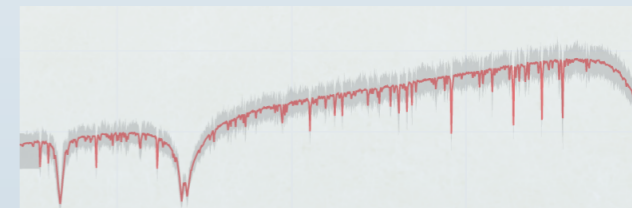
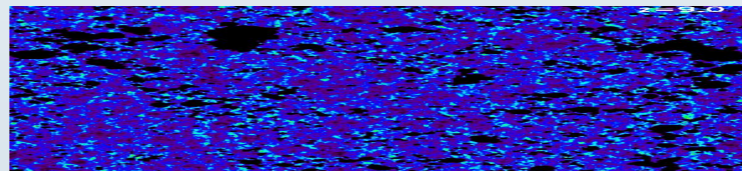
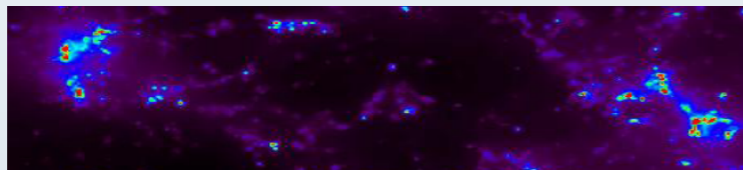


Networks Learning the Universe: From 3D (hydrogen tomography) to 1D (classification of spectra)



Caroline Heneka

Hamburg Observatory & Excellence Cluster Quantum Universe, Universität Hamburg

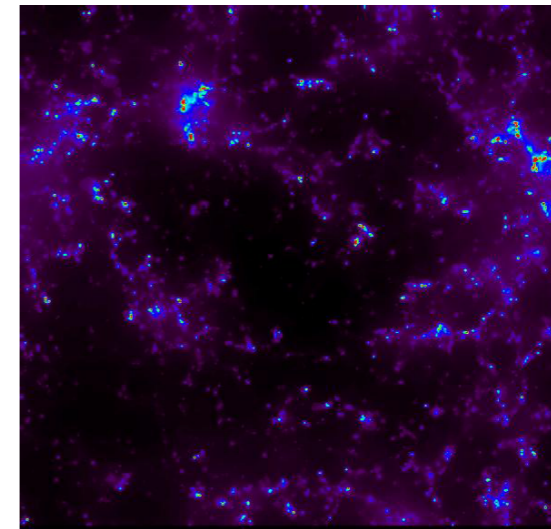
ESA/ESO SciOps Workshop 2022, May 17th 2022

Learning the Universe: Advances

Driven by large-scale + high-resolution surveys

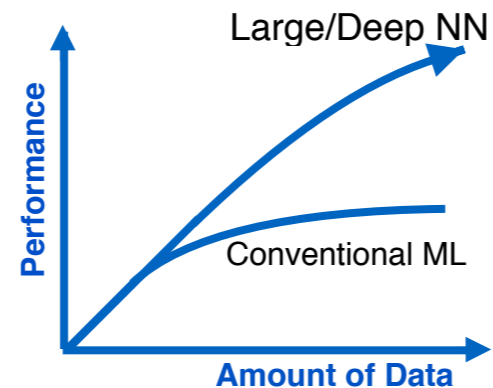


Example: Intensity Mapping



Ly α emission < 1 billion years after Big Bang

Example: Deep Learning
Driven by ability to improve
with large datasets



Extract more & less biased (?) information
Data mining

Efficient data reduction
Automation

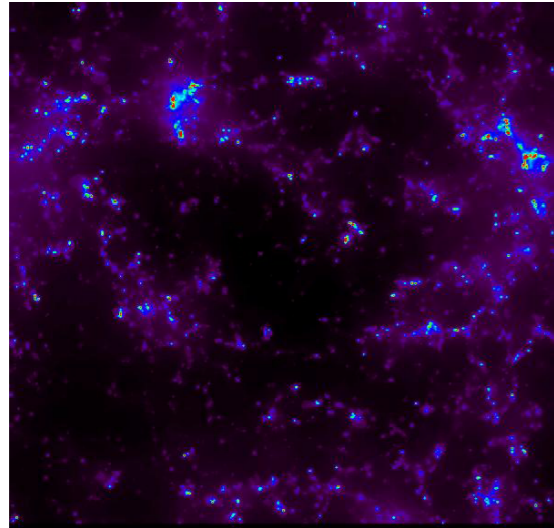
Complementarity to
previous probes + methods

Learning the Universe: Intensity Mapping (IM)

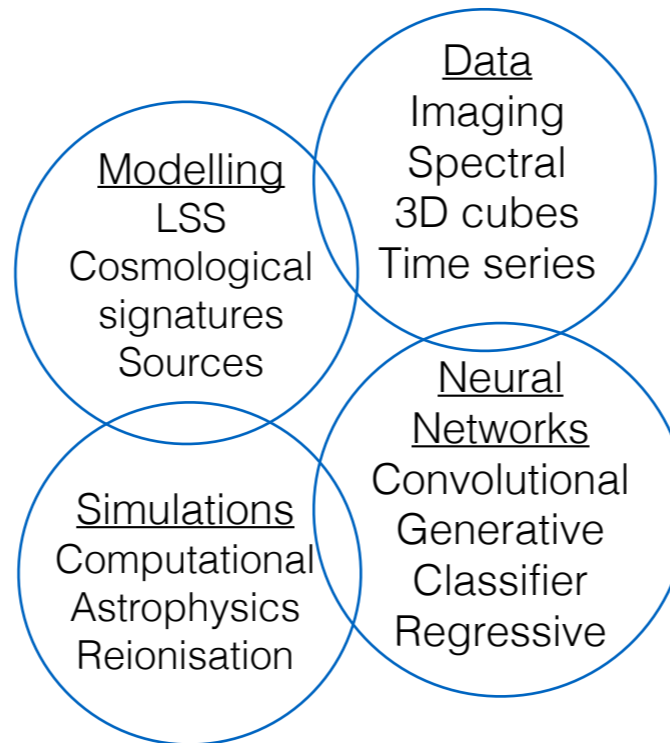
Astrophysics & Cosmology



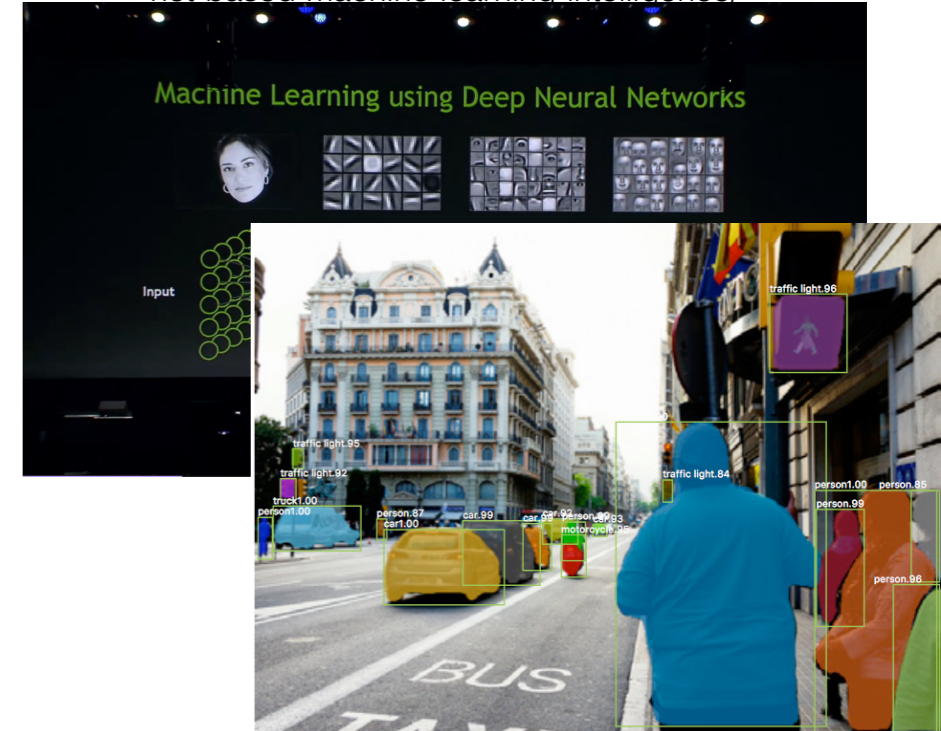
AI and Computer Vision



Ly α emission < 1 billion years after Big Bang



<https://wccftech.com/nvidia-demo-skynet-gtc-2014-neural-net-based-machine-learning-intelligence/>



https://medium.com/@umerfarooq_26378/from-r-cnn-to-mask-r-cnn-d6367b196cfd

Intensity Mapping



Deep Learning

full-sky multi-line mappings pixel-by-pixel

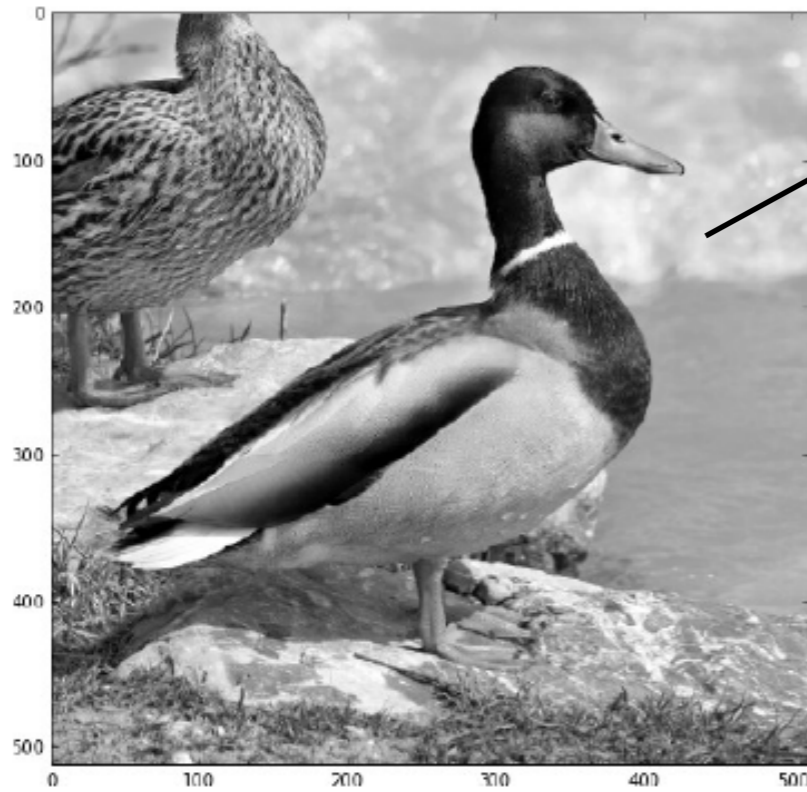
1D, 2D, 3D treatment pixel-by-pixel



novel
scientific life
cycles

Moving on from summary statistics. Why deep learning?

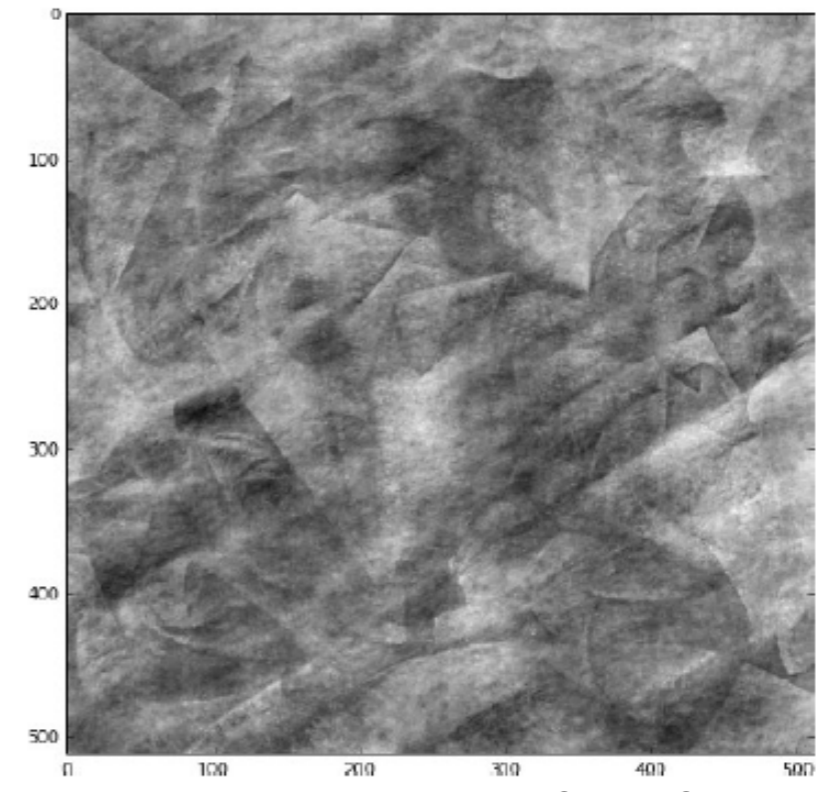
The duck example of (Non-)Gaussianity



The duck: highly non-Gaussian

parameters
(size, color, background)

randomise phases



The Gaussian duck

Credit: G. Bernardi

Same 2D
power spectrum

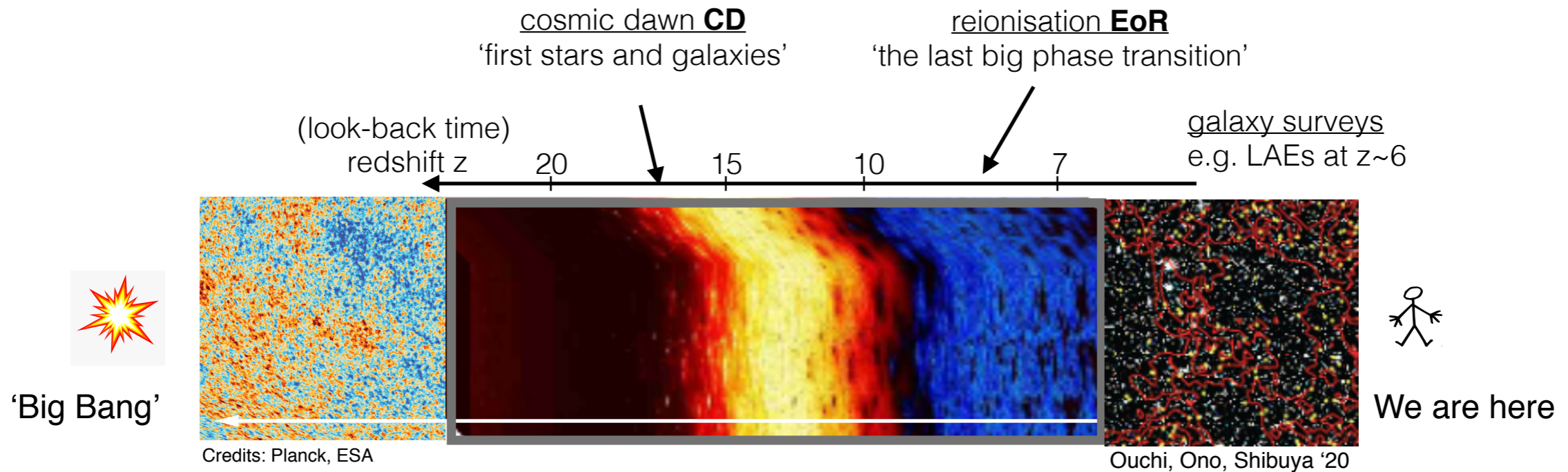
- Picks up non-Gaussian information
- Representation learning

Applications:

1. Detect the duck (or galaxy, or signature)
2. **Inference** (what duck? what properties? what shapes?)

Learning the Universe: Setting sail to the first galaxies

3D imaging to track the history of the Universe



SKA - 21cm signal (neutral hydrogen)

21-cm* 3D imaging**

* neutral hydrogen line

** blue = emission

red / yellow = absorption

+ multi-line intensity mapping
(21cm + H α , Ly α , OIII, H β , CII, ..)

SKA EoR working group, synergies sub-group

Inference from 3D tomographic cubes

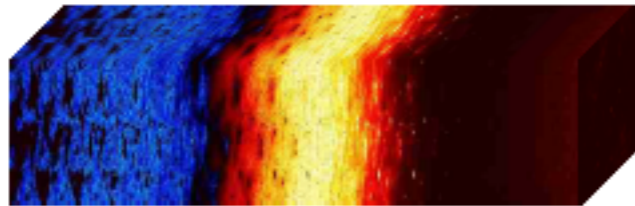
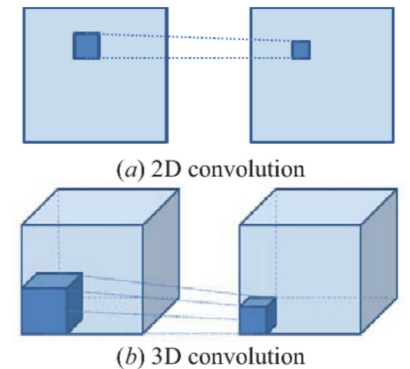
Direct likelihood-free inference from 3D tomographic cubes (21cm IM)

Various Options:

- Slicing and treatment with 2D CNN as image → 'standard' **2D CNN**, residual (skip connections) **ResNet**
- Time series (frequency) of co-eval images → **LSTM** network
- Full 3D convolution → 3D CNN:

[see e.g. Prelogovic+
arXiv: 2107.00018,
Gillet+2019]

Moving from **2D to full 3D convolution**



Inference from 3D tomographic cubes

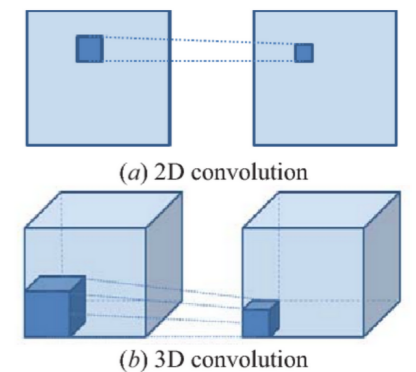
Direct likelihood-free inference from 3D tomographic cubes (21cm IM)

Various Options:

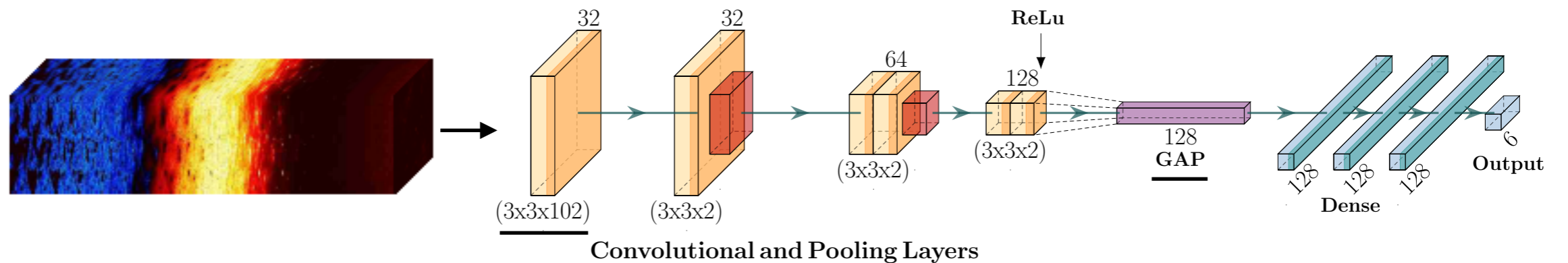
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- Full 3D convolution → **3D CNN**:

[see e.g. Prelogovic+ arXiv: 2107.00018, Gillet+2019]

Moving from **2D to full 3D convolution**



Best-performing: simple Conv3D architecture



Database of ~5000 lightcones
 140x140x2350 pix, 1.4 Mpc resolution
 Training (single K80 GPU): ~20min/epoch, ~30 epochs

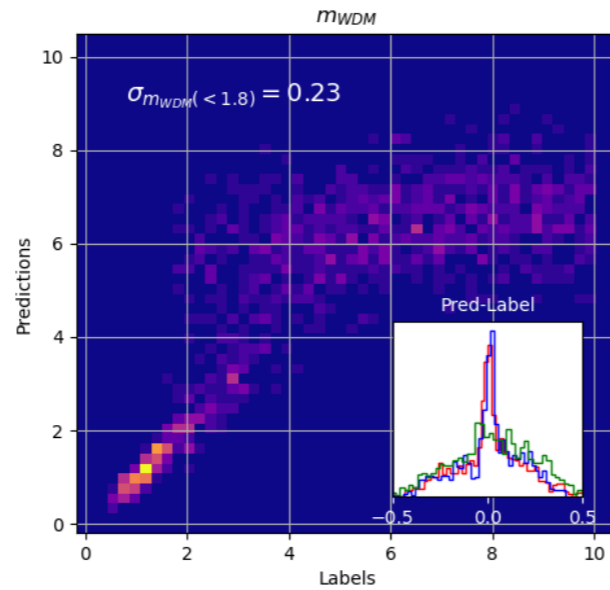
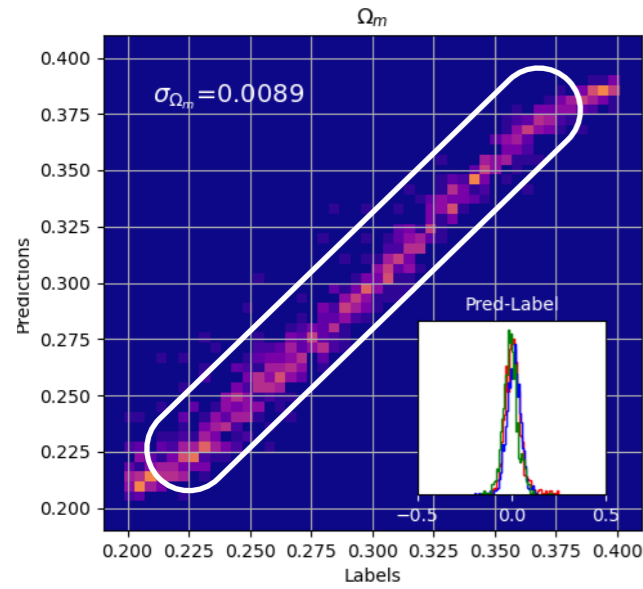
3D-21cmPIE-Net

Neutsch, Heneka, Brüggem
 MNRAS (2022)
 arXiv:2201.07587

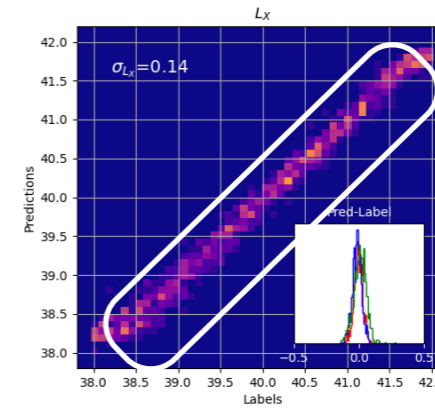
Inference from 3D tomographic cubes

Direct likelihood-free inference from 3D tomographic mock cubes (21cm IM)

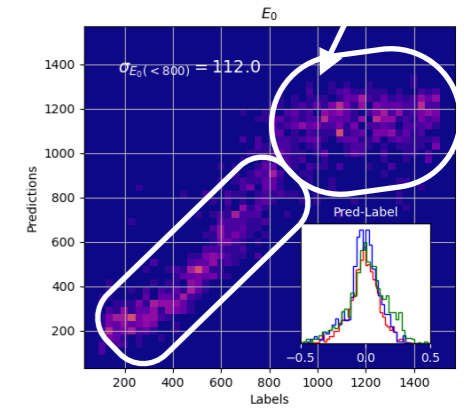
$$(\Omega_m, \zeta, T_{\text{vir}}, L_X, E_0, m_{\text{WDM}})$$



Cosmic Dawn



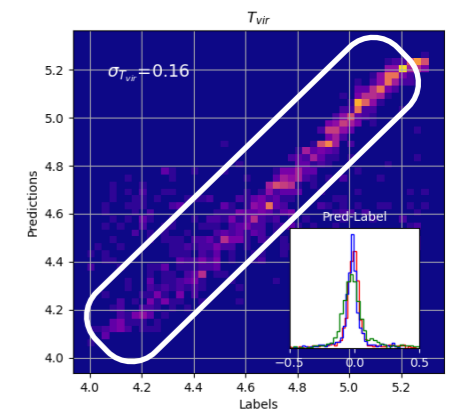
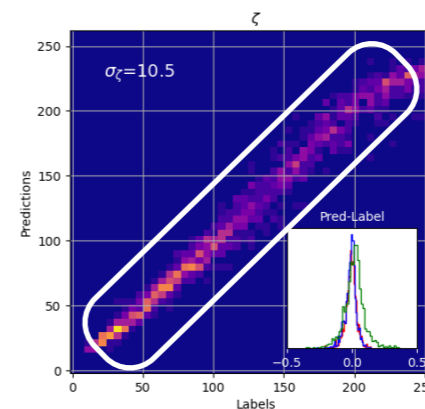
high E0, difficulty to escape



Cosmology

Reionisation

Directly constrain cosmology, CD & EoR
astrophysics
astrophysics
Mostly: small scatter, unbiased

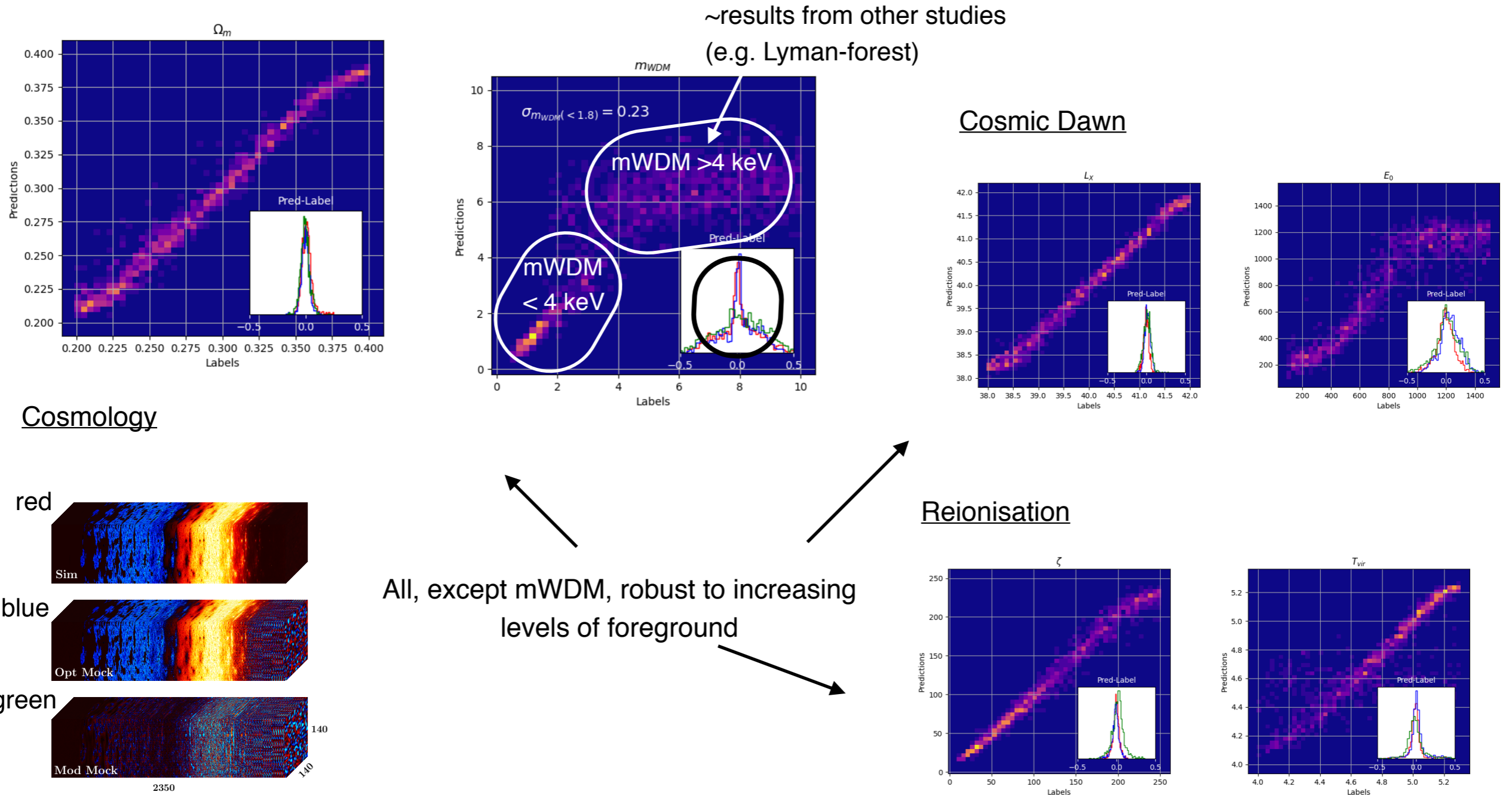


arXiv:2201.07587

Inference from 3D tomographic cubes

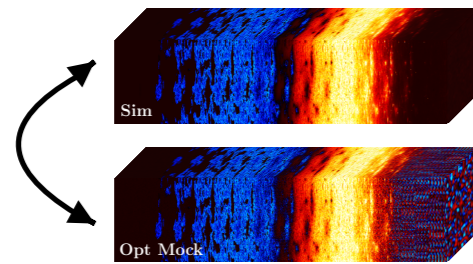
Direct likelihood-free inference from 3D tomographic mock cubes (21cm IM)

$$(\Omega_m, \zeta, T_{\text{vir}}, L_X, E_0, m_{\text{WDM}})$$



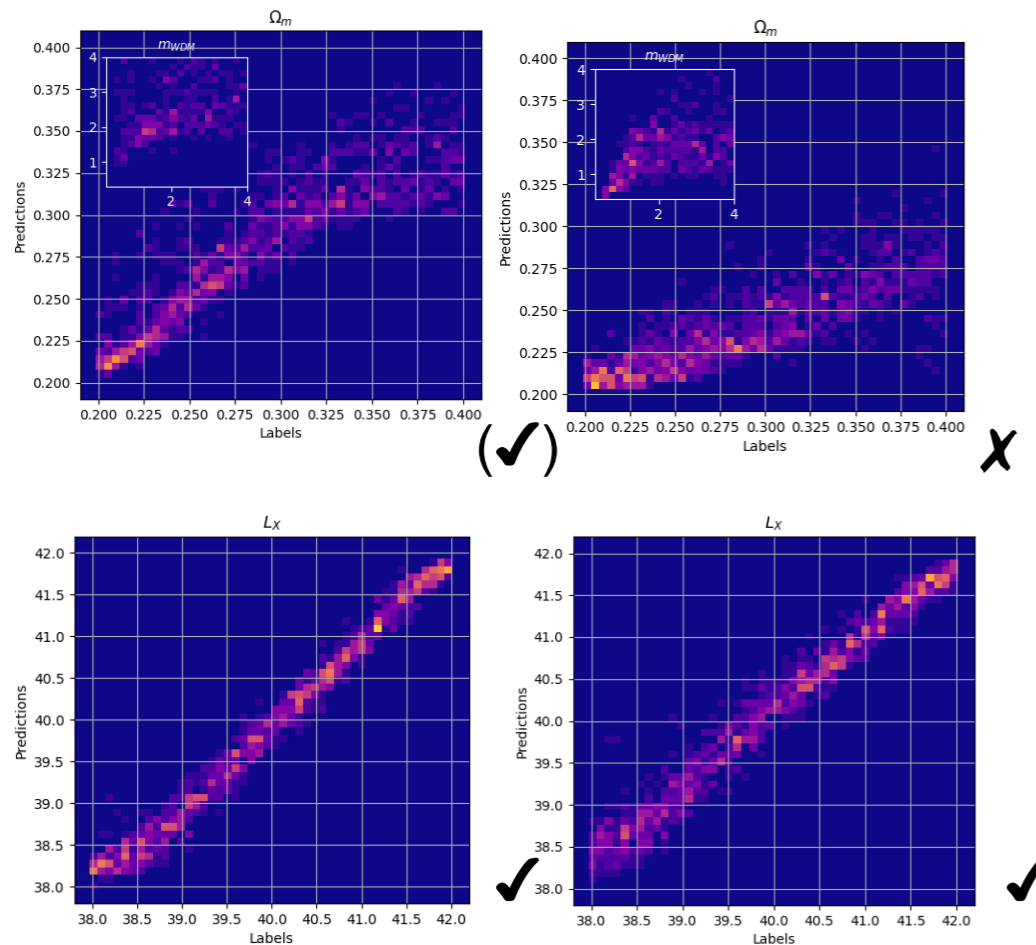
Testing robustness & interpretability

1) Transfer learning Sims & Mocks

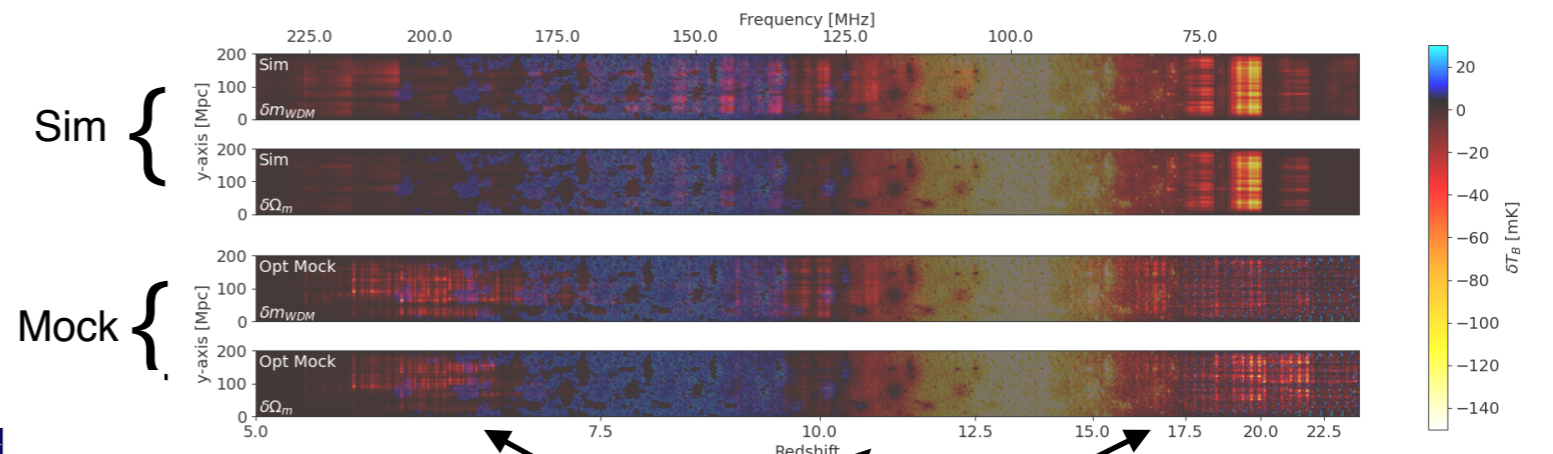


Sim -> Mock

Mock -> Sim



2) Gradient-based saliency maps



'transitions'

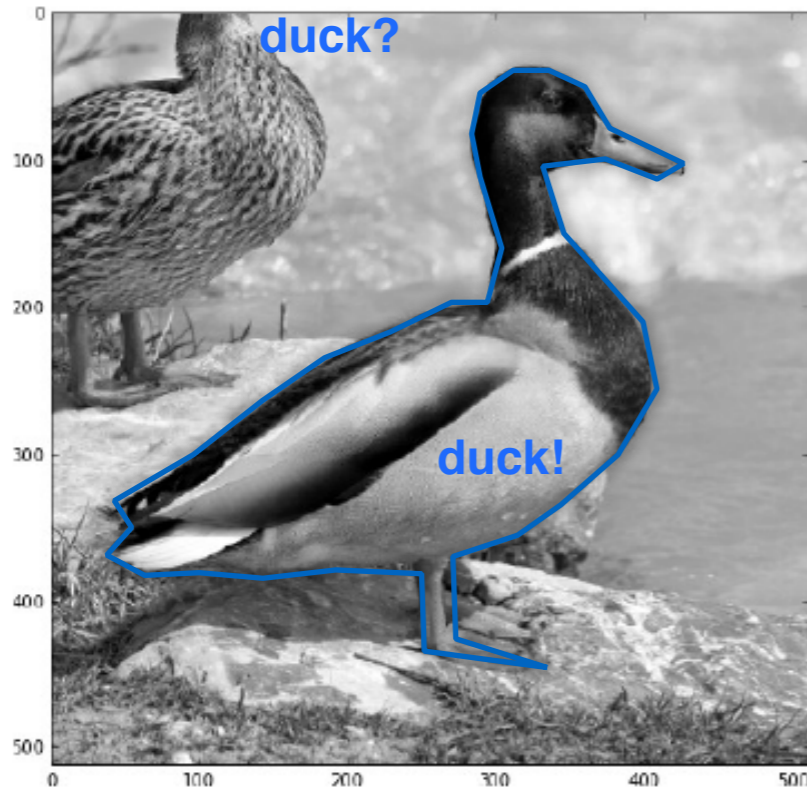
also seen for Fisher forecasts:
Heneka & Amendola 2018
Liu, Heneka, Amendola 2020

✓ Robust to foregrounds & systematics

arXiv:2201.07587

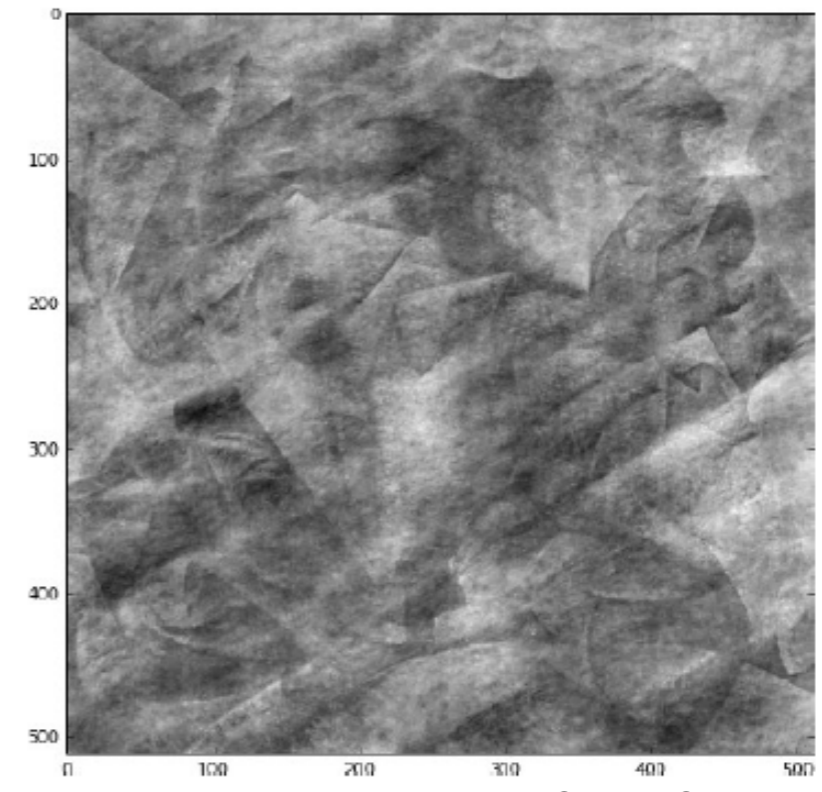
Moving on from summary statistics. Why deep learning?

The duck example of (Non-)Gaussianity



The duck: highly non-Gaussian

randomise phases



Credit: G. Bernardi

The Gaussian duck

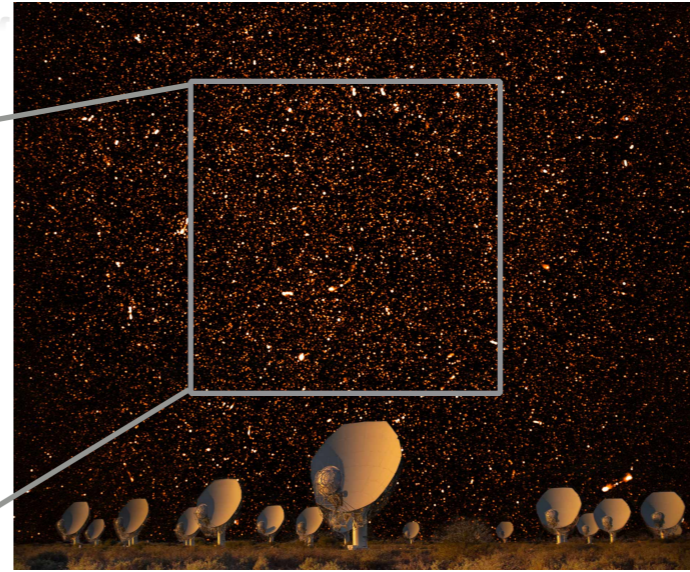
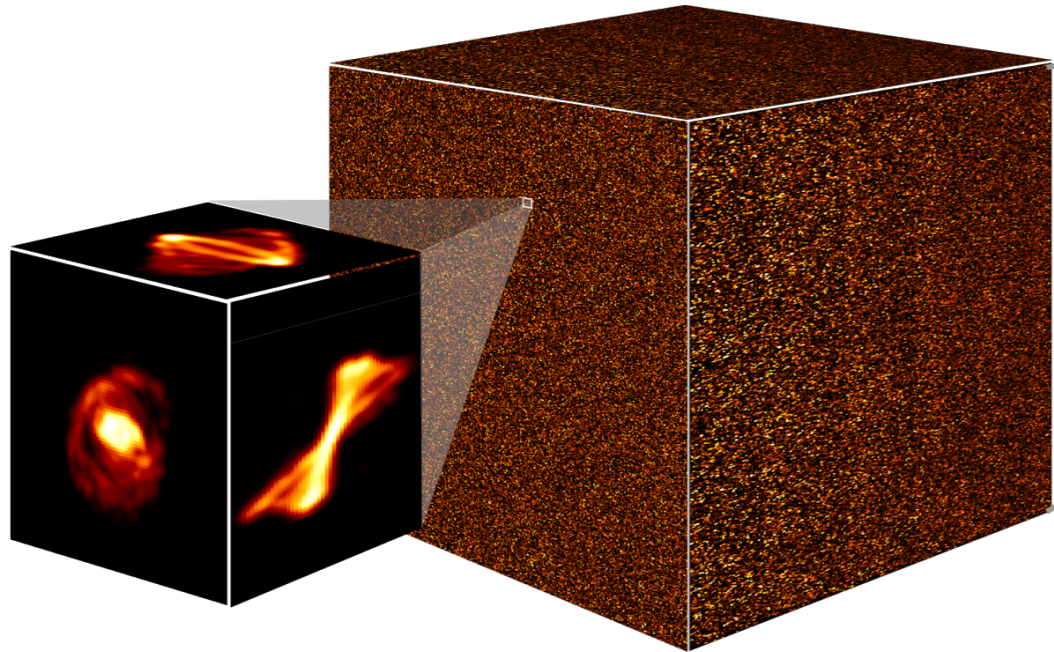
Same 2D
power spectrum

- Picks up non-Gaussian information
- Representation learning

Applications:

1. **Detect** the duck (or galaxy, or signature)

Detection in 3D: SKA Science Data Challenge



Composite MeerKAT dishes and observations.
Credit: South African Radio Astronomy Observatory (SARAO)

SKA -
The Square Kilometre Array

An international effort to build the world's largest radio telescope

Expected data rate in full operation: 1 TB/s

Key science goals include:
Galaxy Evolution, Reionisation, Cosmology, Astroparticles

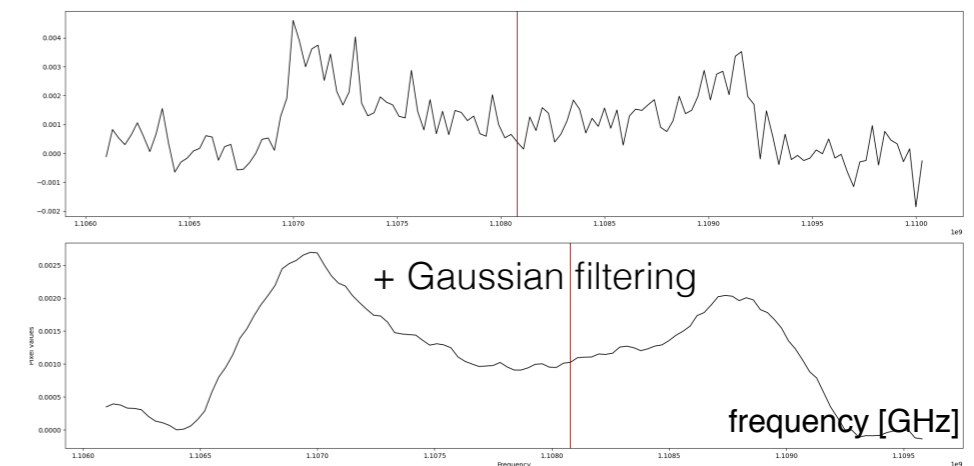
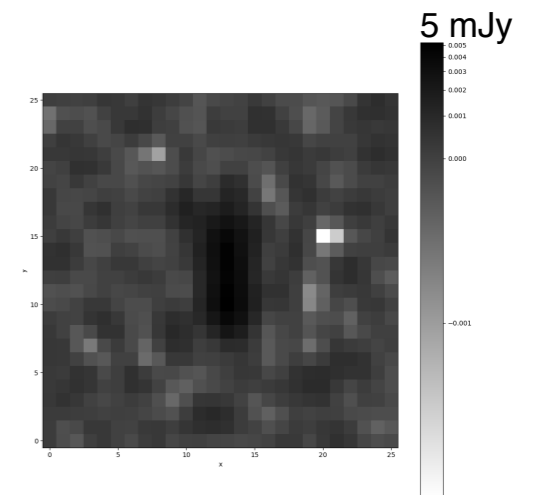
Credit: <https://sdc2.astronomers.skatelescope.org/sdc2-challenge/data>

**Goal is both source finding and characterisation
& test for new SKAO Regional Data Centers**

The challenging HI sources:

- low S/N
- small spatial size
- systematics

The brightest HI source



Detection in 3D: SKA Science Data Challenge

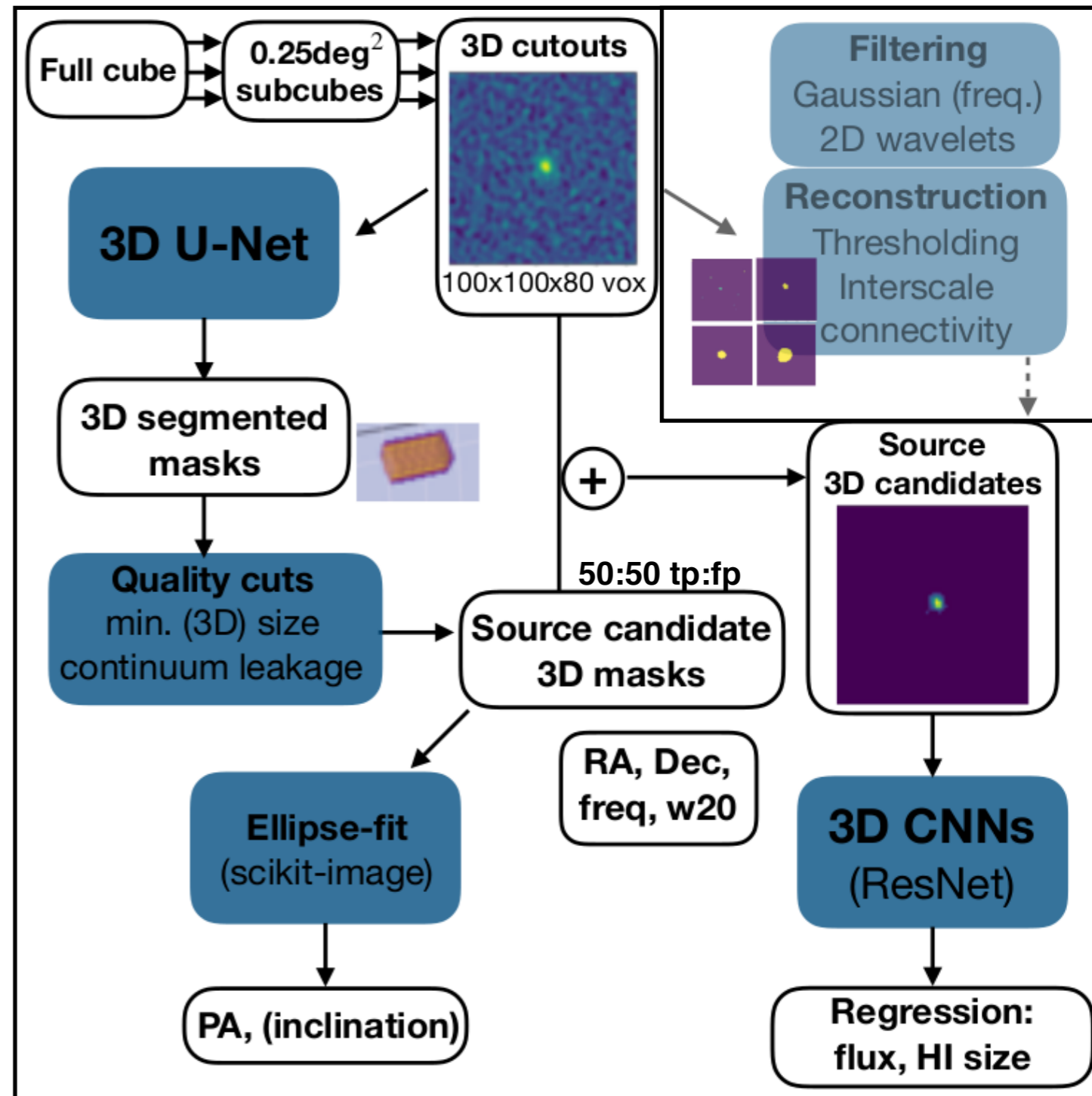
Machine learning and deep learning come together?

Team: Michelle delli Veneri, Andrew Soroka, Bernardo Fraga, Fedor Gobanov, Clecio de Bom, Alex Meshcheryakov

DL source detection & characterisation:

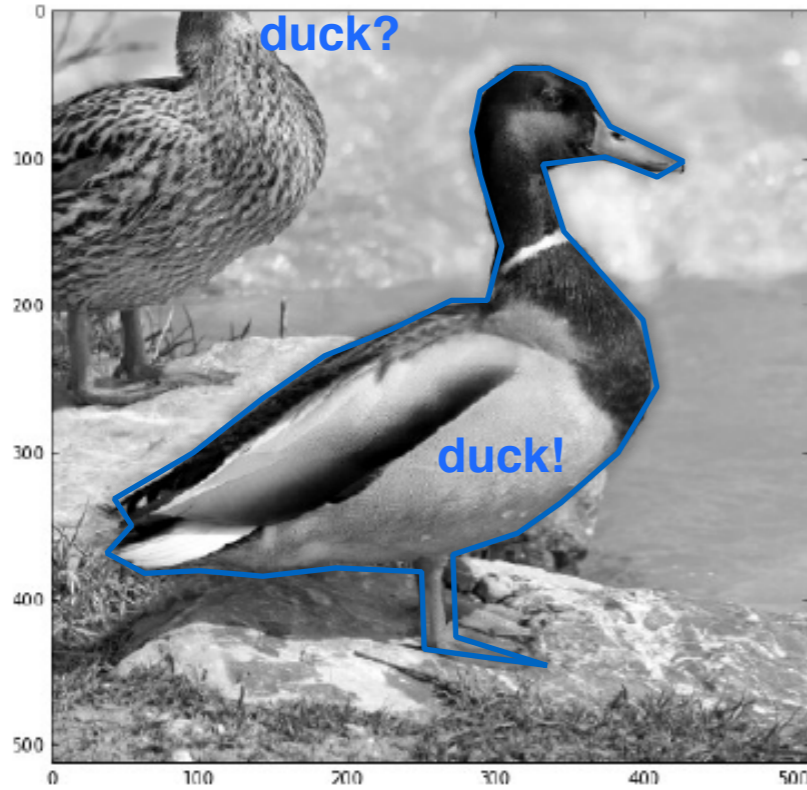
Pitfalls & Take-aways:

- Pre-processing, noise model(s)
- High sparsity
- **Choice of training set**
- **self-supervised**
- **Multi-step and/or ensemble decision**



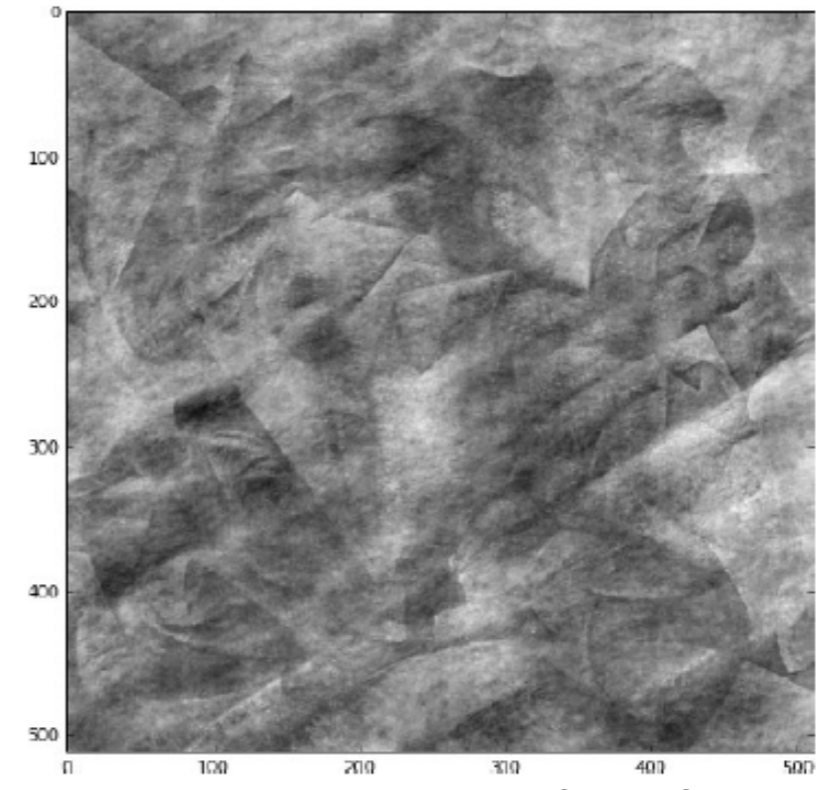
Why deep learning?

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randomise phases



Credit: G. Bernardi

The Gaussian duck

Same 2D
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- Picks up non-Gaussian information
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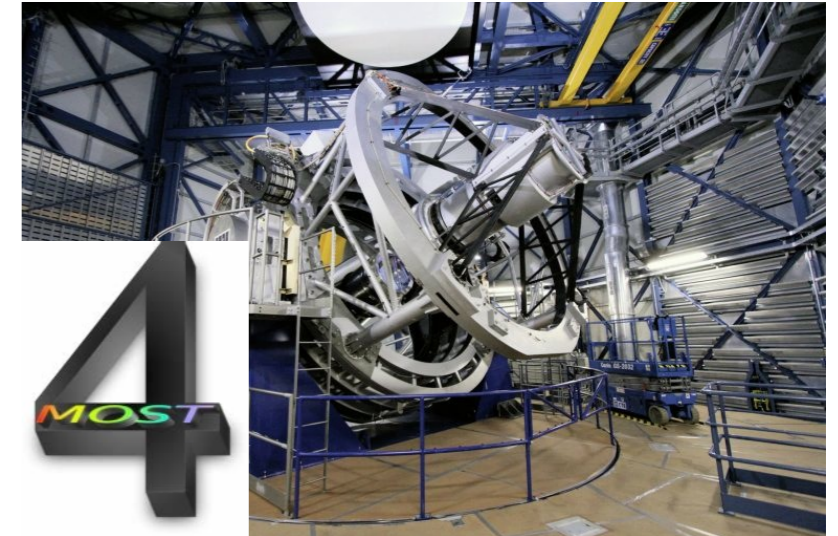
Applications:

1. ~~Detect~~ the duck (or galaxy, or signature)
duck! classify.

Classification in 1D: Spectroscopy

Building a classifier for 4MOST - Classification IWG9

- 5-year survey
- wide-field, fibre-fed, optical spectroscopy
- on ESO's 4-m-class telescope VISTA
- 2.5-degree diameter field-of-view, 2436 fibres
- HRS $R \approx 18000 - 21000$, LRS $R \approx 4000 - 7500$
- 20mio. (LRS), 3mio. (HRS) sources



Credit: ESO

<https://www.4most.eu>

Goal: Data-driven classification layer between L1 and L2 pipelines

- **Basic target classification.**
Classes: star, galaxy, AGN, quasar, ..



Probabilistic multiclassifier
also: lowres vs. highres
(low S/N vs. high S/N)

- **Galactic & extragalactic source classification.**
Sub-classes matching L2 sub-pipeline
galactic: FGKM, OBA, WD sub-pipelines
supplement to metadata based decision



Probabilistic multiclassifier II
(sub-classes)

- **Feedback on a) targets, b) 'unknown' class**
Currently set-up:
4MOST explorer t-SNE
(Gregor Traven, Gal Matijevic)
arXiv: 1612.02242



- a) match with expectation
- b) clustering, dimensionality reduction



Classification in 1D: Spectroscopy

Benchmark tests with SDSS spectra

Convolutional network

Random Forest

Support Vector Machine

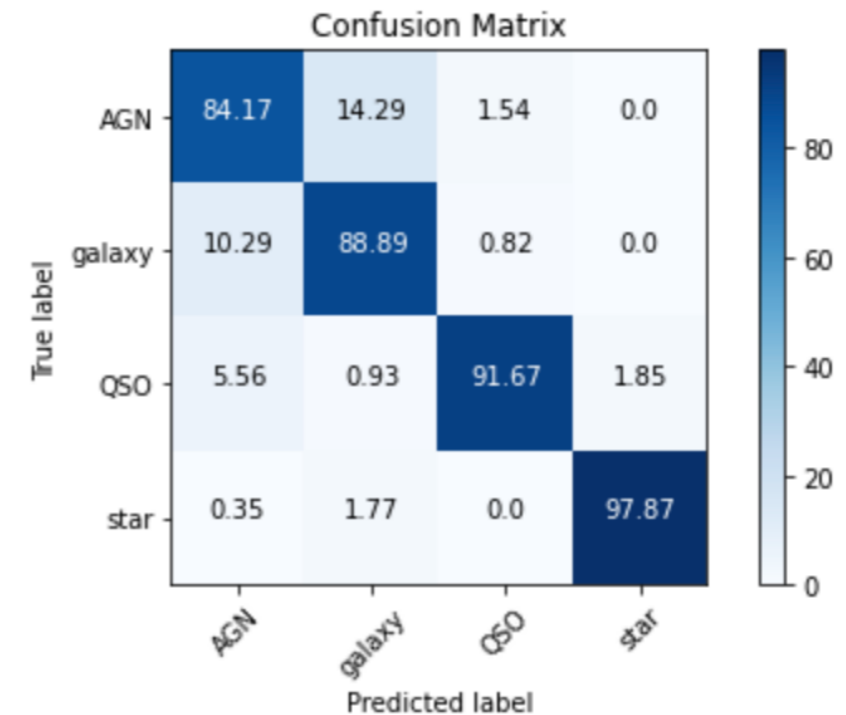
Logistic Regression

Gaussian Naive Bayes

2 convolutional + 2 dense
Currently: softmax-output
Ongoing: 'true' probabilistic

Advantage:

- complements template-based approaches
- once trained, extremely fast evaluation
- transfer of learning - training on archival data

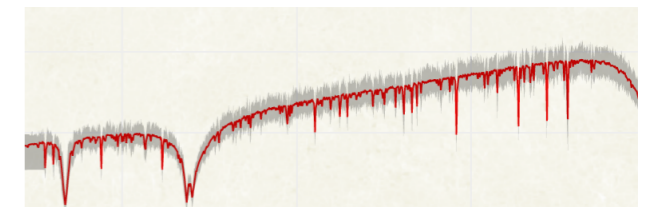


A supervised classifier (to start with) relies on 'good' training data..
Classification working group was re-activated in 2021,
under discussion: focus sub-group for training data

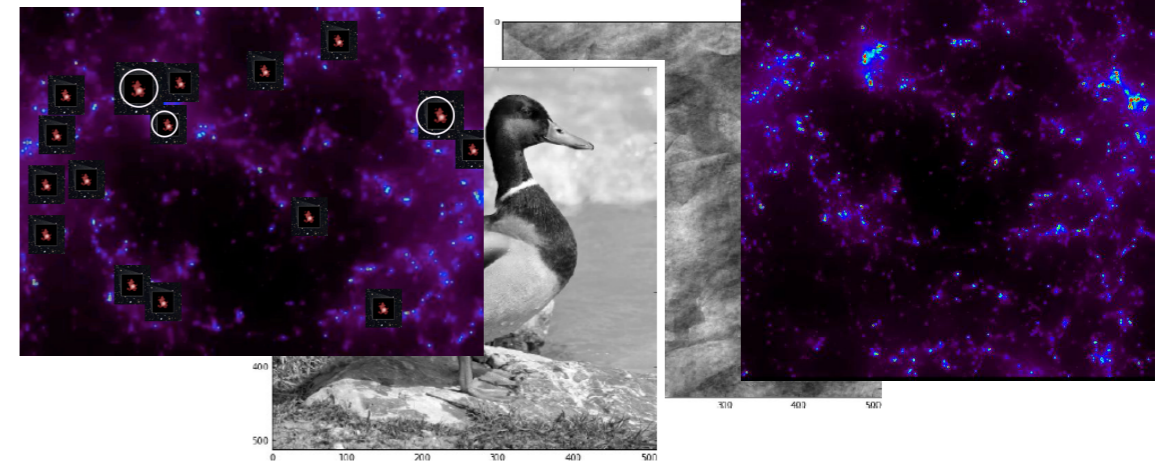
Training sets
(not connected
to daily data-flow,
but subject to updates)

Options:

SDSS, SDSS superset, GALAH, APOGEE, WEAVE (start '22)
templates / synthetic spectra, OpR simulated spectra



Learning the Universe from 3D to 1D



Main take-aways:

- Exploit techniques and methods such as intensity mapping and deep learning
- Avenue to jointly constrain astrophysics and cosmology (at Cosmic Dawn and Reionization)
- ..and more: exploit synergies and complementarity with e.g. galaxy surveys

Ongoing:

- Public on Github: [3D-21cmPIE-Net](#)
- Test of posterior estimate, probabilistic inference
- Test on data from e.g. SKA precursors

Goals:

Map-based approach to astrophysics
Representation learning
Beyond summary 'let the net choose'
Automated, fast, effective
New signatures?

Interesting open questions:

When does ML improve over 'traditional' methods?
What needs to be done in terms of architecture, reproducibility, interpretability?
Training data vs. self-supervised?
Knowledge of uncertainties (epistemic & aleatoric)

Thank you!

caroline.heneka@uni-hamburg.de