Astrophysics & ML/DL (At least some examples)



Caroline Heneka ITP Heidelberg

Machine Learning in Particle Theory, Mainz/Oppenheim, July 17th 2023



DIERF

Who am I? Caroline Heneka Institute for Theoretical Physics, Heidelberg University

• B.Sc. and M.Sc. Physics in Heidelberg (+ Erasmus NPAC Paris)



- 2017-2019: DFG Transregio 33 Fellowship (Heidelberg), Postdoc SNS Pisa
- ca. 1.5 yrs: DLR (German Aerospace Center) Headquarters Cologne, Executive Board Area Space, Programme Strategy Space
- 2020-2022: Senior Postdoc Hamburg University
- Since Oct 2022: back in HD Junior Group Leader & Freigeist (Volkswagen Foundation) Fellow 'Computer Vision Astrophysics and Cosmology'











My Research Interests

Line Intensity Mapping

(also: radio galaxy clustering, cross-correlation studies, galaxy clusters, ..)

High-redshift astrophysics & Epoch of Reionization:

Modelling of 21cm background and further high-redshift lines (Lya, Ha, ..)

 The modern machine learning toolkit with 'Computer Vision Astrophysics + Cosmology', specifically for intensity mapping of large-scale backgrounds:



- Inference

Also:

- Classification (e.g. 4MOST spectra)
- Detection (SKA preparation)







Where we stand: New frontiers in astronomy and astrophysics



Galaxy surveys as an astronomical probe



Test astrophysics of galaxy evolution, the intergalactic medium (IGM) as well as cosmological structure formation from the Epoch of Reionisation (EoR) to the present.

Modelling challenges



APOD, NASA, License & Credit: Wikipedia, Pablo Carlos Budassi

Observable Universe: d ~ 28 Gpc (x3 Glyr) 80% if this: d ~ 22 Gpc Let's say we resolve (only) ~Mpc about 3-4 orders of magnitude about 10⁹-10¹⁰ modes!

... at some point we sub-grid model and/or change modelling approach



ML/DL for astrophysics









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ML/DL for astrophysics



ML/DL for astrophysics



Example: Segmentation & regression, representations

z1

Goal: 'Good' photometry for surveys with high blended fraction (expected), e.g. SDSS, LSST and Euclid

Add-on: Galaxy segmentation and morphology / shape (also prior for 'classic' methods)

z2

Challenge: Galaxies are 'transparent', separating flux in overlapping regions is difficult

CANDELS field Hubble Space Telescope ••

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'Classic':
Fit ellipse(s)
and profile(s)

e.g. Einasto ('65):

 $\frac{d\log(\rho)}{d\log(r)} = -2\left(\frac{r}{r_s}\right)^{\alpha}$





Goal: 'Good' photometry for surveys with high blended fraction (expected), e.g. SDSS, LSST and Euclid - avoid bias!

low stellar density (Ross et al. 2012a). The correlation of galaxy density with stellar density is the most significant known bias on measured clustering, likely caused by incomplete deblending of detected objects in crowded fields of the SDSS imaging data. On the other hand, no significant correlation is seen between number density and potential



CANDELS field

Hubble Space Telescope

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CANDELS field



Artificially blended CANDELS data 18 < mag < 24 (https://github.com/aboucaud/candels-blender) Get photometry of blended galaxies..

Goals for our deep NNs





..Derive galaxy masks (shape measurements)

Boucaud et al., COIN collaboration MNRAS 491,2 (2020)

..do so bias-free

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Histograms of photometric errors





Histogram of IoU (Intersection over Union - Jaccard index)



2 a) *U-net* masks, no photometry



2 b) *blend2mask2flux* photometry + masks



Boucaud et al., COIN collaboration MNRAS 491,2 (2020)

Dispersion broadens when optimised for photometry

Galaxy deblending with nets: Take-aways

The deblending problem

- Large fraction of blends for deep photometric surveys
- Non-trivial to disentangle single galaxies
- Causes bias

Photometry

- Nets recover flux: low bias and high precision
- A 'simple' CNN blend2flux performs well
- Slight improvement when simultaneously constraining masks

Mask Segmentation

- U-Net architecture suitable to recover shapes
- Pitfall: Train photometry + shapes end-to-end



Needed for 'precision-cosmology'

... prepared for Euclid satellite

Example: Classification

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 ≈ 18000 21000, LRS R ≈ 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.

Probabilistic multiclassifier

- Galactic & extragalactic source classification.

Benchmark tests with SDSS spectra

- Feedback on a) targets, b) 'unknown' class

Currently set-up: 4MOST explorer t-SNE (Gregor Traven, Gal Matijevic) arXiv: 1612.02242





Predicted label

Confusion Matrix

20

Classification in 1D — spectroscopy

Benchmark tests with SDSS spectra





Star or galaxy? Which type?

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ML-for-Astro-tutorial

Computer Vision Astrophysics & Cosmology

Monday: Introduction, Deblending (regression, segmentation), classification



Example: Inference, higher-order correlations

https://camels.readthedocs.io

CAMELS

= Cosmology and Astrophysics with MachinE Learning Simulations

Туре	Code	Subgrid model	Simulations
Hydrodynamic	Arepo	IllustrisTNG	1,092
Hydrodynamic	Gizmo	SIMBA	1,092
Hydrodynamic	MP-Gadget	Astrid	1,092
N-body	Gadget-III	-	3,049

https://camels.readthedocs.io

p1, e.g. : Ωm

Parameter set:

$0.1 \leq$	$\Omega_{ m m}$	≤ 0.5
$0.6 \leq$	σ_8	≤ 1.0
$0.25 \leq$	$A_{\rm SN1}$	≤ 4.0
$0.50 \leq$	A_{SN2}	≤ 2.0
$0.25 \leq$	A _{AGN1}	≤ 4.0
$0.50 \leq$	A_{AGN2}	≤ 2.0

. . .

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. . .

From one galaxy to global parameters

https://camels.readthedocs.io

How many galaxies do we need to constrain e.g. Ω_m ? Let's start with one!

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From one galaxy to global parameters

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Loss based on moment density networks (MDN) Jeffrey & Wandelt 2011 arXiv:2011.05991

MDN idea: hierarchy of neural regression models (mean \rightarrow variance \rightarrow skewness \rightarrow ...)

We begin by noting that if we find some function of our data $\mathcal{F}(x)$ that minimizes an L_2 loss over the distribution of possible training examples $\{x_i, \theta_i\}$,

$$J_0 = \int ||\boldsymbol{\theta} - \mathcal{F}(\boldsymbol{x})||^2 p(\boldsymbol{x}, \boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}\boldsymbol{\theta} \quad , \tag{4}$$

then \mathcal{F} , which we represent as a neural network, evaluated for the observed data is the mean of the posterior distribution $\mathcal{F}(x_{obs}) = \langle \theta \rangle_{\theta | x_{obs}}$. It is therefore possible to create a hierarchy of networks

In practice we minimise the following loss function:

$$\begin{aligned} \mathcal{L} &= \sum_{i=1}^{6} \log \left(\sum_{j \in \text{batch}} \left(\theta_{i,j} - \mu_{i,j} \right)^2 \right) \\ &+ \sum_{i=1}^{6} \log \left(\sum_{j \in \text{batch}} \left(\left(\theta_{i,j} - \mu_{i,j} \right)^2 - \sigma_{i,j}^2 \right)^2 \right) \end{aligned}$$

Our model F(x):
CNN layers (19)
+ dense (2)
Villaggeuge Neverre

Villaescusa-Navarro+ arXiv:2109.10915

From one galaxy to global parameters

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https://camels.readthedocs.io

 M_*

Κ

 $M_{\rm g}$

 $Z_{\rm g}$

 V_{max}

 Z_*

g

 σ_v

 R_*

 $M_{\rm t}$

U

 $R_{\rm t}$

 $R_{\rm max}$

SFR

J

V

 $M_{\rm bh}$

From one galaxy to the matter density

From one galaxy to the matter density

recovery of matter density for random galaxy in random simulation

Robustness: Matter density and galaxy mass

also: holds for redshifts other than z=0

Only take into account relation input & predictions for attribution. Show importance of feature on predictions via one-by-one retraining.

Example: SHAP values https://arxiv.org/abs/1705.07874 SHAP = SHapley Additive exPlanations

Approach from Game Theory: Assign to each input feature a value. A larger value indicates higher importance for the output prediction.

Do so via optimal credit allocation of possible 'coalitions'.

- \cdot difference in output by including/excluding feature
- \cdot average over N! orderings
- \cdot repeat: all subsets of remaining features

Computer Vision Astrophysics & Cosmology

Example: Generation / Simulation

Scientific use case:

Fast, reliable way to simulate galaxy cluster images (in X-rays, at different cosmologies)

See arXiv:1701.07875 for a comprehensive mathematical introduction of the WGAN

Real vs. simulated vs. WGAN-generated?

..explore different failure modes of GANs

Radio interferometry - imaging in Fourier space

'The' inverse problem in astronomy/astrophysics

New frontiers in astronomy and astrophysics

 $T(x,y) = \int \int V(u,v) e^{-2\pi i (ux+vy)} du dv$

complex visibility V(u,v) = interferometer response

Radio interferometry: an inverse problem

The Square Kilometre Array (SKA)

SKA in numbers

- Currently 16 member countries, >100 member organisations
- Routine science observations are expected to start in the late 2020s
- Consists of thousands of dishes and up to 1 million antennas, >1km² collecting area
- Expected data rate in full operation: 1 TB/s

SKA-LOW SKA-MID

Credits: SKAO

SKA1-mid

the SKA's mid-frequency instrument

SKA1-low

the SKA's low-frequency instrument

Frequency range: 50 MHz to 350 MHz

The Square Kilometre Array (SKA)

https://doi.org/10.1093/mnras/staa3837

Example: Denoising, detection

Goal for individual HI sources:

Source finding

Location in RA, Dec, central frequency (Hz)

Characterisation

- Integrated line flux (Jy Hz)
- Line width (km/s)
- HI major axis diameter (arcsec)
- Position angle (degrees)
- Inclination angle (degrees)

The challenging HI sources:

- low S/N
- small spatial size
- systematics

Deep learning for source detection and characterisation

3D U-Net

- 3D better than stitching of 2D + 1D
- High-fidelity 3D reconstructions

Good prior for characterisation tasks via 3D CNN:

SDC2 results, Hartley+, under review

Recovery across wide range in HI flux and size

(also in terms of S/N)

Pushing to low S/N recovery came at a cost (FPs)

Detection & Inference in 3D: SDC2

Deep learning for source detection and characterisation

Pitfalls:

- High sparsity
- Choice of training set choose high (enough) S/N sub-sample
- Avoid or mitigate false positives

Top 3 SDC2 models

• Minerva: ensemble of

1)YOLO (you-only-look-once), Redmon+15,16

Turning classification into regression with probability maps

2) CHADHOC, 'traditional' detection + CNN(s)

- FORSKA-Sweden: U-Net segmentation, Ronneberger+15, pre-trained + SoFiA
- Team SoFia: SoFiA (Source Finding Application, in 3D), Serra+15, Westmeier+21

Thresholding of peaks and reliability estimate

Take-aways:

- Choice of training set
 - pre-training (see also YOLO-approach) let the network choose!?
- Multi-step and/or ensemble decision

Ongoing: SDC3 foreground challenge

The complete SDC3a dataset consists of a visibility measurement set (MS) and imaging products derived from it, as well as ancillary data. Teams can decide whether they want to analyse the MS or the imaging products, depending on their pipelines.

Details of the data products are as follows:

General

- Observation track length HA = -2 to +2 hours
- Thermal noise equivalent 1000 [h]
- Field of View: one SKA1-Low pointing at RA, Dec = 0h, -30deg

Measurement sets

- Size 5.4 [TB] (3.3 TB if concatenated)
- Integration time 10 [s]
- Channel width 100 [kHz]
- Frequency coverage 106 196 [MHz]

Image cube

- Weighting: Natural
- Pixel size [arcsec]: 16x16 arcsec
- Number of pixels in RA/Dec 2048x2048

Ancillary data

Synthesised beam and primary beam at each frequency

Non-blind validation data

Example: Discovery

Example clustering: Open Cluster identification

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