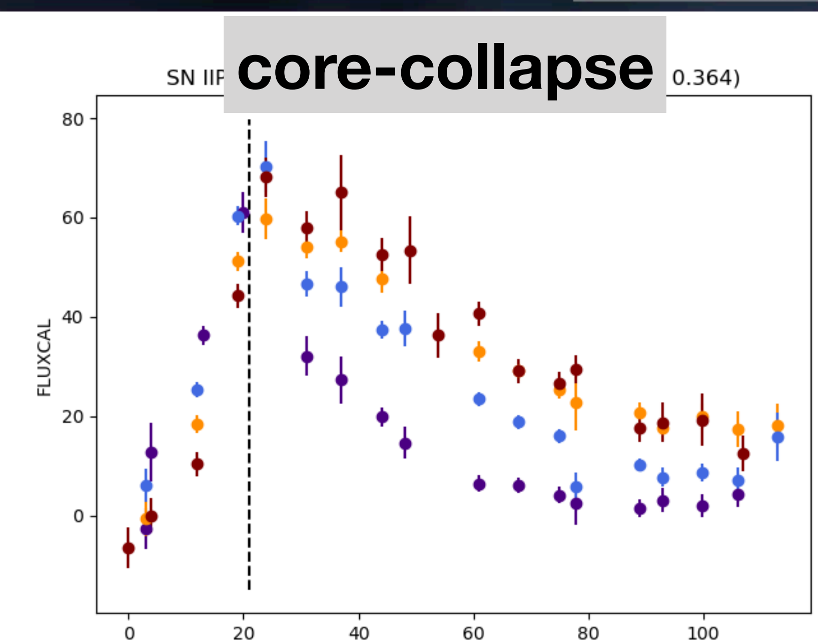
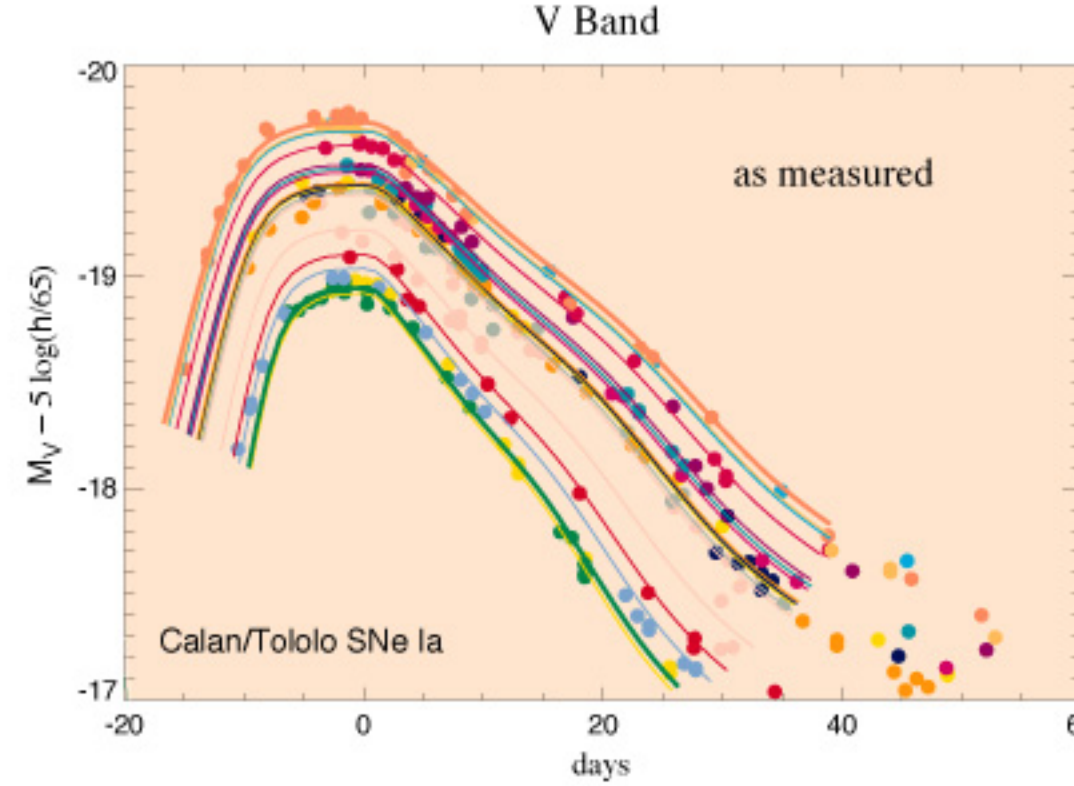




- types:
  - Ia (thermonuclear)
  - II, Ib, Ic (core-collapse)

type Ia supernovae (SNe Ia)

- very luminous
- homogeneous spectral and photometric properties



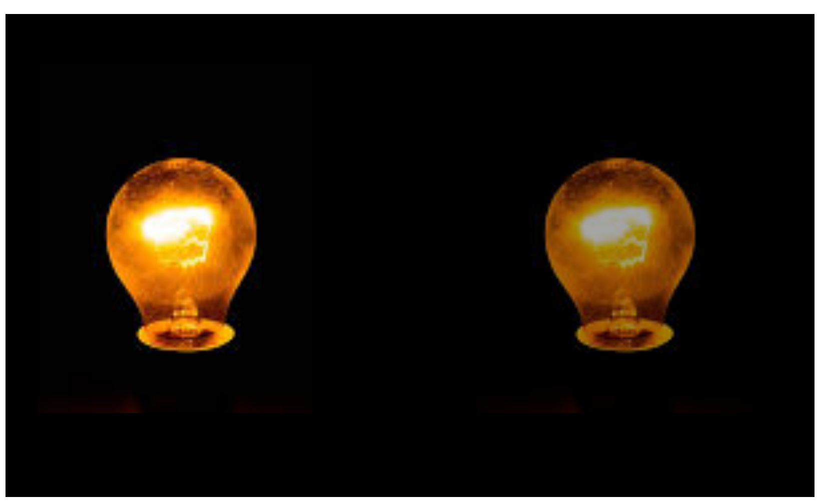
type Ia supernovae (SNe Ia)

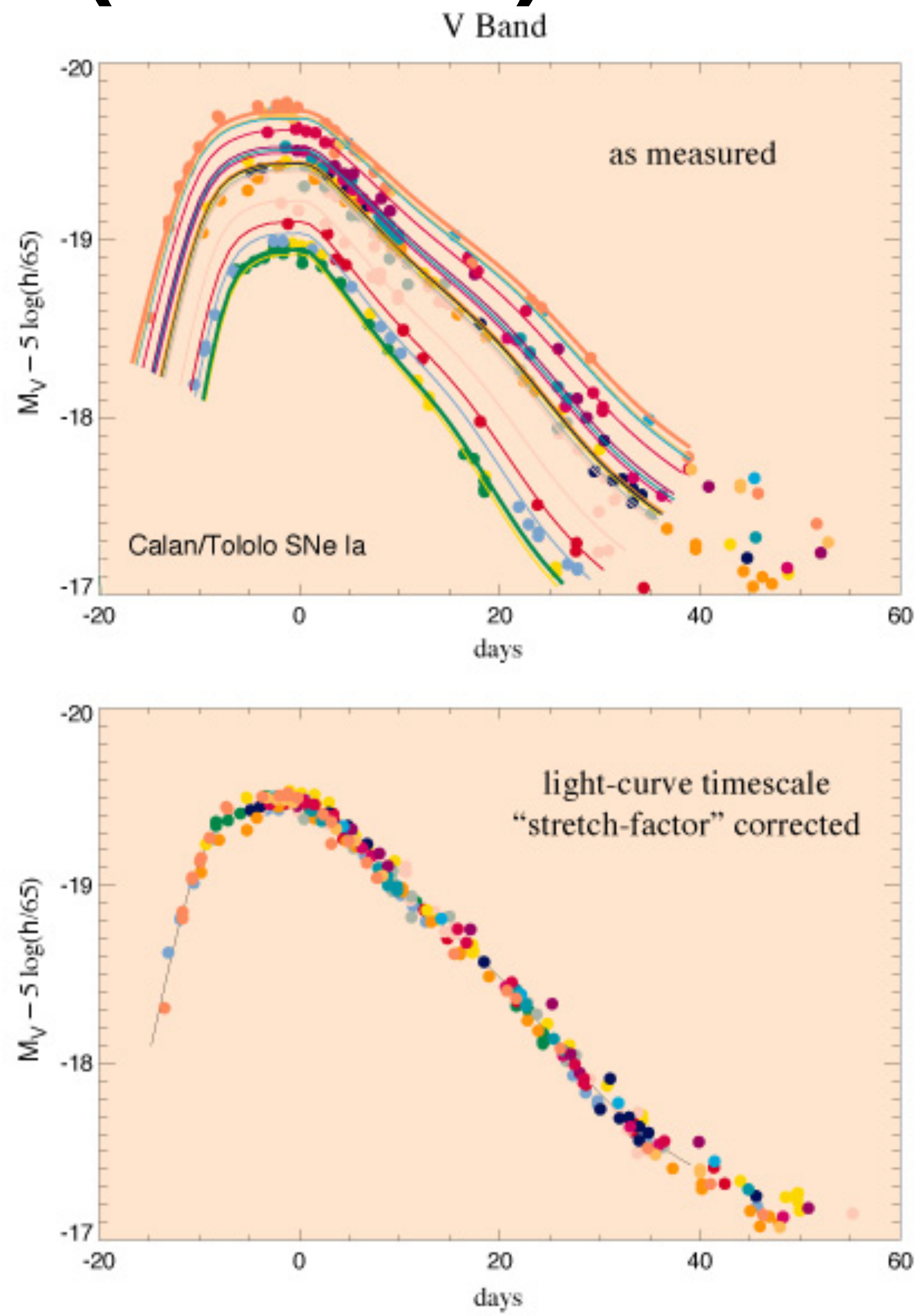
distance modulus:

$$\mu_B = m_B^* - M_B + \underbrace{\alpha\, x_1 - \beta\, C}_{\text{correction shape \& color}}$$

observed brightness

absolute brightness





current surveys

THE DARK ENERGY SURVEY

In numbers:

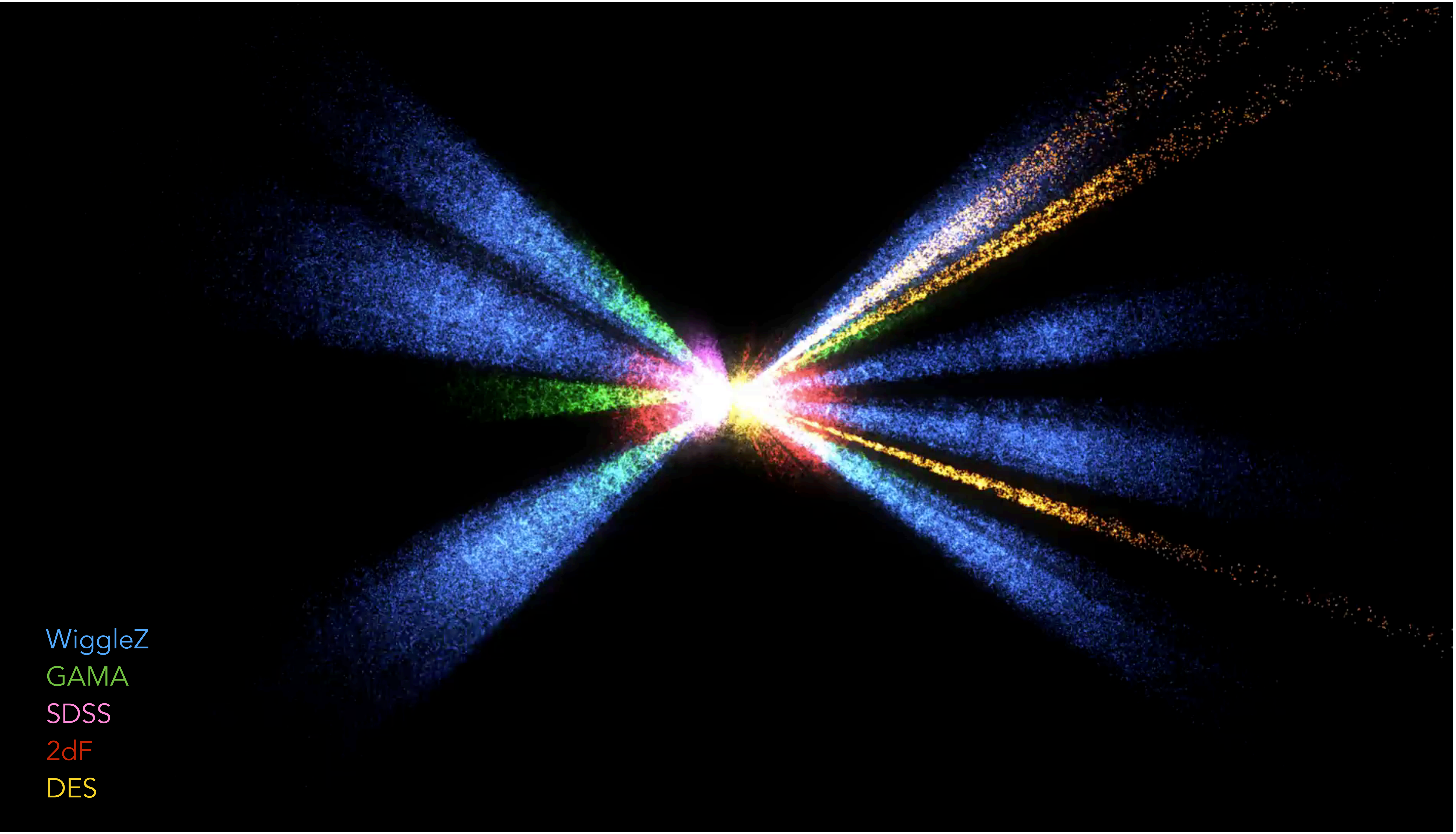
* 5-year survey, started 2013

* 4 primary probes: galaxy clusters, weak lensing, large scale structure, type Ia SNe

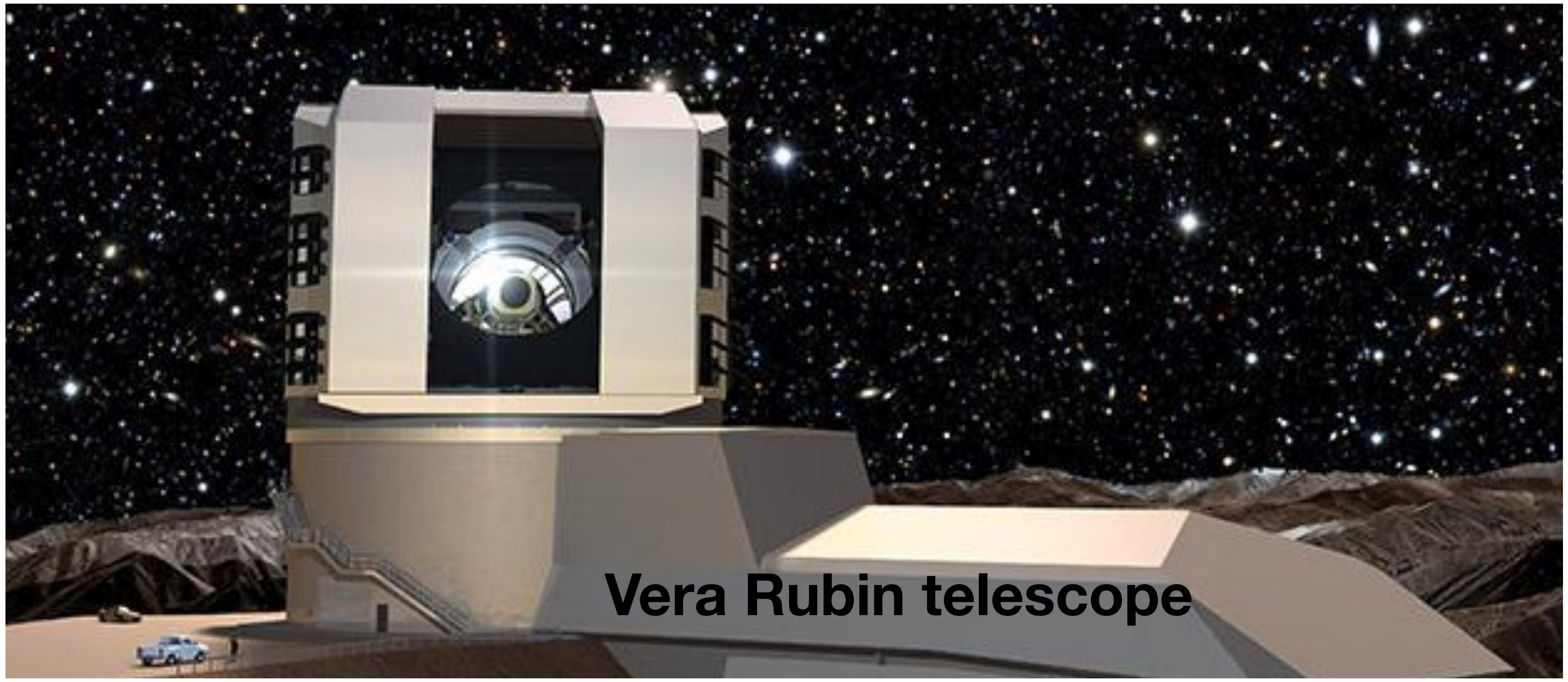
* <2,000 well measured SNe Ia

current surveys

THE DARK ENERGY SURVEY



future surveys: LSST



In numbers:

* 10-year survey, starting 2022

* 1,000 images/night = 15 TB/night

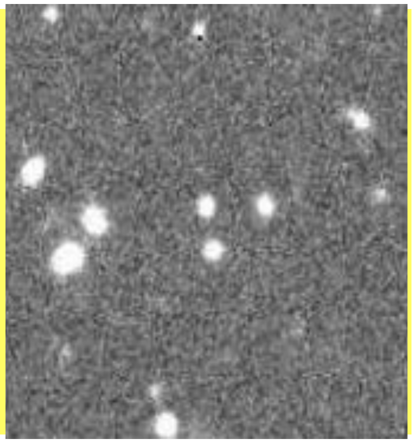
* 10,000 alerts/30 seconds = 1 GB / 30 s

* >4,000 well measured SNe Ia

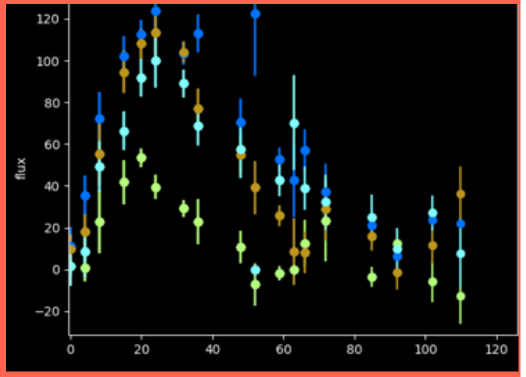
outline

Machine learning in supernova cosmology: classification tasks

Part I: real vs. bogus



Part II: typing with photometry



1. Datasets: PLAsTiCC
2. ML classification issues
    1. Representativity
    2. Incompleteness
    3. “probabilities” for cosmology
3. FINK broker

outline

Machine learning in supernova cosmology: classification tasks

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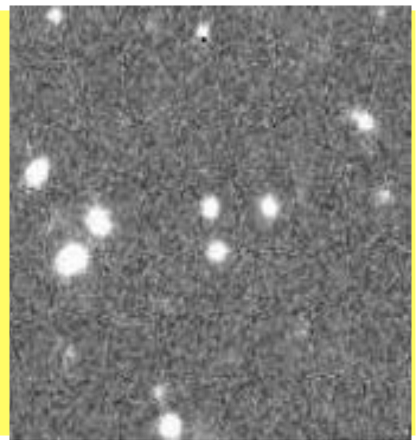
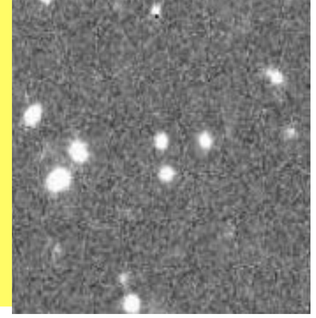
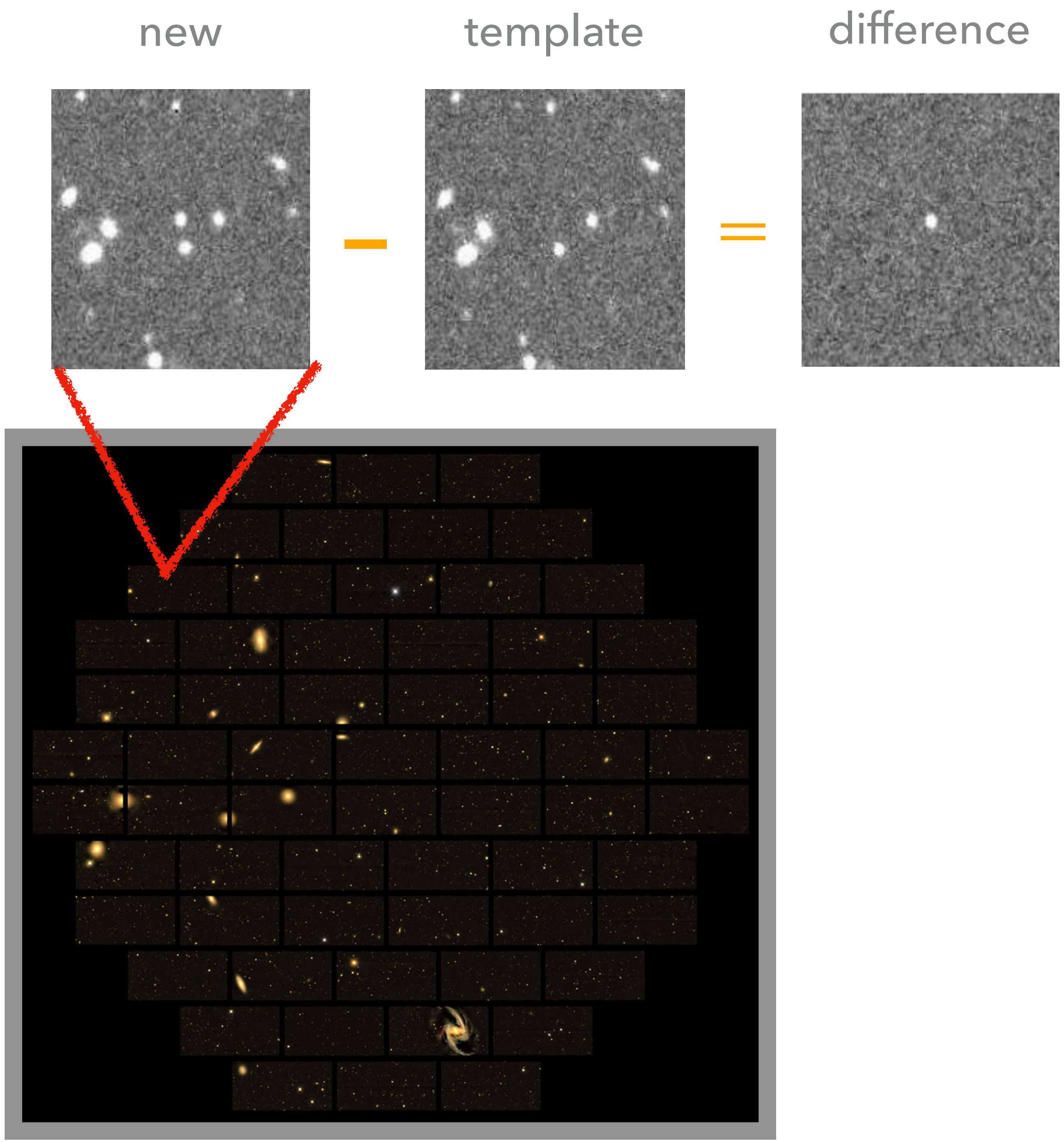




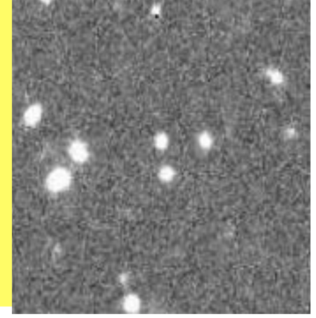
Finding transients



Difference imaging

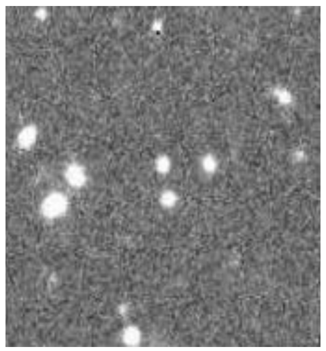
Kessler + 2015
Goldstein + 2015

Part I: real vs. bogus



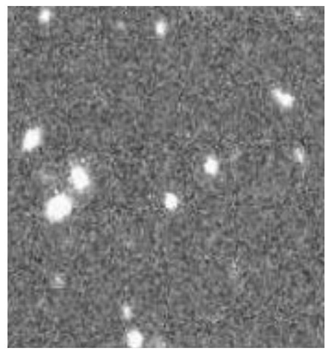
Finding transients

new



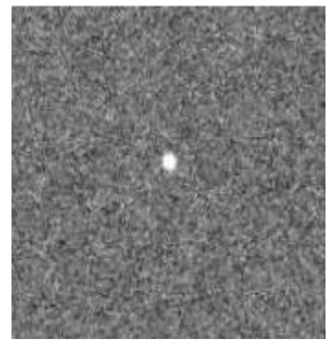
-

template



=

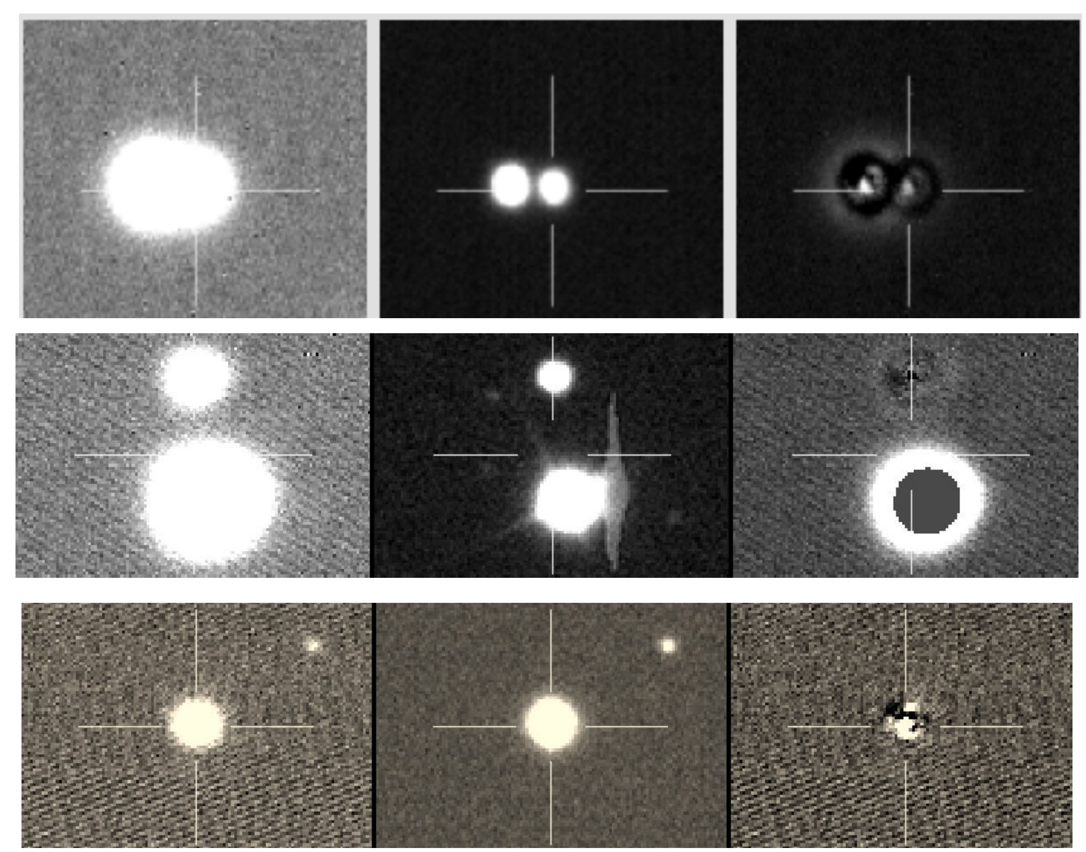
difference



Difference imaging

Kessler + 2015
Goldstein + 2015

Bogus detections



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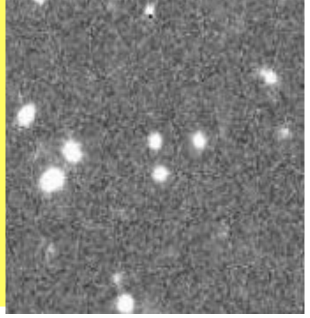
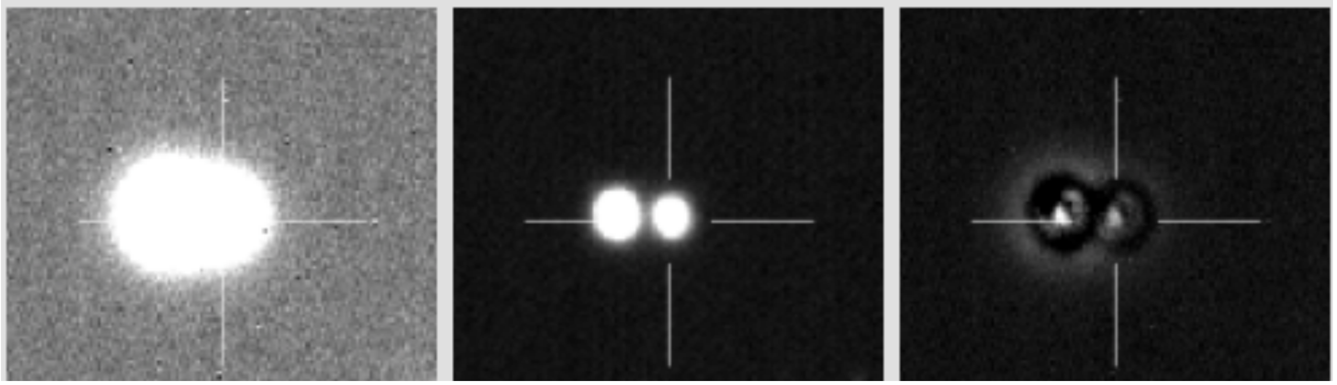


Eliminating bogus

1. Humans

Your team

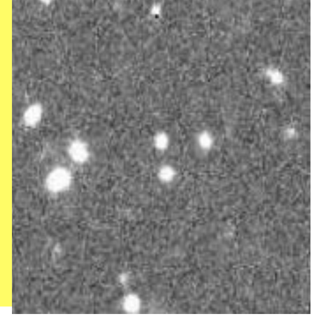


Citizen scientists

ZOONIVERSE

AM, Tucker, Armstrong & the SkyMapper Transient team 2017-2018

Part I: real vs. bogus

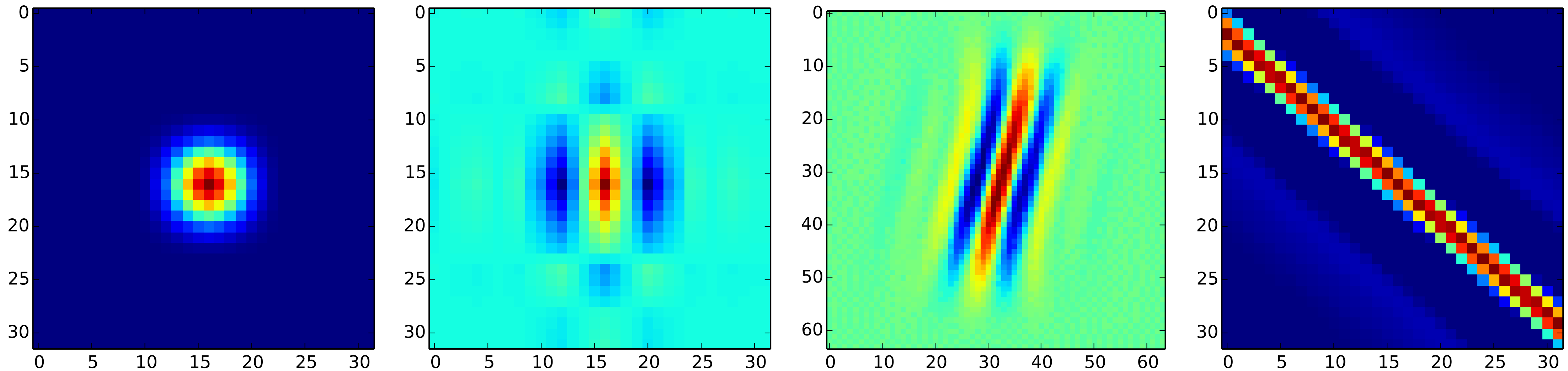


Eliminating bogus

2. Signal Processing

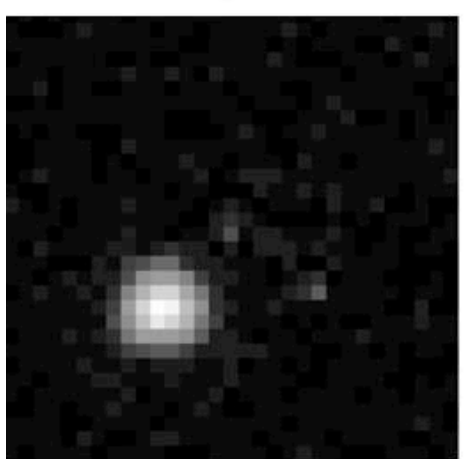
Möller+2015 dictionaries where chosen based on SN-like and artifact studies:

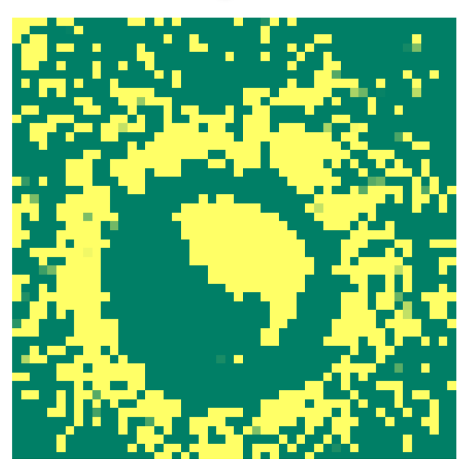
dictionaries

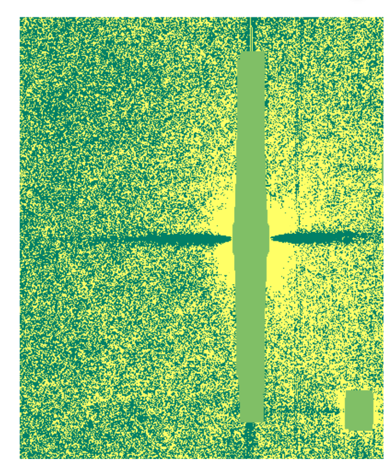


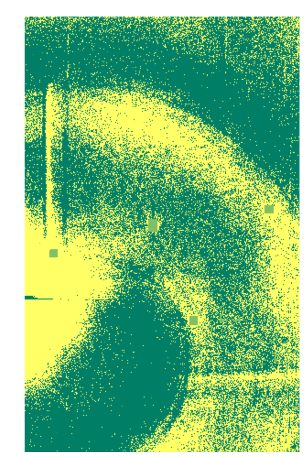
(A) Starlet (B) Bi-orthogonal (C) Curvelet (D) Ridgelet

objects

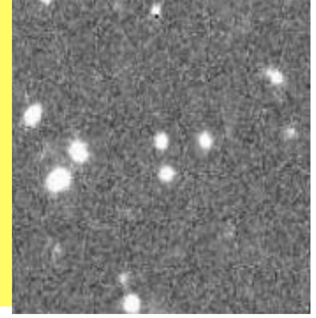








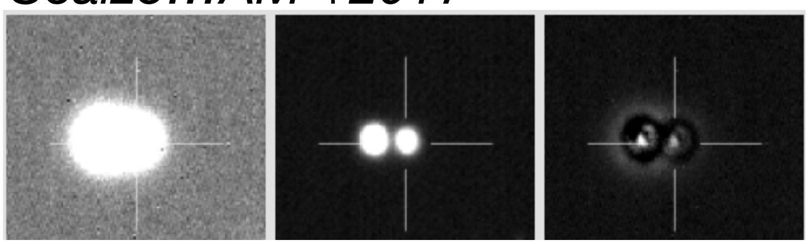
SN-like dipoles saturated star, optical ghost,…



Eliminating bogus

3. Machine learning

Scalzo…AM +2017



SkyMapper images

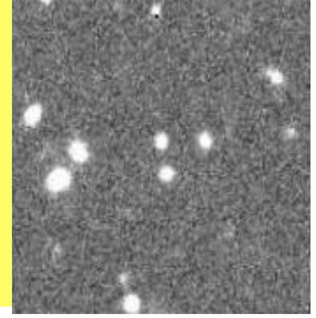
Features

`eref`	ellipticity of source on template image
`thref`	semi-major axis of source on template image
`fwhmref`	full width at half maximum of all template image sources
`f4ref`	flux within 4-pixel aperture in template image
`flagref`	SEXTRACTOR source flags in template image

ML classifier

Random Forest

Part I: real vs. bogus



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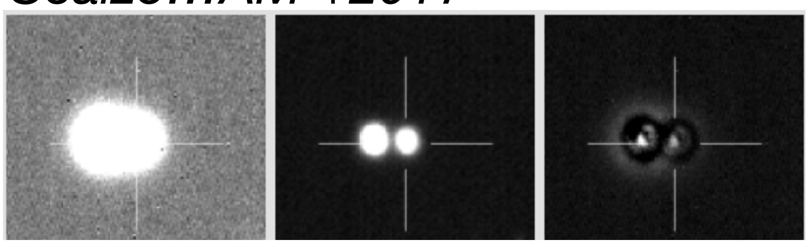

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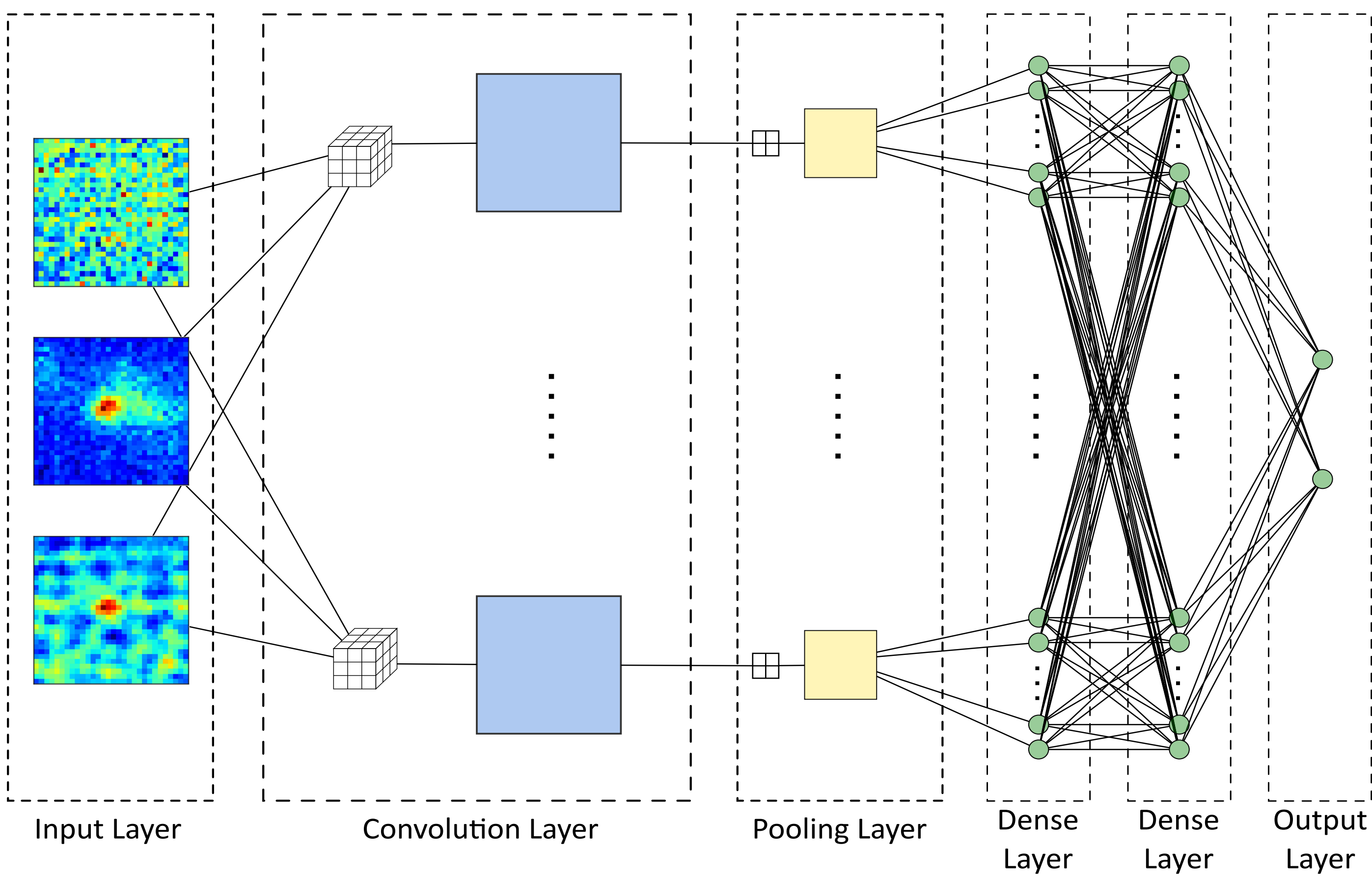
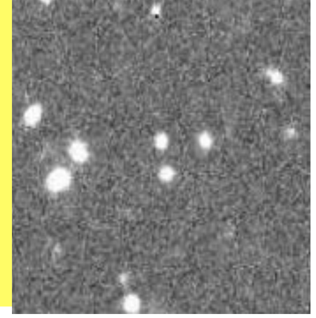
Gieseke…AM+ 2017

SkyMapper images augmented for training



Model	AUC
Random forest	0.9907
Net1(32,64)	0.9914
Net3	0.9972
E2	0.9946

Part I: real vs. bogus

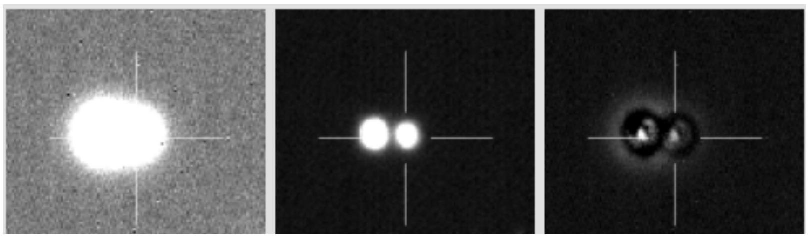


Eliminating bogus

limitations: training sets! feature extraction

3. Machine learning

Scalzo…AM +2017



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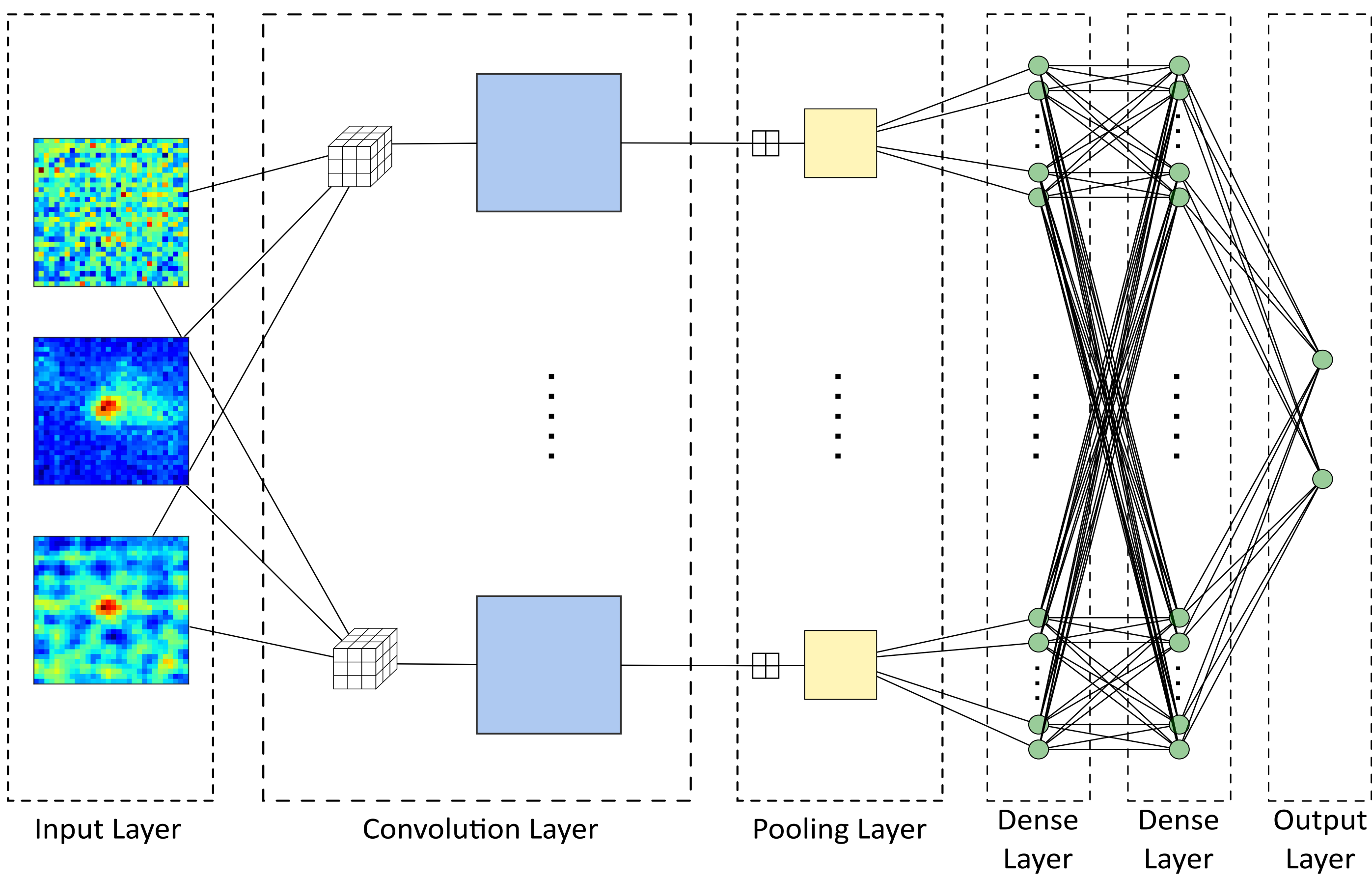

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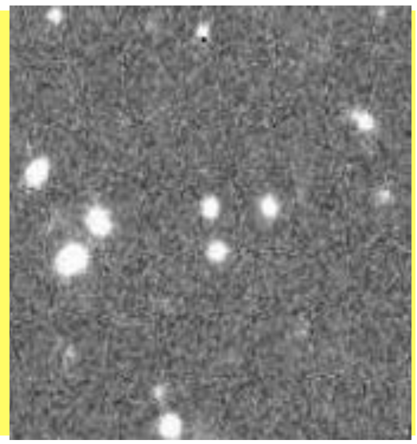

Is it a supernova? Which type?

Part II: typing with photometry

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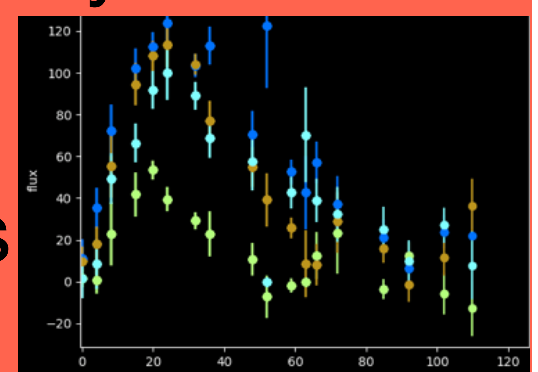
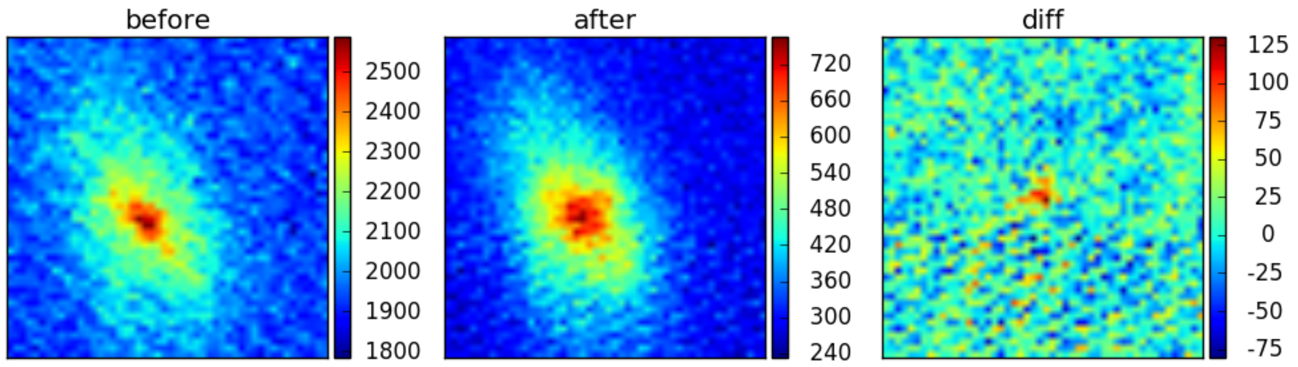
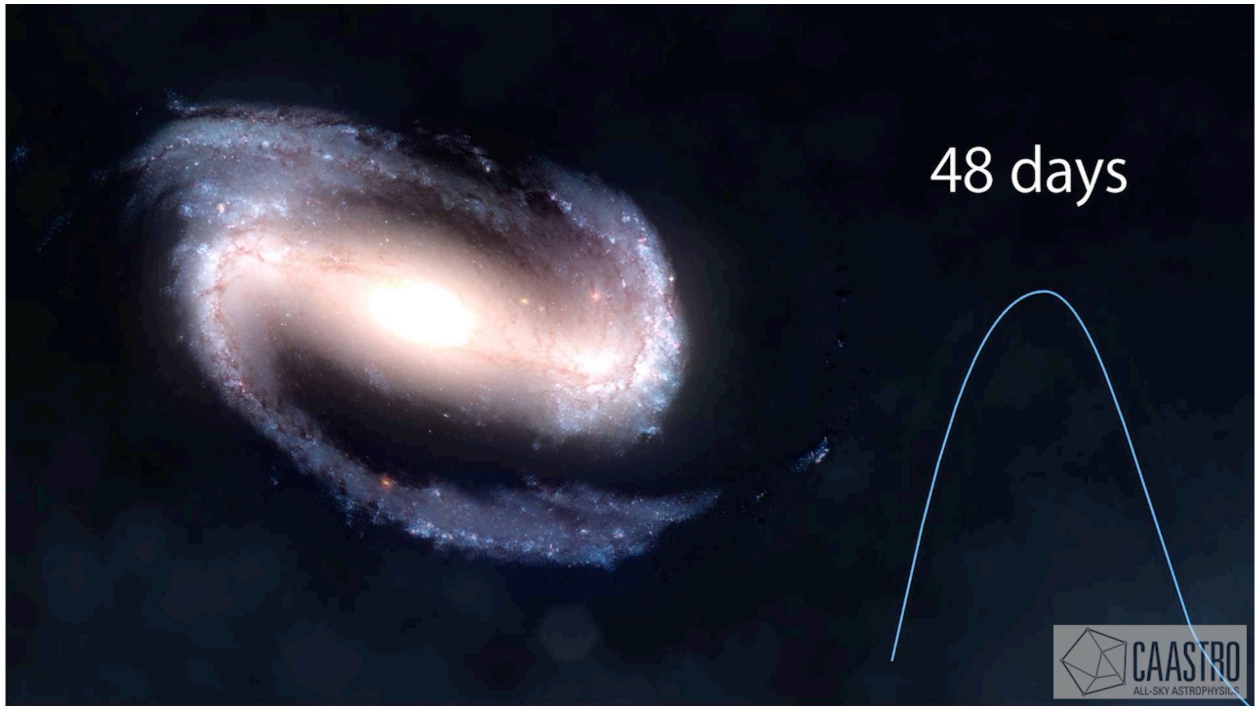


typing supernovae with spectroscopy





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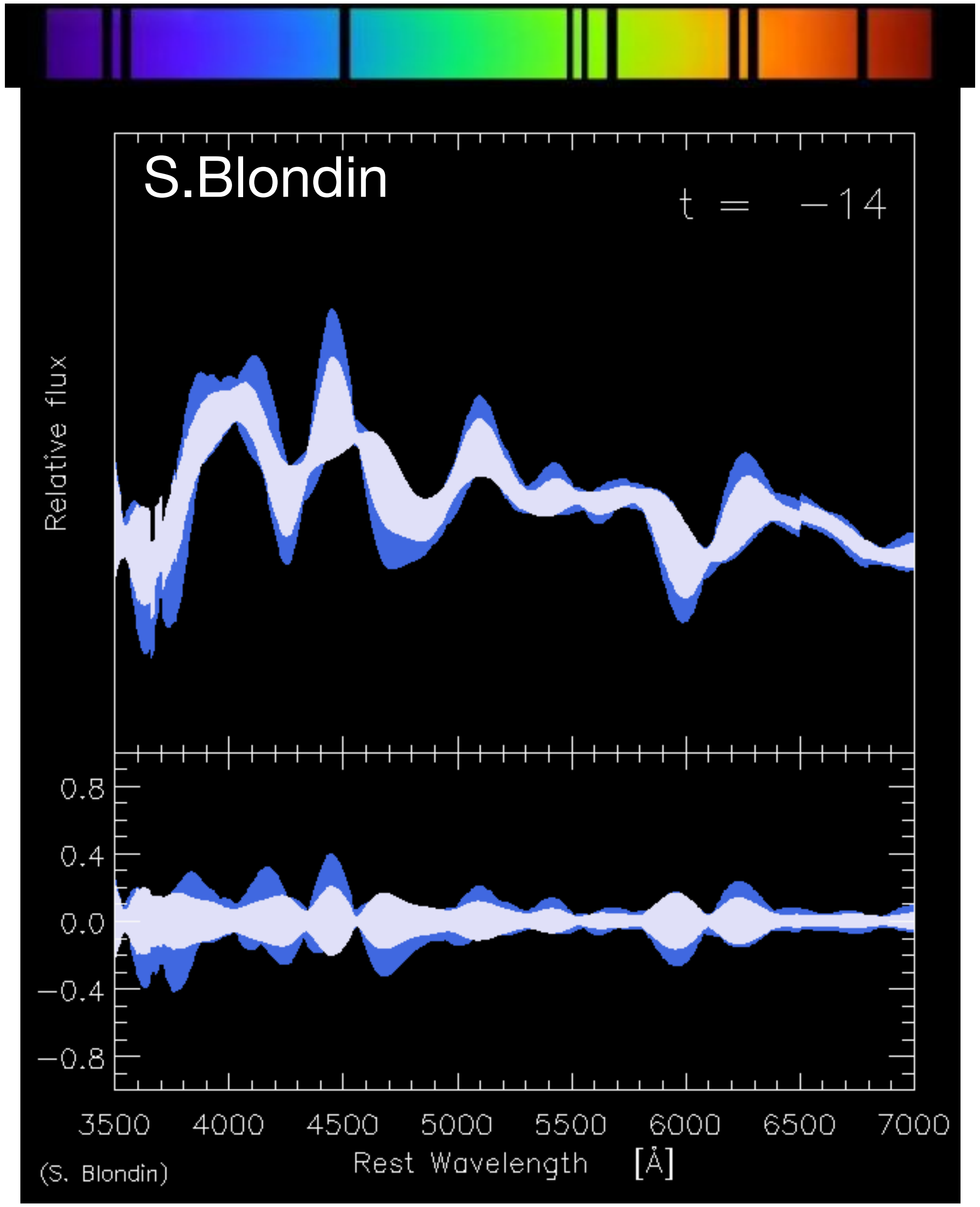
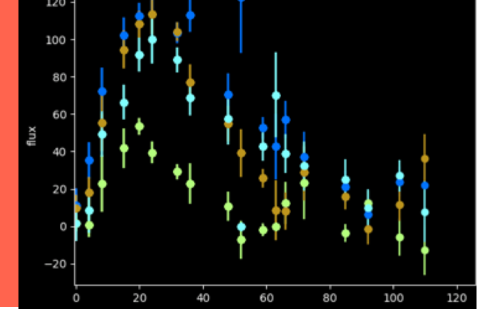
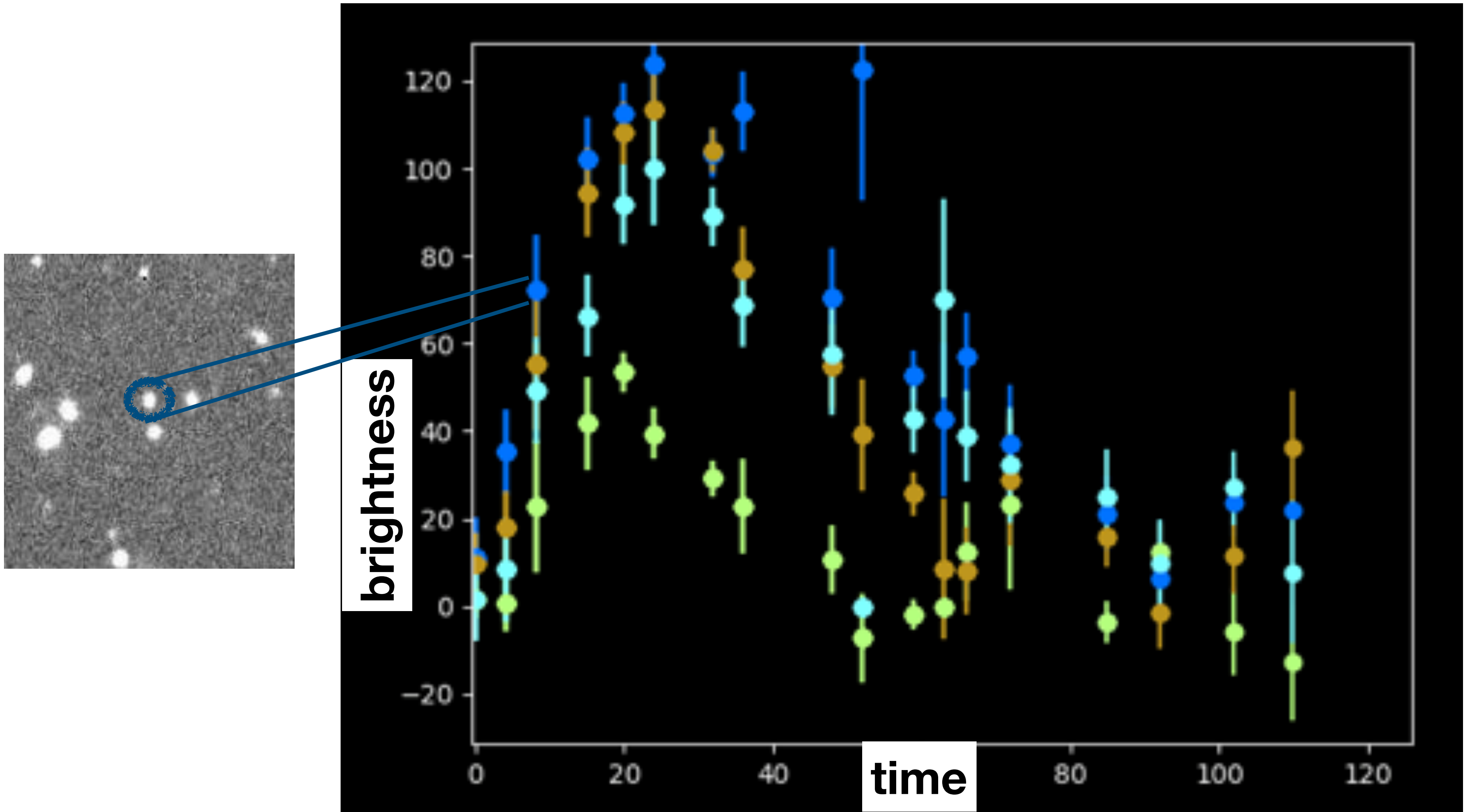




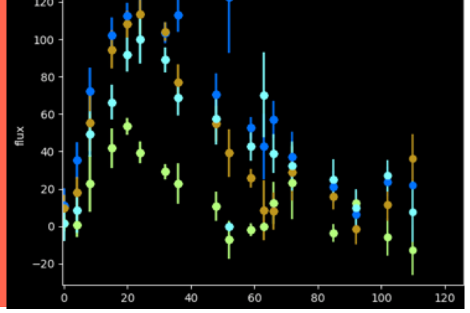
Our goal



classification of SN types

Instead of spectra, we just see the evolution on brightness in some wavelengths

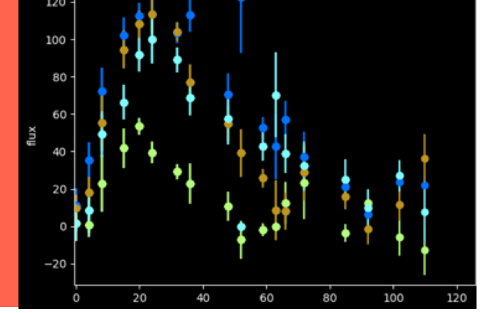
Part II: typing with photometry



we need “simulated” datasets:

- to evaluate our methods
- to train ML classifiers

Part II: typing with photometry



Datasets: PLAsTiCC

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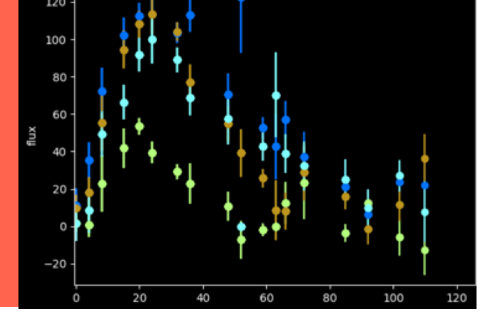
The Photometric LSST Astronomical Time-series Classification Challenge (PLAsTiCC): Data set

The PLAsTiCC team:,[1] Tarek Allam Jr.,[2] Anita Bahmanyar,[3] Rahul Biswas,[4] Mi Dai,[5] Lluís Galbany,[6] Renée Hložek,[3] Emille E. O. Ishida,[7] Saurabh W. Jha,[5] David O. Jones,[8] Richard Kessler,[9] Michelle Lochner,[10, 11] Ashish A. Mahabal,[12, 13] Alex I. Malz,[14, 15] Kaisey S. Mandel,[16, 17] Juan Rafael Martínez-Galarza,[18] Jason D. McEwen,[2] Daniel Muthukrishna,[16] Gautham Narayan,[19] Hiranya Peiris,[4, 20] Christina M. Peters,[3] Kara Ponder,[21] and Christian N. Setzer[4]
(LSST Dark Energy Science Collaboration and the LSST Transients and Variable Stars Science Collaboration)

Part II: typing with photometry



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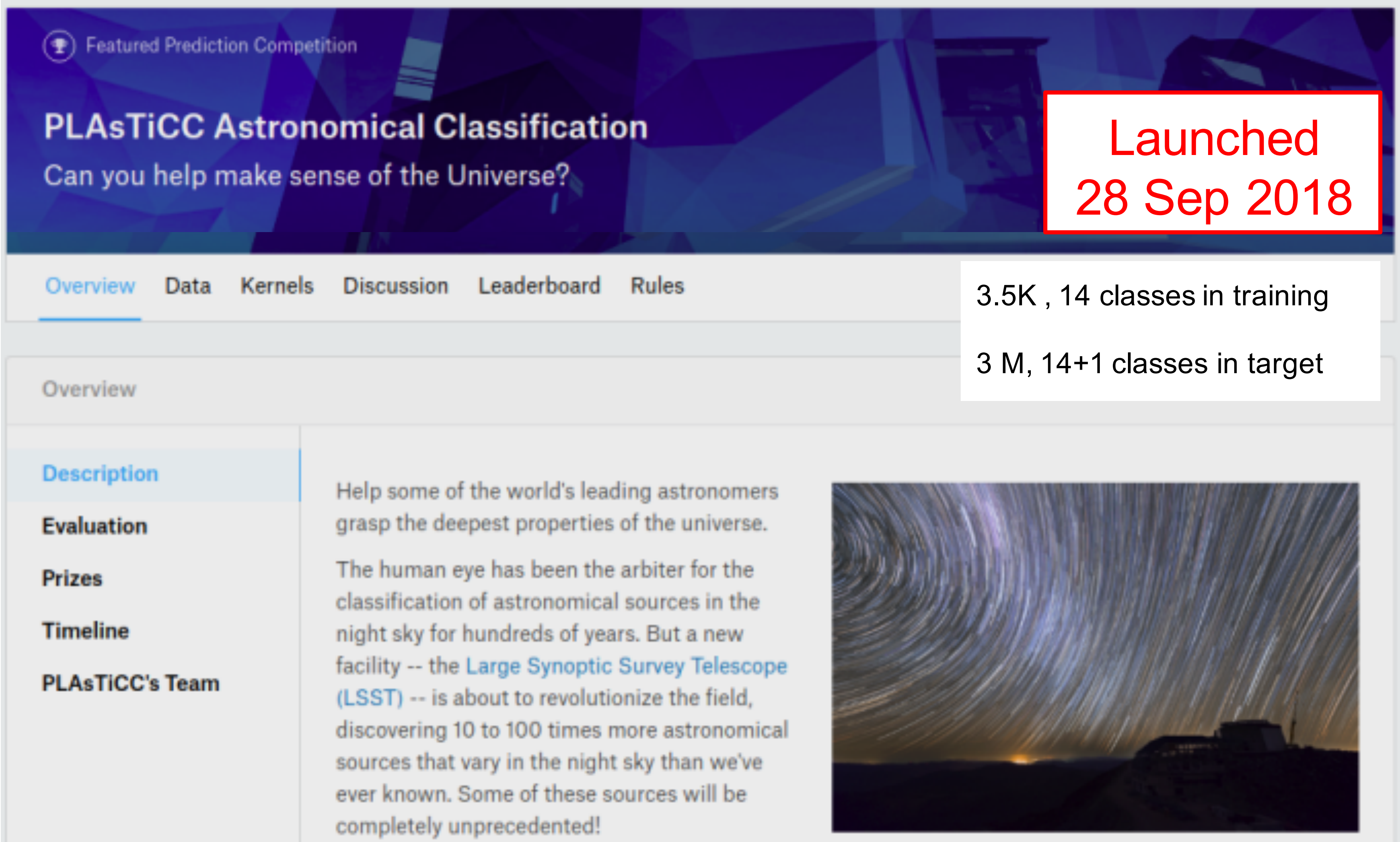


Featured Prediction Competition

PLAsTiCC Astronomical Classification

Can you help make sense of the Universe?

Overview Data Kernels Discussion Leaderboard Rules

Overview

Description
Evaluation
Prizes
Timeline
PLAsTiCC's Team

Help some of the world's leading astronomers grasp the deepest properties of the universe.

The human eye has been the arbiter for the classification of astronomical sources in the night sky for hundreds of years. But a new facility -- the Large Synoptic Survey Telescope (LSST) -- is about to revolutionize the field, discovering 10 to 100 times more astronomical sources that vary in the night sky than we've ever known. Some of these sources will be completely unprecedented!

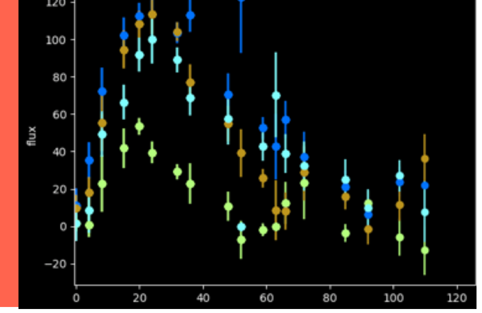
Launched
28 Sep 2018

3.5K , 14 classes in training

3 M, 14+1 classes in target

credit: E. Ishida

Part II: typing with photometry



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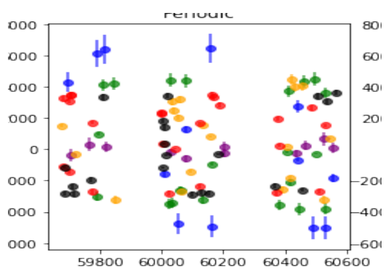
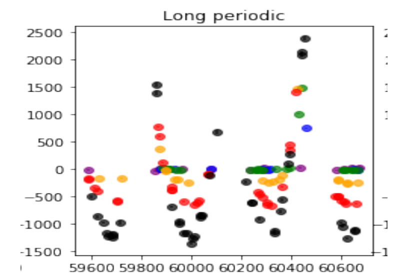
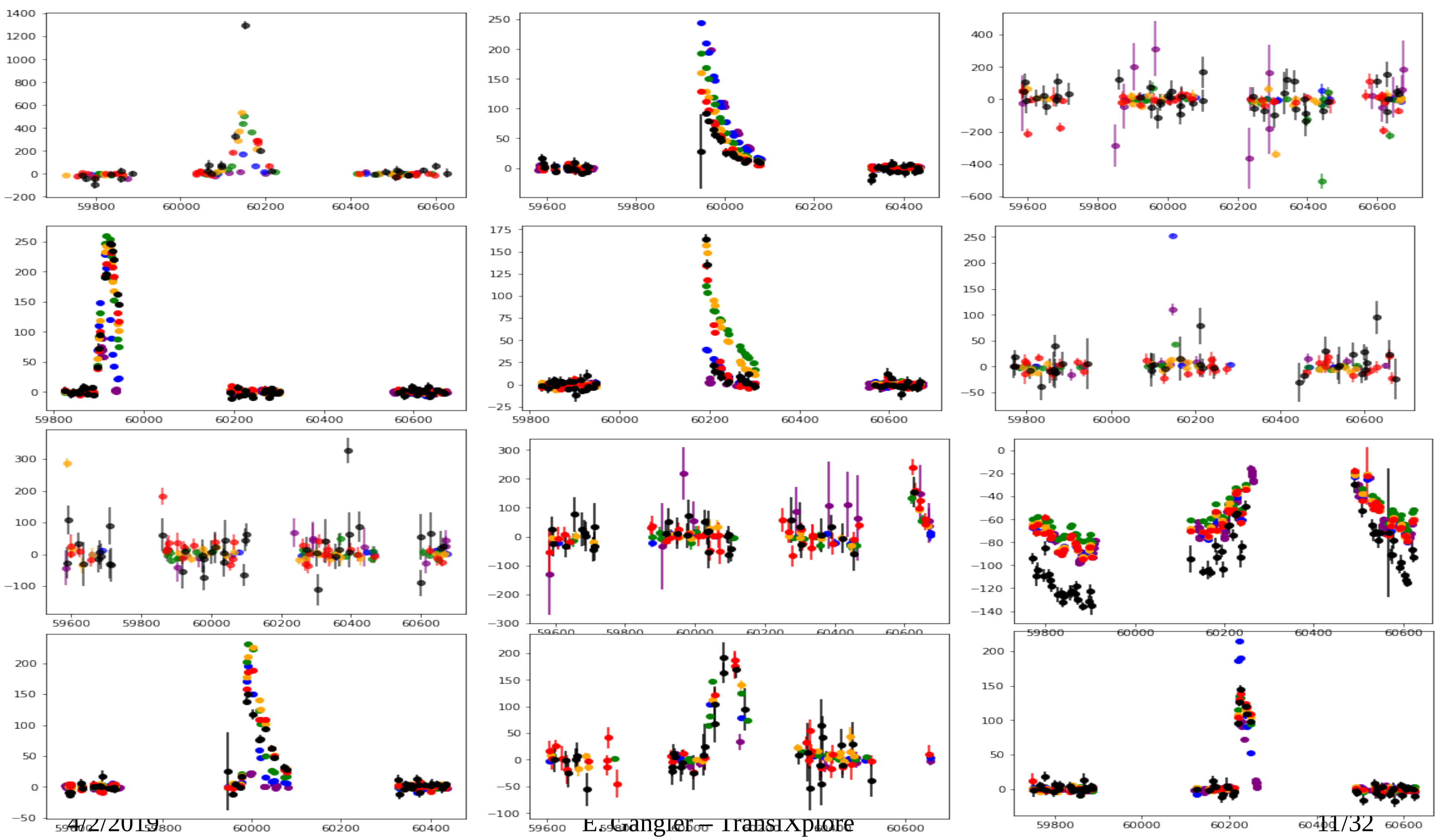


14 classes…





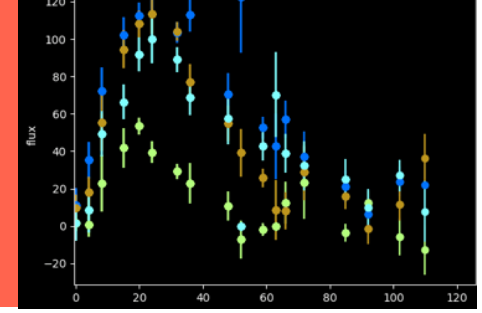
credit: E. Gangler

metric:
each class is roughly equally important for the final score.

$$\text{Log Loss} = -\left(\frac{\sum_{i=1}^{M} w_i \cdot \sum_{j=1}^{N_i} \frac{y_{ij}}{N_i} \cdot \ln p_{ij}}{\sum_{i=1}^{M} w_i} \right)$$

model class num[a]: name	model description
90: SNIa	WD detonation, Type Ia SN
67: SNIa-91bg	Peculiar type Ia: 91bg
52: SNIax	Peculiar SNIax
42: SNII	Core Collapse, Type II SN
62: SNIbc	Core Collapse, Type Ibc SN
95: SLSN-I	Super-Lum. SN (magnetar)
15: TDE	Tidal Disruption Event
64: KN	Kilonova (NS-NS merger)
88: AGN	Active Galactic Nuclei
92: RRL	RR lyrae
65: M-dwarf	M-dwarf stellar flare
16: EB	Eclipsing Binary stars
53: Mira	Pulsating variable stars
6: μLens-Single	μ-lens from single lens
991: μLens-Binary	μ-lens from binary lens
992: ILOT	Intermed. Lum. Optical Trans.
993: CaRT	Calcium Rich Transient
994: PISN	Pair Instability SN
995: μLens-String	μ-lens from cosmic strings
TOTAL	Sum of all models

Part II: typing with photometry



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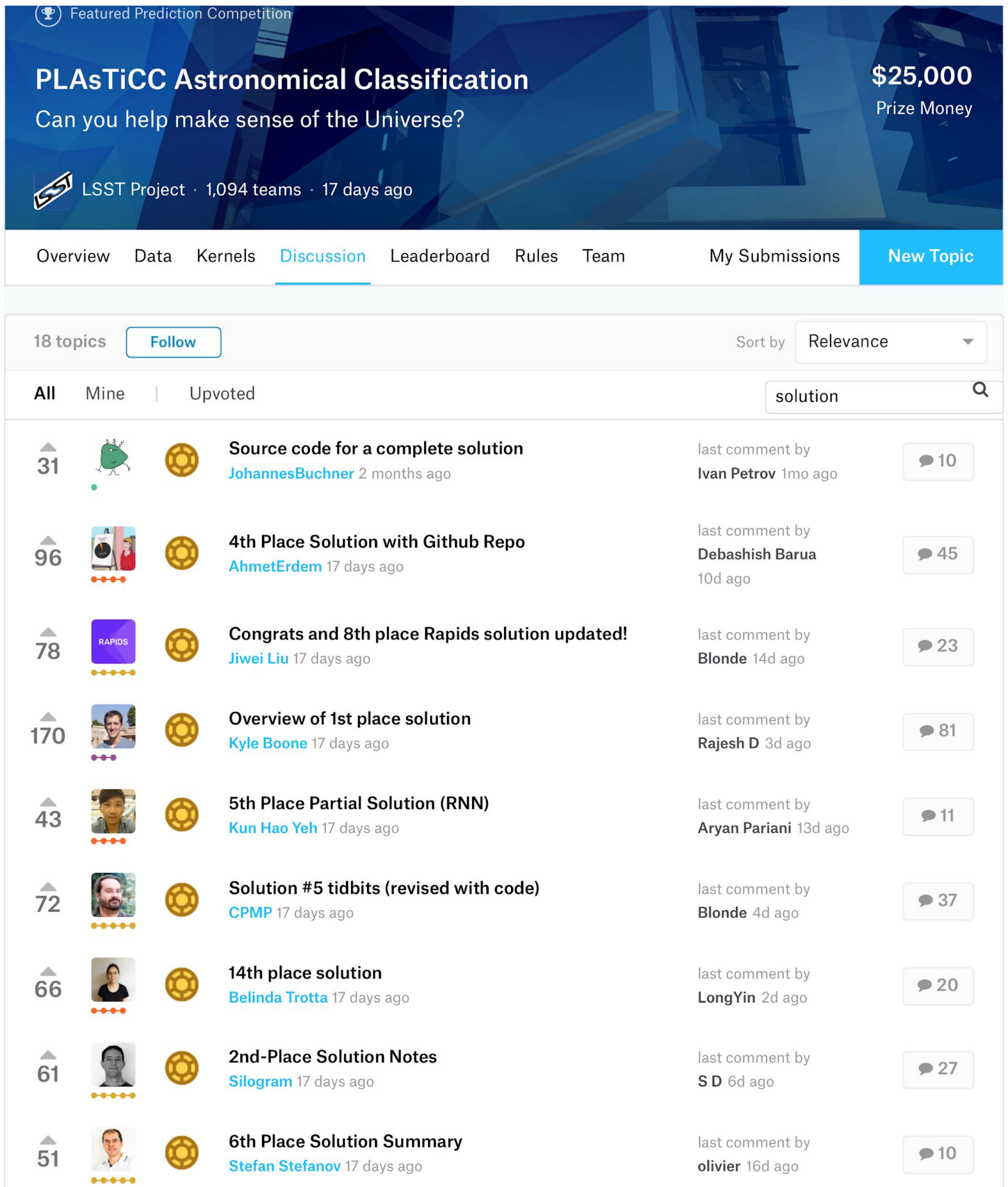
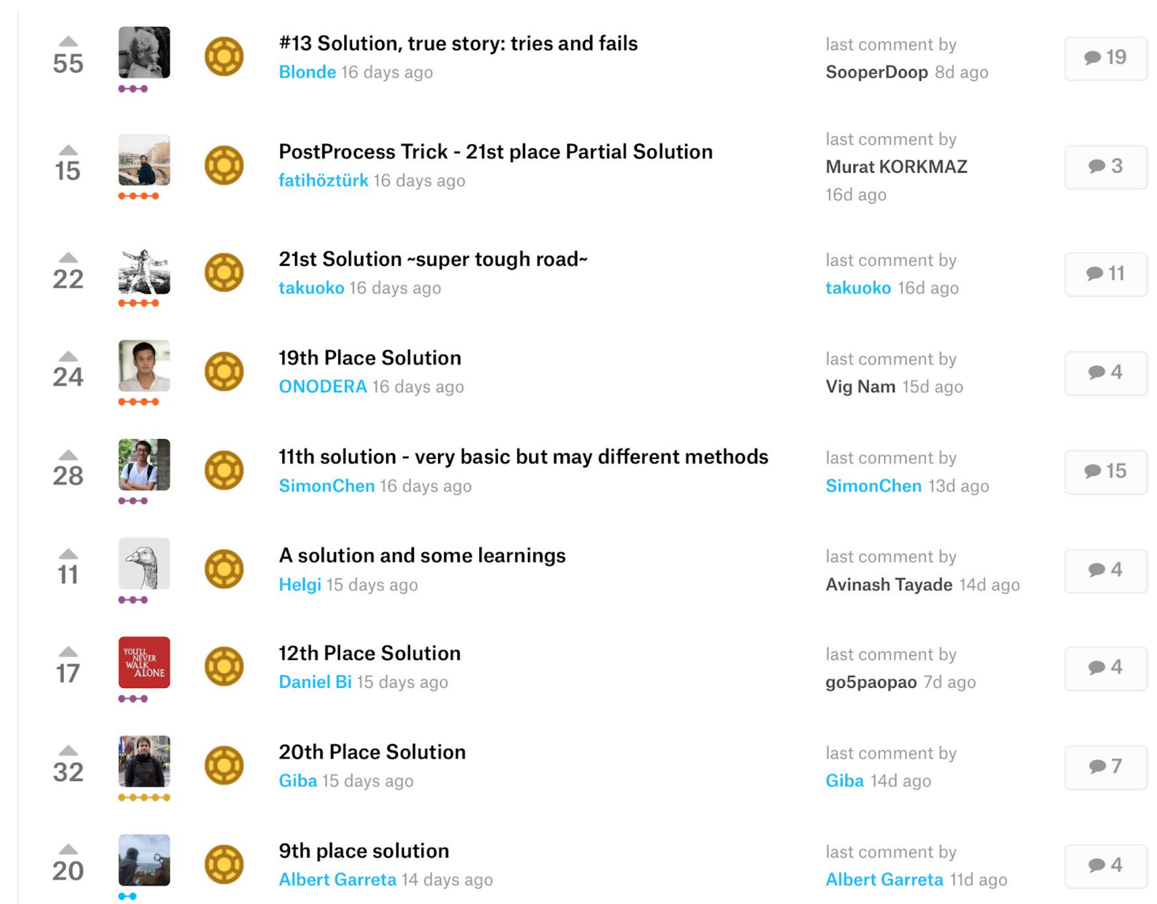
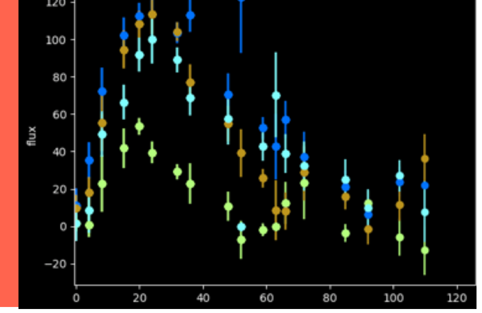


Solutions posted on Kaggle



credit: M. Dai

Part II: typing with photometry



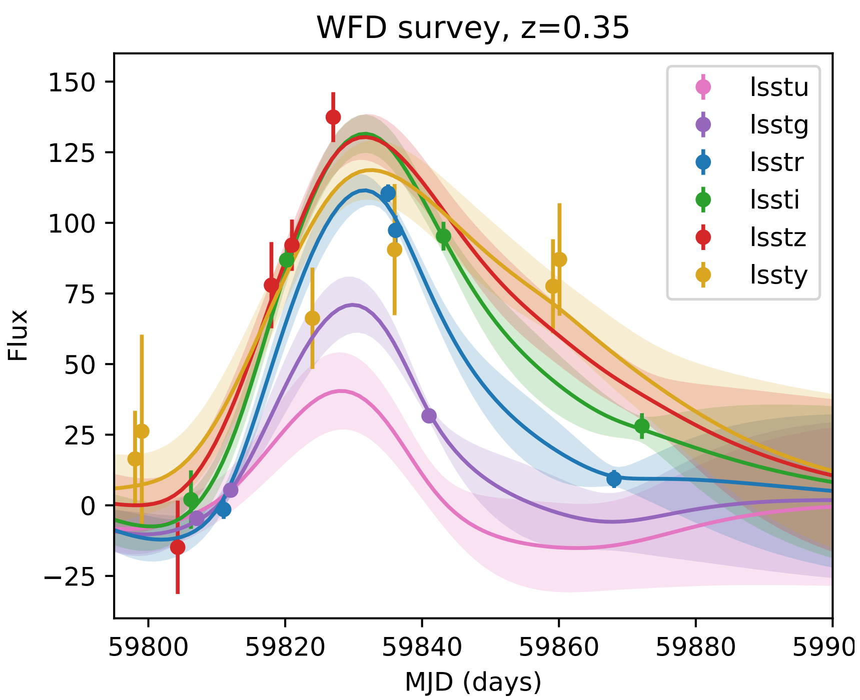
Datasets: PLAsTiCC

Avocado: Photometric Classification of Astronomical Transients with Gaussian Process Augmentation

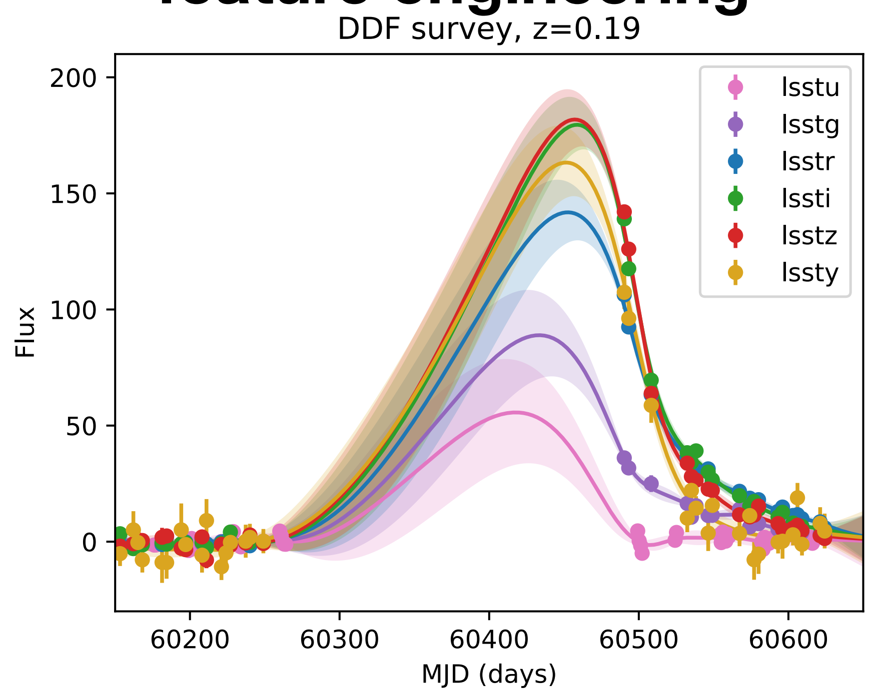
Winning solution

Kyle Boone[1,2]

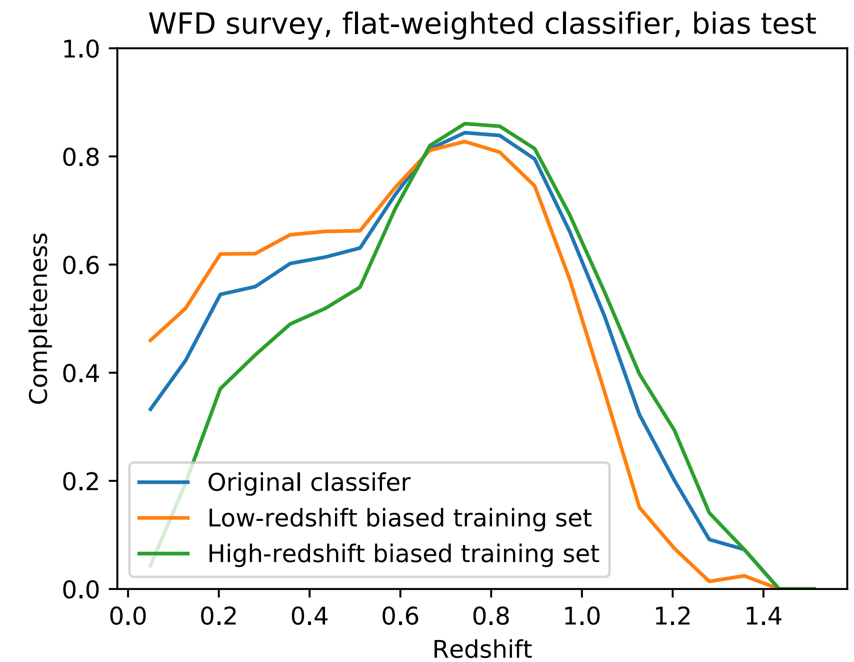
GP modelling



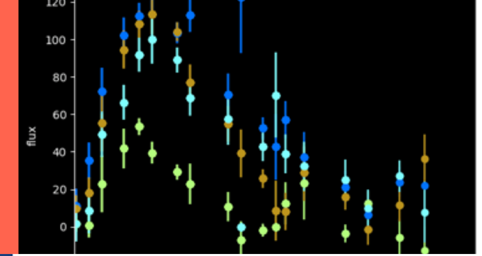
feature engineering



data augmentation



+ boosted decision tree



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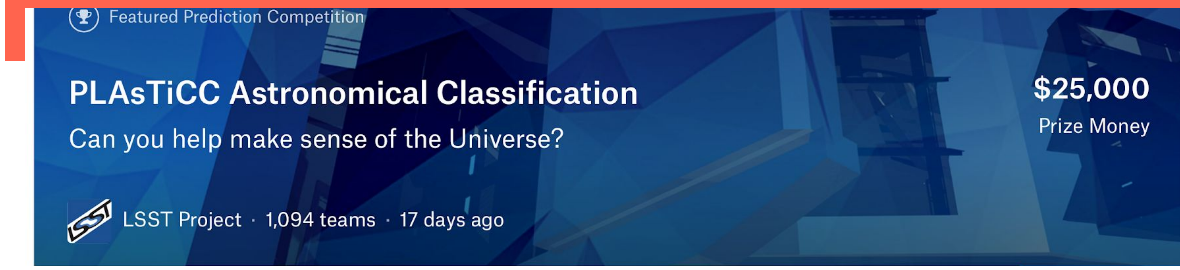


Solutions posted on Kaggle

Useful Features

- Light curve fitting -- Bazin, GP, template fitting (SALT2, SN templates)
- Flux ratio (color)
- Flux difference
- Host galaxy photo-z
- flux * distance ** 2

Popular Models among Kagglers

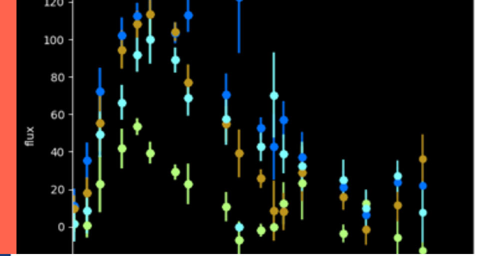
Gradient Boosting
- LightGBM
- XGBoost
- CatBoost

Neural Net
- Convolutional Neural Networks (CNN)
- Recurrent Neural Networks (RNN)
- Multi Layer Perceptron (MLP)
- Autoencoders

Binary Classification

Credit M. Dai

Part II: typing with photometry



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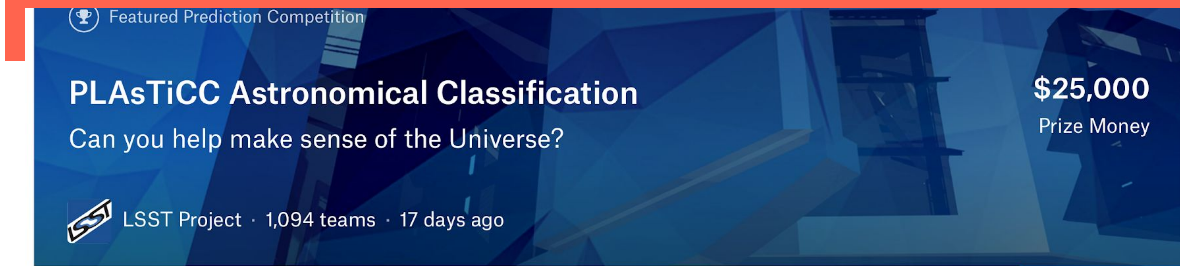

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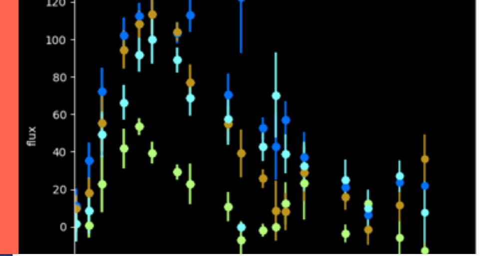
Binary Classification

Credit M. Dai

- common algorithms perform great, e.g. BDTs
- feature extraction is key (domain knowledge + irregular time series)
- labeled set (for training) was crucial, not large nough, not representative of the test set

Part II: typing with photometry



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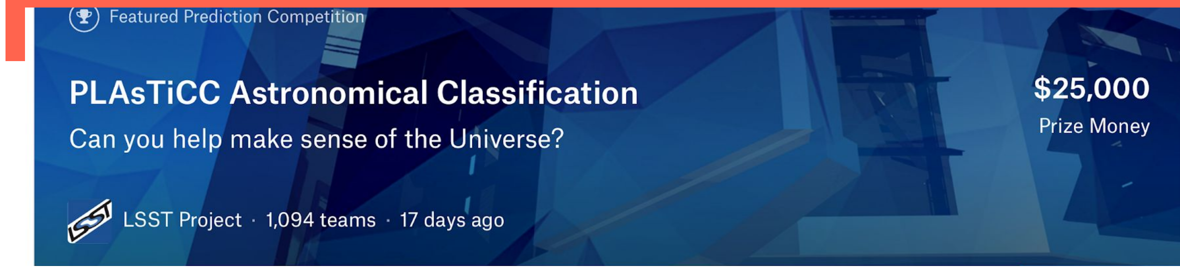

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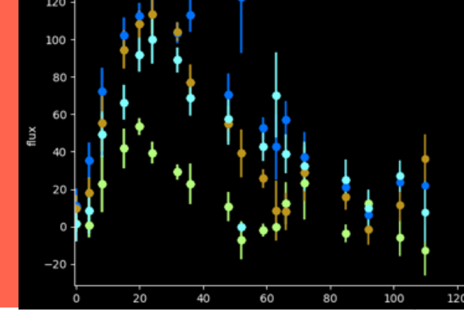
Binary Classification

Credit M. Dai

But feature extraction biases samples!

- common algorithms perform great, e.g. BDTs
- feature extraction is key (domain knowledge + **irregular time series**)
- labeled set (for **training**) was crucial, not large nough, **not representative** of the test set

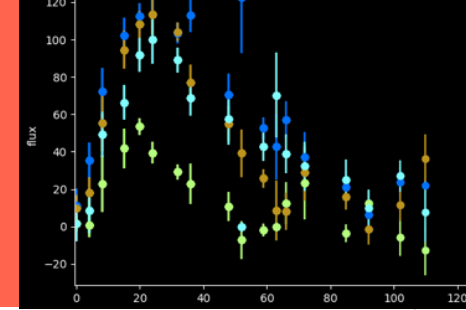
Part II: typing with photometry



SuperNNova
open source photometric classification

Möller & de Boissière 2019

Part II: typing with photometry



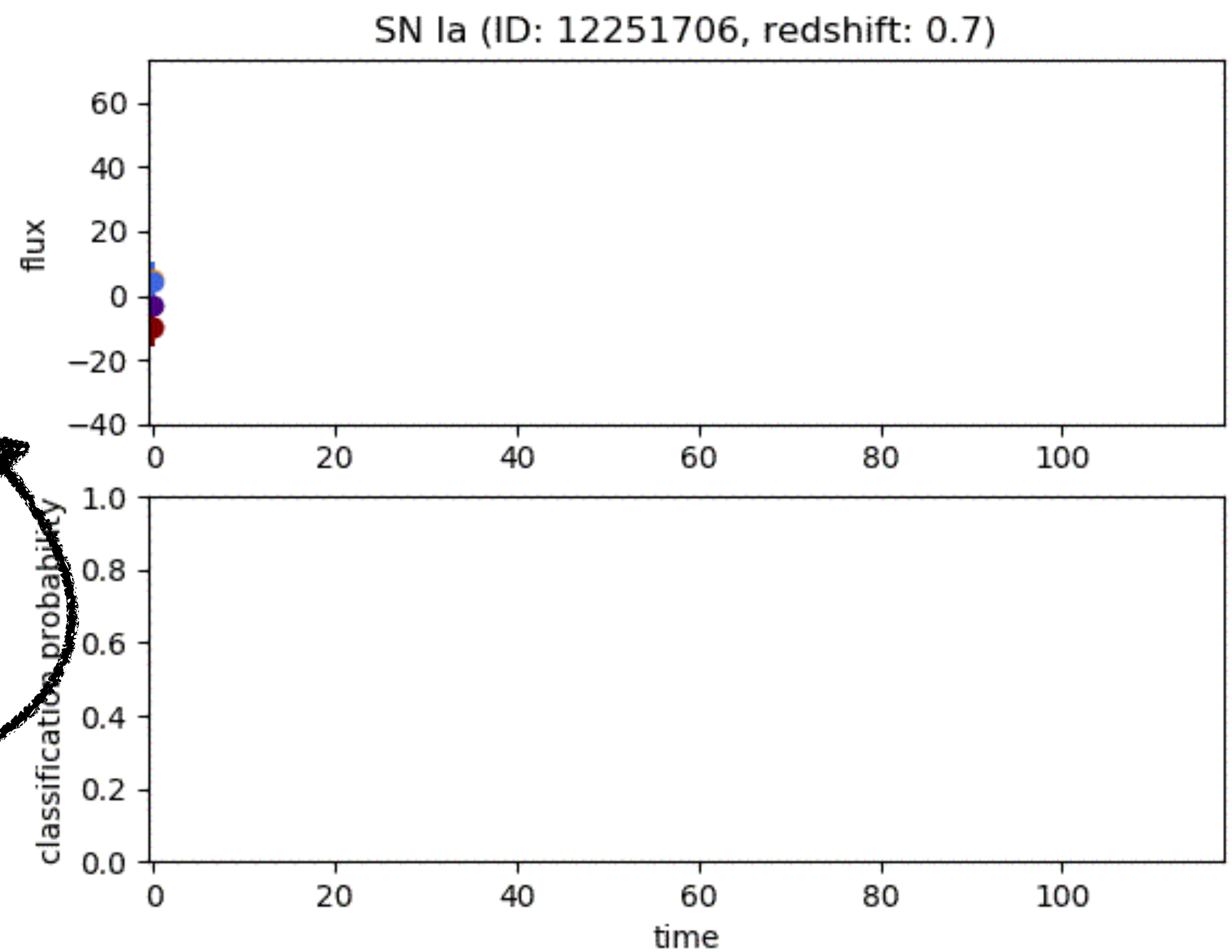
SuperNNova
open source photometric classification

Möller & de Boissière 2019

Inputs:

- Flux in different band-passes
- Flux measurement errors
- Time-step between measurements
- Optional: other features (e.g. host-redshift)

Allows using irregular time series without extrapolation!



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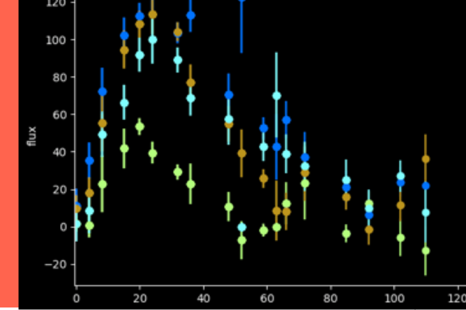
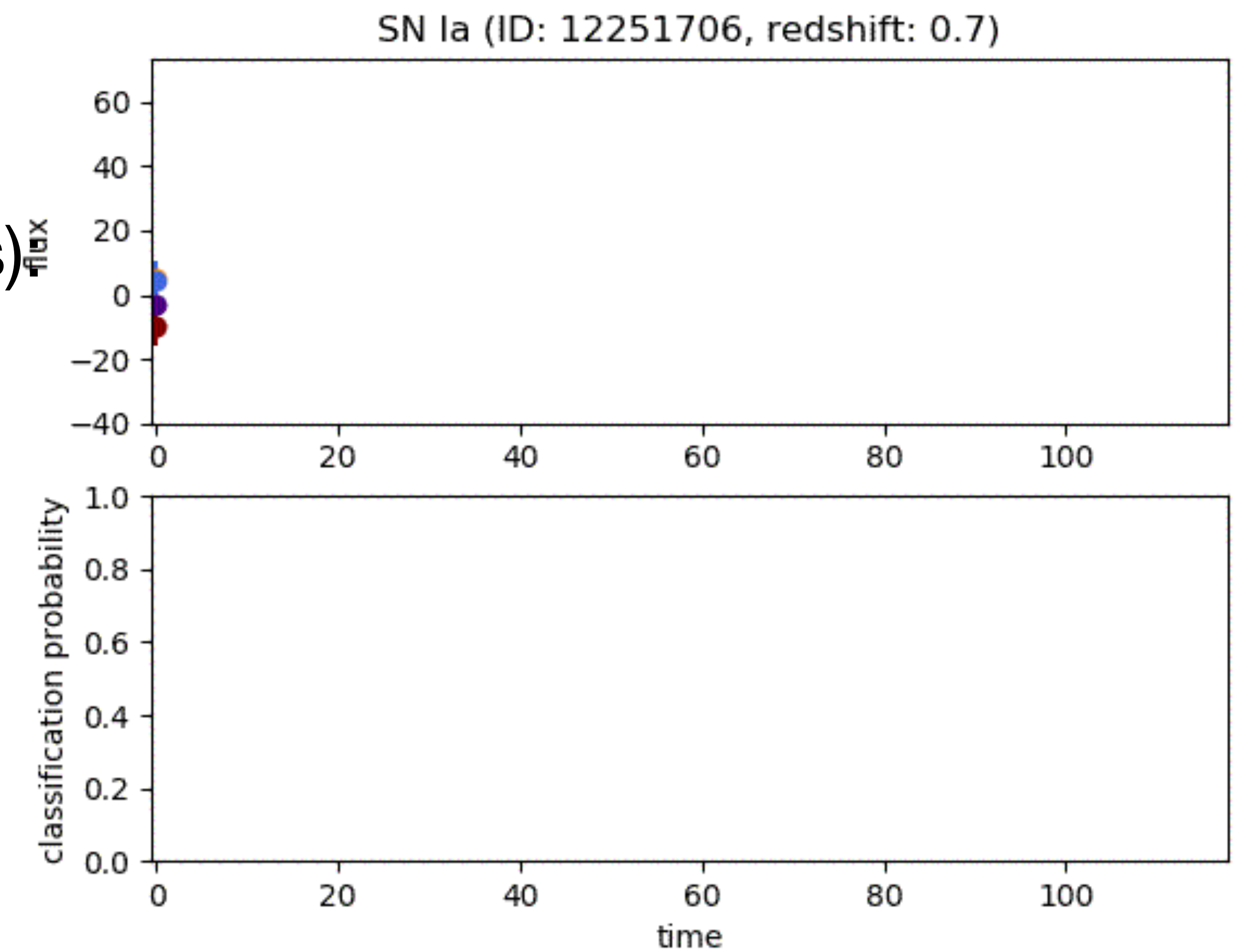


SuperNNova
open source photometric classification

Möller & de Boissière 2019

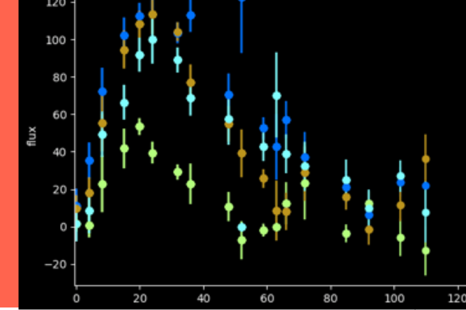
Deep learning for cosmology

- Recurrent Neural Networks (RNNs):
  - LSTM
  - GRU
- Bayesian RNNs
  - Variational (Gal+2016)
  - Bayes by Backprop (Fortunato+2017)
- Convolutional NN



Other time-series applications with:
RNNs: Charnock & Moss 2016, Muthukrishna+2019
CNN: Kimura +2017

Part II: typing with photometry



SuperNNova
open source photometric classification

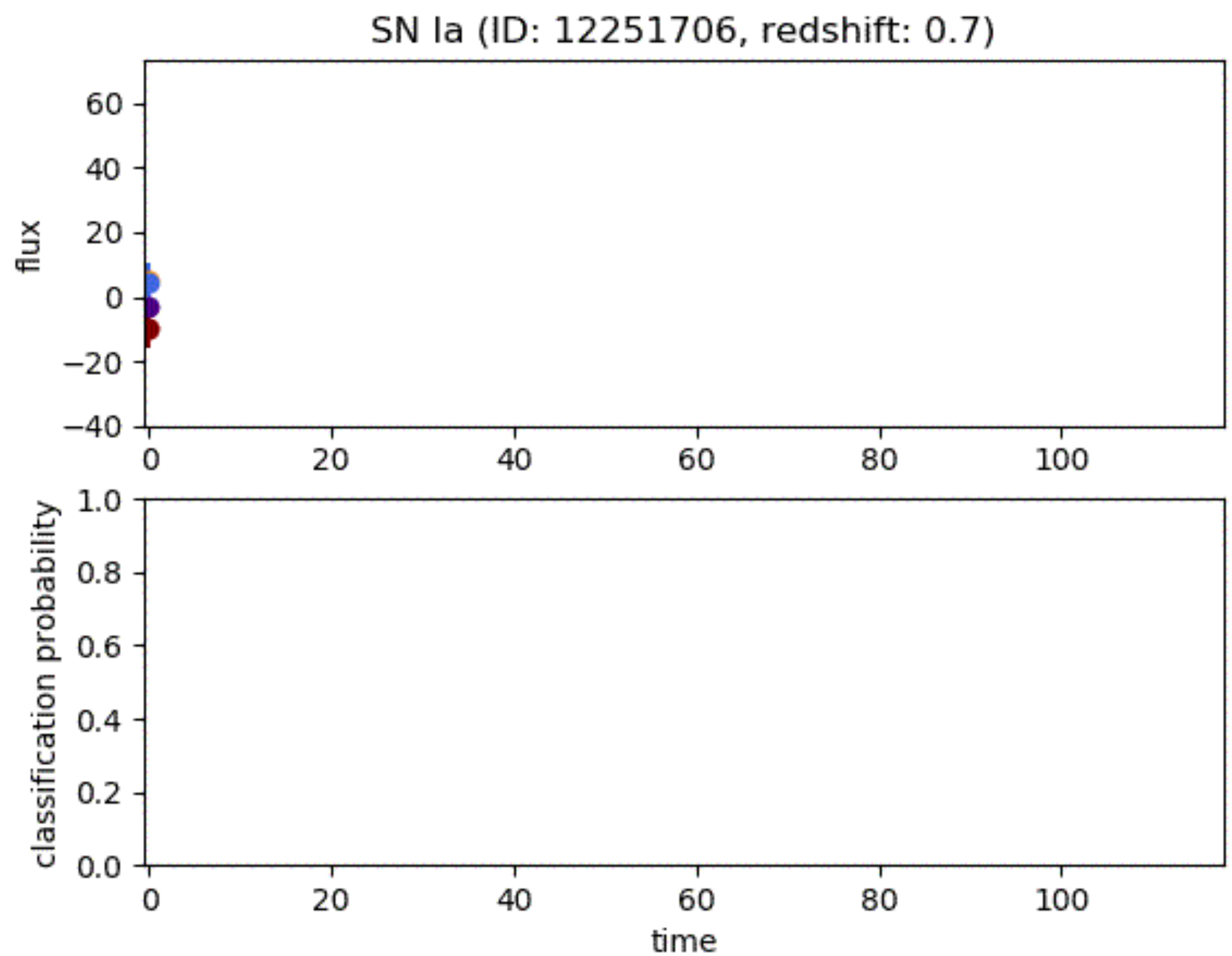
Möller & de Boissière 2019

Accuracy

early classification 87.59 ± 0.13

for:
- brokers
- follow-up for promising candidates

reproducible selection functions
Improving trying samples *e.g. Ishida + 2018*



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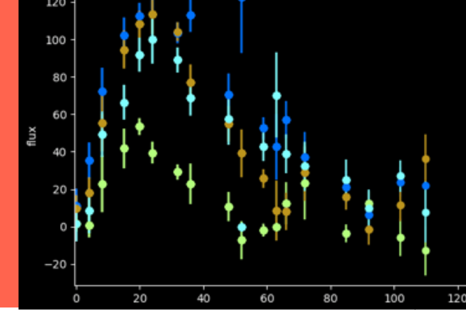


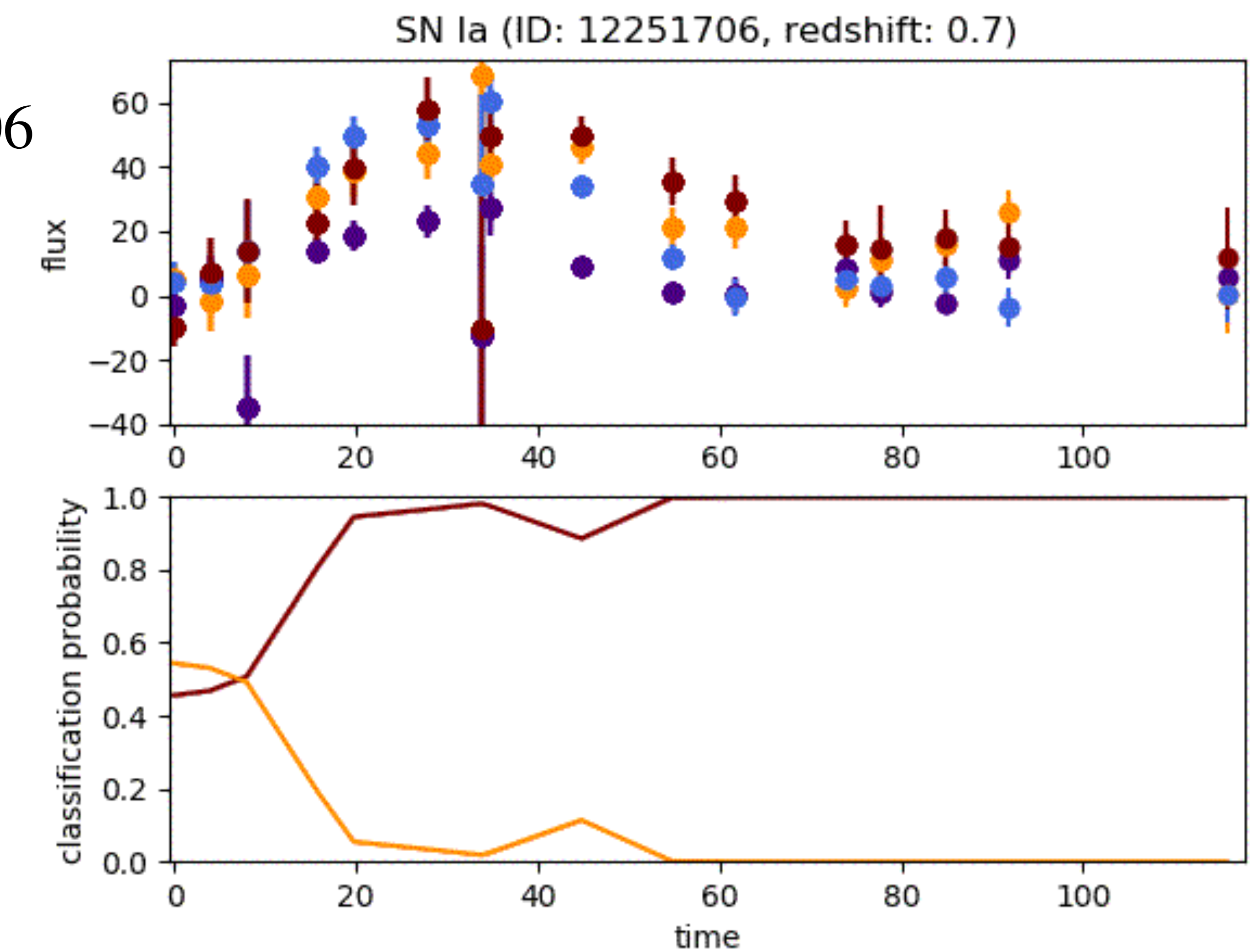
SuperNNova
open source photometric classification

Möller & de Boissière 2019

Accuracy

early classification	87.59 ± 0.13
complete	96.97 ± 0.06

for:
- larger & more reliable samples
- probing new parameter space



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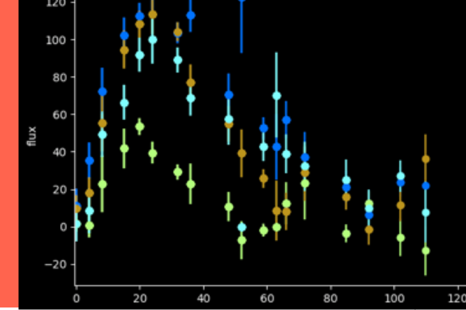

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open source photometric classification

Möller & de Boissière 2019

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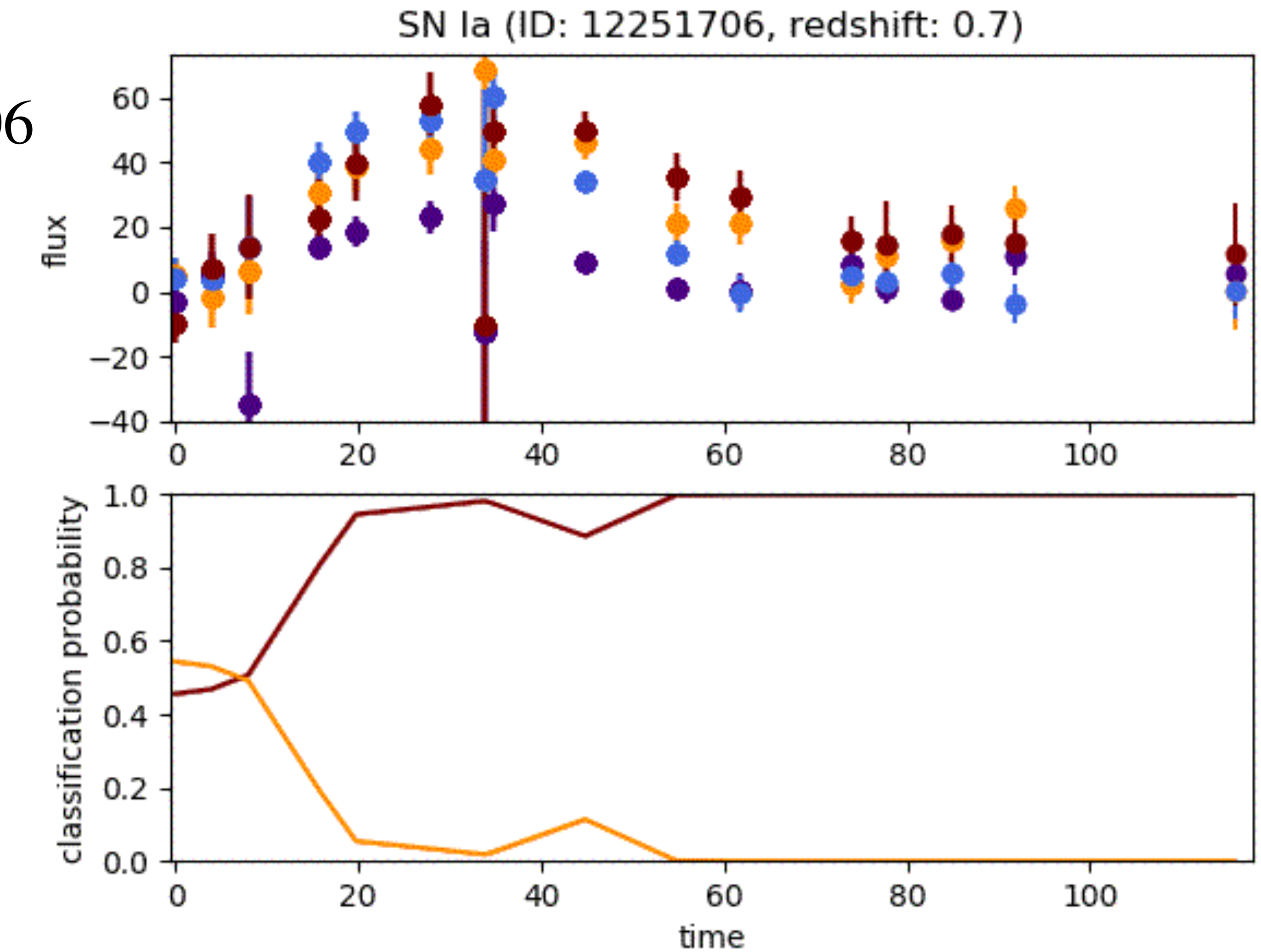
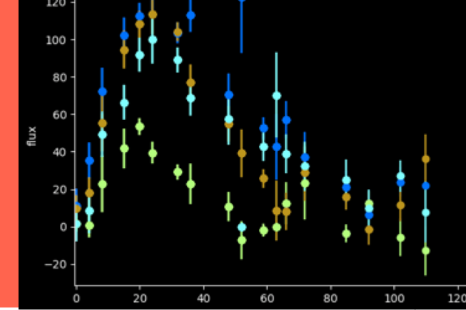


for:
- larger & more reliable samples
- probing new parameter space

cosmology, systematic studies
e.g. Hlozek + 2012, Jones+2016

Cosmology limitation:
Modelling core-collapse contamination

Current efforts include Hinton + 2018, Vincenzi + 2019



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open source photometric classification

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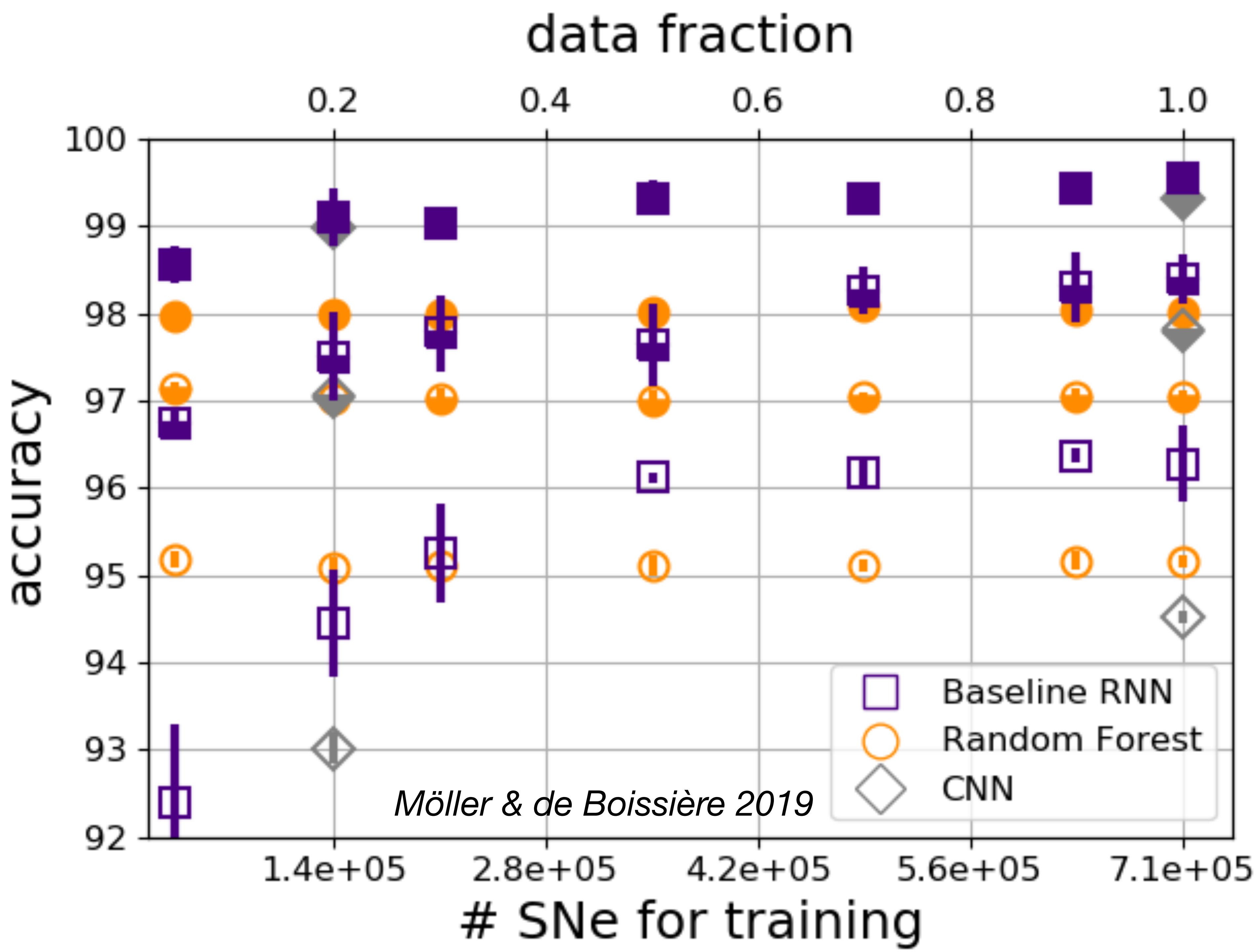
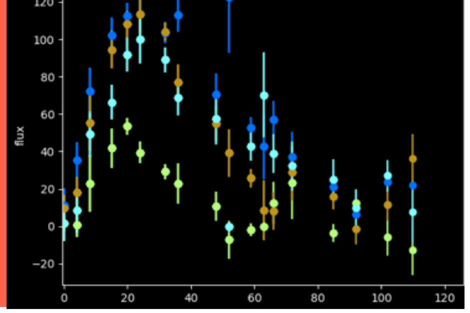


Beware, features in RF are very tuned for Its!

Part II: typing with photometry



Bayesian NNs

$$\mathcal{P}\left(\mathbf{y}|\mathbf{X},\mathbf{w}\right)$$

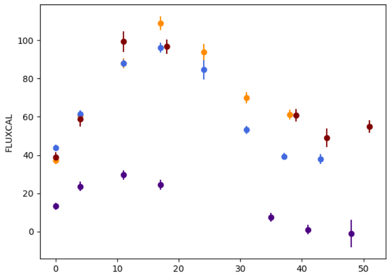
Categorical distribution

Target
(SN type)

data
(lightcurves)

Network weights

Ia vs. Non Ia



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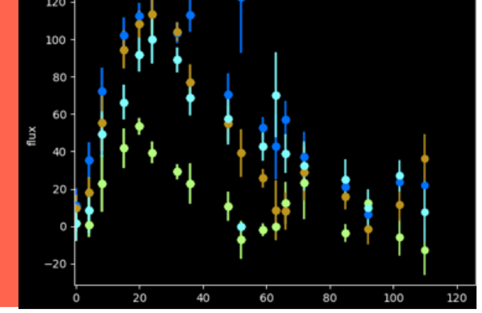

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Categorical distribution

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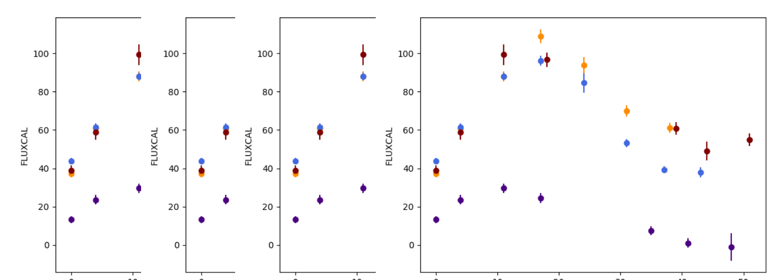
Network weights

data $$\mathcal{D} = (\mathbf{X}_k, \mathbf{y}_k)_{k=1\ldots K}$$



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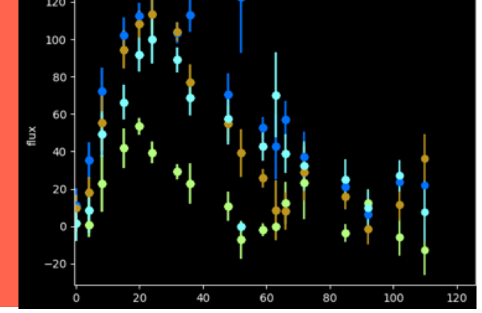

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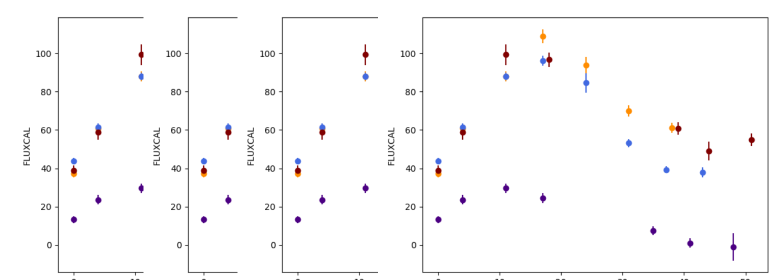
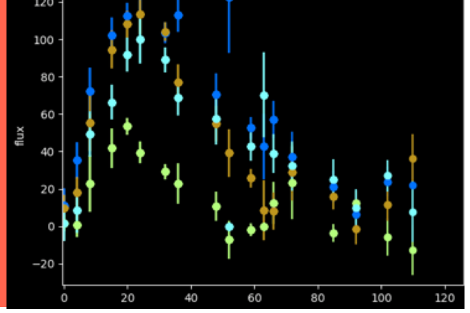


Training minimisation $NLL = \min_{\mathbf{w}} \sum_{k=1}^{K} -\log \mathcal{P}(\mathbf{y_k}|\mathbf{X}_k, \mathbf{w})$

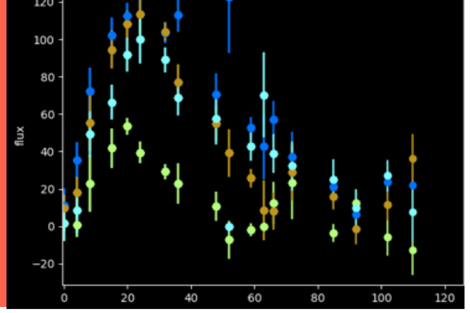
Part II: typing with photometry



Bayesian NNs

$$\mathscr{P}(\hat{\mathbf{y}} \,|\, \mathbf{x}) = \int \mathscr{P}(\hat{\mathbf{y}} \,|\, \mathbf{x}, \mathbf{w}) \mathscr{P}\left(\mathbf{w} \,|\, \mathscr{D}\right) d\mathbf{w}$$

Bayesian: distribution of weights



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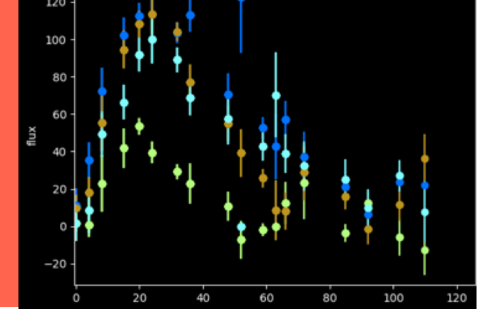
posterior is intractable for deep neural networks

Part II: typing with photometry

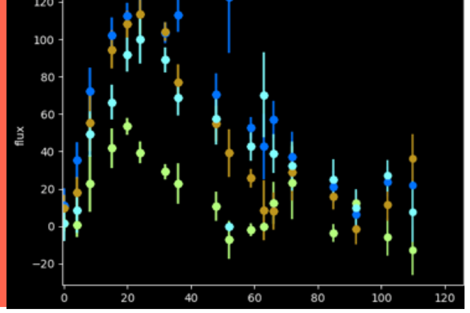


Bayesian NNs

$$\mathscr{P}(\hat{\mathbf{y}} \mid \mathbf{x}) = \int \mathscr{P}(\hat{\mathbf{y}} \mid \mathbf{x}, \mathbf{w}) \mathscr{P}\left(\mathbf{w} \mid \mathscr{D}\right) d\mathbf{w}$$

$$\mathscr{P}(\mathbf{w} \mid \mathscr{D}) \approx q(\mathbf{w} \mid \theta)$$ variational distribution

Part II: typing with photometry



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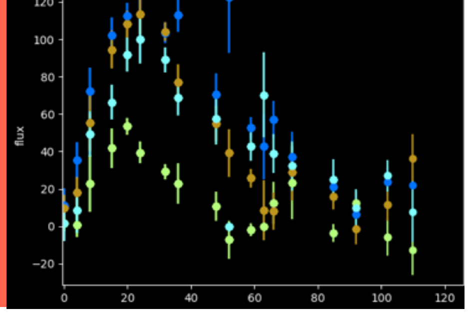
Training minimisation $$\hat{\theta} = \min_{\theta} \mathbf{KL}\left(q(\mathbf{w} \,|\, \theta) \,||\, \mathscr{P}(\mathbf{w} \,|\, \mathscr{D})\right)$$

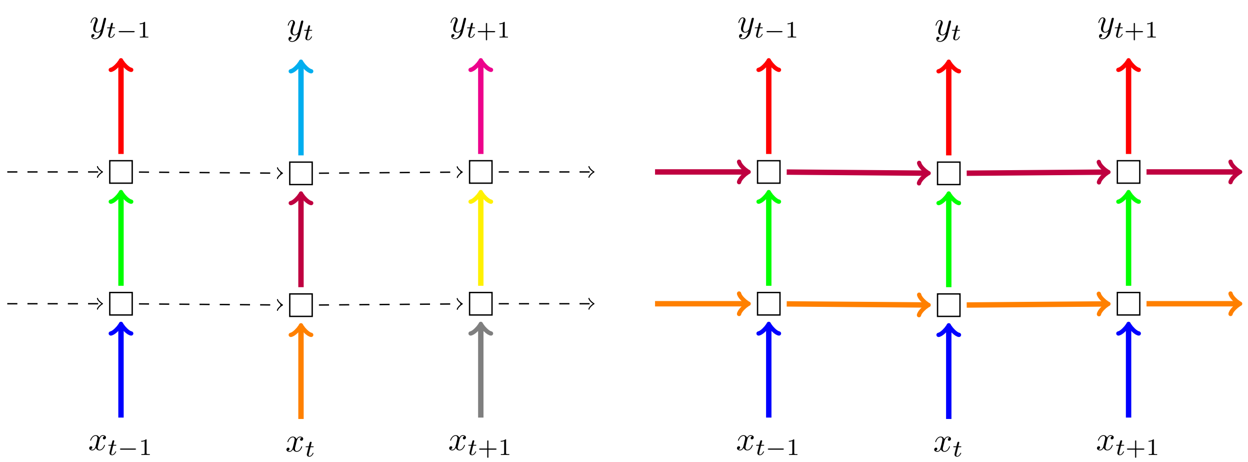


Bayesian NNs

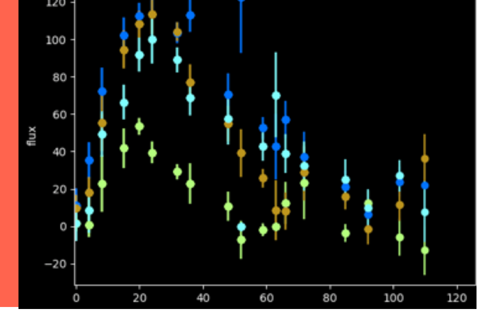
Approximating the variational distribution $q(\mathbf{w}|\theta)$

1. MC dropout

Gal & Ghahramani 2016



(a) Naive dropout RNN (b) Variational RNN



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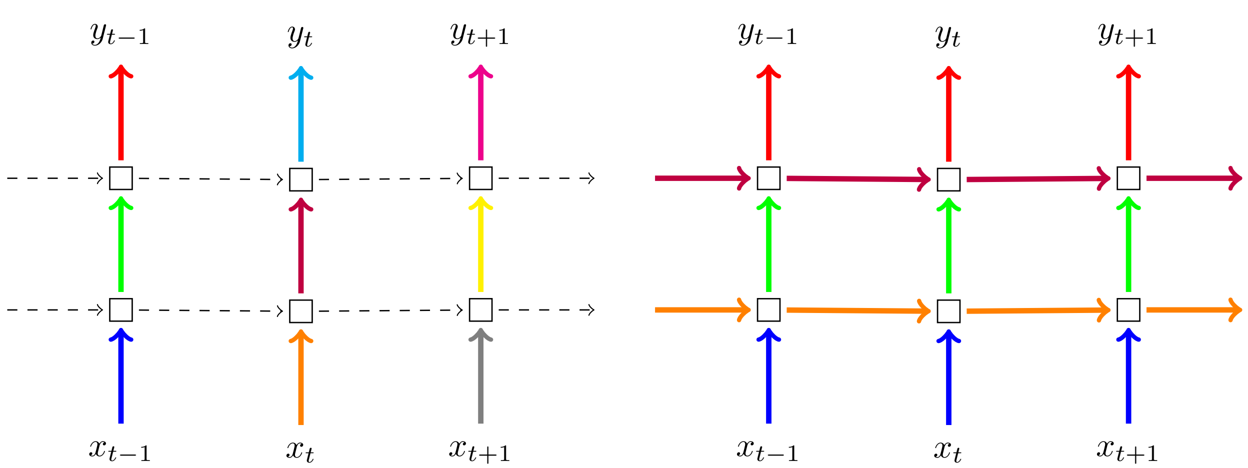
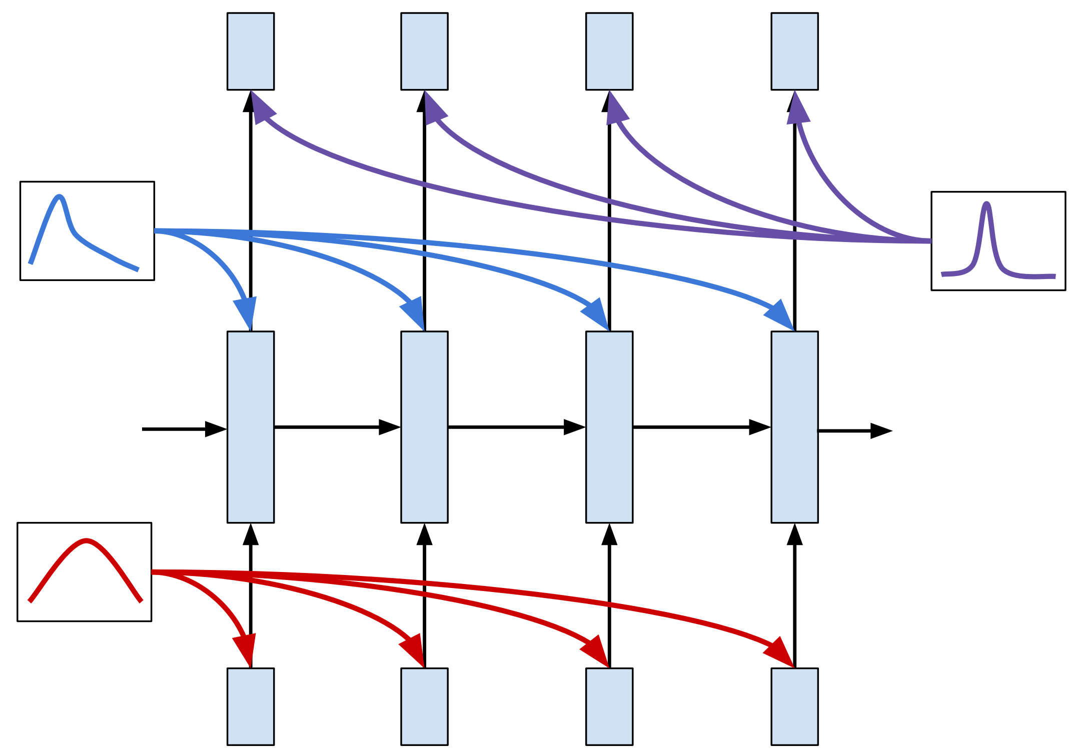


(a) Naive dropout RNN

(b) Variational RNN

2. Bayes by Backprop
Fortunato+ 2017



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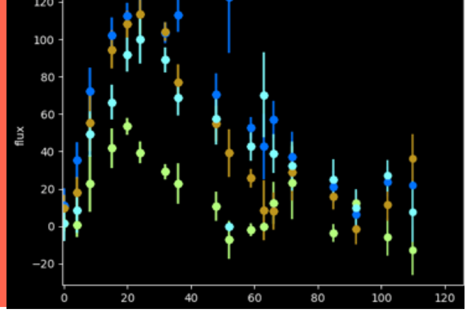
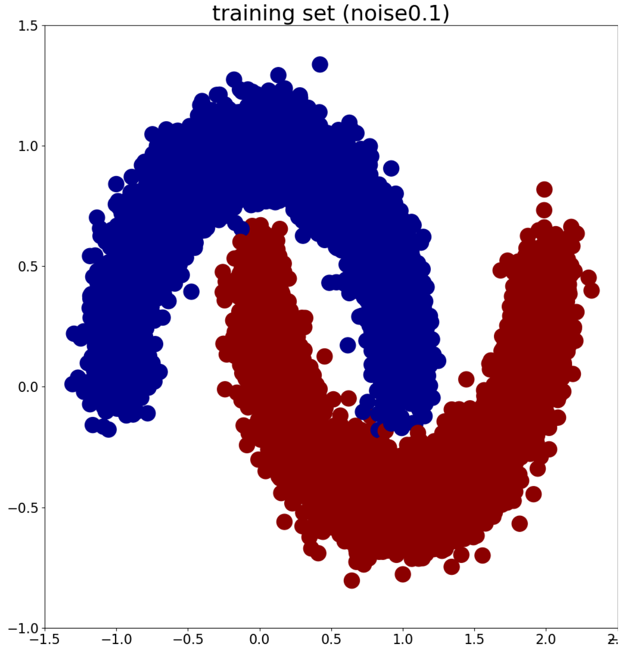


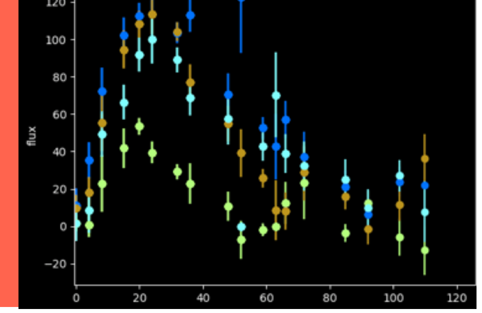
Bayesian NNs

training



classification probability

Part II: typing with photometry



Bayesian NNs

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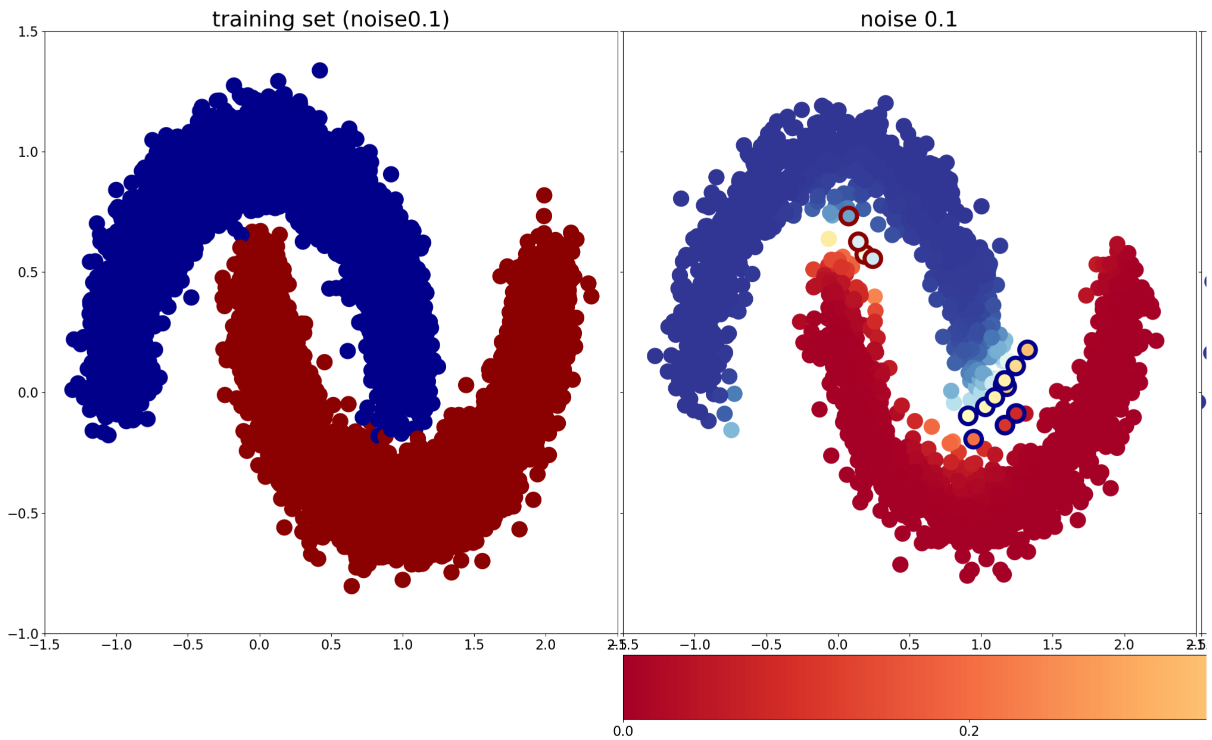

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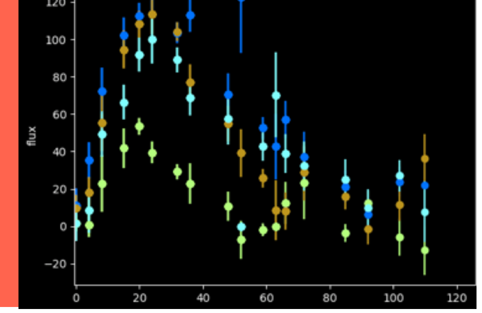

Bayesian NNs

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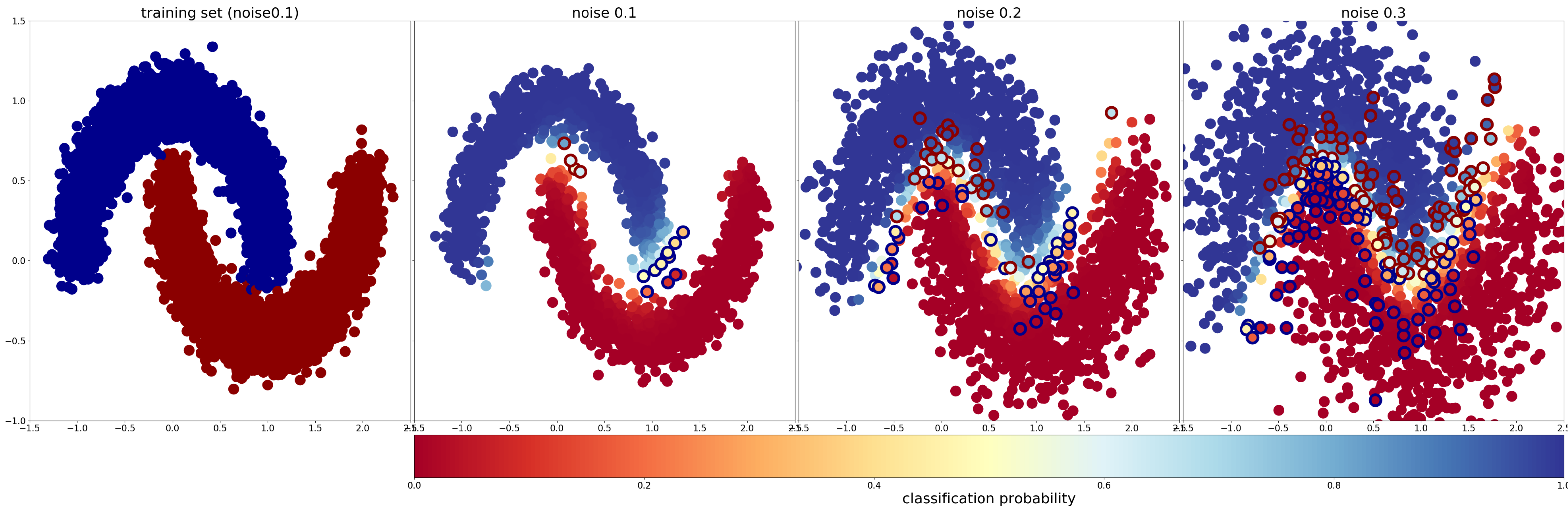

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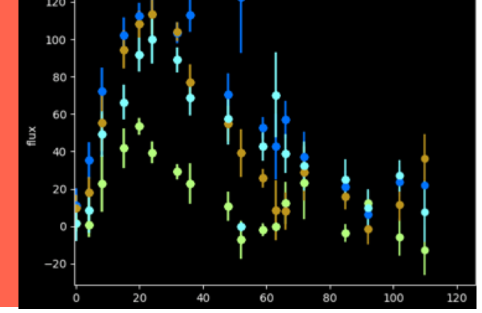
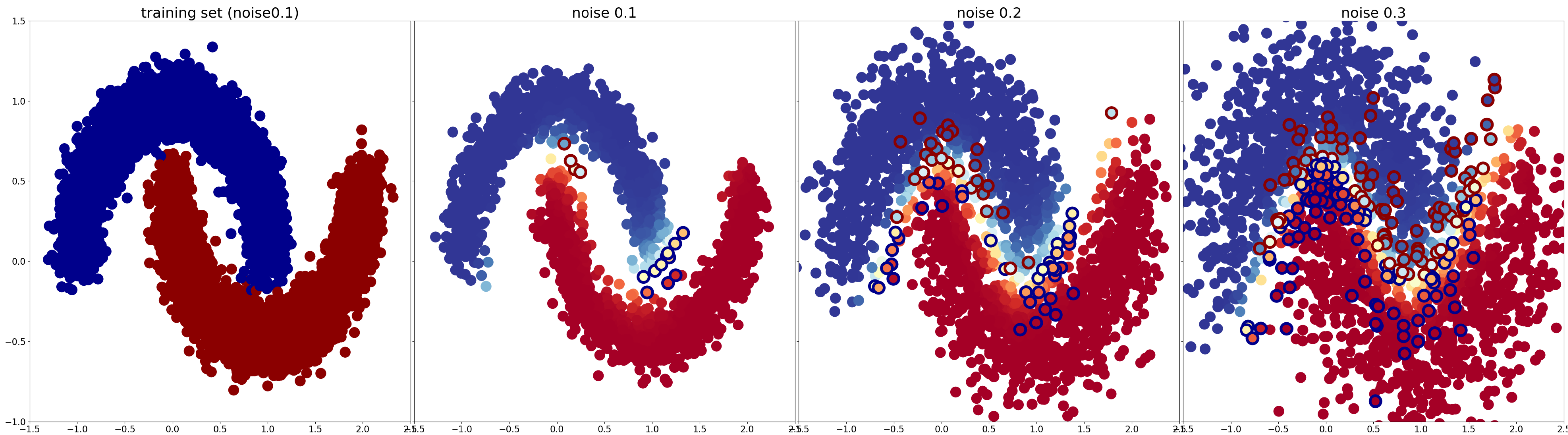


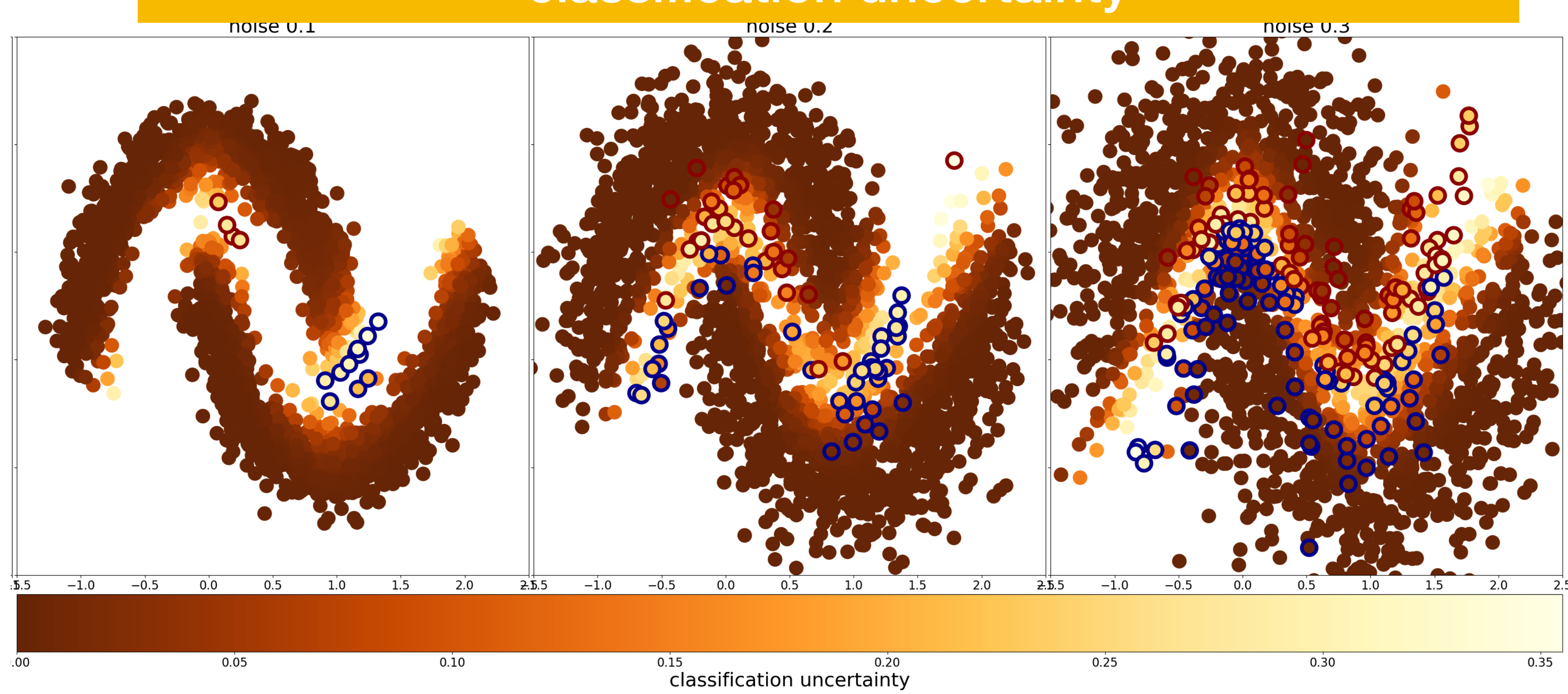
Bayesian NNs

training

classification probability



classification uncertainty



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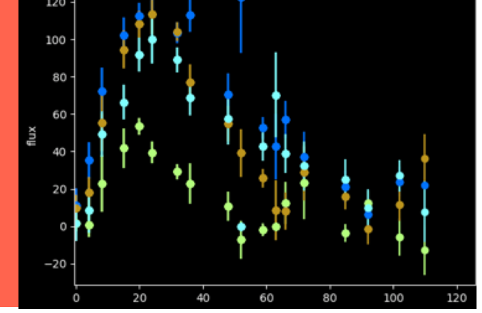

Bayesian NNs

SuperNNova
open source photometric classification

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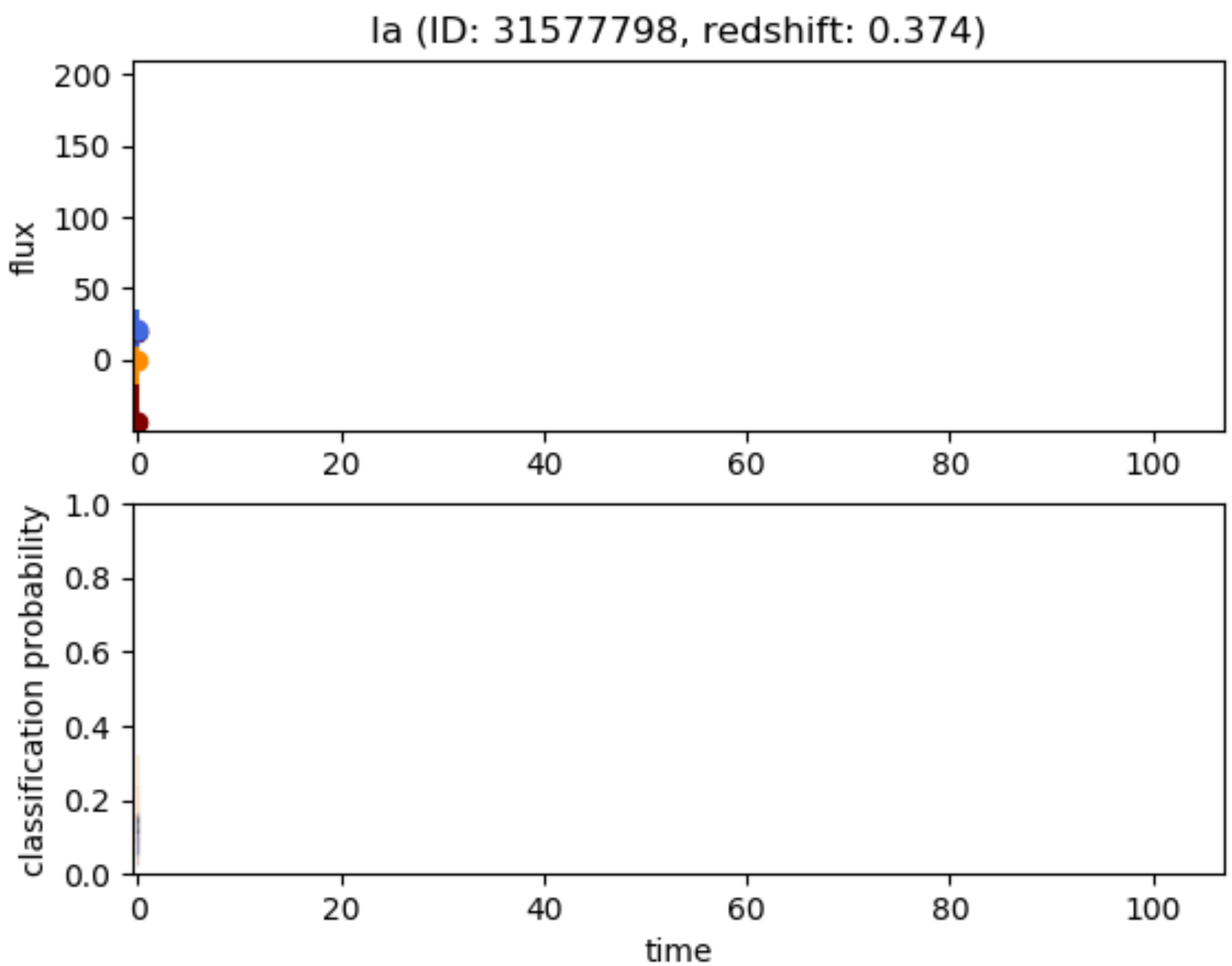
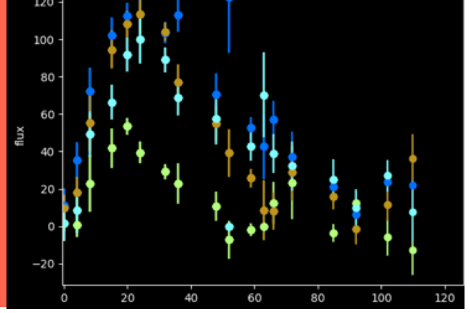


2. Bayes by Backprop
Fortunato+ 2017

Posterior that provides epistemic uncertainties

Epistemic uncertainties:

express our <u>ignorance about the model</u> that generated the data.



ML limitations

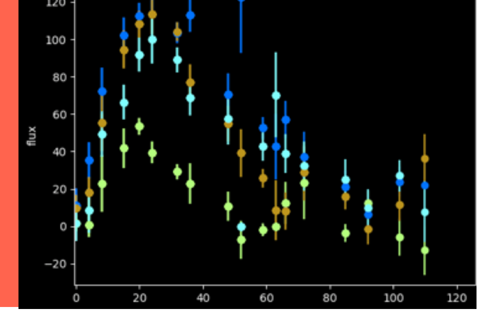
Training sets are:

! not representative

! incomplete (we don't know/can't simulate)

? *Can we use output from ML classifiers for cosmology or any statistical analyses?*

Part II: typing with photometry



ML limitations
representativity

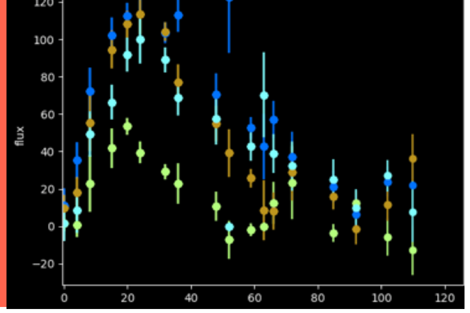
simulation

peak brightness *i*

data

peak brightness *i*

Distribution of properties of SNe



ML limitations
representativity

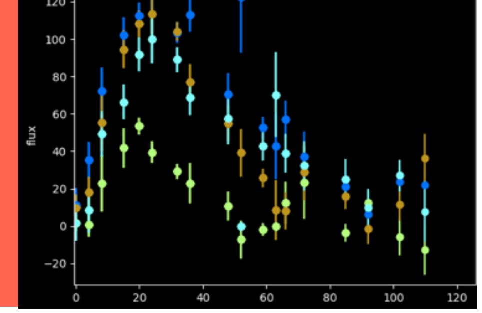
simulation

peak brightness *i*

→ train classification algorithm

data

peak brightness *i*



ML limitations
representativity

simulation

peak brightness *i*

train classification algorithm

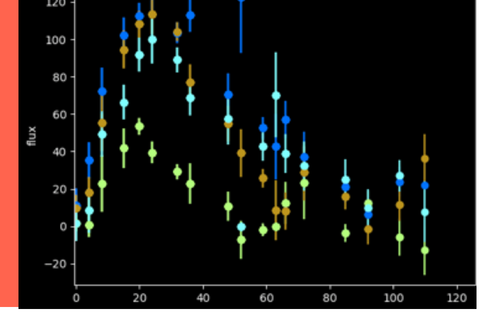
data

peak brightness *i*

classify the data

accuracy decreases (*Lochner+ 2015, Charnock+2017*)

Part II: typing with photometry



ML limitations
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simulation

peak brightness *i*

train classification algorithm

data

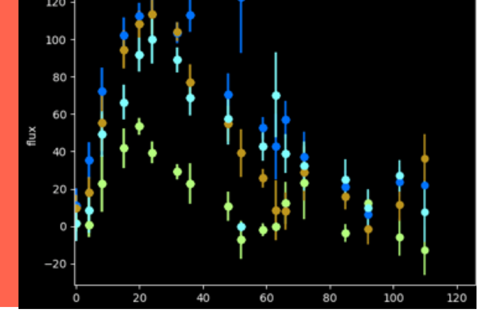
peak brightness *i*

classify the data

Either we improve our training sets or search for robust methods!

Pasquet+ 2019, Möller+ 2019

Part II: typing with photometry



ML limitations
representativity

SuperNNova
open source photometric classification

BNNs

Simplistic simulation

peak brightness *i*

classify

representative simulation

peak brightness *i*

representative simulation

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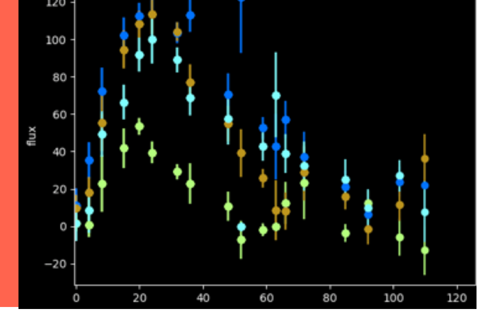

ML limitations
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Simplistic simulation

peak brightness *i*

representative simulation

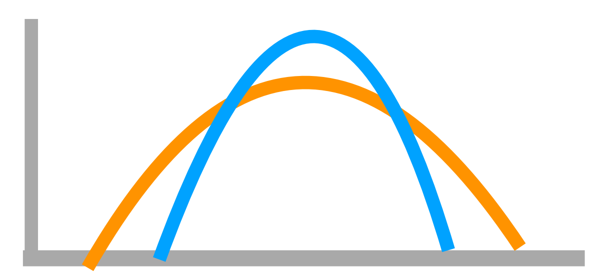
peak brightness *i*

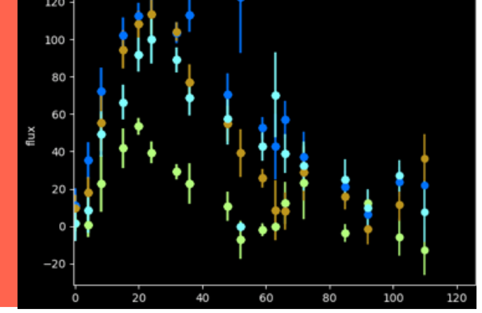
classify

representative simulation

accuracy changes slightly (<prob> are not the most indicative)

non-representative models give larger uncertainties!



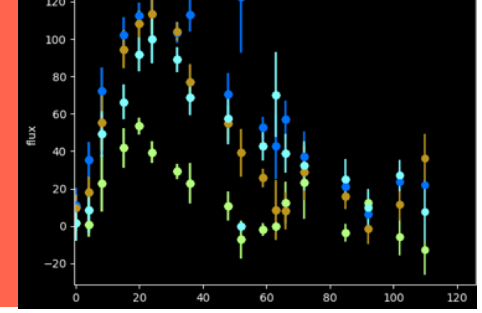


ML limitations
incompleteness

training set

to classify

Part II: typing with photometry



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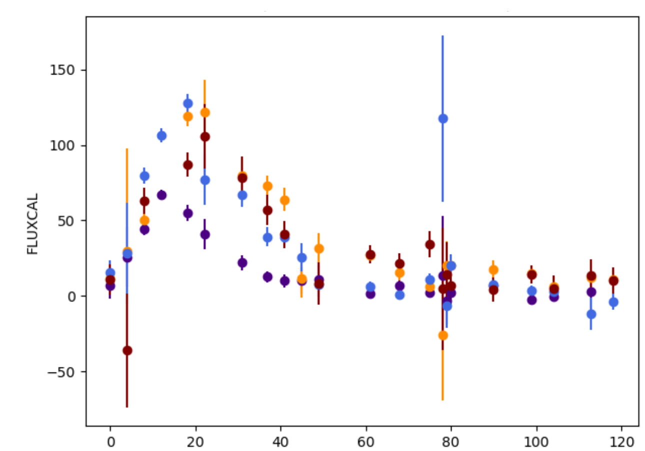

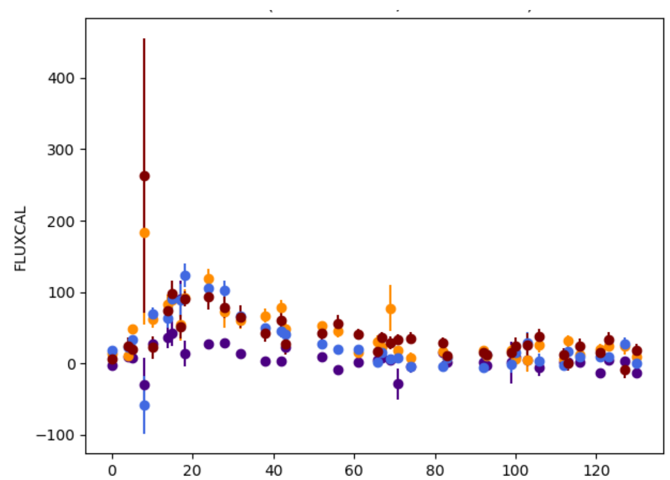

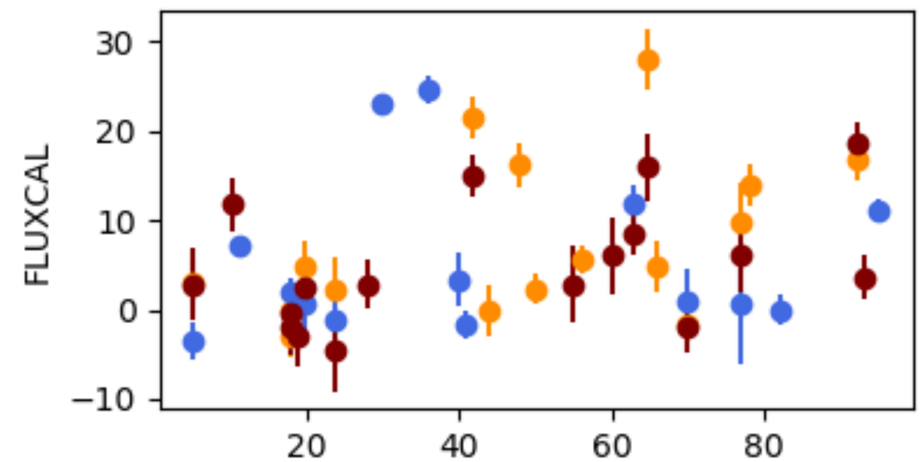

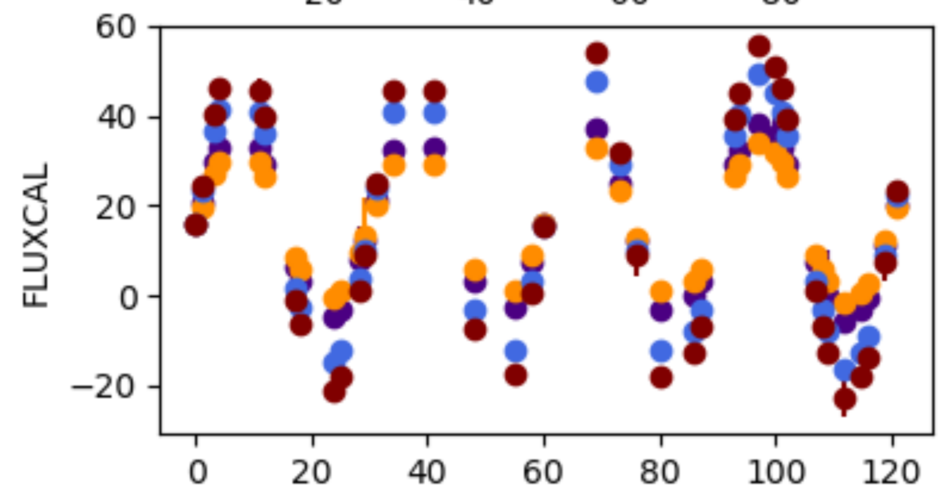

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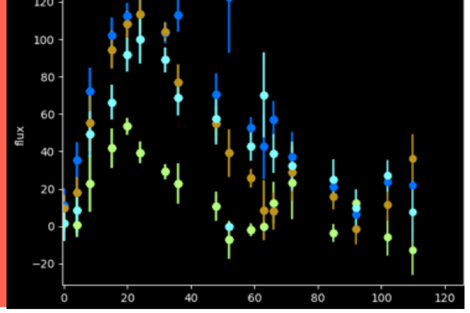

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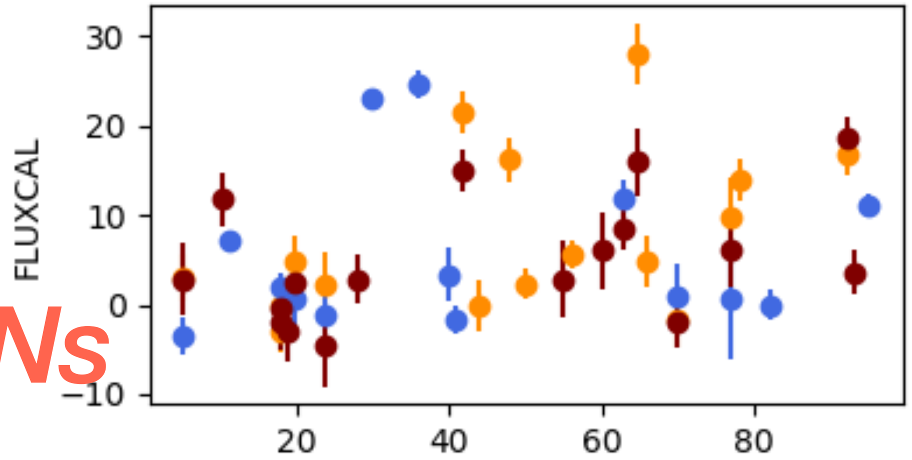
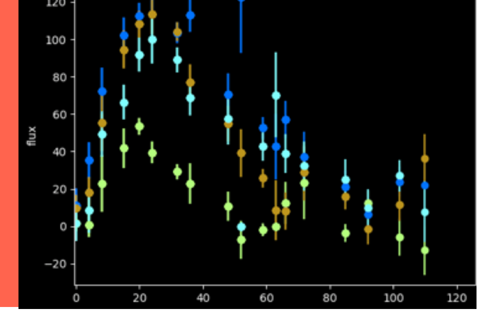


SuperNNova *with BNNs*

open source photometric classification

Part II: typing with photometry



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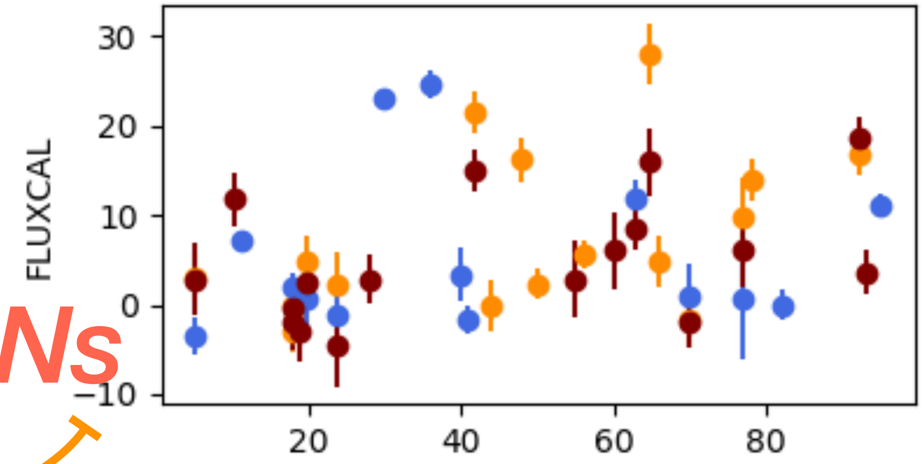
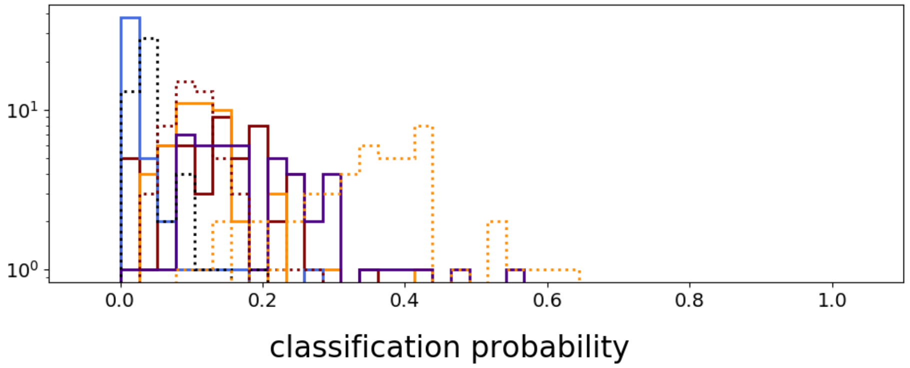


SuperNNova *with BNNs*

open source photometric classification

low probability for any class



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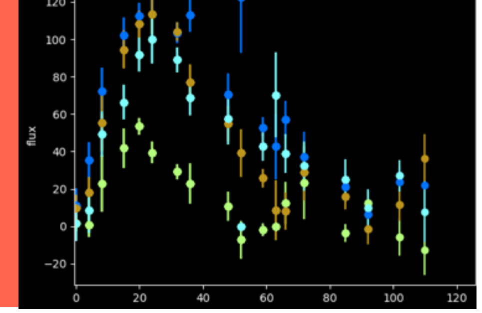

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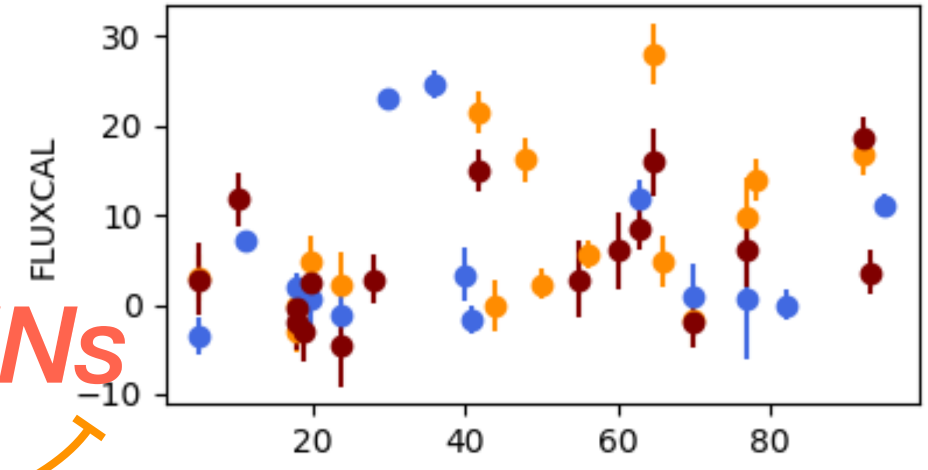

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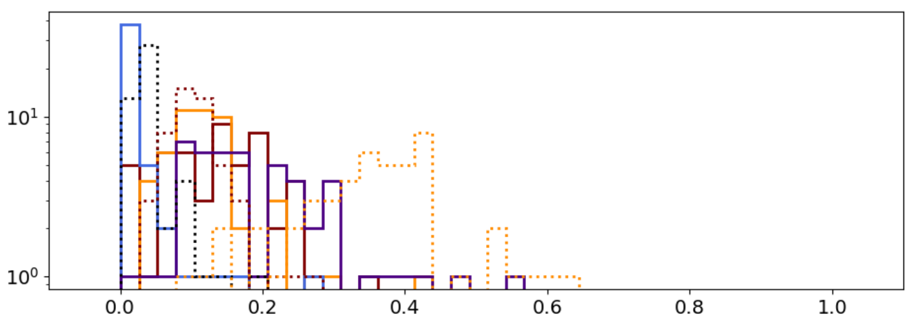
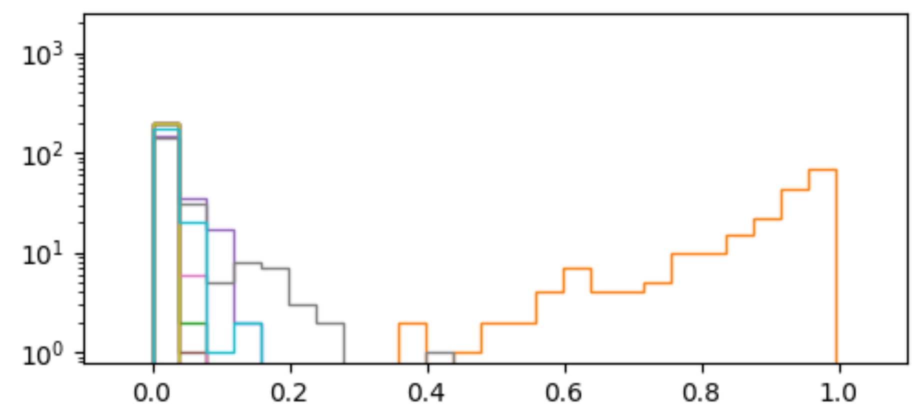
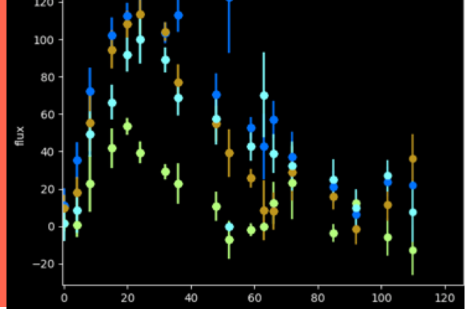


high probability for “less-known” class



but… BNNs can give us high-probability but large uncertainty

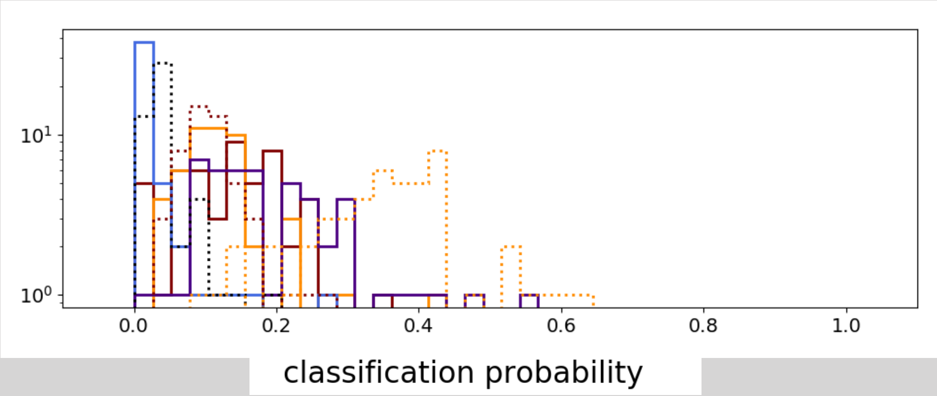
“an increase in average classification uncertainties for these anomalies” Möller + 2019



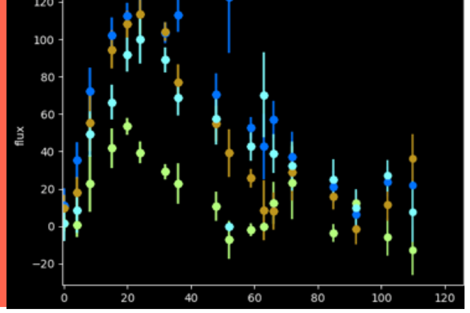
ML probabilities for statistical analyses?

Selecting a SN Ia sample:

cutting on "classification probabilities" for selection

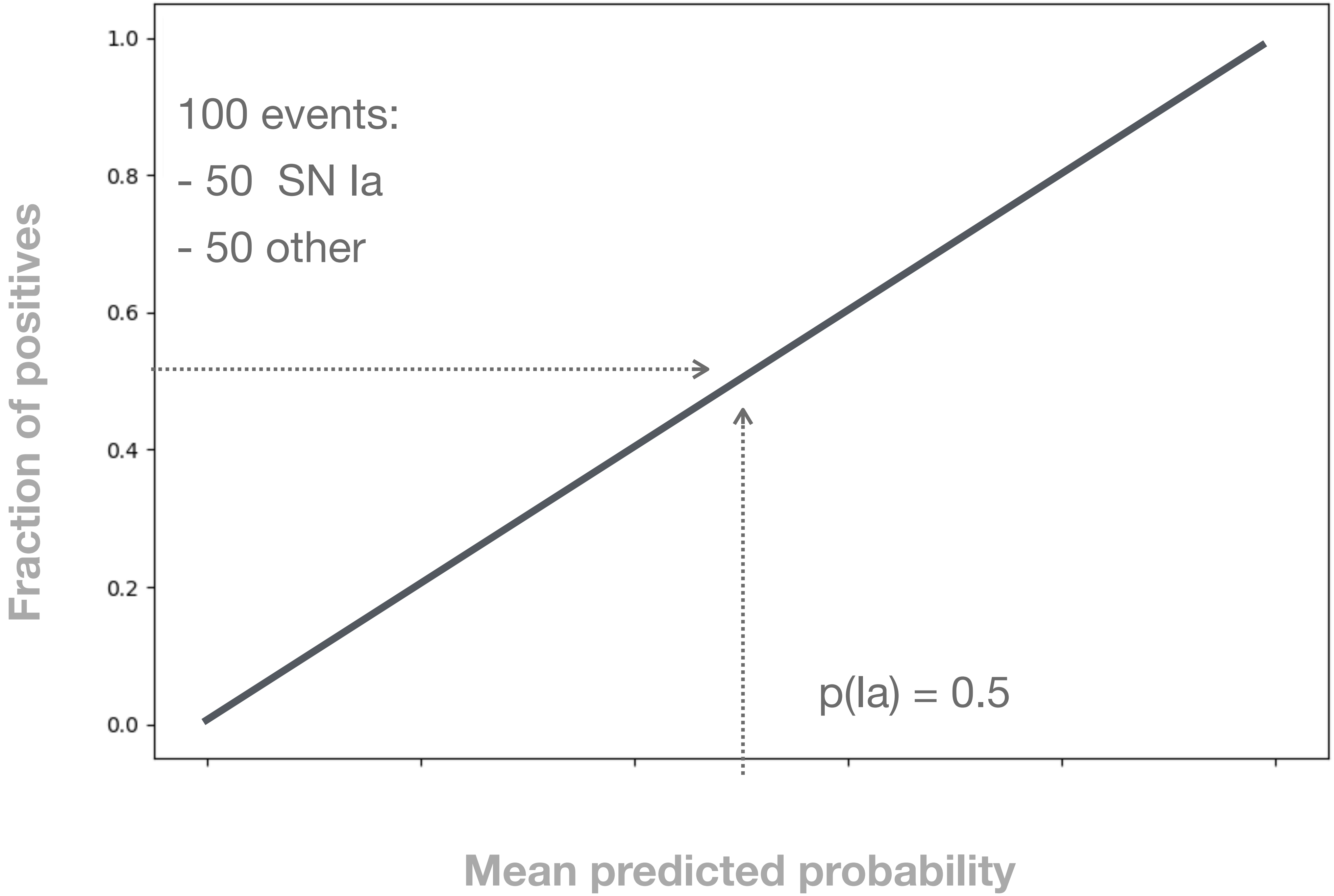


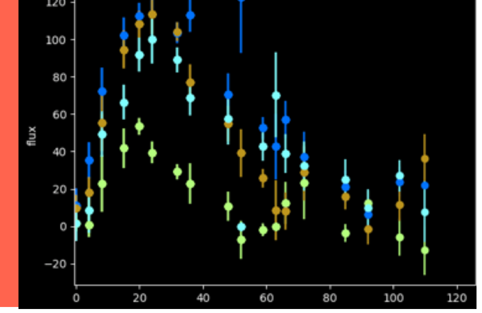
Can use a "weight" in the analysis using these "classification probabilities" *Jones+2018, Hinton+2018*



ML probabilities for statistical analyses?

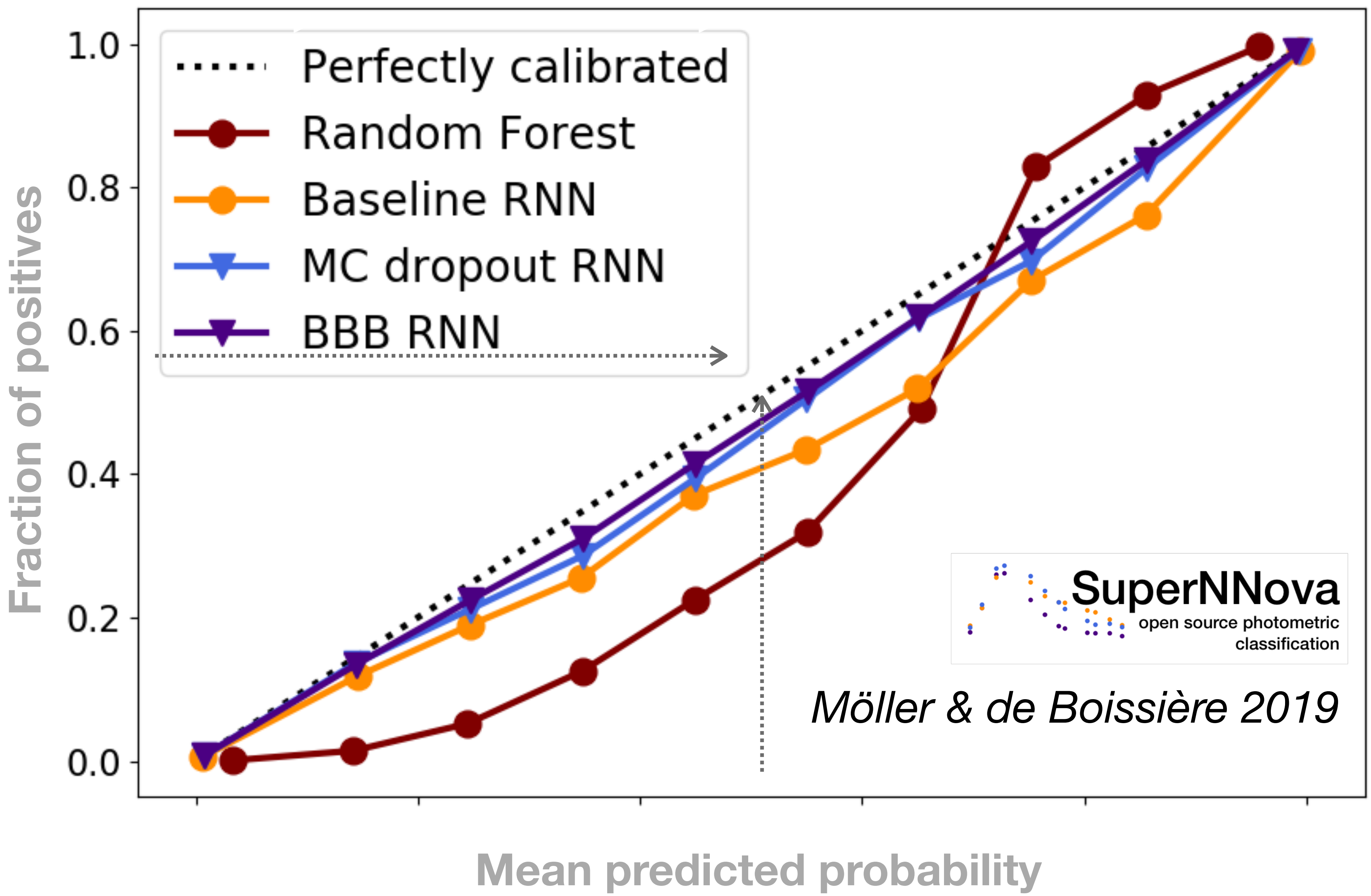
De Groot+ 1983, Niculezcu-Mizil+ 2005, Guo+ 2017





ML limitations

ML probabilities for statistical analyses?



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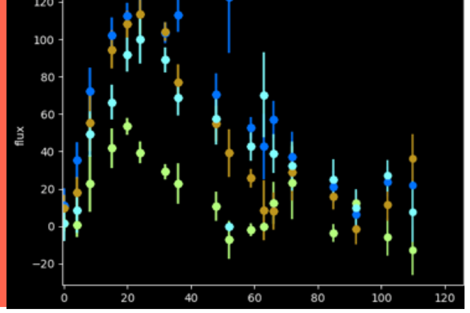
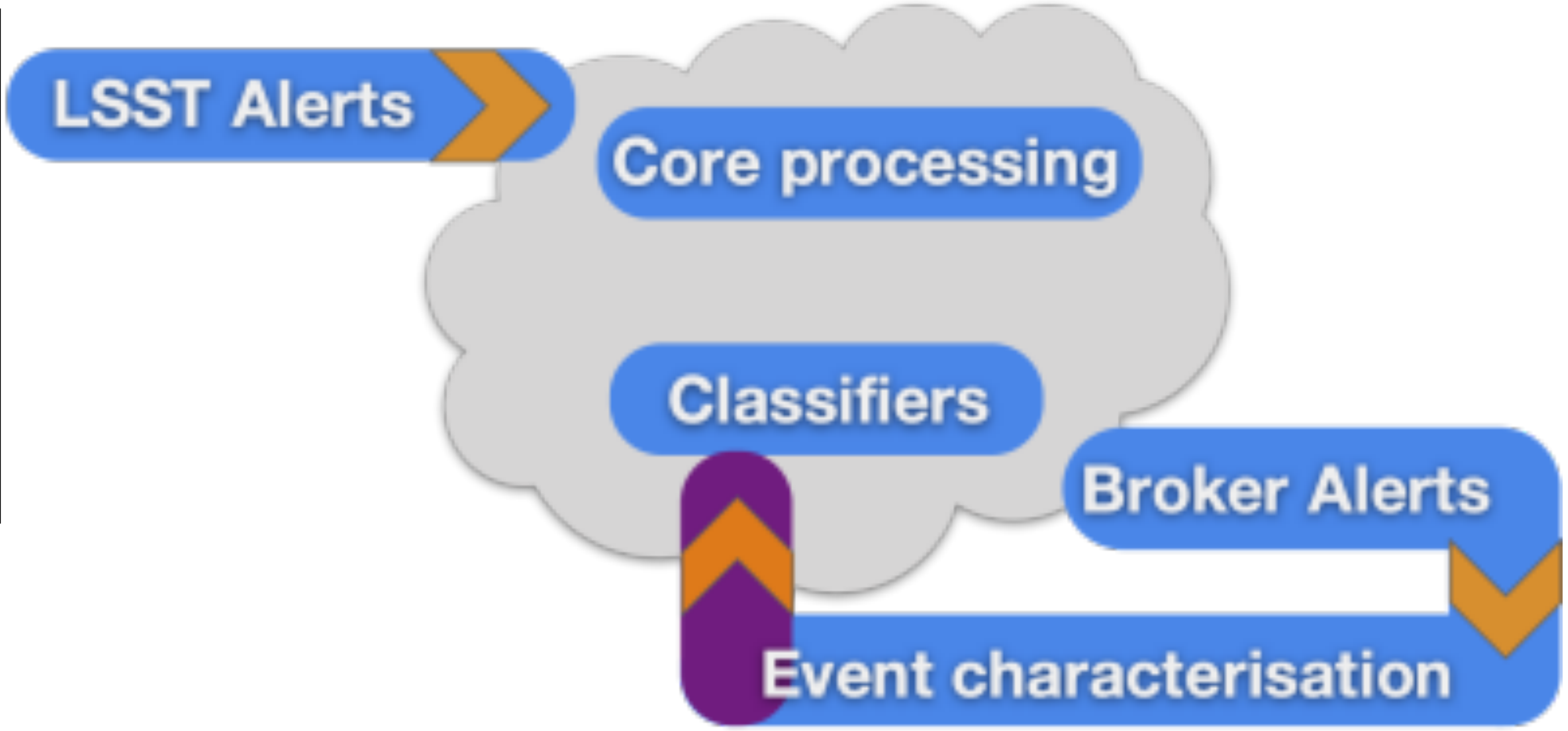


FINK

find, classify, improve

- 10 IN2P3/CNRS labs and centers
- Big data (15 TB/night)
- **ML on data stream**
- Automatized decision making
- Minimum duration of 10 years
- Connection across experiments

J. Peloton, E. Ishida, A. Möller
+28 signatories



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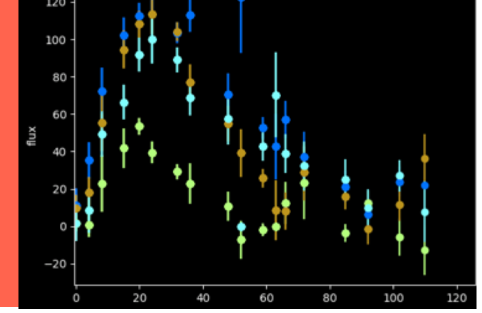

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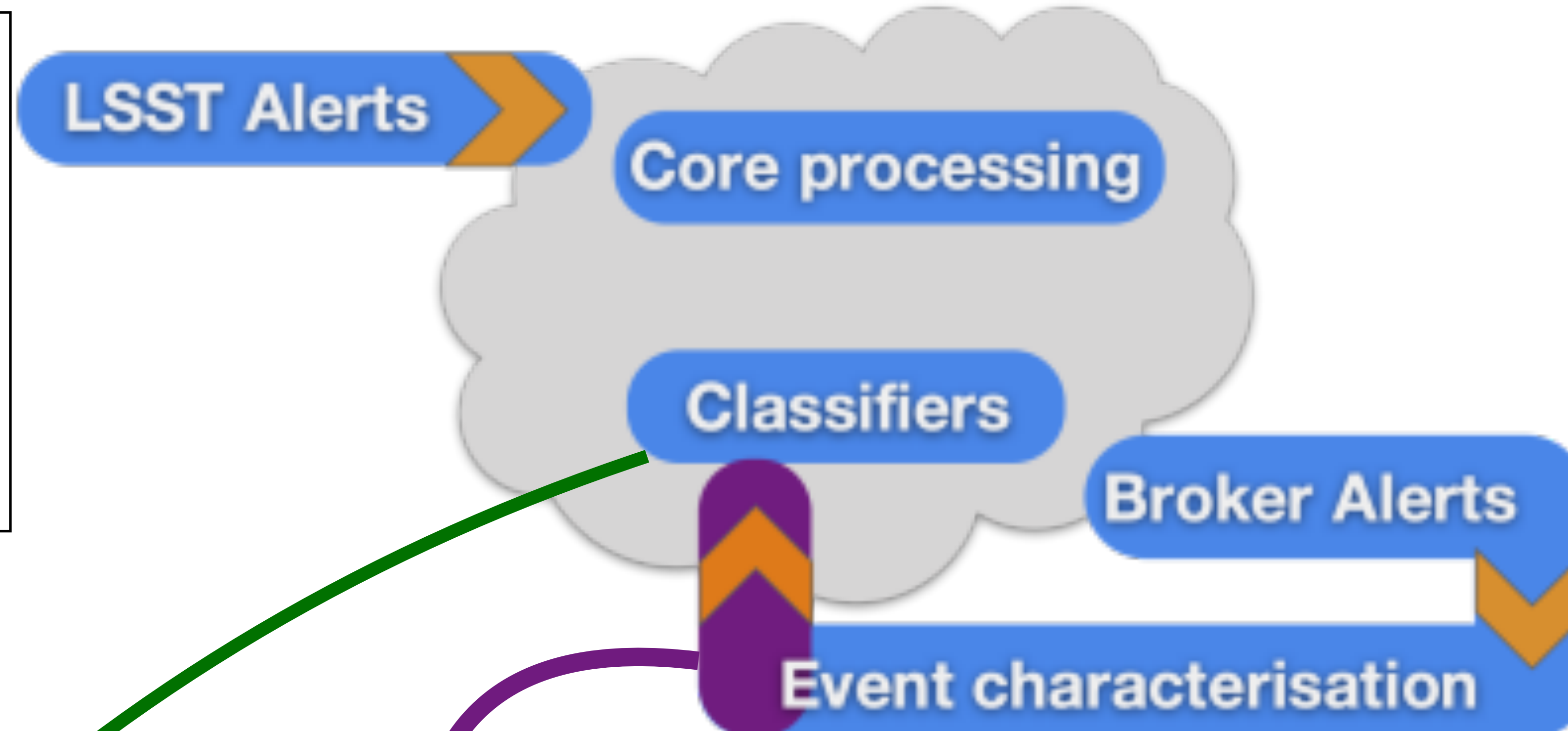
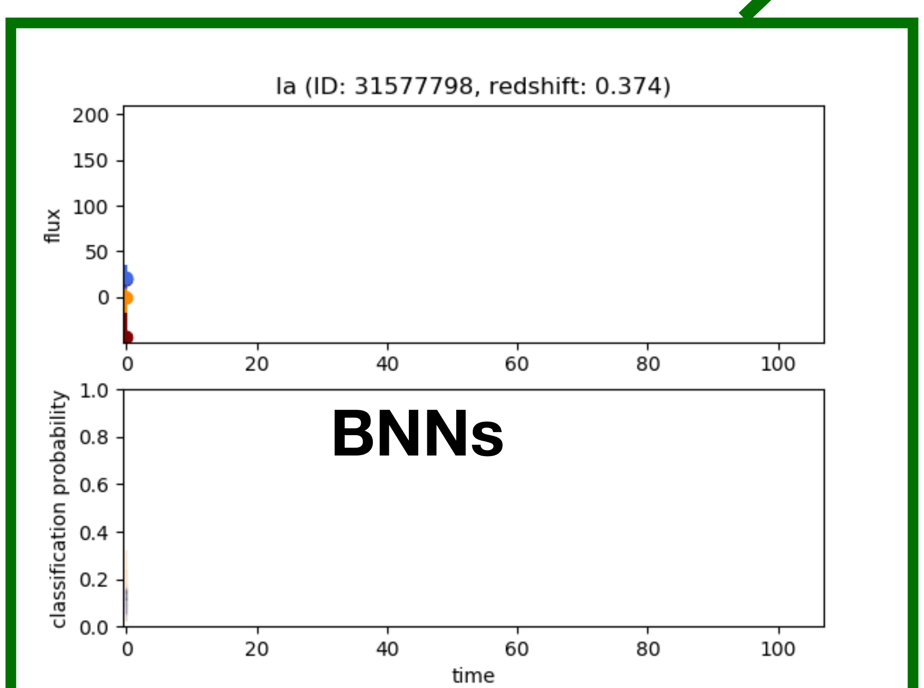
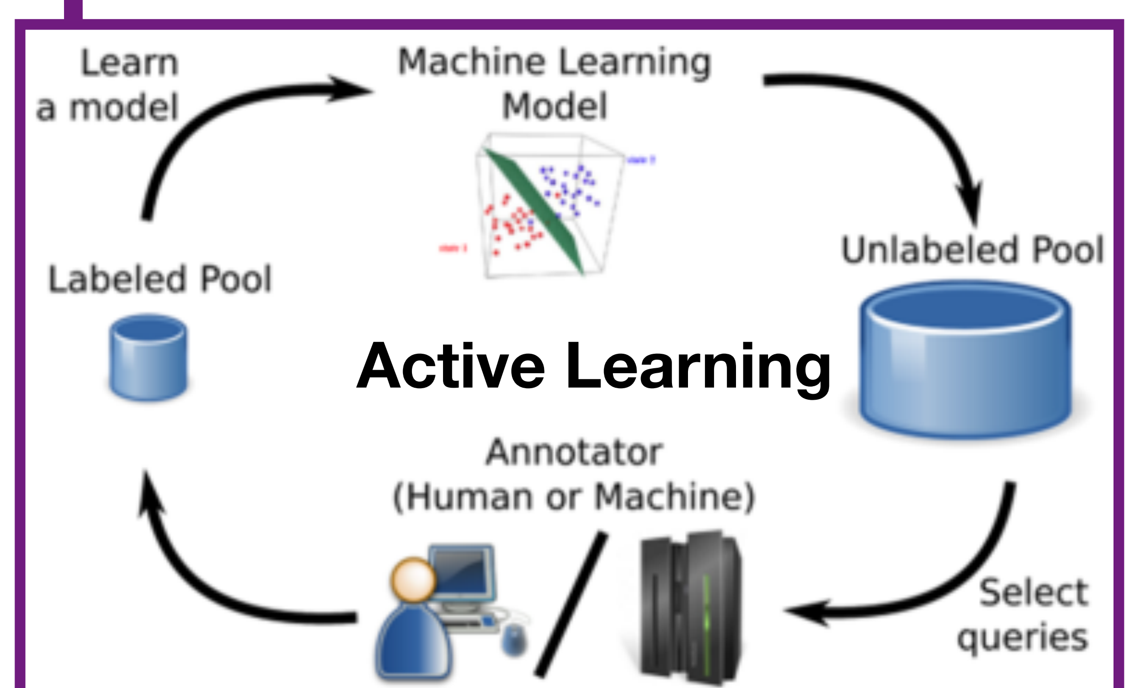




Möller + 2019



Ishida + 2018

take away

- The big *astronomical* data era requires the use of ML methods
- Machine learning is key for supernova cosmology.
- The last decade we have seen large advancements on problems like real vs. bogus & photometric classification.
- To exploit our large SN samples we need to start evaluating the robustness as one of the key components of our classifiers.
- Bayesian Neural Networks are promising for statistical analyses.

github: supernnova/SuperNNova