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Constructing Impactful Machine Learning Research for Astronomy

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Machine Learning Papers in Astronomy



Key challenges: trust, robustness, interpretability







6 Rules for Constructing Impactful Machine Learning in Astronomy

Today



Box Loop for Machine Learning in Astronomy

Conceptualise Model

Why does this problem exist, and what do good solutions look like? (Rule 2.1)
What is the current best domain reference? (Rule 2.1)
How does a potential ML solution fit into the broader context of existing solutions? (Rule 2.1)

- What is the target problem, and what data can be used to solve it? How can model inputs be derived from idealised or realistic observations? (Rule 2.4)

Build and Test Model

- What is the added value of the current best ML solution compared to the standard in the field? (<u>Rule 2.1</u>)

- What trade-offs does my new solution require in terms of interpretability? (<u>Rule 2.1</u>)

- Where can I apply best practices from the ML community, and where do these not make sense? (<u>Rule</u> <u>2.2</u>)

- How can I best diagnose and visualise the model and its outputs? (<u>Rule 2.3</u>)





Did you write a paper that showcases a rule? Do you know someone who did? Please send it to me!



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Rule 1: Compare against a domain reference and put result into larger context











1. Decrease the computational time and costs associated with scalability to larger data sets and samples



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- 2. Improve the robustness or precision of solutions to astrophysical questions



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What value is added by implementing a machine learning model, compared to the trade-offs (e.g. interpretability, biases in population inference)

cINN (MAP) vs. Template fitting (lit)

Literature







Bolometric luminosity

- J-band mag (HAWK-I, VISTA)
- extinction (A_{v}) ٠
- Colors and bolometric • correction = $f(T_{eff})$
- Average stellar age: 0.7Myr
- Two stellar populations ٠
 - Youna: ~ 0.7Mvr •

Da Eun Kang's talk: Conditional Invertible Neural Networks for enhanced analysis of young, low-mass stars in Trumpler 14





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cINN (MAP) vs. Template fitting (lit)



Da Eun Kang

Templates used in literature: M9.5 – G8.0

- No templates higher than G8 (5430K)
- No templates between K6 and K4 (ΔT ~360K)

cINN training range: 2600K – 7000K

Da Eun Kang's talk: Conditional Invertible Neural Networks for enhanced analysis of young, low-mass stars in Trumpler 14







Rule 2: Adopt best practices from the ML community











Designing and preparing data sets



Designing and preparing data sets

2. Choosing algoriothms



- Designing and preparing data sets
- 2. Choosing algoriothms
- 3. Choosing evaluation metrics



- 1. Designing and preparing data sets
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- 4. Exploring and reporting outputs

1. 2. 3.

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Machine learning is not just a set of algorithms, but a community of practice with rules, conventions and best practices to guard against challenges (e.g. overfitting, lack of generalisation)

K-fold cross-validation

- time
 - Run 1
 - Run 2
 - Run 3
 - Run 4
 - Run 5



We only have 101 finetuning samples, or ~20 samples for testing Train the model k times, reserving different data for testing each



Rule 3: Interpret, Diagnose and/or Visualise Models











Monitor in-distribution validation of ML models



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Check for outliers



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Visualize model output beyond summary statistics



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ML models have numerous algorithmic failure modes, and blindly trusting their output may lead to biased inferences about astrophysical problems

PHANGS-ML: dissecting multiphase gas and dust in nearby galaxies using machine learning









Rule 4: Explore limits and scope of the model











Determine target problem and data with which it can be solved





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- Generate training data from idealised or realistic observations





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- Don't forget about rare, previously unseen events!







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In many situations where training data is imperfect or incompletely understood, it may be impossible to build unbiased models: transparency if crucial to be able to apply results







Francesco Belfiore's talk yesterday: A domain-adaptation approach to classify ionised nebulae in nearby galaxies



ancesco Belfiore

Rule 5: Share and Discuss Lessons Learned











Adapting ML to astronomical problems involves both successes and informative failures

















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- Publications are biased towards successes

















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Biasing publication exclusively towards successful approaches could discourage model exploration to avoid risk of failure, an deprive the literature of these examples





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Rule 6: Make Software and Data Publicly Available











Enables others to reproduce research results, verify correctness



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- Enables reuse of model architectures, loss functions or whole pipelines





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But: data and model sharing rights might be complicated!





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- Enables reuse of model architectures, loss functions or whole pipelines
- 3. Provides a foundation for new projects
- 4. But: data and model sharing rights might be complicated!

Benchmarking new models against existing ones, and publishing the results, are best done when existing models are public!



EMBER: emulating baryons from dark matter-only simulations over cosmic time

Bernadini et al (2022)

See talk on Wednesday morning!







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About The Project

This repository provides the network implementation and training routines for the paper "From EMBER to FIRE: predicting high resolution baryon fields from dark matter simulations with Deep Learning". The code is written using the Tensorflow2 API, is easy to use and supports parallel training on multiple GPUs. Simulations are part of the FIRE project.

Networks

Pretrained networks and prediction maps can be found at Google Drive.

Prerequisites and Usage

Note that the you may need to modify the code for your specific project application.

Application

for enriching large dark matter simulations with baryons



Rules are meant to be broken!









a. Which of the rules resonate with you?b. Which do you disagree with? Why?c. What did we miss?

- Think on your own (2 minutes)
- Discuss with a partner (4 minutes)
- Discuss in group of 4 (8 minutes)
- Share with full group (6 minutes)

Which of the rules resonate with you? Which do you disagree with? Why? What did we miss?

a.

b.

C.

- Think on your own (2 minutes)
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a.

- 1. Compare against a domain reference and put result into larger context
- 2. Adopt best practices from the ML community
- 3. Interpret, Diagnose and/or Visualise Models
- 4. Explore limits and scope of the model
- 5. Share and Discuss Lessons Learned
- 6. Make Software and Data Publicly Available

Which of the rules resonate with you? Which do you disagree with? Why? What did we miss?

Interactive Activity: Share-Out a. Which of the rules resonate with you?b. Which do you disagree with? Why?c. What did we miss?

Notes

• Start here





Questions?

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