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MACHINE LEARNING IN ASTROPHYSICS





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MODERN COSMOLOGY AND ASTROPHYSICS





TMT 2.4 billion USD

SKA 2.3 billion USD



ALMA 1.3 billion USD WFIRST 3.2 billion USD ATHENA 1 billion USD Euclid 0.7 billion USD





JWST 10 billion USD LSST 2 billion USD





DATA IS GETTING MORE AND MORE COMPLEX! THIS MEANS: NEW OPPORTUNITIES BUT ALSO NEW CHALLENGES











AI ASSISTED PROGRAMMING

GitHub Copilot

LARGE LANGUAGE MODELS IN ASTROPHYSICS

A public-friendly visualization of the 2d manifold of galaxy evolution papers created with UMAP+stable diffusion that shows the different areas of the astro-ph literature corpus. Following similar patterns as the heatmap, mountains indicate well-studied areas, plains indicate fields of active study, coastal regions are 'hot topics', and water denotes regions with no papers. Similar to a world map, the axes here do not hold a particular meaning. Regions close to each other have semantic similarity, while distant regions do not.





1. Unsupervised Learning A. Clustering **B.** Representation Learning 2. Inference / Bayesian Modelling C. Modeling Complex Prob. Distributions **D. Simulation-Based Inference 3. Forward Models and Emulators** F. Neural ODEs and Operator Learning and PINNs

OUTLINE

E. Model Comparison & Model Misspecification





Unsupervised Clustering



CLUSTERING AND DIMENSIONALITY REDUCTION

most of the time we think in categories: stars vs. galaxies, elliptical vs. spirals, halos vs. filaments vs. voids how to find/exploit structure in the data?



https://astrolink.readthedocs.io

- unsupervised clustering: Gaussian Mixture Models, k-means, HDBSCAN, ... in general any halo finder

ASTROLINK







CLUSTERING AND DIMENSIONALITY REDUCTION



https://fuzzycat.readthedocs.io

- most of the time we think in categories: stars vs. galaxies, elliptical vs. spirals, halos vs. filaments vs. voids
 - how to find/exploit structure in the data?
 - What about measurement uncertainties or time evolving data?





CLUSTERING AND DIMENSIONALITY REDUCTION



- most of the time we think in categories: stars vs. galaxies, elliptical vs. spirals, halos vs. filaments vs. voids
 - how to find/exploit structure in the data?
 - What about measurement uncertainties or time evolving data?



https://fuzzycat.readthedocs.io



Oliver+ in prep.

representation learning seeks to automatically discover the representations needed for feature detection or classification from raw data.



Cat by Martin LEBRETON, Dog by Serhii Smirnov from the Noun

image credit: https://blog.fastforwardlabs.com/2020/11/15/representation-learning-101-for-software-engineers.html

1. Self-supervised contrastive representation learning







REPRESENTATION LEARNING FOR STELLAR SPECTRA

multi-modal data: Gaia RVS spectra and Gaia XP coefficients plus contrastive loss



Buck+2024 in prep., see also Parker+2024 for AstroCLIP





REPRESENTATION LEARNING FOR STELLAR SPECTRA

regression



cross-modal generation

Buck+2024 in prep.





REPRESENTATION LEARNING FOR STELLAR SPECTRA



cross-modal generation: AspGap

Li,Wong,Hogg+2024



A brief review of contrastive learning applied to astrophysics

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Accepted XXX. Received YYY; in original form ZZZ

ABSTRACT

Reliable tools to extract patterns from high-dimensionality spaces are becoming more necessary as astronomical datasets increase both in volume and complexity. Contrastive Learning is a self-supervised machine learning algorithm that extracts informative measurements from multi-dimensional datasets, which has become increasingly popular in the computer vision and Machine Learning communities in recent years. To do so, it maximizes the agreement between the information extracted from augmented versions of the same input data, making the final representation invariant to the applied transformations. Contrastive Learning is particularly useful in astronomy for removing known instrumental effects and for performing supervised classifications and regressions with a limited amount of available labels, showing a promising avenue towards Foundation Models. This short review paper briefly summarizes the main concepts behind contrastive learning and reviews the first promising applications to astronomy. We include some practical recommendations on which applications are particularly attractive for contrastive learning.

Key words: methods: data analysis – methods: statistical – methods: miscellaneous – techniques: miscellaneous

Literature: Huertas-Company & Sarmiento 2023

Inference and Bayesian Modelling



MODELING COMPLEX PROBABILITY DISTRIBUTIONS

Bayesian inference aims at determining $p(\theta | \mathbf{x}_0)$

$p(\theta \,|\, \mathbf{x_0}) = \frac{p(\mathbf{x_0} \,|\, \theta) p(\theta)}{p(\mathbf{x_0})} \propto p(\mathbf{x_0} \,|\, \theta) p(\theta)$

In astrophysics, x_o typically results from a large number of mechanisms/effects that transform the data and involve a large number of latent variables z, hence the marginal likelihood $p(\mathbf{x}_0 | \theta)$ is intractable.

$p(\mathbf{x}_0 | \theta) = \left[p(\mathbf{x}_0 | \theta, z) p(z) dz \right]$



MODELING COMPLEX PROBABILITY DISTRIBUTIONS

How can we approximate high-dimensional, complex probability distributions $p(\theta | \mathbf{x}_0)$?

Goal:

- effectively: learn a model from the data!
- model $p(\theta | \mathbf{x}_0)$ explicitly or implicitly
- sample and evaluate $p(\theta | \mathbf{x}_0)$

Options:

- normalizing flows
- VAEs
- GANs
- score matching / flow matching
- and possibly more

implicit model: architectural constraints explicit model: prone to mode collapse

GENERATIVE AI FLAVOURS

- GANs: Sample noise z from a known p(z) and use a generator G(z) to get data. VAEs: Sample noise z from a prior p(z) and use a decoder p(x | z) to sample data. f to get data, $x = f^{-1}(z)$
- Normalizing Flows: Sample noise z from a base distribution p(z) and use an invertible transformation
- score matching: Sample noise z from a Gaussian distribution p(z) and use Langevin dynamics to denoise

"Creating noise from data is easy; creating data from noise is generative modeling." (Song+2020)

don't forget good old Gaussian Processes







SCORE MATCHING AND DIFFUSION MODELS

- Idea: Learn $p(\mathbf{x})$ solely from data samples, then sample new instances.



Target

Target

distribution

Simple distribution Langevin equation

De-noise according to the backward distribution adapted from: slides by Laurence Perrault Levasseur and blog post by https://jmtomczak.github.io/blog/16/16 score matching.html

- What is the score $s(\mathbf{x})$ of a pdf $p(\mathbf{x})$?
 - $s(\mathbf{x}) = \nabla_{\mathbf{x}} \log p(\mathbf{x})$
- But how does this work? \rightarrow Langevin dynamics (Welling&Teh 2011) $x_{t+1} = x_t + \alpha \nabla_{x_t} \log p_{\text{real}}(x) + \eta \epsilon$
 - Add noise according to the forward Langevin equation

Simple (Gaussian) distribution



SCORE MATCHING AND DIFFUSION MODELS

Learn generative model purely from data!

Smith+2021



http://www.mjjsmith.com/thisisnotagalaxy/



SCORE MATCHING AND DIFFUSION MODELS

- Posterior p(x | y) with observation y is given by Bayes' theorem:
 - $\log p(x | y) = \log p(y | x) + \log p(x) \log p(y)$
 - with p(y | x) being the likelihood and p(x) the prior.
 - hence the score is given by:

To a good approximation, we can calculate the likelihood score analytically if we assume it's Gaussian.

Posterior samples with score-based priors





SCORE MATCHING AND DIFFUSION MODELS calculate the likelihood score This is the score we analyti Postérior sample's of source galaxies in strong gravitational and we know A. Ienses with score-based priors



Adam+2022



SCORE MATCHING AND DIFFUSIO

Posterior samples for out-of-distribution galaxies





Adam+2022



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Normalizing Flows



NORMALIZING FLOWS

How can we approximate high-dimensional, complex probability distributions $p(\theta | \mathbf{x_0})$?

Goal:

- model $p(\theta | \mathbf{x_0})$ explicitly
- sample and evaluate $p(\theta | \mathbf{x}_0)$

Idea:

Transform a simple base distribution through a series of invertible transformations.

NORMALISING FLOW: APPLICATION I







NORMALISING FLOW: APPLICATION III

- Normalizing flows for random fields in cosmology (Rouhiainen+2021)
- Bayesian Stokes inversion with normalizing flows (Baso+2022)
- A Hierarchy of Normalizing Flows for Modelling the Galaxy-Halo Relationship (Lovell+2023)
- HIFlow: Generating Diverse Hi Maps and Inferring Cosmology while Marginalizing over Astrophysics Using Normalizing Flows (Hassan+2022)
- Normalizing Flows as an Avenue to Studying Overlapping Gravitational Wave Signals (Langendorff+2023)
- Charting Galactic Accelerations: When and How to Extract a Unique Potential from the Distribution Function (An+2021)
- Charting galactic accelerations II: how to 'learn' accelerations in the solar neighbourhood (Naik+2021)
- many many more...

Simulation-based Inference





SIMULATION-BASED INFERENCE - SBI $p(\theta \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid \theta)p(\theta)}{p(\mathbf{x})} \propto p(\mathbf{x} \mid \theta)p(\theta)$

- likelihood $p(\mathbf{x} \mid \theta)$
- (review: Cranmer+2020)
- recent progress thanks to deep learning algorithms, e.g. conditional normalizing flows (Papamarkios+2019, Greenberg+2019, Hermans+2020, ...)

• Insight: running a stochastic simulator with input θ gives an output x that is drawn from an implicit

• "simulation-based inference" or "likelihood-free inference" or "implicit likelihood inference" or …



SBI: NEURAL X ESTIMATION

• Use neural networks to approximate some quantities in Bayes' formula

$$p(\theta \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid \theta)}{p(\mathbf{x})} p(\theta) = \frac{p(\mathbf{x} \mid \theta)}{p(\mathbf{x})} p(\theta)$$

Neural Posterior Estimation (NPE)

Neural Likelihood Estimation (NLE)

Neural Ratio Estimation (NRE)

SBI: (CONDITIONAL) DENSITY ESTIMATION

- NLE and NPE both estimate normalised probability densities, hence:
 - restricted network architectures, e.g. normalizing flows or mixture density models. potentially difficult to train (Papamarkios+2021)
 - for high-dimensional data, compression/embedding network needed.
- but: restriction can be a good inductive bias, especially if posterior or likelihood is "perturbation" around Gaussian distribution"
- automatic marginalization possible

swyft Miller+2021,2022

https://simulation-based-inference.org/ https://github.com/smsharma/awesome-neural-sbi for references to software and applications

- c.f. pydelfi Alsing+2018,2019; moment networks Jeffrey+Wandelt 2020, SBI Jakob Macke, ItU-ili Ho+2024, Bayesflow Radev+2020,2023,



kSZ $Z \times CIB$ Planck 100A100B43B217A

217B

: APPLICATION IN COSMOLOGY



Cole+2022



SBI: APPLICATION FOR STELLAR STREAMS



TRUNCATED MARGINAL NEURAL RATIO ESTIMATION (TMNRE) FOR STELLAR STREAMS

STEP 1: (RE-) SIMULATE

- Sample parameters θ from (truncated) prior $p(\theta)$
- Simulate data $x \sim p(x \mid \theta)$

 $\theta \equiv (t_{\text{age}}, \sigma_v, \ldots) \rightarrow x = \text{stream} + \text{bkg}.$



STEP 4: TRUNCATION

- Use ratios $r(x_0; \theta_i)$ to remove regions with extremely low posterior density
- If this leads to a reduction in prior volume, resimulate from **Step 1** with truncated prior
- Repeat until converged across all parameters, then obtain resulting posterior

STEP 2: RATIO ESTIMATION

• Train ratio estimators $r(x; \theta_i)$ on simulated data to approximate the posterior-to-prior ratio $r(x; \theta_i) \sim p(\theta_i | x) / p(\theta_i)$ for each parameter of interest θ_i



- Obtain a prior sample from $p(\theta_i)$

LBATROSS

- Target a specific observation x_0 and compute the ratios $r(x_0; \theta_i)$ across the prior sample
- Weight the samples according to this ratio





SBI: APPLICATION FOR GALACTIC CHEMICAL ENRICHMENT







SBI: APPLICATION IN COSMOLOGY



slide from Cole



SBI: APPLICATION IN STRONG LENSING

Searching light DM halos



Halo mass function cutoff

Image credit: Wagner-Carena+ 2203.00690

Alternative to: HMC, parameter reduction, ABC, ...

Probing **population effects of light dark matter halos** rather than individual detections



Related work: He+ 2010.13221 (similar in spirit, using ABC)

Wagner-Carena+ 2203.00690 (constraining subhalo mass function normalization)



SBI: APPLICATION IN STRONG LENSING

30°

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Astrometry Mishra-Sharma+ 2110.01620



Single frequency CMB B-mode inference with realistic foregrounds from a single training image

Niall Jeffrey,^{1,2}* François Boulanger,¹ Benjamin D. Wandelt,^{3,4} Bruno Regaldo-Saint Blancard,^{1,5} Erwan Allys,¹ François Levrier¹ slide from Cole



GW parameters

Delaunoy+ 2010.12931, Dax+ 2106.12594, ...



Stellar streams Hermans+ 2011.14923







Dax+2021,2023,2024

Bayesian Model Comparison





Bayesian model selection assigns posterior probabilities $p(\mathcal{M}_k | \mathbf{d})$ to models $\mathcal{M}_k \in$ $\{\mathcal{M}_1, \ldots, \mathcal{M}_N\}$ (instead of to values of their parameters θ_k), conditional on observed data d. The conventional approach is to compute the marginal likelihood (or *evidence*) $p(\mathbf{d} \mid \mathcal{M}_k)$, which is the average likelihood $p(\mathbf{d} | \boldsymbol{\theta}_k)$ of parameters distributed according to the prior $p(\boldsymbol{\theta}_k)$:

$$p(\mathbf{d} \mid \mathcal{M}_k) = \int_{\mathcal{M}_k} \int$$

(where the presence of \mathcal{M}_k 's parameters θ_k implies conditioning on \mathcal{M}_k in the right-hand side). The prior belief in the model, $p(\mathcal{M}_k)$, is then updated to its posterior probability in accordance with Bayes' theorem: $p(\mathcal{M}_k \mid \mathbf{d}) \propto p(\mathbf{d} \mid \mathcal{M}_k) p(\mathcal{M}_k)$, normalised over all models considered.

$$\int p(\mathbf{d} | \boldsymbol{\theta}_k) p(\boldsymbol{\theta}_k) d\boldsymbol{\theta}_k$$



Methods

- Jeffrey+Wandelt 2023: loss functions for two-way model comparison with an emphasis on recovering accurate extreme Bayes factors
- Radev+2021: estimate a Dirichlet distribution over an arbitrary number of models using a NN and variational optimisation
- Elsemüller+2023 and Karchev+2024: use a cross-entropy loss for multi-class posterior probabilities
- Macciò+2022: Model selection for star formation prescriptions in cosmo sims
- Zhou+2024: Model misspecification plus model comparison for low simulation budget applications
- Jin+2024: Model comparison of cosmo sims via GANomaly scores



Idea:

- Train embedding network on ~600.000 SDSS images, then encode simulated SDSS images
- Train simulation classifiers on embeddings, apply to real SDSS images

UMAP projection of k-sparse encoding of sims and Jobs



Zhou, Buck+2024 subm.







Zhou, Buck+2024 subm.



MODEL COMPARISON/SELECTION

SimSIMS: Simulation-based Supernova Ia Model Selection with thousands of latent variables



Christoph Weniger⁵ **Roberto Trotta**^{1,2,3,4} dM M0dMposterior odds posterior odds local local local 1:1001:101:110:1 100:1 100:1 1:10 1:1 10:1 0.5 0.4 0.3 6 0.2 0.1 0.0 -0.2 -0.1 0.1 3 0.0 0.2 2 5 6 4 ΔM μ_R







LEARNING THE SOLUTION OF ODES AND PDES — **NEURAL ODES, OPERATOR LEARNING AND PINNS**

- ODEs are good for:
 - population models
 - motion of the planets
 - structural integrity of a bridge
 - fluid dynamics
 - •

ODEs are kind of easy — only derivatives with respect to one variable

PDEs are more complicated — derivatives with respect to many variables and differential equations are local while solutions exhibit non-local properties

• Traditional solution: discretisation (in time and space) and iterative solution



NEURAL ODES, OPERATOR LEARNING **AND PINNS**

Neural ODE:

 $\frac{df}{dt} = h_{\theta}(x_0, t, p)$

Neural Operator:

 $G_{\theta}: X \to Y \quad u \mapsto G_{\theta}(u)$ with X, Y function spaces (infinite dimensional)

PINN:

 $f(x,t) = h_{\theta}(x,t,p)$ with $\frac{df}{dt} = \frac{dh_{\theta}}{dt}$, $\frac{df}{dx} = \frac{dh_{\theta}}{dx}$ need to fulfil the diff eq.

(neural net = right hand side of diff eq.

solution: integrate entire neural net.)

(neural net approximates the operator i.e. the map between function space)

(solution is given by neural net, autodiff and diff eq. are used in loss)











• Traditional solution: discretisation (in time and space) and iterative solution

Euler discretization

$$h_{t+1} = h_t + f_t(h_t, \theta_t)$$
$$h(t + \Delta t) = h(t) + \Delta t \cdot f(t, h(t), \theta)$$
$$\frac{h(t + \Delta t) - h(t)}{\Delta t} = f(t, h(t), \theta)$$

NEURAL ODES



Chen+2019



NEURAL ODES IN ASTROPHYSICS

- Neural Astrophysical Wind Models (Nguyen 2023)
- Neural ODEs as a discovery tool to characterize the structure of the hot galactic wind of M82 (Nguyen+2023)
- 2023)



Speeding up astrochemical reaction networks with autoencoders and neural ODEs (Sulzer+Buck)



PHYSICS INFORMED NEURAL NETS

Loss function for PINNs

Differential Equation: $\mathcal{F}[u(x, y)] = f(x, y)$

Dataset: (x_i, y_i, u_i) ; $i = 1, ..., N_{data}$

Collocation points: $(x_j, y_j); j = 1, ..., N_C$

Initial Condition: (x_0, y_0, u_0)



$$L_{DiffEq} = \frac{1}{N_c} \sum_{j=1}^{N_c} (\mathcal{F}[u(x_j, y_j)] - f(x_j, y_j))^2$$



PINNS IN ASTROPHYSICS

- Physics-informed neural networks for modeling astrophysical shocks (Moschou+2023)
- Probing the solar coronal magnetic field with physicsinformed neural networks (Jarolim+2022)
- Physics-informed neural networks in the recreation of hydrodynamic simulations from dark matter (Dai+2023)
- Physics informed neural networks for simulating radiative transfer (Mishra+Molinaro 2021)
- Neural networks: solving the chemistry of the interstellar medium (Branca+Pallottini 2023)



DEEP OPERATORS IN ASTROPHYSICS

- Systems (Mao+2023)
- Emulating the interstellar medium chemistry with neural operators (Branca+Pallottini 2024)
- CODES Benchmark for neuralODEs and Operator Learning for astrochemistry (Janssen, Sulzer+Buck 2024)



• PPDONet: Deep Operator Networks for Fast Prediction of Steady-State Solutions in Disk-Planet

SUMMARY & CONCLUSION

My personal message:

Write better code! Share more data! Build more open-source software!

This will accelerate research cycles and lets you engage with peers early on!

Main take away:

scientific motivated inductive bias helps to be more robust, more data efficient and better interpretable

Differentiable Simulators

DIFFERENTIABLE SIMULATORS