Paris workshop on Bayesian Deep Learning for Cosmology and Time Domain Astrophysics

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ML inference & uncertainties
ML in the next decades
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Bayesian Time Series Analysis with TFP on JAX
Probabilistic Deep Learning with TFP and JAX/Flax
Likelihood-Free Inference and Application to Cosmology
Breakout session over lunch

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Introduction to Bayesian thinking

Cosmology / 54

Deblending Galaxies with Generative Adversarial Networks

Auteur: Shoubaneh Hemmati¹

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Deep generative models including generative adversarial networks (GANs) are powerful unsupervised tools in learning the distributions of data sets. Various applications of GANs such as image generation, data/image to image translation, feature transfer, or super resolution could notably enhance astronomical data sets. Building a simple GAN architecture in PyTorch and training on the CANDELS data set, we generate galaxy images with the Hubble Space Telescope resolution starting from a noise vector. We proceed by modifying the GAN architecture to improve the Subaru Hyper Suprime-Cam ground-based images by increasing their resolution to the HST resolution. We use the super resolution GAN on a large sample of blended galaxies which we create using CANDELS cutouts. In our simulated blend sample, $\sim 20\%$ would unrecognizably be blended even in the HST resolution cutouts. In the HSC-like cutouts this fraction rises to $\sim 90\%$. With our modified GAN we can lower this value to $\sim 50\%$. We quantify the blending fraction in the high, low and GAN resolutions over the whole manifold of angular separation, flux ratios, sizes and redshift difference between the two blended objects. The two peaks found by the GAN deblender result in ten times improvement in the photometry measurement of the blended objects. Modifying the architecture of the GAN, we also train a Multi-wavelength GAN with seven band optical+NIR HST cutouts. This multi-wavelength GAN improves the fraction of detected blends by another $\sim\,10\%$ compared to the single-band GAN. This is most beneficial to the current and future precision cosmology experiments (e.g., LSST, SPHEREx, Euclid, Roman), specifically those relying on weak gravitational lensing, where blending is a major source of systematic error.

Time Domain Astrophysics / 55

Searching for changing-state AGNs in massive datasets with anomaly detection

Auteur: Paula Sanchez Saez¹

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The classic classification scheme for Active Galactic Nuclei (AGNs) was recently challenged by the discovery of the so-called changing-state (changing-look) AGNs (CSAGNs). The physical mechanism behind this phenomenon is still a matter of open debate and the samples are too small and of serendipitous nature to provide robust answers. In order to tackle this problem, we need to design methods that are able to detect AGN right in the act of changing-state.

In this talk I will present an anomaly detection (AD) technique designed to identify AGN light curves with anomalous behaviors in massive datasets, in preparation for the upcoming Vera Rubin Observatory. The main aim of this technique is to identify CSAGN at different stages of the transition, but it can also be used for more general purposes, such as cleaning massive datasets for AGN variability analyses. To test this algorithm, we used light curves from the Zwicky Transient Facility data release 5 (ZTF DR5), containing a sample of 230,458 AGNs of different classes. The ZTF DR5 light

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curves were modeled with a Variational Recurrent Autoencoder (VRAE) architecture, that allowed us to obtain a set of attributes from the VRAE latent space that describes the general behaviour of our sample. These attributes were then used as features for an Isolation Forest (IF) algorithm. We used the VRAE reconstruction errors and the IF anomaly score to select a sample of 8810 anomalies. These anomalies are dominated by bogus candidates, but we were able to identify promising CSAGN candidates.

Cosmology / 56

Galaxies and Halos on Graph Neural Networks: Deep Generative Modeling Scalar and Vector Quantities for Intrinsic Alignment

Auteur: Yesukhei Jagvaral^{None}

Co-auteurs: Campbell Duncan; Siamak Ravanbakhsh; Francois Lanusse ¹; Rachel Mandelbaum ²; Singh Sukhdeep

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In order to prepare for the upcoming wide-field cosmological surveys, large simulations of the Universe with realistic galaxy populations are required. In particular, the tendency of galaxies to naturally align towards overdensities, an effect called intrinsic alignments (IA), can be a major source of systematics in the weak lensing analysis. As the details of galaxy formation and evolution relevant to IA cannot be simulated in practice on such volumes, we propose as an alternative a Deep Generative Model. This model is trained on the IllustrisTNG-100 simulation and is capable of sampling the orientations of a population of galaxies so as to recover the correct alignments. In our approach, we model the cosmic web as a set of graphs, where the graphs are constructed for each halo, and galaxy orientations as a signal on those graphs. The generative model is implemented on a Generative Adversarial Network architecture and uses specifically designed Graph-Convolutional Networks sensitive to the relative 3D positions of the vertices. Given (sub)halo masses and tidal fields, the model is able to learn and predict scalar features such as galaxy and dark matter subhalo shapes; and more importantly, vector features such as the 3D orientation of the major axis of the ellipsoid and the complex 2D ellipticities. For correlations of 3D orientations the model is in good quantitative agreement with the measured values from the simulation, except for at very small and transition scales. For correlations of 2D ellipticities, the model is in good quantitative agreement with the measured values from the simulation on all scales. Additionally, the model is able to capture the dependence of IA on mass, morphological type and central/satellite type.

Lightning talks / 57

Bayesian planetary numerical ephemerides B-INPOP with MCMC

Auteur: Vincenzo Mariani¹ **Co-auteur:** Agnès Fienga ¹

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The INPOP planetary ephemerides are worldwide references for Planetary Ephemerides for almost twenty years now, and the subject proposed in this poster is devoted to continue this development

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in investigating a rigorous mathematical set-up of a Bayesian approach for the determination of IN-POP parameters involved in the ephemerides computation.

It has been already shown in several publications that testing gravity with the orbits of solar system objetcs is affected by heavy correlations between parameters and can e highly improved by using alternative methods to the classic optimization methods like the Least Squares. The construction of INPOP following a full Bayesian characterization would overcome this kind of correlation problems.

The work presented here had been developed in the frame of measuring the mass of the graviton with planetary ephemerides. Untill now we tried to asses model uncertainty, and to proceed with Bayesian inference, using MCMC methods and the Likelihood values obtained from the classical INPOP fit for the remaining parameters involved.

An additional important difficulty for our specific problem is that obtaining the Likelihood is computationally expensive (in terms of time) since we integrate equations of motions for the whole Solar System. Therefore we cannot use it directly in the Bayesian algorithm but we can use interpolated values of the Likelihood using Gaussian Process (GP).

The GP is used for:

- i) estimating interpolated values,
- ii) assessing the uncertainty of the approximated-Likelihood computation.

Using as parameter of the Bayesian inference the mass of the graviton is the first step, afterwards we will proceed with the computation of PPN parameters and the masses of the asteroids exploiting more advanced MCMC and Bayesian Deep Learning methods. The INPOP planetary ephemerides are involved in the design of several space missions (like JUICE, BepiColombo and GAIA), for fundamental physics and Solar System dynamics investigations (for short-term and long-term integration of the equations of motion) therefore improving the precision of the INPOP ephemerides by a Bayesian approach can also influence the final outcome of all these missions and researches.

Ethics of large scale machine learning / 58

Goodness-of-fit Evaluation: Toward Trustworthy Probabilistic Machine Learning

Auteur: Arya Farahi¹

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Likelihood-based and machine learning-based probabilistic classifiers are utilized by astronomers to classify astronomical objects and events. Simultaneously, these models are increasingly deployed to guide consequential decision-making tasks in our society (resource allocation, admission recommendation, etc). While the applications of these models have been rapidly increasing, we have not seen a corresponding leap in developing validation methodologies that can verify the trustworthiness of these models. Typically, the performance of a probabilistic classifier is assessed with metrics, such as accuracy, precision, and Area under the ROC curve, among others. Except in trivial cases, where a model can perfectly identify class members, neither of these performance metrics can evaluate the goodness-of-fit. To fill this gap, we have developed a novel kernel-based, distribution-free method that (1) evaluates the goodness-of-fit of a probabilistic classifier and (2) quantifies its distance from the oracle classifier. This tool, that is initially developed to evaluate the trustworthiness of classifiers in decision-support systems, has ample applications in astronomical settings. In this talk, I will introduce this novel tool, present theoretical guarantees, and its application to trustworthy ML. Then, I will illustrate the performance of the proposed test statistic by applying it to a set of controlled simulated data; and finally, demonstrate its application to astronomical data analysis.

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Enhancing gravitational-wave population inference with deep learning

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Gravitational-wave population studies have become a common approach to learn about the astrophysical distribution of merging stellar-mass binary black holes. The goal is to map the source properties (e.g., masses and spins) of events observed by ground-based interferometers —which have been filtered through detection biases— to the true parameter distributions as a whole across the population. In practice, this requires us to construct models for the population and detection biases, which feed into a hierarchical Bayesian inference to measure the properties of the population. I will present our approach to solving this problem, the key ingredient being the use of machine learning models. We employ a simulation-based approach which, when enhanced with deep neural networks, allows us to compare astrophysical models directly with gravitational-wave data while fully mapping the Bayesian posterior. Applying our deep learning population framework to the case of dynamical formation, in which components in binary black hole mergers may already be the remnants of previous mergers, we show that features in the mass and spin distributions can be explained by this repeated-merger scenario. Our approach readily applies to realistic simulations of various astrophysical formation channels.

Lightning talks / 61

A Bayesian Convolutional Neural Network for Robust Galaxy Ellipticity Regression

Auteurs: Amedeo Napoli^{None}; Claire Theobald¹; Bastien Arcelin²; Brieuc Conan-Guez^{None}; Frédéric Pennerath^{None}; Miguel Couceiro^{None}

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Cosmic shear estimation is an essential scientific goal for large galaxy surveys. It refers to the coherent distortion of distant galaxy images due to weak gravitational lensing along the line of sight. It can be used as a tracer of the matter distribution in the Universe. The unbiased estimation of the local value of the cosmic shear can be obtained via Bayesian analysis which relies on robust estimation of the galaxies ellipticity (shape) posterior distribution. This is not a simple problem as, among other things, the images may be corrupted with strong background noise. For current and coming surveys, another central issue in galaxy shape determination is the treatment of statistically dominant overlapping (blended) objects. We propose a Bayesian Convolutional Neural Network based on Monte-Carlo Dropout to reliably estimate the ellipticity of galaxies and the corresponding measurement uncertainties. We show that while a convolutional network can be trained to correctly estimate well calibrated aleatoric uncertainty, – the uncertainty due to the presence of noise in the images – it is unable to generate a trustworthy ellipticity distribution when exposed to previously unseen data (i.e. here, blended scenes). By introducing a Bayesian Neural Network, we show how to reliably estimate the posterior predictive distribution of ellipticities along with robust estimation of epistemic uncertainties. Experiments also show that epistemic uncertainty can detect inconsistent predictions due to unknown blended scenes.

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Lightning talks / 62

There's no difference: Convolutional Neural Networks for transient detection without template subtraction

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We present a Convolutional Neural Network (CNN) model for the separation of astrophysical transients from image artifacts, a task known as "real-bogus" classification, that does not rely on Difference Image Analysis (DIA) which is a computationally expensive process involving image matching on small spatial scales in large volumes of data. We explore the use of CNNs to (1) automate the "real-bogus" classification, (2) reduce the computational costs of transient discovery. We compare the efficiency of two CNNs with similar architectures, one that uses "image triplets" (templates, search, and the corresponding difference image) and one that adopts a similar architecture but takes as input the template and search only. Without substantially changing the model architecture or retuning the hyperparameters to the new input, we observe only a small decrease in model efficiency (97% to 92% accuracy). We further investigate how the model that does not receive the difference image learns the required information from the template and search by exploring the saliency maps. Our work demonstrates that (1) CNNs are excellent models for "real-bogus" classification that rely exclusively on the imaging data and require no feature engineering task; (2) high-accuracy models can be built without the need to construct difference images. Since once trained, neural networks can generate predictions at minimal computational costs, we argue that future implementations of this methodology could dramatically reduce the computational costs in the detection of genuine transients in synoptic surveys like Rubin Observatory's Legacy Survey of Space and Time by bypassing the DIA step entirely.

Time Domain Astrophysics / 63

A Convolutional Neural Network Approach to Classifying Supernova Time-Series Photometry

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The use of type Ia supernovae (SNe Ia) as standardizable candles led to the Nobel Prize-winning discovery of the accelerating expansion of the universe and cemented their role in the quest to understand the nature of dark energy. Accurate cosmological parameter estimation requires a sample of pure SNe Ia with minimal non-Ia contamination, but supernova type confirmation using spectroscopy is logistically infeasible in most cases. Thus, a reliable algorithm for supernova classification with photometry (image data) alone is vital to expanding the set of cosmologically useful SNe Ia beyond the spectroscopic sample. In this talk, I will present SCONE (Supernova Classification with a Convolutional Neural Network), a novel deep learning-based method for photometric supernova classification. While traditional photometric classification algorithms rely on extracting handcrafted features from supernova photometry, deep learning methods bypass this requirement by identifying and using features optimized for the classification task. SCONE is a convolutional neural network (CNN), an architecture prized in the deep learning community for its state-of-the-art image recognition capabilities. Supernova time-series photometry is preprocessed into 2D "images" using Gaussian processes in both wavelength and time dimensions to generate the input to the model. This alleviates the issue of irregular sampling between filters and, along with the choice of an asymmetric convolutional kernel covering the full wavelength range, allows the CNN to learn from information in all

filters simultaneously. In addition, our model requires raw photometric data only, precluding the necessity for accurate redshift approximations. SCONE has achieved 99.73 \pm 0.26% test set accuracy differentiating SNe Ia from non-Ia, as well as 98.18 \pm 0.3% test accuracy performing 6-way classification of supernovae by type. SCONE also exhibits impressive performance classifying supernovae by type as early as the second detection with very few epochs of photometric observations. SCONE achieved 60% average accuracy across 6 supernova types at the date of trigger and 70% accuracy 5 days after trigger. The incorporation of redshift information improves these results significantly to 75% accuracy at the date of trigger and 80% accuracy 5 days after trigger. The model also has relatively low computational and dataset size requirements without compromising on performance – the above results are from models trained on a ~10^4 sample dataset in around 15 minutes on a GPU. SCONE's ability to produce impressive early-time classification results as well as perform highly accurate SNe Ia vs. non-Ia classification makes it an excellent choice for spectroscopic targeting as well as the development of photometric SNe Ia samples for cosmology.

Lightning talks / 64

Improvement of the statistical model of a photoz bayesian estimator hybridizing a SED template fitting and a gaussian process

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We propose an improvement of the statistical model of the Delight code, which proposes a Bayesian estimation of the photometric redshift PhotoZ of target galaxies from training galaxies data.

The peculiarity of this estimator is that it combines a template fitting estimator capable of extrapolation to large redshift with a more accurate machine learning estimator but with a low extrapolation capability.

The Gaussian likelihood function of the observed target fluxes in different bandwidths is computed on a predictive model built on a multivariate Gaussian process Y = f(X) on a multidimensional space represented by X = (band indexes, redshift, template indexes), where Y is the vector of fluxes in the different bands and to which we add a nuisance parameter I corresponding to the relative scaling factor of luminosity between the target and training galaxies.

The Gaussian process is implemented on a mean flux prediction computed from the SED templates (latent SED) while the covariance matrix (kernel) encodes only the physical flux-redshift relation independently of any reference to a SED. The role of the kernel is to learn from the training galaxies the presence of variable features such as a continuum related to dust absorption or emission lines and to find these features in the targets while they are absent from the latent SED. The interpretation of this kernel is to evaluate a weighting coefficient that selects the training galaxies that present characteristics close to those of the target galaxies in the likelihood function.

This Photoz estimator is built around a hierarchical Bayesian model with hyperparameters that need to be optimised either on simulations or on data.

We compared the performance of this hybrid estimator with other estimators such as a Random Forest Tree and the LePhare code of SED Template Fitting with standard Photoz metrics on DESC DC2 simulations.

The results suggest that there is room for improvement for Delight compared to pure machine learning results, while Delight and LePhare show similar performance.

We consider that an optimizations of Delight's hyperparameters would be facilitated if the flux-redshift model constructed from the SEDs and spectral bands were corrected beforehand for the photodetection bias induced by the sample selection.

The hyperparameter optimization could be performed later with a self-differentiated version of the marginal likelihood function.

Cosmology / 65

Graph-Convolutional Neural Networks for large-scale structure clustering

Auteur: Farida Farsian¹

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One of the most important challenges in modern Cosmology will be to deal with enormous amount of data which will be produced by future cosmological and astrophysical surveys. Therefore, new methodologies such as Artificial Intelligence and Deep Learning (DL) should come to play to handle the computational expensive operations, automation and extracting of non explored data features and statistics.

On the other hand, there are plenty of cosmological models, in particular in the dark energy field, which have to be tested and explored. The latter would be essential to analyse the data provided e.g. by the Euclid satellite.

Up to now, standard cosmological analyses based on abundances, two-point and higher-order statistics have been widely used to investigate the properties of the large-scale structure of the Universe. However, these statistics can only exploit a sub-set of the whole information content available.

Along these lines, we aim at extracting clustering information of large-scale structures with various dark energy equation of state parameters by only considering the coordinates and masses of galaxy clusters. We introduce a new representation of the cosmic web data in form of graphs, in which the clustering information of cosmic tracers would be automatically included. This form of data can be fed to the fascinating branch of DL, Graph-Convolutional Neural network (GCNN).

GCNNs has been recently designed to deal with irregular and sparse data, and moreover they are built to capture the graph structure of data which is often very rich. In order to create a graph-structured data from dark matter halo catalogues, we consider different sets of Quijote simulations for different values of w0, and to build our appropriate GCNN, we utilise Spektral package which is based on Tensorflow and Keras.

In this work, we show that the built model is able to distinguish different dark energy models with very high accuracy, in both manner of Binary classification (acc = 99%) and Multi-class classifications (acc = 97%). Moreover, changing the problem to the regression, the model is able to predict the value of w0 with high precision.

Furthermore this method can be applied on any kind of astrophysical data which are characterised by point clouds, because Graph Neural Networks in general are suitable to apprehend global permutation invariant quantities.

Lightning talks / 66

Attention-based modeling of AGN light curves

Auteur: Matthew Lowery¹

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With large heaps of time-domain active galactic nuclei (AGN) data in multiple broadband wavelengths anticipated from upcoming surveys such as the Vera C. Rubin Observatory's Legacy Survey of Space and Time, statistical models must be equipped to process this irregularly sampled light curve data at scale and better represent the optical and UV variability of the compact region near the central black hole without making any underlying assumptions. Attention-based architectures have quickly become the de facto standard in deep learning models for sequential data due to their

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ability to bridge long-term temporal dependencies and added allowance for intra-training example parallelization that is fundamentally not possible in recurrent models like LSTMs. We consider a particular time-based attention model for this problem, HeTVAE (Heteroscedastic Temporal Variational Autoencoder; Shukla and Marlin 2021), which poses notable promise by propagating uncertainty through a 'sparsity-aware'heteroscedastic output layer in its interpolation of a sparse and multivariate time series with significantly shorter run times than Gaussian Process Regression-based methods that reflect uncertainty through posterior inference. An appropriate and scalable means of reconstructing the light curves gives way to more adequately exploring the underlying process of the AGN's variability and the black hole's physical properties in the LSST era, specifically with regard to estimating time lags from the UV and optical reprocessing of X-ray variability close to the black hole.

ML Methodology / 68

Fast Inference of Star Formation Histories of Galaxies with Spectra and Simulation-Based Inference (SBI)

Auteur: Gourav Khullar¹

Co-auteurs: Fei Xu ²; Brian Nord ³; Aleksandra Ciprijanovic ³; Jason Poh ²; Michael Gladders ²; Alexander Ji

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A pressing question in the field of cosmological structure formation is how the long-term assembly and evolution of baryonic matter occurs in galaxies. Galaxies take different pathways to assemble their stellar mass, signatures of which can be derived from galaxy star formation histories via stellar population synthesis (SPS) modeling. Today, we are approaching the age of trillion-galaxy surveys (DECaLS, DESI, Rubin surveys) containing photometry and spectroscopy (describing a given galaxy' s spectral energy distribution, or SED). It is imperative that fast and efficient methods —beyond traditional Bayesian MCMC methods —are built to constrain galaxy parameters such as stellar age, metallicity, dust attenuation, stellar mass, and star formation rates for these large samples. The combination of machine learning (ML) and simulation-based inference (SBI) is a promising path forward. SBI allows a) efficient analysis of galaxy SEDs and inference of galaxy parameters with physically interpretable uncertainties; and b) amortized calculations of posterior distributions of said galaxy parameters at the modest cost of a few galaxy fits with MCMC methods. In this work, we show initial results from our SBI analysis using the Python package 'sbi'to perform Sequential Neural Posterior Estimation (SNPE) to obtain 1- and 2-parameter SED fits. In our proof-of-concept analysis on simulated galaxy photometry and spectroscopy, we demonstrate that SBI - with its combination of fast and amortized posterior estimations - is capable of inferring galaxy stellar masses and metallicities with accuracy and precision comparable to traditional inverse-modeling with MCMC. We compare SBI to Bayesian Neural Network-based inference of these parameters. We also demonstrate the efficacy of our framework with photometry of cluster galaxies and gravitationally lensed systems; observations of these galaxies in the next decade are bound to help solve the question of stellar mass assembly.

Lightning talks / 69

Applying Likelihood-Free Inference to LISA parameter estimation: a project

Auteur: Ivan Martin Vilchez¹

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The Laser Interferometer Space Antenna (LISA) is an ESA mission for a future space-based Gravitational Wave detector. Work is currently underway on establishing a ground segment data processing and data analysis pipelines, from the raw instrumental data to astrophysical catalogs. A central part of this are the LISA Data Challenges (LDCs), which consist of simulated LISA data to be analyzed by the participants. Over time, more realistic, complicated challenges will be released, incentivizing the development of new algorithms.

Among the different sources expected to be found by LISA, one of the main ones are the coalescence of Massive Black Hole Binaries (MBHBs). Their Signal to Noise Ratio (SNR) is expected to be very large, making their detection relatively easy, but the parameters that describe them can be confused, resulting in a multimodal posterior.

Parameter estimation of these sources is typically done with Bayesian sampling methods, like Parallel Tempered Markov Chain Monte Carlo (PTMCMC). These are generally reliable, but very computationally expensive as they require many forward simulations to produce samples and compute the likelihood function. We are looking to approach the problem by using Likelihood-Free Inference (LFI) methods to estimate the posterior distribution. In this poster we describe our current efforts in this project, which is still in its early stages, and future plans.

Cosmology / 70

COSMOPOWER: Deep Learning - accelerated Bayesian inference from next-generation cosmological surveys

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Next-generation Large-Scale Structure (LSS) and Cosmic Microwave Background (CMB) surveys will provide us with unprecedented levels of precision in the final constraints on our cosmological model. However, the computational challenges posed by these enormous datasets dangerously hinder their analysis within a Bayesian framework for rigorous uncertainty propagation –a condition necessary to ensure correspondingly high levels of accuracy in the final constraints.

In my talk I will present COSMOPOWER, an open-source Python framework for Deep Learning accelerated Bayesian inference from next-generation CMB and LSS surveys. COSMOPOWER provides orders-of-magnitude acceleration to the inference pipeline by training Deep Learning emulators of matter and CMB power spectra. I will show how these emulators meet the accuracy requirements for application to both currently available cosmological data, such as from the Kilo-Degree Survey (KiDS), as well as to simulated, next-generation data from e.g. a Euclid-like survey. The emulators always recover the fiducial cosmological constraints, while providing a speed-up factor up to O(10^4) to the complete inference pipeline. Bayesian parameter contours can thus be recovered in just a few seconds on a common laptop, as opposed to the many hours, days or months of runtime on computer clusters required by standard methods. I will conclude with an outlook on extensions of this software that are currently being developed to extend COSMOPOWER into a fully differentiable library for cosmology.

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HARMONIC: Bayesian model comparison for simulation-based inference

Auteurs: Alessio Spurio Mancini¹; Matthew Docherty²

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Simulation-based inference techniques will play a key role in the analysis of upcoming astronomical surveys, providing a statistically rigorous method for Bayesian parameter estimation. However, these techniques do not provide a natural way to perform Bayesian model comparison, as they do not have access to the Bayesian model evidence.

In my talk I will present a novel method to estimate the Bayesian model evidence in a simulation-based inference scenario, which makes use of the learnt harmonic mean estimator. We recently implemented this method in a public software package, HARMONIC, which allows one to obtain estimates of the evidence from posterior distribution samples, irrespective of the method used to sample the posterior distribution. I will showcase the performance of HARMONIC in multiple simulation-based inference scenarios where the estimated evidence can be compared with exact analytical results, including an example of model selection in the analysis of gravitational waveforms.

The versatility of the model evidence estimation framework provided by HARMONIC, coupled with the robustness of simulation-based inference techniques, creates a new complete Bayesian pipeline for parameter estimation and model comparison from next-generation astronomical surveys.

Gravitational Waves / 72

Fast Parameter Estimation for Massive Black Hole Binaries with Normalising Flows

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One of the sources which Laser Interferometer Space Antenna (LISA) will observe are the signals from the Massive Black Hole Binaries (MBHBs) during their inspiral, merged and ringdown phases. To estimate physical parameters of these systems and their localisations one has to perform some form of Bayesian Inference. The most common approach to do this is through defining the likelihood function and producing posterior samples with some form of sampling technique. The disadvantage of the sampling methods is that they are slow. We propose the Bayesian parameter estimation method which is based on the Normalising flows a technique which allows to make an extremely fast mapping from the base sample distribution to the posterior conditioned on the data. This is implemented by learning this mapping in advance on the training dataset and then applying the trained map to the real data. We apply this method to the data from the first LISA Data Challenge (LDC) in order to evaluate how the estimated posteriors agree with the standard approaches. The main purpose of the fast parameter estimation is to use it for the multi-messenger observations and to be able to alert other observatories to perform follow-ups.

Cosmology / 73

The Extended LSST Astronomical Time Series Classification Challenge (ELAsTiCC)

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The original Photometric LSST Astronomical Time-Series Classification Challenge (PLAsTiCC) established the gold-standard reference dataset of Rubin light curves and catalyzed the development of several deep learning algorithms for classification. However, to truly simulate LSST operations, we must simulate not light curves, but real-time alert streams, complete with the contextual information an astrophysicist would receive from Rubin. This dataset will allow the Rubin ML community to prepare for the start of commissioning, as well as provide a new reference sample for cosmological investigations with LSST. The key goal of ELAsTiCC to prepare LSST's Science Collaborations working in the time-domain for Rubin Operations. In creating this successor to PLAsTiCC, we have incorporated deep-learning in generating the simulations, and we expect the simulations to become the basis for many novel ML methods that encode both light curves and contextual information into a complex feature space. I will discuss the ELAsTiCC team's work in building this dataset, and progress towards launching the challenge, and discuss several of the studies that we have envisioned for this dataset.

Time Domain Astrophysics / 74

SNAD: anomaly detection for large scale time-domain astronomy

Auteurs: Konstantin Malanchev¹; Patrick Aleo²; Emille Ishida³; Matwey Kornilov⁴; Vladimir Korolev⁵; Maria Pruzhinskaya⁴; Etienne Russeil³; Sreevarsha Sreejith⁶; Alina Volnova⁷

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Modern large scale astronomical surveys scan wide areas of the sky following a predetermined cadence. As a result, their data sets contain records of both, known and unknown (or not yet observationally confirmed) astrophysical phenomena. Such datasets hold an immense potential for discovery, however, their volume and complexity makes successfully identifying such events a far from trivial task. The challenge will be orders of magnitude greater with the arrival of the Vera Rubin Observatory Large Survey of Space and Time (LSST), expected to collect 15 TB per night of observation for at least ten years. In this new paradigm, serendipitous discoveries are unlikely to happen and new physics can easily hide in plain sight if we do not have the proper tools and knowledge framework necessary to characterize them.

In preparation for this new era in data intensive astronomy, since 2018 SNAD group has been developing efficient methods for time-domain anomaly detection. In this talk I will give an overview of the SNAD tools and strategies which enabled the treatment of a variety of light curve data sets: from a few thousands objects of the Open Supernova Catalog to a few millions light curves of the Zwicky Transient Facility (ZTF) data release. Their employed anomaly detection approach is centered in the combination of machine learning methods and expert analysis of the data. Two of the main SNAD products, currently widely in use by the community are: a high-performant feature extraction toolbox "light-curve" – now used by three ZTF/LSST alert brokers; and the SNAD ZTF viewer which allows experts to efficiently evaluate the output of the machine learning pipeline. Last but not least, the team also developed an active anomaly detection pipeline, which implements a machine-expert

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interactive loop and gives significantly better performance in both detecting unusual astrophysical objects and filtering bogus data. I will briefly go through these tools, discuss their scalability and strategies to optimize the incorporation of domain knowledge to machine learning algorithms in the era of LSST.

Based on:

https://ui.adsabs.harvard.edu/abs/2019MNRAS.489.3591P/abstract https://ui.adsabs.harvard.edu/abs/2021A%26A...650A.195I/abstract https://ui.adsabs.harvard.edu/abs/2021MNRAS.502.5147M/abstract https://ui.adsabs.harvard.edu/abs/2021arXiv211111555A/abstract https://ztf.snad.space https://github.com/light-curve/

Lightning talks / 75

SNAD miner: Finding Missed Transient Events in ZTF DR4

Auteurs: Patrick Aleo¹; Konstantin Malanchev¹; Maria Pruzhinskaya²; Emille Ishida³; Matwey Kornilov²; Vladimir Korolev⁴; Etienne Russeil³; Sreevarsha Sreejith⁵; Alina Volnova⁶; Gautham Narayan¹

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We report the automatic detection of 11 transients (7 possible supernovae and 4 active galactic nuclei candidates) within the Zwicky Transient Facility fourth data release (ZTF DR4), all of them observed in 2018 and absent from public catalogs. Among these, three were not part of the ZTF alert stream. Our transient mining strategy employs 41 physically motivated features extracted from both real light curves and four simulated light curve models (SN Ia, SN II, TDE, SLSN-I). These features are input to a k-D tree algorithm, from which we calculate the 15 nearest neighbors. After pre-processing and selection cuts, our dataset contained approximately a million objects among which we visually inspected the 105 closest neighbors from seven of our brightest, most well-sampled simulations, comprising 89 unique ZTF DR4 sources. Our result illustrates the potential of coherently incorporating domain knowledge and automatic learning algorithms, which is one of the guiding principles directing the SNAD team. It also demonstrates that the ZTF DR is a suitable testing ground for data mining algorithms aiming to prepare for the next generation of astronomical data.

Lightning talks / 76

Inferring Cosmological parameters using Normalizing Flows and Gravitational Waves (CosmoFlow)

Auteur: Federico Stachurski1

Co-auteurs: Christopher Messenger ²; Martin Hendry ²

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The idea of using Gravitational Wave (GW) detections to learn about the characteristics of our universe was first proposed by Schutz (1984), where they proposed GW signals from compact binary coalescences (CBCs) can be used to infer cosmological parameters of the universe. This is because GW signals give us information about the calibrated luminosity distance of the event without the use of the cosmological distance ladder or any prior knowledge or assumptions of the universe. To estimate the cosmological parameters, such as the Hubble constant (H_0) , we implement a machine learning approach, called Normalizing Flows (NFs), which allows for a fast computation of the posterior distributions over one or multiple cosmological parameters, conditioned on the observed GW signals detected by the LIGO/VIRGO ground based interferometric detectors. Normalizing Flows are generative models, which allow to sample from and evaluate complex probability distribution functions by learning how to map points from the complex distribution to a simple one, such as a normal distribution. In this work we present CosmoFlow, a python based code which trains a Normalizing Flow model with simulated GW events, generated with varying values of the cosmological parameters, outputting the evaluated posterior distribution over the parameters.

Cosmology / 77

Unraveling the role of cosmic velocity field in dark matter halo mass function using deep learning

Auteurs: Saba Etezad Razavi¹; Erfan Abbasgholinezhad²

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Understanding dark matter halo formation is essential for understanding the formation of galaxies to test our cosmological model.

In the last decades, there has been a continued effort to investigate large-scale structure formation using the LSS surveys and large cosmological simulations.

Despite the success of newly developed simulations to predict halo formation, they usually lack the profound insight that we could get from analytical models. On the other hand, the well-developed analytical models have failed to predict the formation of smallest and largest halos accurately. One of the crucial questions that arise in this field is what are the main features in the early universe that are essential to predict the dark matter halo formation?

We discuss an implementation of a deep learning framework to gain insight into dark matter (DM) structure formation directly from N-body relativistic simulation, gevolution.

We investigate the impact of velocity and density field information on the construction of halo mass function (HMF) through cosmological N-body simulations.

We train a Convolutional Neural Network (CNN) on the initial snapshot of an only DM simulation to predict the Halo mass that individual particles fall into at z=0, in the halo mass range of $10.5 < \log(M/M_{\odot}) < 14$. Our results show a negligible improvement from including the velocity in addition to the density information when considering simulations based on (Λ CDM) with the amplitude of initial scalar perturbations $A_s = 2 \times 10^{-9}$.

To investigate the ellipsoidal collapse models to study the effect of velocity in smaller mass ranges, we increase the initial power spectrum such that we see the effect of velocities in larger halos. The CNN model trained on the simulation snapshots with large A_s shows a considerable improvement in the HMF prediction when adding the velocity field information. Eventually, for the simulation with $A_s=8\times 10^{-8}$, the model trained with only density information shows at least 80% increase in the mean squared error relative to the model with both velocity and density information, which indicates the failure of the density-only model to predict the HMF in this case.

Our results indicate that the effect of the velocity field on the halo collapse is scale-dependent with a negligible effect for the mass scales $10.5 < \log(M/M_{\odot}) < 14$. The very same machinery can be used to investigate the effect of other phenomena such as neutrino physics on the formation of dark matter halos.

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Time Domain Astrophysics / 78

Adapting to big data: active anomaly detection on ZTF

Auteur: Maria Pruzhinskaya1

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In order to explore the potential of adaptive learning techniques to big data sets, the SNAD team used Active Anomaly Detection (AAD) as a tool to search for new supernova (SN) candidates in the photometric data from the first 9.4 months of the Zwicky Transient Facility (ZTF) survey -between 2018 March 17 and December 31 (58194 ≤ MJD ≤ 58483). We analyzed 70 ZTF fields with high galactic latitude and visually inspected 2100 outliers. As a result, 100 supernova-like objects were found, 54 of which are discovered for the first time and 46 are previously mentioned in other catalogues either as supernovae with known types or as supernova candidates. After the visual inspection of multicolour light curves of non-catalogued transients and their fit with different supernova models (Ia, Ib/c, IIP, IIL, IIn), 48 supernova, 4 AGN candidates and 2 possible novae are identified. A few of the newly discovered SNe are the good candidates to the theoretical class of the pair-instability supernovae. All transients were sent to the Transient Name Server (TNS) and received an official TNS identifier as well as an internal SNAD name. Among the known supernovae there are 14 SNe Ia, 12 possible SNe, 7 SNe II, 3 SNe Ic, 2 SNe IIP, 1 SN Ib. The remaining 7 catalogued supernovae belong to the rare supernova classes, i.e. 2 SNe IIb, 1 SN Ia Pec, 1 SN Ia-91bg, 1 SN Ic BL, 1 SN IIn, 1 SLSN-I. In this talk, I will describe how the expert knowledge is introduced into the algorithm and discuss how it can be optimized. Using as example the task of supernova search, the SNAD efforts have shown that the concept of human-machine interaction underlying the AAD is effective. The algorithm can be applied to the directed search of other type of transients. The particular transient-oriented use of the AAD do still allow to discover the anomalies, which is confirmed by the pair-instability supernova candidates found in this work.

ML Methodology / 79

Amortized variational inference for supernovae light curves

Auteur: Alexis Sánchez¹

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Markov Chain Monte Carlo (MCMC) methods are widely used for Bayesian inference in astronomy. However, when applied to data coming from next-generation telescopes, inference requires a significant amount of resources. An alternative is to use amortized variational inference, which consists of introducing a function that maps the observations to the parameters of an approximate posterior

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distribution. We evaluate this approach on a set of type Ia supernovae light curves from the Zwicky Transient Facility and show that amortization with a recurrent neural network is significantly faster than MCMC while providing competitive estimates of the predictive distribution. To the best of our knowledge, this is the first time this fast amortized framework is applied to supernova light curves. This approach will be essential when estimating the posterior of astrophysical parameters for thousands of light curves which will be observed by next-generation instruments such as the Vera Rubin Observatory.

ML Methodology / 80

Self-Supervised Machine Learning; Detecting Galaxy Tidal Features in HSC-SSP

Auteur: Alice Desmons¹

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With the advent of the Rubin Observatory's Legacy Survey of Space and Time (LSST), which will reach the petabyte data regime, it is imperative that we refine our methods of detecting and classifying images of interest within this myriad of data. In this talk I will present promising results from a Self-Supervised Machine Learning Algorithm, specifically the SimSiam Contrastive Learning model, regarding the detection of galaxies possessing low surface-brightness tidal features such as streams or shells. The algorithm has been tested on a sample of tens of thousands of galaxies drawn from the Hyper Suprime-Cam Subaru Strategic Program (HSC-SSP) Ultradeep survey. I will describe the methods involved in isolating these galaxies and how the same methods can be applied to larger future surveys such as LSST. With such automated detection, LSST offers the first opportunity to study a large, statistical sample of these important features to answer outstanding questions regarding galaxy evolution.

Lightning talks / 81

Search for ultra-fast radio bursts

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Gaussian phase noise of radio intensity time series is reduced by a factor of n when the raw voltage data are digitally filtered through n orthornormal bandpass eigen-filters, sharing the same intensity bandwidth, and the resulting intensity series are co-added. (Lieu et al. 2020) The algorithm is designed to enhance the sensitivity of detecting ultra-fast radio bursts that would otherwise be smoothed out by time averaging and too faint to be visible in a noisy unaveraged time series. We define ultra-fast to be a timescale on the order of the coherence time of the filtered radiation. We propose to use FETCH, a deep-learning based fast transient classifier, created by Agarwal et al. (2020). Here we present our progress on this front.

References Lieu, R., et al., CQG, 37, 165001, 2020

Lightning talks / 82

Deep Learning Techniques for Time Series Analysis in the context of Gravitational Waves Detection

Auteur: Vlad-Andrei Basceanu¹

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Here we present the results of our tests involving different Deep Learning (DL) algorithms in order to detect Gravitational waves (GW) in time-domain data from Massive Black Hole Binaries (MBHB) mergers. We selected three different neural networks (Shallow Multilayer Perceptron, Deep Multilayer Perceptron and a Deep Convolutional Neural Network) which are trained with simulated GW signals and noise produced in-house. The dataset consists of GW signals with the component masses ratios (q) in the range of 1-1501, GW signals injected into Gaussian Noise in the same ratio range and Gaussian Noise. The whole dataset is split into 5 classes as follows: A (q = 1-300), B (q = 301-749), C (q = 750-1200), D (q = 1201-1501) and the fifth class representing just noise (N). The results have direct implications to future ground like Einstein Telescope or space-based GW observatories such as LISA.

Cosmology - Tableau: 42 / 83

Interpreting non-Gaussian posterior distributions of cosmological parameters with normalizing flows

Auteur: Cyrille Doux1

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Modern cosmological experiments yield high-dimensional, non-Gaussian posterior distributions over cosmological parameters. These posteriors are challenging to interpret, in the sense that classical Monte-Carlo estimates of summary statistics, such as tension metrics, become numerically unstable. In this talk, I will present recent work where normalizing flows (NF) are used to obtain analytical approximations of posterior distributions, thus enabling fast and accurate computations of summary statistics as a quick post-processing step. First (arXiv:2105.03324), we develop a tension metric, the shift probability, and an estimator based of NFs, that work for non-Gaussian posteriors of both correlated and uncorrelated experiments. This allows us to test the level of agreement between two experiments such as the Dark Energy Survey (DES) and Planck using their full posteriors, but also the internal consistency of DES measurements. Second (arXiv:2112.05737), we use the NF differentiable approximation to define a local metric in parameter space. This allows us to define a covariant decomposition of the posterior, which is useful to characterize what different experiments truly measure. As an application, we estimate the Hubble constant, 🖾0, from large-scale structure data alone. These tools are available in the Python package tensiometer.

Lightning talks / 84

Background Estimation in Fermi Gamma-ray Burst Monitor lightcurves through a Neural Network

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The aim of this work is to provide a data-driven approach to estimate a background model for the Gamma-Ray Burst Monitor (GBM) of Fermi satellite. We employ a Neural Network (NN) to estimate each detector background signal given the information of the satellite: position, velocity, direction of the detectors, etc.

The estimated background can be employed into a triggering algorithm to discover significant long/weak events that are not previously detected by other approaches.

We show the potential of the model by estimating the background on GBM data for Gamma-Ray Bursts (GRBs) present in GBM cataloge, the long GRB 190320 and ultra-long GRB 091024.

The proposed approach is straightforwardly generalizable to estimate the background model of other satellites.

Cosmology / 85

Maximum-A-posteriori estimate with Deep generative NEtworks for Source Separation (MADNESS)

Auteur: Biswajit Biswas¹

Co-auteurs: Eric Aubourg ¹; Alexandre Boucaud ²; Axel GUINOT ³; Junpeng Lao ⁴; Cécile Roucelle ¹

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Next-generation of astronomical surveys such as the Large Survey of Space and Time (LSST) and Euclid will collect massive amounts of data. It will present challenges not only because of the sheer volume of data but also because of its complexity. As these surveys will detect fainter objects, the increased object density will lead to more overlapping sources. In LSST, for example, we expect around 60% of galaxies to be blended. In order to better constrain Dark Energy parameters, mapping the matter content of our Universe with weak gravitational lensing is one of the main probes for the upcoming large cosmological surveys and one of the major systematics is expected to be the blending of objects. Classical methods for solving the inverse problem of source separation, so-called "deblending", either fail to capture the diverse morphologies of galaxies or are too slow to analyze billions of galaxies. To overcome these challenges, we propose a deep learning-based approach to deal with the size and complexity of the data.

Taking forward the work on Debvader that uses a slightly modified form of Variational Autoencoders, our algorithm called MADNESS deblends galaxies from a field by finding the Maximum-A-posteriori solution parameterized by latent space representation of galaxies generated with deep generative models. We first train a VAE as a generative model and then model the underlying latent space distribution so that can it be sampled to simulate galaxies. To perform deblending, we do a gradient descent to find the MAP estimate.

In my talk, I will outline the methodology of our algorithm and evaluate its performance and compare it against state-of-the-art techniques, using flux reconstruction and runtime as metrics.

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Complete inference for binary-black hole gravitational wave data analysis

Auteur: Alex Kolmus^{None}

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When merging, two black holes spiral each other before coalescing into a bigger compact object, distorting the fabric of space-time and emitting gravitational waves. These can be detected and analyzed. Most of the analysis techniques rely on computationally-expensive Bayesian inference software. Recently, machine-learning-based techniques have emerged. These have the advantage that the computational burden is moved upstream; the model needs to be trained once in a more expensive step but is then able to produce samples very rapidly. That way, the analysis of gravitational wave data can be done faster during the observation periods. Since the detection rate increases each time the detectors are upgraded, it means that it will be more and more complicated to keep up the pace to analyze the data. Therefore, fast techniques such as machine-learning-based ones are very interesting. In addition, it is desirable to extract as much information as possible out of the observed events. This requires accounting for the lower mass binary black holes but also probing the higher-order mode content present in the signal. To analyze the entire possible spectrum of binary black hole signals and to extract as much information as possible, we present a deep-learning-based algorithm able to analyze merging compact objects down to a chirp mass of 3 solar masses. Using this method would facilitate the analysis of the increasing amount of gravitational wave events to analyze.

Uncertainties / 88

When (not) to use uncertainties for ML in particle physics

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Uncertainties / 93

Sampling high-dimensional posterior with a simulation based prior

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Time Domain Astrophysics / 95

Bayesian DL methods in extragalactic, time-domain studies

Time Domain Astrophysics / 96

Searching for changing-state AGNs in massive datasets with anomaly detection

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A Convolutional Neural Network Approach to Classifying Supernova Time-Series Photometry

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Time Domain Astrophysics / 98

SNAD: anomaly detection for large scale time-domain astronomy

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Gravitational Waves / 99

Fast Parameter Estimation for Massive Black Hole Binaries with Normalising Flows

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ML Methodology / 100

Fast Inference of Star Formation Histories of Galaxies with Spectra and Simulation-Based Inference (SBI)

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ML Methodology / 101

HARMONIC: Bayesian model comparison for simulation-based inference

Auteur: Matthew Docherty¹

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ML Methodology / 102

Amortized variational inference for supernovae light curves

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ML Methodology / 103

Self-Supervised Machine Learning; Detecting Galaxy Tidal Features in HSC-SSP

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Ethics of large scale machine learning / 105

Goodness-of-fit Evaluation: Toward Trustworthy Probabilistic Machine Learning

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ML Methodology - Tableau: 60 / 106

Enhancing gravitational-wave population inference with deep learning

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ML Methodology / 107

Scalable Bayesian Workflows in JAX

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Cosmology / 110

Artificial Intelligence: a game-changer for large scale structure cosmology

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In large scale structure cosmology, the information about the cosmological parameters governing the evolution of the universe is contained in the complex and rich structure of dark matter density field.

To date, this information was probed using simple human-designed statistics, such as the 2-pt functions, which are not guaranteed or expected to capture the full information content of the LSS maps. Recently, multiple AI-based methods have been proposed to work with this highly complex data: both for parameter inference and to aid the generation of simulations.

In this talk I will review the progress of practical appliacations of AI to the LSS inference and modelling and highlight with the focus on areas in which AI can be a "game-changer".

I will discuss the recent applications of AI to weak lensing analysis, probe combination, mass map emulators and the creation multi-field simulations.

I will present upcoming simulation sets available to the community that can be used to further advance these techniques.

Cosmology / 111

Deblending Galaxies with Generative Adversarial Networks

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Cosmology / 112

Graph-Convolutional Neural Networks for large-scale structure clustering

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Cosmology / 113

COSMOPOWER: Deep Learning - accelerated Bayesian inference from next-generation cosmological surveys

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Cosmology / 114

The Extended LSST Astronomical Time Series Classification Challenge (ELAsTiCC)

Cosmology / 115

Maximum-A-posteriori estimate with Deep generative NEtworks for Source Separation (MADNESS)

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Cosmology / 116

Interpreting non-Gaussian posterior distributions of cosmological parameters with normalizing flows

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Ethics of large scale machine learning / 117

Keynote

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Gravitational Waves / 118

Simulation-based inference for gravitational waves

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Lightning talks / 121

Bayesian planetary numerical ephemerides B-INPOP with MCMC

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Lightning talks / 122

A Bayesian Convolutional Neural Network for Robust Galaxy Ellipticity Regression

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Lightning talks / 123

There's no difference: Convolutional Neural Networks for transient detection without template subtraction

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Improvement of the statistical model of a photoz bayesian estimator hybridizing a SED template fitting and a gaussian process

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Lightning talks / 125

Attention-based modeling of AGN light curves

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Lightning talks / 126

SNAD miner: Finding Missed Transient Events in ZTF DR4

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Lightning talks / 127

Applying Likelihood-Free Inference to LISA parameter estimation: a project

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Inferring Cosmological parameters using Normalizing Flows and Gravitational Waves (CosmoFlow)

Auteur correspondant f.stachurski.1@research.gla.ac.uk

Cosmology / 129

Unraveling the role of cosmic velocity field in dark matter halo mass function using deep learning

Auteur: Saba Etezad Razavi¹

Co-auteur: Erfan Abbasgholinezhad ²

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Time Domain Astrophysics / 130

¹ Sharif University of Technology

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Adapting to big data: active anomaly detection on ZTF

Lightning talks / 131

Search for ultra-fast radio bursts

Auteur correspondant klackeos@mpifr-bonn.mpg.de

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Deep Learning Techniques for Time Series Analysis in the context of Gravitational Waves Detection

Auteur correspondant vabasceanu@spacescience.ro

Cosmology / 133

Galaxies and Halos on Graph Neural Networks: Deep Generative Modeling Scalar and Vector Quantities for Intrinsic Alignment

Auteur correspondant yjagvara@andrew.cmu.edu

ML Methodology / 134

Neural Posterior Estimation with Differentiable Simulators

Auteur correspondant zeghal@apc.in2p3.fr

Cosmology / 135

Hybrid Physical-Neural ODEs for fast differentiable N-body Simulations

Auteur correspondant denise.lanzieri@cea.fr

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ML inference & uncertainties

Chair: François Lanusse - AIM/CEA/CNRS/Paris-Saclay University/Paris Cite University

Panel:

Yvonne Becherini - Université de Paris, APC, diiP Emille Ishida - CNRS/LPC-Clermont Colin Carroll - Google Benjamin Wandelt - Institut d'Astrophysique de Paris

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ML in the next decades

Jean-Gabriel Ganascia - Sorbonne Université Laurent Daudet - LightOn Anja Butter - IPT Heidelberg

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Introduction to Bayesian Modeling

Tutorials / 139

Bayesian Time Series Analysis with TFP on JAX

Tutorials / 140

Probabilistic Deep Learning with TFP and JAX/Flax

Auteur correspondant francois.lanusse@cea.fr

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Likelihood-Free Inference and Application to Cosmology

Auteur correspondant wandelt@iap.fr

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Breakout session over lunch