

PHYSTAT - Statistics meets ML



Report of Contributions

Contribution ID: 1

Type: **Poster**

Uncertainty-aware machine learning for the LHC

Estimating uncertainties is a fundamental aspect in every physics problem, no measurements or calculations comes without uncertainties. Hence it is crucial to consider the effect of training a neural network to problems in physics. I will present our work on amplitude regression, using loop amplitudes from LHC processes, as an example to examine the impact of different uncertainties on the outcome of the network. We test the behavior of different neural networks with uncertainty estimation, including Bayesian neural networks and repulsive ensembles.

Primary Field of Research

Particle Physics

Primary authors: FAVARO, Luigi; ELMER, Nina; PLEHN, Tilman

Presenter: ELMER, Nina

Contribution ID: 2

Type: **Poster**

Generative models: their evaluation and their limitations

I will present and discuss several proposed metrics, based on integral probability measures, for the evaluation of generative models (and, more generally, for the comparison of different generators). Some of the metrics are particularly efficient to be computed in parallel, and show good performances. I will first compare the metrics on toy multivariate/multimodal distributions, and then focus on HEP examples from the JetNet jet dataset. I will discuss the power of the tests and their implementation in TensorFlow2, taking the opportunity to discuss, more generally, the limitations in the usage of generative models in HEP.

To be presented by Samuele Grossi

Primary Field of Research

Particle Physics

Primary authors: TORRE, Riccardo (INFN e Universita Genova (IT)); Dr GROSSI, Samuele (University of Genova)

Presenter: TORRE, Riccardo (INFN e Universita Genova (IT))

Contribution ID: 3

Type: **Poster**

Limits to classification performance by relating Kullback-Leibler divergence to Cohen's Kappa

The performance of machine learning classification algorithms are evaluated by estimating metrics, often from the confusion matrix, using training data and cross-validation. However, these do not prove that the best possible performance has been achieved. Fundamental limits to error rates can be estimated using information distance measures. To this end, the confusion matrix has been formulated to comply with the Chernoff-Stein Lemma. This links the error rates to the Kullback-Leibler divergences between the probability density functions describing the two classes. This leads to a key result that relates Cohen's Kappa to the Resistor Average Distance which is the parallel resistor combination of the two Kullback-Leibler divergences. The Resistor Average Distance has units of bits and is estimated from the same training data used by the classification algorithm, using kNN estimates of the Kullback-Leibler divergences. The classification algorithm gives the confusion matrix and Kappa. Theory and methods are discussed in detail and then applied to Monte Carlo data and real datasets. Four very different real datasets - Breast Cancer, Coronary Heart Disease, Bankruptcy, and Particle Identification - are analysed, with both continuous and discrete values, and their classification performance compared to the expected theoretical limit. In all cases this analysis shows that the algorithms could not have performed any better due to the underlying probability density functions for the two classes. Important lessons are learnt on how to predict the performance of algorithms for imbalanced data. Preprint available at arXiv:2403.01571.

Primary Field of Research

Particle Physics

Primary authors: Dr CROW, Lisa; Prof. WATTS, Stephen (University of Manchester)

Presenter: Prof. WATTS, Stephen (University of Manchester)

Contribution ID: 4

Type: **Poster**

Precision-Machine Learning for the Matrix Element Method

The matrix element method is the LHC inference method of choice for limited statistics, as it allows for optimal use of available information. We present a dedicated machine learning framework, based on efficient phase-space integration, a learned acceptance and transfer function. It is based on a choice of INN and diffusion networks, and a transformer to solve jet combinatorics. We showcase this setup for the CP-phase of the top Yukawa coupling in associated Higgs and single-top production.

Primary Field of Research

Particle Physics

Primary authors: BUTTER, Anja (Centre National de la Recherche Scientifique (FR)); HUETSCH, Nathan (Heidelberg University, ITP Heidelberg); WINTERHALDER, Ramon (UCLouvain); HEIMEL, Theo (Heidelberg University); PLEHN, Tilman (Heidelberg University)

Presenter: HUETSCH, Nathan (Heidelberg University, ITP Heidelberg)

Contribution ID: 5

Type: **Contributed Talk**

Lorentz-Equivariant Geometric Algebra Transformers for High-Energy Physics

Extracting scientific understanding from particle-physics experiments requires solving diverse learning problems with high precision and good data efficiency. We propose the Lorentz Geometric Algebra Transformer (L-GATr), a new multi-purpose architecture for high-energy physics. L-GATr represents high-energy data in a geometric algebra over four-dimensional space-time and is equivariant under Lorentz transformations, the symmetry group of relativistic kinematics. At the same time, the architecture is a Transformer, which makes it versatile and scalable to large systems. L-GATr is first demonstrated on regression and classification tasks from particle physics. We then construct the first Lorentz-equivariant generative model: a continuous normalizing flow based on an L-GATr network, trained with Riemannian flow matching. Across our experiments, L-GATr is on par with or outperforms strong domain-specific baselines.

Primary Field of Research

Machine Learning

Primary authors: SPINNER, Jonas; BRESÓ PLA, Víctor (University of Heidelberg)

Co-authors: THALER, Jesse (MIT); BREHMER, Johann (CERN); DE HAAN, Pim; PLEHN, Tilman

Presenter: SPINNER, Jonas

Contribution ID: 6

Type: **Poster**

Graph neural networks on the test bench in HEP applications

Data analyses in the high-energy particle physics (HEP) community more and more often exploit advanced multivariate methods to separate signal from background processes. In this talk, a maximally unbiased, in-depth comparison of the graph neural network (GNN) architecture, which is of increasing popularity in the HEP community, with the already well-established technology of fully connected feed-forward deep neural networks (DNNs) is presented. When it comes to choosing a suitable machine-learning model, it is not a priori clear, what model this should be to benefit from inherent properties of the task. Also, the design of a fair and unbiased benchmark is non-trivial. This GNN vs. DNN comparison is insightful in terms of the details it reveals as to which aspects of GNNs are superior to DNNs - and which are not. The study is performed on a typical data set of a complex challenge recently faced at the Large Hadron Collider: the classification of events with top quark-antiquark pairs with additional heavy flavour jets originating from gluon splittings, Z or Higgs bosons.

The study is documented in the paper “A Case Study of Sending Graph Neural Networks Back to the Test Bench for Applications in High-Energy Particle Physics” published in *Computing and Software for Big Science*, <https://doi.org/10.1007/s41781-024-00122-3>.

Primary Field of Research

Machine Learning

Primary author: PFEFFER, Emanuel Lorenz (KIT - Karlsruhe Institute of Technology (DE))

Presenter: PFEFFER, Emanuel Lorenz (KIT - Karlsruhe Institute of Technology (DE))

Contribution ID: 7

Type: **not specified**

Intro to statistics (Speaker TBC)

Session Classification: Talks

Contribution ID: 8

Type: **not specified**

Intro to ML (Speaker TBC)

Session Classification: Talks

Contribution ID: 9

Type: **not specified**

Astro/Cosmology for others

Presenter: MAKINEN, Lucas (Imperial College London)

Session Classification: Talks

Contribution ID: **10**

Type: **not specified**

ML in Astro/Cosmology (speaker TBC)

Session Classification: Talks

Contribution ID: 11

Type: **not specified**

Particle physics for others

Presenter: WINTERBOTTOM, Daniel (Imperial College (GB))

Session Classification: Talks

Contribution ID: 12

Type: **not specified**

ML in Particle Physics

Presenter: LANGFORD, Jonathon Mark (Imperial College (GB))

Session Classification: Talks

Contribution ID: 13

Type: **not specified**

Welcome

Tuesday 10 September 2024 09:00 (15 minutes)

Session Classification: Talks

Contribution ID: 14

Type: **not specified**

ML in Particle Physics

Tuesday 10 September 2024 09:15 (45 minutes)

Machine learning and AI have quickly turned into indispensable tools for modern particle physics. They both greatly amplify the power of existing techniques - such as supercharging supervised classification - and enable qualitatively new ways of extracting information - such as anomaly detection and likelihood-free inference. Accordingly, the underlying statistical machinery needs to be understood in greater detail or in some cases newly developed.

After briefly introducing the environment of collider based particle physics, this talk will review key developments in machine learning applied to data analysis with a special eye on statistical challenges.

Primary Field of Research

Presenter: KASIECZKA, Gregor (Hamburg University (DE))

Session Classification: Talks

Contribution ID: 15

Type: **not specified**

Cosmology and machine learning

Tuesday 10 September 2024 11:00 (45 minutes)

Cosmologists strive to uncover the mysteries of the origin, composition, evolution, and fate of the cosmos from all the information the sky has to offer: the cosmic microwave background, galaxy surveys, exploding stars, and reverberations of space-time caused by colliding black holes and neutron stars. I will discuss new ways to connect cosmological theory and simulation with these data sets. Novel cosmological tests promise insights to classical cosmological questions; and Artificial Intelligence (AI) and Machine Learning are revolutionizing our ability to confront computational models with data, enabling end-to-end, quantitative Bayesian reasoning for problems that were previously deemed intractable. Very recently, AI has even begun to inspire novel cosmological insights. I will discuss the current status, promises, and challenges and outline a path towards achieving the goals of reconstructing the detailed initial conditions of the universe at its cosmic beginning and understanding the formation of cosmic structures much more completely than ever before.

Primary Field of Research

Presenter: WANDEL, Ben**Session Classification:** Talks

Contribution ID: 16

Type: **not specified**

Simulation-based machine learning for gravitational-wave analysis

Tuesday 10 September 2024 11:45 (45 minutes)

Gravitational waves (GWs) provide a unique window to the universe, enabling us to study mergers of black holes and/or neutron stars. In my talk, I will highlight how machine learning can address critical limitations in GW data analysis. I will present key innovations in this field, driven by unusually high requirements for accuracy, reliability and interpretability. Finally, I will discuss how insights gained from GW science transfer to other application domains of machine learning.

Primary Field of Research

Presenter: DAX, Maximilian

Session Classification: Talks

Contribution ID: 17

Type: **not specified**

[Contributed talk]

Session Classification: Talks

Contribution ID: 18

Type: **not specified**

Interpretable Machine Learning for Particle Physics

Tuesday 10 September 2024 14:00 (45 minutes)

The term “interpretability” encompasses various strategies to scrutinize the decisions made by machine learning algorithms. In this talk, I argue that interpretability, at least in the context of particle physics, should be considered as part of the broader goal of assessing systematic uncertainties. I provide examples from my own research on jet physics at the Large Hadron Collider, where some of the goals of interpretability can be achieved through modified machine learning architectures and training paradigms. I also comment on the growing interest in foundation models, which are forcing us to rethink how we specify machine learning tasks and whether there can be statistical gains from incorporating auxiliary information.

Primary Field of Research

Presenter: THALER, Jesse (MIT/IAIFI)

Session Classification: Talks

Contribution ID: 19

Type: **not specified**

Understanding and mitigating failures in anomaly detection: a probabilistic perspective

Tuesday 10 September 2024 14:45 (45 minutes)

In this talk, we present an overview of anomaly detection from a probabilistic machine learning perspective, with a focus on work emerging from the machine learning literature. First, we discuss empirical failures of deep generative models for anomaly detection and why they occur, as well as their implications for deep generative modeling and anomaly detection. Then, we discuss the endeavor of robust anomaly detection and what is required to achieve it. We conclude with recent work that applies these insights to jet anomaly detection in high-energy physics.

Primary Field of Research

Presenter: ZHANG, Lily

Session Classification: Talks

Contribution ID: 20

Type: **not specified**

Anomalies

Primary Field of Research

Presenter: ZHANG, Lily

Session Classification: Talks

Contribution ID: 21

Type: **not specified**

Statistical tests for anomaly detection at the LHC

Tuesday 10 September 2024 16:00 (45 minutes)

Signal-agnostic data exploration could unveil very subtle statistical deviations of collider data from the expected Standard Model of particle physics. However, the extreme size, rate and complexity of the datasets generated at the Large Hadron Collider (LHC) pose unique challenges for data analysis. Making assumptions about what is relevant becomes unavoidable to scale the information down to a human readable level.

Machine learning can be exploited at multiple stages in the experimental pipeline to reduce these assumptions, trading assumed knowledge for a richer basis of acquired experimental evidence. In this talk I will discuss the main challenges behind the design of efficient, robust and at the same time interpretable statistical tests for anomaly detection at the LHC, such as model selection, uncertainty quantification and scalability. I will present recent solutions and future prospects based on existing literature, and examples from my own research on the Neyman-Pearson strategy for signal-agnostic likelihood-ratio-test.

Primary Field of Research

Presenter: GROSSO, Gaia

Session Classification: Talks

Contribution ID: 22

Type: **not specified**

Detecting New Physics as data anomalies at the LHC: Transitioning from small-scale toy datasets to millions of complex proton collisions

Tuesday 10 September 2024 16:45 (25 minutes)

Anomaly detection has emerged as a promising technique for identifying subtle New Physics signals amidst a dominant Standard Model background. Due to the novelty of these techniques, they are often proposed and demonstrated on toy datasets that mimic real LHC data before being deployed in actual experiments. In this talk, we will discuss the challenges encountered during the transition from research and development to practical implementation in experiments, highlighting lessons learned and future prospects. Various techniques will be compared, including outlier detection versus over-density detection, along with different levels of supervision, ranging from weakly supervised to semi-supervised and unsupervised methods. We will address the statistical challenges involved in applying these methods for data analysis and ultra-fast event filtering in the CMS Experiment at CERN. The discussion will focus on the robustness of these methods and the challenges associated with validating them.

Presenter: AARRESTAD, Thea (ETH Zurich (CH))

Session Classification: Talks

Contribution ID: 23

Type: **not specified**

Theoretical and Societal Topics in AI and Deep Learning for Physicists

Wednesday 11 September 2024 09:00 (45 minutes)

I plan to touch on several theoretical topics (overparameterization, neural balance, attention and transformers) and their applications in physics and end on a proposal to solve some of the societal issues raised by AI inspired by physics.

Primary Field of Research

Presenter: BALDI, Pierre

Session Classification: Talks

Contribution ID: 24

Type: **not specified**

AI Benchmarks and Science

Wednesday 11 September 2024 09:45 (25 minutes)

Primary Field of Research

Presenter: THIYAGALINGAM, Jeyan (Rutherford Appleton Laboratory, Science and Technology Facilities Council)

Session Classification: Talks

Contribution ID: 25

Type: **not specified**

Simulation-based Inference (SBI)

Wednesday 11 September 2024 11:00 (45 minutes)

A powerful class of statistical inference methods are starting to be used in across fields that leverage the power of machine learning (ML) to perform inference directly from high-dimensional data. They can be used, for instance, to estimate fundamental physics parameters from data collected in high energy physics experiments, or cosmological / astrophysics observations and work with both Bayesian and frequentist settings. In these application cases, the exact likelihood itself is typically intractable, but it can be sampled from using sophisticated forward simulation software. ML models can then learn to estimate statistical quantities such as posteriors, likelihoods or likelihood ratios from simulated samples and also exploit additional knowledge available at intermediate steps of the simulation, which are inaccessible in real data. This talk will focus on important statistical questions with regard to the application of SBI, with a bias towards frequentist statistical framework typically used in high-energy physics.

Primary Field of Research

Presenter: GHOSH, Aishik (University of California Irvine (US))

Session Classification: Talks

Contribution ID: 26

Type: **not specified**

[Contributed talk]

Session Classification: Talks

Contribution ID: 27

Type: **not specified**

[Contributed talk]

Session Classification: Talks

Contribution ID: 28

Type: **not specified**

[Contributed talk]

Session Classification: Talks

Contribution ID: 29

Type: **Contributed Talk**

lsbi: linear simulation based inference

Wednesday 11 September 2024 14:25 (25 minutes)

Simulation-based inference is undergoing a renaissance in statistics and machine learning. With several packages implementing the state-of-the-art in expressive AI [mackelab/sbi] [undark-lab/swyft], it is now being effectively applied to a wide range of problems in the physical sciences, biology, and beyond.

Given the rapid pace of AI/ML, there is little expectation that the implementations of the future will resemble these current first generation neural network-based approaches. This talk will present a new framework for simulation-based inference, linear simulation-based inference (lsbi), which abstracts the core principles of SBI from the specific details of machine learning, implementing a plug-and-play framework of linear and mixture models. lsbi has several use-cases:

1. It is pedagogically helpful to separate out the general principles of SBI from the specific details of neural networks (particularly for ML skeptics).
2. It is practically useful for producing expressive examples with known ground truths.
3. It is pragmatically useful, since in many cases, lsbi is competitive with neural approaches in terms of accuracy, whilst being faster and more interpretable.

An evolving code-driven PyPI/conda research package is available at: <https://github.com/handleylab/lsbi>

Primary Field of Research

Presenter: Dr HANDLEY, William

Session Classification: Talks

Contribution ID: 30

Type: **Contributed Talk**

Fairness Methods in Particle Physics Event Classification

In social sciences, fairness in Machine Learning (ML) comprises the attempt to correct or eliminate algorithmic bias of gender, ethnicity, or sexual orientation from ML models. Many high-energy physics (HEP) analyses that search for a resonant decay of a particle employ mass-decorrelated event classifiers, as the particle mass is often used to perform the final signal extraction fit. These classifiers are designed to maintain fairness with respect to the mass, which is accomplished primarily by retaining mass-correlated information during training.

Our studies present a first proof-of-concept for systematically applying, testing and comparing fairness methods for ML-based event classifiers in HEP analyses. We explore techniques that mitigate mass correlation during and after training. Through simulations and a case studies, we demonstrate the effectiveness of these methods in maintaining fairness while preserving the classifier performance.

Presenter: RIEGER, Oliver (Nikhef National institute for subatomic physics (NL))

Session Classification: Talks

Contribution ID: 31

Type: **not specified**

Robust signal detection with classifiers decorrelated via optimal transport

Wednesday 11 September 2024 14:50 (25 minutes)

New physics searches are usually done by training a supervised classifier to separate a signal model from the known Standard Model physics (also called the background model). However, even when the signal model is correct, systematic errors in the background model can influence supervised classifiers and might adversely affect the signal detection procedure. To tackle this problem, one approach is to use the (possibly misspecified) classifier only to perform a signal-enrichment step and then to carry out a model-agnostic search in the signal-rich region using only the real experimental data. For this procedure to work, we need a classifier constrained to be decorrelated with one or more protected variables used for the signal detection step. We do this by considering an optimal transport map of the classifier output that makes it independent of the protected variable(s) for the background. We then fit a semi-parametric mixture model to the distribution of the protected variable after making cuts on the transformed classifier to detect the presence of a signal. We compare and contrast this decorrelation method with previous approaches, show that the decorrelation procedure is robust to background misspecification, and analyse the power of the signal detection test.

Primary Field of Research

Presenter: Dr CHAKRAVARTI, Purvasha (UCL)

Session Classification: Talks

Contribution ID: 32

Type: **Contributed Talk**

Feldman-Cousins' ML Cousin

The statistical treatment of sterile neutrino searches suffers from the fact that Wilks' theorem, a beneficial simplifying assumption, does not hold across all regions of parameter space. The alternative, the Feldman-Cousins algorithm, suffers from expensive computational runtimes that prohibit its application into many-experiment global fits. This contribution introduces a deep learning-based method (which does not assume Wilks' theorem) that can fit electron (anti)neutrino disappearance experiments in a tractable amount of time. Though this procedure's utility for sterile neutrino searches are presented here, it will be useful for a variety of particle physics analyses.

Primary Field of Research

Presenter: VILLARREAL, Josh

Session Classification: Talks

Contribution ID: 33

Type: **not specified**

Systematics: Misery or Muse?

Wednesday 11 September 2024 16:55 (45 minutes)

Systematic uncertainties usually have a negative connotation since they reduce the sensitivity of an experiment. However, the practical and conceptual challenges posed by various types of systematic uncertainty also have a long track record of motivating new ideas. I will outline some examples for my own career where systematics were my muse for innovation.

Primary Field of Research

Presenter: CRANMER, Kyle Stuart (University of Wisconsin Madison (US))

Session Classification: Talks

Contribution ID: 34

Type: **not specified**

Model misspecification meets ML: a HEP perspective

Thursday 12 September 2024 09:00 (45 minutes)

The field of high energy physics (HEP) benefits immensely from sophisticated simulators and data-driven techniques to perform measurements of nature at increasingly higher precision. Using the example of HEP, I will describe how and where uncertainties are incorporated into data analysis to address model misspecification concerns. My focus will be how machine learning (ML), in the variety of ways it is employed in practice, affects considerations around mis-modeling.

Primary Field of Research

Presenter: HELD, Alexander (University of Wisconsin Madison (US))

Session Classification: Talks

Contribution ID: 35

Type: **Contributed Talk**

Learned harmonic mean estimation of the Bayesian evidence with normalizing flows

Thursday 12 September 2024 09:45 (30 minutes)

Computing the Bayesian evidence is an important task in Bayesian model selection, providing a principled quantitative way to compare models. In this work, we introduce normalizing flows to improve the learned harmonic mean estimator of the Bayesian evidence. This recently presented estimator leverages machine learning to address the exploding variance problem associated with the original harmonic mean. The improved method provides an accurate, robust and scalable estimator of the Bayesian evidence. Moreover, it is agnostic to the sampling strategy, meaning it can be combined with various efficient MCMC sampling techniques or variational inference approaches. We present numerical experiments demonstrating the effectiveness of the use of normalizing flows for the learned harmonic mean. We also apply the method to practical cosmological examples, including a 37-dimensional cosmic shear analysis using CosmoPower-JAX, a JAX-based implementation of the CosmoPower framework that accelerates cosmological inference by building differentiable neural emulators of cosmological power spectra, observing significant speed-up compared to the conventional method. We also successfully perform a 3x2pt analysis in a 157-dimensional setting, where using conventional methods is not feasible. This shows that the scalability CosmoPower-JAX and the learned harmonic mean estimator offer could allow for the comparison between models of unprecedented complexity, thus unlocking the full potential of Bayesian analysis even in high-dimensional settings.

Presenter: POLANSKA, Alicja (University College London)

Session Classification: Talks

Contribution ID: 36

Type: **not specified**

pop-cosmos: investigating the explainability of a high-dimensional, data-driven generative model in cosmology

Thursday 12 September 2024 11:15 (30 minutes)

I will present a perspective that explainability —model interrogation and validation rooted in domain knowledge—is a more important desideratum in fundamental science than interpretability in its strict meaning. In order to illustrate this point, I will draw on our recent work on pop-cosmos: a forward modelling framework for photometric galaxy survey data, where galaxies are modelled as draws from a population prior distribution over redshift, mass, dust properties, metallicity, and star formation history. After showing how the model is composed in terms of a diffusion model population prior and calibrated using simulation-based optimal-transport optimisation, I will discuss how to view this type of approach from a hierarchical Bayesian perspective. I will showcase the parallels between validating this type of model and standard practices in validating any complex physics-based parametric model in the field.

Primary Field of Research

Presenter: PEIRIS, Hiranya

Session Classification: Talks

Contribution ID: 37

Type: **not specified**

Identifying Tau Neutrinos in IceCube

Thursday 12 September 2024 11:45 (25 minutes)

Astrophysical tau neutrinos were predicted for a long time, but only recently has IceCube been able to identify those at the 5 sigma significance level. The key to this discovery was using machine learning methods to analyse the data. In this talk, I will first give a brief overview of the analysis and results before we dive deeper into the neural nets. We will try to understand how they work and discuss what surprising things we learned.

Primary Field of Research

Presenter: ELLER, Philipp (Wisconsin)

Session Classification: Talks

Contribution ID: 38

Type: **not specified**

Conditional generation

Thursday 12 September 2024 12:10 (25 minutes)

“If you can simulate it, you can learn it.” The concept of conditional generation is powerful and versatile. The heavy lifting is distributed over a generator of a latent distribution of interest and an embedding network to encode the information contained in the data. Concrete applications to the reconstruction of neutrino kinematics in LHC collisions and associated interpretability questions will be presented.

Primary Field of Research

Presenter: GOLLING, Tobias (Universite de Geneve (CH))

Session Classification: Talks

Contribution ID: 39

Type: **not specified**

Interpretability in Semi-Supervised Classifier Tests for Model-Independent Searches of New Physics

Thursday 12 September 2024 10:45 (30 minutes)

Many model-independent search methods can be understood as performing a high-dimensional two-sample test. The test is typically performed by training a neural network over the high-dimensional feature space. If the test indicates a significant deviation from the background, it would be desirable to be able to characterize the “signal” the network may have found. In this talk, I will describe our work on interpreting semi-supervised classifier tests using active subspaces to understand the properties of the detected signal. Additionally, I will show how to extract the signal strength parameter from the trained classifier.

Primary Field of Research

Presenter: KUUSELA, Mikael (Carnegie Mellon University (US))

Session Classification: Talks

Contribution ID: 40

Type: **not specified**

Highlights, Statistics

Thursday 12 September 2024 14:45 (45 minutes)

Primary Field of Research

Presenter: KUUSELA, Mikael (Carnegie Mellon University (US))

Session Classification: Talks

Contribution ID: 41

Type: **not specified**

Highlights, ML

Thursday 12 September 2024 14:00 (45 minutes)

Primary Field of Research

Presenters: LOUPPE, Gilles; LOUPPE, Gilles

Session Classification: Talks

Contribution ID: 42

Type: **not specified**

Highlights, Astro/Cosmo

Thursday 12 September 2024 16:00 (45 minutes)

Primary Field of Research

Presenter: LUCIE-SMITH, Luisa

Session Classification: Talks

Contribution ID: 43

Type: **not specified**

Highlights, Particle Physics

Thursday 12 September 2024 16:45 (45 minutes)

Primary Field of Research

Presenter: HEINRICH, Lukas Alexander (Technische Universitat Munchen (DE))

Session Classification: Talks

Contribution ID: 44

Type: **not specified**

Closing discussion

Thursday 12 September 2024 17:30 (15 minutes)

Session Classification: Talks

Contribution ID: 45

Type: **not specified**

Astro/Cosmology for others

Monday 9 September 2024 14:00 (25 minutes)

Presenter: TSAPRAZI, Eleni

Session Classification: Introductory talks. These optional talks are aimed at people who feel that they would like more background introductory material, before the next 3 days' talks.

Contribution ID: 46

Type: **not specified**

Particle Physics for others

Monday 9 September 2024 14:25 (35 minutes)

Presenter: WINTERBOTTOM, Daniel (Imperial College (GB))

Session Classification: Introductory talks. These optional talks are aimed at people who feel that they would like more background introductory material, before the next 3 days' talks.

Contribution ID: 47

Type: **not specified**

Introduction to Machine Learning

Monday 9 September 2024 15:00 (45 minutes)

Primary Field of Research

Presenter: MAKINEN, Lucas (Imperial College London)

Session Classification: Introductory talks. These optional talks are aimed at people who feel that they would like more background introductory material, before the next 3 days' talks.

Contribution ID: 48

Type: **not specified**

Types of ML in Astro/Cosmology

Monday 9 September 2024 16:15 (40 minutes)

Presenter: Dr JEFFREY, Niall (University College London)

Session Classification: Introductory talks. These optional talks are aimed at people who feel that they would like more background introductory material, before the next 3 days' talks.

Contribution ID: 49

Type: **not specified**

Particle Physics for others

Presenter: WINTERBOTTOM, Daniel (Imperial College (GB))

Session Classification: Introductory talks. These optional talks are aimed at people who feel that they would like more background introductory material, before the next 3 days' talks.

Contribution ID: 50

Type: **not specified**

Types of ML in Particle Physics

Monday 9 September 2024 16:55 (40 minutes)

Presenter: LANGFORD, Jonathon Mark (Imperial College (GB))

Session Classification: Introductory talks. These optional talks are aimed at people who feel that they would like more background introductory material, before the next 3 days' talks.

Contribution ID: 51

Type: **Contributed Talk**

Feldman-Cousins' ML Cousin

The statistical treatment of sterile neutrino searches suffers from the fact that Wilks' theorem, a beneficial simplifying assumption, does not hold across all regions of parameter space. The alternative, the Feldman-Cousins algorithm, suffers from expensive computational runtimes that prohibit its application into many-experiment global fits. This contribution introduces a deep learning-based method (which does not assume Wilks' theorem) that can fit electron (anti)neutrino disappearance experiments in a tractable amount of time. Though this procedure's utility for sterile neutrino searches are presented here, it will be useful for a variety of particle physics analyses.

Primary Field of Research

Particle Physics

Primary author: VILLARREAL, Josh**Presenter:** VILLARREAL, Josh

Contribution ID: 52

Type: **Poster**

The Landscape of Unfolding with Machine Learning

Recent innovations from machine learning allow for data unfolding, without binning and including correlations across many dimensions. We describe a set of known, upgraded, and new methods for ML-based unfolding. The performance of these approaches are evaluated on the same two datasets. We find that all techniques are capable of accurately reproducing the particle-level spectra across complex observables. Given that these approaches are conceptually diverse, they offer an exciting toolkit for a new class of measurements that can probe the Standard Model with an unprecedented level of detail and may enable sensitivity to new phenomena.

Primary Field of Research

Particle Physics

Primary authors: HUETSCH, Nathan (Heidelberg University, ITP Heidelberg); MARIÑO VILLADAMIGO, Javier (Institut für Theoretische Physik - University of Heidelberg); SHMAKOV, Alexander (University of California Irvine (US))

Co-authors: DIEFENBACHER, Sascha (Lawrence Berkeley National Lab. (US)); MIKUNI, Vinicius Massami (Lawrence Berkeley National Lab. (US)); HEIMEL, Theo (Heidelberg University); FENTON, Michael James (University of California Irvine (US)); GREIF, Kevin Thomas (University of California Irvine (US)); NACHMAN, Ben (Lawrence Berkeley National Lab. (US)); WHITESON, Daniel (University of California Irvine (US)); BUTTER, Anja (Centre National de la Recherche Scientifique (FR)); PLEHN, Tilman

Presenter: MARIÑO VILLADAMIGO, Javier (Institut für Theoretische Physik - University of Heidelberg)

Contribution ID: 53

Type: **Contributed Talk**

Learned harmonic mean estimation of the Bayesian evidence with normalizing flows

Computing the Bayesian evidence is an important task in Bayesian model selection, providing a principled quantitative way to compare models. In this work, we introduce normalizing flows to improve the learned harmonic mean estimator of the Bayesian evidence. This recently presented estimator leverages machine learning to address the exploding variance problem associated with the original harmonic mean. The improved method provides an accurate, robust and scalable estimator of the Bayesian evidence. Moreover, it is agnostic to the sampling strategy, meaning it can be combined with various efficient MCMC sampling techniques or variational inference approaches. We present numerical experiments demonstrating the effectiveness of the use of normalizing flows for the learned harmonic mean. We also apply the method to practical cosmological examples, including a 37-dimensional cosmic shear analysis using CosmoPower-JAX, a JAX-based implementation of the CosmoPower framework that accelerates cosmological inference by building differentiable neural emulators of cosmological power spectra, observing significant speed-up compared to the conventional method. We also successfully perform a 3x2pt analysis in a 157-dimensional setting, where using conventional methods is not feasible. This shows that the scalability CosmoPower-JAX and the learned harmonic mean estimator offer could allow for the comparison between models of unprecedented complexity, thus unlocking the full potential of Bayesian analysis even in high-dimensional settings.

Primary Field of Research

Astro/Cosmo

Primary authors: Dr SPURIO MANCINI, Alessio (Department of Physics, Royal Holloway, University of London); POLANSKA, Alicja (Mullard Space Science Laboratory, University College London); Dr PIRAS, Davide (Centre Universitaire d'Informatique, Universite de Geneve); MCEWEN, Jason (Mullard Space Science Laboratory, University College London); Dr PRICE, Matthew (Mullard Space Science Laboratory, University College London)

Presenter: POLANSKA, Alicja (Mullard Space Science Laboratory, University College London)

Contribution ID: 54

Type: **Contributed Talk**

Development of systematic-aware neural network trainings for binned-likelihood-analyses at the LHC

We demonstrate a neural network training, capable of accounting for the effects of systematic variations of the utilized data model in the training process and describe its extension towards neural network multiclass classification. We show the importance of adjusting backpropagation to be able to handle derivatives of histogram bins during training and add an interpretation of the optimization process itself, highlighting the differences between the systematic aware and conventional training strategies. Trainings for binary and multiclass classification with seven output classes are performed, based on a comprehensive data model with 86 nontrivial shape-altering systematic variations, as used for a previous measurement. The neural network output functions are used to infer the signal strengths for inclusive Higgs boson production, as well as for Higgs boson production via gluon-fusion (r_{ggH}) and vector boson fusion (r_{qqH}). With respect to a conventional training, based on cross-entropy, we observe improvements of 12 and 16 %, for the sensitivity in r_{ggH} and r_{qqH} , respectively.

Primary Field of Research

Machine Learning

Primary authors: MONSCH, Artur (KIT - Karlsruhe Institute of Technology (DE)); KLUTE, Markus (Karlsruhe Inst. of Technology (GER)); SOWA, Lars (KIT - Karlsruhe Institute of Technology (DE)); WOLF, Roger (KIT - Karlsruhe Institute of Technology (DE))

Presenter: MONSCH, Artur (KIT - Karlsruhe Institute of Technology (DE))

Contribution ID: 55

Type: **Poster**

Interpolated Likelihoods for Fast Reinterpretations

We present a method to accelerate Effective Field Theory reinterpretations using interpolated likelihoods. By employing Radial Basis Functions for interpolation and Gaussian Processes to strategically select interpolation points, we show that we can reduce the computational burden while maintaining accuracy. We apply this in the context of the Combined Higgs Boson measurement at CMS, a complex statistical model with many thousands of parameters requiring large computing power to evaluate.

Primary Field of Research

Particle Physics

Primary author: RUNTING, Tom (Imperial College (GB))

Presenter: RUNTING, Tom (Imperial College (GB))

Contribution ID: 56

Type: **Poster**

How to Unfold Top Decays

Many physics analyses at the LHC rely on algorithms to remove detector effect, commonly known as unfolding. Whereas classical methods only work with binned, one-dimensional data, Machine Learning promises to overcome both problems. Using a generative unfolding pipeline, we show how it can be build into an existing LHC analysis, designed to measure the top mass. We discuss the model-dependence of our algorithm, i.e. the bias of our measurement towards the top mass used in simulation and propose a method to reliably achieve unbiased results.

Primary Field of Research

Particle Physics

Primary authors: PAASCH, Alexander (Hamburg University (DE)); SCHWARZ, Dennis (Austrian Academy of Sciences (AT)); FAVARO, Luigi; KOGLER, Roman (DESY (DE)); PALACIOS SCHWEITZER, Sofia (ITP, University Heidelberg); PLEHN, Tilman

Presenter: PALACIOS SCHWEITZER, Sofia (ITP, University Heidelberg)

Contribution ID: 57

Type: **Poster**

Efficient machine learning for statistical hypothesis testing

Traditional statistical methods are often not adequate to perform inclusive and signal-agnostic searches at modern collider experiments delivering large amounts of multivariate data. Machine learning provides a set of tools to enhance analyses in large scale regimes, but the adoption of these methodologies comes with new challenges, such as the lack of efficiency and robustness, and potential hidden biases. In this talk, I will discuss these aspects in the context of a recent proposal for a likelihood-ratio-based goodness-of-fit test powered by large-scale implementations of kernel methods, nonparametric learning models that can approximate any continuous function given enough data.

Primary Field of Research

Machine Learning

Primary author: Dr LETIZIA, Marco (University of Genoa and INFN)

Co-authors: WULZER, Andrea (IFAE and ICREA – Barcelona, Spain); Dr GROSSO, Gaia (IAIFI, MIT); Prof. ROSASCO, Lorenzo (University of Genoa); ZANETTI, Marco (Universita e INFN, Padova (IT)); PIERINI, Maurizio (CERN)

Presenter: Dr LETIZIA, Marco (University of Genoa and INFN)

Contribution ID: 58

Type: **Poster**

Integrating Explainable AI in Modern High-Energy Physics (the MUCCA Project)

The Multi-disciplinary Use Cases for Convergent new Approaches to AI explainability (MUCCA) project is pioneering efforts to enhance the transparency and interpretability of AI algorithms in complex scientific endeavours. The presented study focuses on the role of Explainable AI (xAI) in the domain of high-energy physics (HEP). Approaches based on Machine Learning (ML) methodologies, from classical boosted decision trees to Graph Neural Nets, are considered to search for new physics models.

A set of use-cases are exploited to highlight the potential of ML, based on studies performed on the ATLAS experiment at the Large Hadron Collider (LHC). Results demonstrate there can be significant enhancements in sensitivity when using ML approaches, affirming the effectiveness of these tools in exploring a broad range of phase space and new physics models that traditional searches may not reach. Maintaining this balance is critical for consistent result interpretation and scientific rigour. The studies performed so far and presented in this talk emphasise this crucial balance in HEP between state-of-the-art ML techniques and transparency achievable through xAI.

Primary Field of Research

Particle Physics

Primary author: CARMIGNANI, Joseph (University of Liverpool (GB))

Presenter: CARMIGNANI, Joseph (University of Liverpool (GB))

Contribution ID: 59

Type: **Poster**

Integrating Energy Flow Networks with Jet Substructure Observables for Enhanced Jet Quenching Studies

The phenomena of Jet Quenching, a key signature of the Quark-Gluon Plasma (QGP) formed in Heavy-Ion (HI) collisions, provides a window of insight into the properties of this primordial liquid. In this study, we rigorously evaluate the discriminating power of Energy Flow Networks (EFNs), enhanced with substructure observables, in distinguishing between jets stemming from proton-proton (pp) and jets stemming from HI collisions. This work is yet another step towards separating significantly quenched jets from relatively unmodified ones on a per-jet basis, which would enable increasingly more precise measurements of QGP properties. We have analyzed simple Energy Flow Networks (EFNs) and subsequently augmented them with global features such as N-Subjettiness observables and Energy Flow Polynomials (EFPs). Our primary objective is to gauge the power of these approaches in the context of Jet Quenching. Initial evaluations using Linear Discriminant Analysis (LDA) set a performance baseline, which is further enhanced through simple Deep Neural Networks (DNNs), capable of capturing non-linear relations in the data. Integrating EFPs and N-Subjettiness observables into EFNs results in the most performant model over this task, achieving state-of-the-art ROC AUC values of approximately 0.84, a very considerable value given that both medium response and underlying event contamination effects are taken into account.

Primary Field of Research

Particle Physics

Primary authors: Dr MILHANO, Guilherme (LIP-Lisbon & CERN TH); A. GONÇALVES, João (LIP - IST)

Presenter: A. GONÇALVES, João (LIP - IST)

Contribution ID: 60

Type: **Poster**

Proximal Nested Sampling with Data-Driven AI Priors

Bayesian model selection provides a powerful framework for objectively comparing models directly from observed data, without reference to ground truth data. However, Bayesian model selection requires the computation of the marginal likelihood (model evidence), which is computationally challenging, prohibiting its use in many high-dimensional Bayesian inverse problems. With Bayesian imaging applications in mind, we introduce the proximal nested sampling methodology to objectively compare alternative Bayesian imaging models for applications that use images to inform decisions under uncertainty. The methodology is based on nested sampling, a Monte Carlo approach specialised for model comparison, and exploits proximal Markov chain Monte Carlo techniques to scale efficiently to large problems and to tackle models that are log-concave and not necessarily smooth (e.g., involving l1 or total-variation priors). Taking one step further, we show how proximal nested sampling can be extended using Tweedie's formula to support data-driven priors, such as deep neural networks learned from training data. We demonstrate our method by carrying out Bayesian model comparison between data-driven and hand-crafted priors in imaging applications like radio-interferometric image reconstruction.

Based on arXiv:2106.03646 and arXiv:2307.00056

Primary Field of Research

Astro/Cosmo

Primary author: Dr LIAUDAT, Tobías (CEA Paris-Saclay)

Co-authors: ALDRIDGE, Henry (UCL); Dr PRICE, Matthew (UCL); Prof. PEREYRA, Marcelo (Heriot-Watt University); Dr CAI, Xiaohao (University of Southampton); Prof. MCEWEN, Jason (UCL)

Presenter: ALDRIDGE, Henry (UCL)

Contribution ID: 61

Type: **Poster**

Generative models of astrophysical fields with scattering transforms on the sphere

Scattering transforms are a new type of summary statistics recently developed for the study of highly non-Gaussian processes, which have been shown to be very promising for astrophysical studies. In particular, they allow one to build generative models of complex non-linear fields from a limited amount of data, and have also been used as the basis of new statistical component separation algorithms. In the context of upcoming cosmological surveys, such as LiteBIRD for the cosmic microwave background polarization or Rubin-LSST and Euclid for study of the large scale structures of the Universe, the extension of these tools to spherical data is necessary. We develop scattering transforms on the sphere and focus on the construction of maximum-entropy generative models of several astrophysical fields. We construct, from a single target field, generative models of homogeneous astrophysical and cosmological fields, whose samples are quantitatively compared to the target fields using common statistics (power spectrum, pixel probability density function and Minkowski functionals). Our sampled fields agree well with the target fields, both statistically and visually. These generative models therefore open up a wide range of new applications for future astrophysical and cosmological studies; particularly those for which very little simulated data is available. We make our code available to the community so that this work can be easily reproduced and developed further.

Primary Field of Research

Astro/Cosmo

Primary author: MCEWEN, Jason

Co-authors: Dr MOUSSET, Louise; Prof. ALLYS, Erwan; Dr PRICE, Matt; Prof. AUMONT, Jonathan; Dr DELOUIS, Jean-Marc; Prof. MONTIER, Ludovic

Presenter: MCEWEN, Jason

Contribution ID: 62

Type: **Poster**

Advanced techniques for Simulation Based Inference in collider physics

We present an application of Simulation-Based Inference (SBI) in collider physics, aiming to constrain anomalous interactions beyond the Standard Model (SM). This is achieved by leveraging Neural Networks to learn otherwise intractable likelihood ratios. We explore methods to incorporate the underlying physics structure into the likelihood estimation process. Specifically, we compare two approaches: morphing-aware likelihood estimation and derivative learning. Furthermore, we illustrate how uncertainty-aware networks can be employed to compare the performance of these methods. Additionally, we demonstrate two new techniques for enhancing the accuracy and reliability of the network training. First, we introduce a new way to treat the outliers in the target reconstruction-level distributions by repeated smearing and modifying their parton-level weights accordingly (dubbed fractional smearing). Second, we utilise Lorentz-equivariant network architectures to exploit the symmetry structure inherent in the underlying particle physics amplitudes.

Primary Field of Research

Particle Physics

Primary author: DE CRESCENZO, Giovanni (University of Heidelberg)**Presenter:** DE CRESCENZO, Giovanni (University of Heidelberg)

Contribution ID: 63

Type: **Poster**

SBI for wide field weak lensing

The standard approach to inference from cosmic large-scale structure data employs summary statistics that are compared to analytic models in a Gaussian likelihood with pre-computed covariance. To overcome many of the idealising assumptions that go into this type of explicit likelihood inference, and to take advantage of the high-fidelity wide field data that Euclid and LSST will provide, we can employ simulation-based inference (SBI). In previous work we have demonstrated the power of SBI in the context of performing a full re-analysis of the KiDS-1000 survey (MvWK & KL 2024) whilst modelling anisotropic observational systematics with forward simulations that significantly impact the outcome of the inference and must be included in the analysis of Euclid and LSST data. We further report on the effects of different levels of Gaussianity imposed on the inference. Our current work explores the use of wavelet summary statistics to construct higher order summary statistics directly from the field without any machine learning. This method thus does not suffer from many of the problems that are associated with using neural methods whilst being fast and capable of extracting large amounts of information. We present here an outlook of how we can tackle the task of SBI applied to upcoming wide field weak lensing surveys.

Primary Field of Research

Astro/Cosmo

Primary author: LIN, Kiyam**Presenter:** LIN, Kiyam

Contribution ID: 64

Type: **Poster**

Exhaustive Symbolic Regression: Learning Astrophysics directly from Data

A key challenge in the field of AI is to make machine-assisted discovery interpretable, enabling it not only to uncover correlations but also to improve our physical understanding of the world. A nascent branch of machine learning – Symbolic Regression (SR) – aims to discover the optimal functional representations of datasets, producing perfectly interpretable outputs (equations) by construction. SR is traditionally done using a “genetic algorithm” which stochastically selects trial functions by analogy with natural selection; I will describe the more ambitious approach of exhaustively searching and evaluating function space.

Coupled to an information-theoretic model selection principle based on minimum description length, our algorithm “Exhaustive Symbolic Regression” (ESR) is guaranteed to find the simple functions that optimally balance accuracy with simplicity on a dataset. This gives it broad application across science. I will detail the method, its relation to Bayesian statistics and an optional language model-based prior on functions designed to enhance their physicality. Then I will use ESR to quantify the extent to which state-of-the-art astrophysical theories – FLRW cosmology, General Relativity and Inflation – are implied by the current data.

Primary Field of Research

Astro/Cosmo

Primary authors: DESMOND, Harry (University of Portsmouth); BARTLETT, Deaglan; FERREIRA, Pedro (University of Oxford)

Presenter: DESMOND, Harry (University of Portsmouth)

Contribution ID: 65

Type: **Poster**

Usage of weakly correlated observables for nuisance parameter fits

Precision measurements at the Large Hadron Collider (LHC), such as the measurement of the top quark mass, are essential for advancing our understanding of fundamental particle physics. Profile likelihood fits have become the standard method to extract physical quantities and parameters from the measurements. These fits incorporate nuisance parameters to include systematic uncertainties. The results depend critically on the selection of observables. Including multiple observables from the measurements is beneficial for precision, as it helps to restrict the nuisance parameters, leading to more reliable fits. Usually, the used observables are assumed to be independent; however, including more observables can introduce correlations that complicate the analysis, as these correlations violate the assumption of independence. At the current precision of the top quark mass measurement, introducing more observables with minor correlations might already lead to a significant distortion of the results of the profile likelihood fit. This project aims to investigate the threshold of correlation at which the accuracy of likelihood fits begins to degrade. We utilize the realistically correlated reconstructed top and W mass, applying an uncorrelated single event likelihood fit for the analysis. To assess the accuracy of our fits, we calculate the pull for the nuisance parameters alongside the top quark mass distribution. Subsequently, we will explore machine learning techniques, such as normalizing flows, that take correlations into account instead of avoiding them.

Primary Field of Research

Machine Learning

Primary author: STIETZ, Lars (Hamburg University of Technology (DE))

Co-authors: STADIE, Hartmut (Hamburg University (DE)); LANGE, Johannes (Hamburg University (DE)); CONNOR, Patrick Louis S (University Hamburg (DE)); SCHLEPER, Peter (Hamburg University (DE))

Presenter: STIETZ, Lars (Hamburg University of Technology (DE))

Contribution ID: 66

Type: **Poster**

Accounting for Selection Effects in Supernova Cosmology with Simulation-Based Inference and Hierarchical Bayesian Modelling

Type Ia supernovae (SNe Ia) are thermonuclear exploding stars that can be used to put constraints on the nature of our universe. One challenge with population analyses of SNe Ia is Malmquist bias, where we preferentially observe the brighter SNe due to limitations of our telescopes. If untreated, this bias can propagate through to our posteriors on cosmological parameters. In this work, we develop a novel technique of using a normalising flow to learn the non-analytical likelihood of observing a SN Ia for a given survey from simulations, that is independent of any cosmological model. The learnt likelihood is then used in a hierarchical Bayesian model with Hamiltonian Monte Carlo sampling to put constraints on different sets of cosmological parameters conditioned on the observed data. The technique is verified on toy model simulations finding excellent agreement with analytically-derived posteriors to within 1σ . We conclude by discussing plans to show the generalisation of our flexible method to real survey selection effects where analytical solutions are intractable.

Primary Field of Research

Astro/Cosmo

Primary author: BOYD, Benjamin (University of Cambridge)

Co-authors: Dr GRAYLING, Matthew (University of Cambridge); Dr THORP, Stephen (Stockholm University); Prof. MANDEL, Kaisey (University of Cambridge)

Presenter: BOYD, Benjamin (University of Cambridge)

Contribution ID: 67

Type: **Contributed Talk**

Fairness Methods in Particle Physics Event Classification

In social sciences, fairness in Machine Learning (ML) comprises the attempt to correct or eliminate algorithmic bias of gender, ethnicity, or sexual orientation from ML models. Many high-energy physics (HEP) analyses that search for a resonant decay of a particle employ mass-decorrelated event classifiers, as the particle mass is often used to perform the final signal extraction fit. These classifiers are designed to maintain fairness with respect to the mass, which is accomplished primarily by retaining mass-correlated information during training.

Our studies present a first proof-of-concept for systematically applying, testing and comparing fairness methods for ML-based event classifiers in HEP analyses. We explore techniques that mitigate mass correlation during and after training. Through simulations and a case studies, we demonstrate the effectiveness of these methods in maintaining fairness while preserving the classifier performance.

Primary Field of Research

Particle Physics

Primary authors: DE VRIES, Karel (Nikhef National institute for subatomic physics (NL)); BRENNER, Lydia (Nikhef National institute for subatomic physics (NL)); RIEGER, Oliver (Nikhef National institute for subatomic physics (NL)); VAN ERVEN, Tim; VERKERKE, Wouter (Nikhef National institute for subatomic physics (NL))

Presenter: RIEGER, Oliver (Nikhef National institute for subatomic physics (NL))

Contribution ID: 68

Type: **Poster**

COMoving Computer Acceleration (COCA): Correcting Emulation Errors for Trustworthy N-Body Simulations

Neural networks are increasingly used to emulate complex simulations due to their speed and efficiency. Unfortunately, many ML algorithms, including (deep) neural networks, lack interpretability. If machines predict something humans do not understand, how can we check (and trust) the results? Even if we could identify potential mistakes, current methods lack effective mechanisms to correct them, limiting the reliability of these emulators. To address these issues, we introduce COMoving Computer Acceleration (COCA), a novel hybrid framework that integrates machine learning with traditional N-body simulators. COCA solves the correct physical equations of motion within an emulated frame of reference, inherently correcting any prediction errors. Our framework significantly reduces emulation errors in particle trajectories but also requires far fewer force evaluations compared to conventional simulations. This method effectively addresses the critical challenges of interpretability and accuracy in cosmological applications of machine learning, ensuring both speed and trustworthiness in complex simulations.

Primary Field of Research

Astro/Cosmo

Primary author: BARTLETT, Deaglan (Institut d'Astrophysique de Paris)

Co-authors: Dr LECLERCQ, Florent (Institut d'Astrophysique de Paris); Mr DOESER, Ludvig (The Oskar Klein Centre, Stockholm University); Mr CHIARENZA, Marco (Institut d'Astrophysique de Paris and Università degli Studi di Milano)

Presenter: BARTLETT, Deaglan (Institut d'Astrophysique de Paris)

Contribution ID: 69

Type: **Poster**

Application of Machine Learning Based Top Quark and \bar{X} Jet Tagging to Hadronic Four-Top Final States Induced by SM as well as BSM Processes

The aim of this work is to solve the problem of hadronic jet substructure recognition using classical subjettness variables available in the parameterized detector simulation package, Delphes. Jets produced in simulated proton-proton collisions are identified as either originating from the decay of a top quark or a W boson and are used to reconstruct the mass of a hypothetical scalar resonance decaying into a pair of top quarks in events where a total of four top quarks are produced. We compare a simple cut-based tagging method for the stacked histograms of a mixture of the Standard Model and new physics processes with a multi-layer perceptron classifier and a gradient boosting classifier. Due to the sufficient amount of data, we applied various undersampling techniques to the training sets. Our findings demonstrate that gradient boosting methods provide better results than the other tested approaches.

Primary Field of Research

Machine Learning

Primary author: Dr KVITA, Jiří (Joint Laboratory of Optics of Palacký University Olomouc and Institute of Physics of Czech Academy of Sciences, Czech Republic)

Co-authors: Dr TOMEČEK, Jan (Department of Mathematical Analysis and Applications of Mathematics, of Palacký University Olomouc, Czech Republic); MACHALOVÁ, Monika (Department of Mathematical Analysis and Applications of Mathematics, of Palacký University Olomouc, Czech Republic); Mr BAROŇ, Petr (Joint Laboratory of Optics of Palacký University Olomouc and Institute of Physics of Czech Academy of Sciences, Czech Republic); Mr PŘÍVARA, Radek (Joint Laboratory of Optics of Palacký University Olomouc and Institute of Physics of Czech Academy of Sciences, Czech Republic); Dr VODÁK, Rostislav (Department of Mathematical Analysis and Applications of Mathematics, of Palacký University Olomouc, Czech Republic)

Presenter: MACHALOVÁ, Monika (Department of Mathematical Analysis and Applications of Mathematics, of Palacký University Olomouc, Czech Republic)

Contribution ID: 70

Type: **Poster**

Emulation of Cosmological Observables under Model Misspecification in the Era of Petascale Cosmology

The modeling of cosmological observables becomes increasingly complex and we need to rely on computationally costly computer models for scalable inference. I will present a current project on advancing current emulation efforts to include functional input like selection functions into the emulation. In particular I will highlight opportunities to include Machine Learning models into the emulator design and discuss the impact of model misspecification error on emulation and inference. I will summarize the basic problem and present prior work and proposals to mitigate the issue.

Primary Field of Research

Astro/Cosmo

Primary author: RAU, Markus Michael**Presenter:** RAU, Markus Michael

Contribution ID: 71

Type: **Contributed Talk**

From galaxies to dark matter and back: addressing model misspecification in cosmology

Machine learning applications in cosmological galaxy surveys face challenges due to our limited understanding of the galaxy distribution within the dark matter cosmic web. This issue reflects a broader problem of model misspecification in simulation-based inference. In astrophysics, fully simulating the universe requires solving for gravity and the evolution of stars, galaxies, and black holes at resolutions currently unattainable. To address this, simulations employ simplified sub-grid models approximating small-scale processes' effects on larger structures, known as baryonic feedback. Our research aims to develop reliable models that remain robust despite these subgrid assumptions.

This talk will demonstrate two probabilistic approaches: using machine learning to robustly reverse-map galaxies to dark matter density (probabilistic debiasing), and learning the forward mapping from dark matter density fields to galaxy point clouds using hydrodynamical simulations and semi-analytical models of galaxy formation. We will present preliminary results on probabilistically debiasing on the CosmicFlows dataset. Furthermore, we'll discuss how leveraging learned representations of baryonic feedback can not only improve cosmological constraints but also deepen our understanding of small-scale physics missing in current simulations, potentially informing the next generation of hydrodynamical simulations.

Primary Field of Research

Astro/Cosmo

Primary author: CUESTA LAZARO, Carolina

Co-authors: PARK, Core Francisco (Harvard); MUDUR, Nayantara (Harvard); NI, Yueying (Harvard); YUAN, Sihan (Stanford)

Presenter: CUESTA LAZARO, Carolina

Contribution ID: 72

Type: **Poster**

Amplitude interpolation with equivariant neural networks

We present a detailed comparison of multiple interpolation methods to characterize the amplitude distribution of several Higgs boson production modes at the LHC. Apart from standard interpolation techniques, we develop a new approach based on the use of the Lorentz Geometric Algebra Transformer (L-GATr). L-GATr is an equivariant neural network that is able to encode Lorentz and permutation equivariant operations into a transformer architecture. Thanks to its symmetry awareness and the attention mechanism, we are able to obtain excellent results for the interpolation at tree-level and one-loop, specially at the low sample limit.

Primary Field of Research

Machine Learning

Primary authors: OLSSON, Anton (KIT); HEINRICH, Gudrun (KIT); MAGERYA, Vitaly; BRESÓ PLA, Víctor (University of Heidelberg)

Presenter: BRESÓ PLA, Víctor (University of Heidelberg)

Contribution ID: 73

Type: **Contributed Talk**

Improved Weak Lensing Photometric Redshift Calibration via StratLearn and Hierarchical Modeling

Discrepancies between cosmological parameter estimates from cosmic shear surveys and from recent Planck cosmic microwave background measurements challenge the ability of the highly successful Λ CDM model to describe the nature of the Universe. To rule out systematic biases in cosmic shear survey analyses, accurate redshift calibration within tomographic bins is key. In this work, we improve photo- z calibration via Bayesian hierarchical modeling of full galaxy photo- z conditional densities, by employing *StratLearn*, a recently developed statistical methodology, which accounts for systematic differences in the distribution of the spectroscopic training/source set and the photometric target set.

Using realistic simulations that were designed to resemble the KiDS+VIKING-450 dataset, we show that *StratLearn*-estimated conditional densities improve the galaxy tomographic bin assignment, and that our *StratLearn*-Bayesian framework leads to nearly unbiased estimates of the target population means. This leads to a factor of ~ 2 improvement upon often used and state-of-the-art photo- z calibration methods. Our approach delivers a maximum bias per tomographic bin of $\Delta\langle z \rangle = 0.0095 \pm 0.0089$, with an average absolute bias of 0.0052 ± 0.0067 across the five tomographic bins.

Primary Field of Research

Statistics

Primary author: Dr AUTENRIETH, Maximilian (Imperial College London)

Co-authors: Dr WRIGHT, Angus H. (Ruhr University Bochum); Prof. TROTTA, Roberto (SISSA –International School for Advanced Studies; Department of Physics, Imperial College London); Prof. VANDYK, David A. (Imperial College London); Prof. STENNING, David (Simon Fraser University); Prof. JOACHIMI, Benjamin (University College London)

Presenter: Dr AUTENRIETH, Maximilian (Imperial College London)

Contribution ID: 74

Type: **Contributed Talk**

Anomaly aware machine learning for dark matter direct detection at the DARWIN experiment

This talk presents a novel approach to dark matter direct detection using anomaly-aware machine learning techniques in the DARWIN next-generation dark matter direct detection experiment. I will introduce a semi-supervised deep learning pipeline that falls under the umbrella of generalized Simulation-Based Inference (SBI), an approach that allows one to effectively learn likelihoods straight from simulated data, without the need for complex functional dependence on systematics or nuisance parameters. I also present an inference procedure to detect non-background physics utilizing an anomaly function derived from the loss functions of the semi-supervised architecture. The pipeline's performance is evaluated using pseudo-data sets in a sensitivity forecasting task, and the results suggest that it offers improved sensitivity over traditional methods.

Primary Field of Research

Particle Physics

Primary author: SCAFFIDI, Andre Joshua**Presenter:** SCAFFIDI, Andre Joshua

Contribution ID: 75

Type: **Poster**

Non-standard boundary behaviour arising in binary mixture problems

Consider a binary mixture model of the form $F_\theta = (1-\theta)F_0 + \theta F_1$, where F_0 is standard normal and F_1 is a completely specified heavy-tailed distribution with the same support. Gaussianity of F_0 reflects a reduction of the raw data to a set of pivotal test statistics at each site (e.g. an energy level in a particle physics context). For a sample of n independent and identically distributed values $X_i \sim F_\theta$, the maximum likelihood estimator $\hat{\theta}_n$ is asymptotically normal provided that $0 < \theta < 1$ is an interior point. This paper investigates the large-sample behaviour for boundary points, which is entirely different and strikingly asymmetric for $\theta = 0$ and $\theta = 1$. On the right boundary, well known results on boundary parameter problems are recovered, giving $\lim \mathbb{P}_1(\hat{\theta}_n < 1) = 1/2$. On the left boundary (which corresponds to no new physics) $\lim \mathbb{P}_0(\hat{\theta}_n > 0) = 1 - 1/\alpha$, where $1 \leq \alpha \leq 2$ indexes the domain of attraction of the density ratio $f_1(X)/f_0(X)$ when $X \sim F_0$. For $\alpha = 1$, which is the most important case in practice, the tail behaviour of F_1 governs the properties of the maximum likelihood estimator and related statistics. Most notably, conditional on the event $\hat{\theta}_n > 0$, the likelihood ratio statistic has a conditional null limit distribution that is not the usual χ_1^2 . In the talk I will omit technical details and focus on the conceptual points with a view to ascertaining whether the formulation is reasonable in a particle physics context. This is joint work with Peter McCullagh and Daniel Xiang at the University of Chicago.

Primary Field of Research

Statistics

Primary author: BATTEY, Heather (Imperial College London)**Co-authors:** MCCULLAGH, Peter; XIANG, Daniel**Presenter:** BATTEY, Heather (Imperial College London)

Contribution ID: 76

Type: **Poster**

Accelerating High-Dimensional Cosmological Inference with COSMOPOWER

A new generation of astronomical surveys, such as the recently launched European Space Agency's *Euclid* mission, will soon deliver exquisite datasets with unparalleled amounts of cosmological information, poised to change our understanding of the Universe. However, analysing these datasets presents unprecedented statistical challenges. Multiple systematic effects need to be carefully accounted for, which would otherwise lead to incorrect physical interpretations. Efficiently navigating the large, complex parameter spaces required for robust systematics modelling is critical to ensuring that the anticipated increase in precision translates into equally enhanced accuracy in the final cosmological measurements.

My software COSMOPOWER tackles this challenge by training neural networks to emulate the computationally intensive calculation of cosmological power spectra. The emulation produces orders-of-magnitude acceleration in the inference pipeline. COSMOPOWER also enables the creation of fully-differentiable pipelines to leverage gradient-based sampling methods, which scale efficiently to high-dimensional parameter spaces. The acceleration provided by COSMOPOWER has led major international collaborations (e.g. *Euclid*, KiDS, ACT, Simons Observatory), working on both large-scale structure and Cosmic Microwave Background data, to adopt this software in their cosmological inference pipelines.

In this talk, I will showcase how recent advancements in COSMOPOWER pave the way for a new paradigm in cosmological inference, allowing for comprehensive Bayesian analyses—including both parameter estimation and model selection—to be conducted in a fraction of the time required by traditional methods, and extracting more information from the data than the traditional approach based on two-point statistics. The framework not only accelerates the inference process but also improves our ability to accurately model the underlying physics, especially for beyond-standard models, making it a critical tool for the future of cosmological research.

Primary Field of Research

Astro/Cosmo

Primary author: SPURIO MANCINI, Alessio (Royal Holloway, University of London)

Presenter: SPURIO MANCINI, Alessio (Royal Holloway, University of London)

Contribution ID: 77

Type: **Poster**

Learning Optimal and Interpretable Summary Statistics of Galaxy Catalogs with SBI

How much cosmological information can we reliably extract from existing and upcoming large-scale structure observations? Many summary statistics fall short in describing the non-Gaussian nature of the late-time Universe and modelling uncertainties from baryonic physics. Using simulation based inference (SBI) with automatic data-compression from graph neural networks, we learn optimal summary statistics for galaxy catalogs in the context of cosmological parameter estimation. By construction these summaries do not require the ability to write down an explicit likelihood. We demonstrate that they can be used for efficient parameter inference, outperforming existing (ML) methods for the same parameter estimation. These summary statistics offer a new avenue for analyzing different simulation models for baryonic physics with respect to their relevance for the resulting cosmological features. The learned summary statistics are low-dimensional, feature the underlying simulation parameters, and are similar across different network architectures. To link our models, we identify the relevant scales associated to our summary statistics (e.g. in the range of modes between $k = 5 - 30h/Mpc$) and we are able to match the summary statistics to underlying simulation parameters across various simulation models. Furthermore, we compare different baryonic feedback models in latent space and find differences in the flexibility of their parametrizations.

Primary Field of Research

Astro/Cosmo

Primary author: LEHMAN, Kai (LMU Munich)**Co-authors:** Dr KRIPPENDORF, Sven (LMU Munich); Prof. WELLER, Jochen (LMU Munich); Prof. DOLAG, Klaus (LMU Munich)**Presenter:** LEHMAN, Kai (LMU Munich)

Contribution ID: 78

Type: **Poster**

Bayesian evidence estimation with normalizing flows

Using *floZ*, an improved Bayesian evidence (and its numerical uncertainty) estimation method based on normalizing flows, we estimate the Bayes factor in favor of gravitational wave overtones in the ringdown of the first detection. We find good agreement with nested sampling. Provided representative samples from the target posterior are available, our method is more robust to posterior distributions with sharp features, especially in higher dimensions. I propose a metric to evaluate the flow training completion using the latent space map of the posterior samples. Finally, I introduce a nested flow technique for improved density estimation.

Primary Field of Research

Astro/Cosmo

Primary author: SRINIVASAN, Rahul**Co-authors:** BARAUSSE, Enrico; Dr CRISOSTOMI, Marco (California Institute of Technology, USA); TROTTA, Roberto**Presenter:** SRINIVASAN, Rahul

Contribution ID: 79

Type: **Poster**

Isbi: linear simulation based inference

Simulation-based inference is undergoing a renaissance in statistics and machine learning. With several packages implementing the state-of-the-art in expressive AI [mackelab/sbi] [undark-lab/swyft], it is now being effectively applied to a wide range of problems in the physical sciences, biology, and beyond.

Given the rapid pace of AI/ML, there is little expectation that the implementations of the future will resemble these current first generation neural network-based approaches. This talk will present a new framework for simulation-based inference, linear simulation-based inference (lsbi), which abstracts the core principles of SBI from the specific details of machine learning, implementing a plug-and-play framework of linear and mixture models.

lsbi has several use-cases:

1. It is pedagogically helpful to separate out the general principles of SBI from the specific details of neural networks (particularly for ML skeptics).
2. It is practically useful for producing expressive examples with known ground truths.
3. It is pragmatically useful, since in many cases, lsbi is competitive with neural approaches in terms of accuracy, whilst being faster and more interpretable.

An evolving code-driven PyPI/conda research package is available at:
<https://github.com/handley-lab/lsbi>

Primary Field of Research

Astro/Cosmo

Primary author: Dr HANDLEY, William

Presenter: Dr HANDLEY, William

Contribution ID: **80**Type: **Poster**

Uncertainty-aware machine learning for the LHC

Estimating uncertainties is a fundamental aspect in every physics problem, no measurements or calculations comes without uncertainties. Hence it is crucial to consider the effect of training a neural network to problems in physics. I will present our work on amplitude regression, using loop amplitudes from LHC processes, as an example to examine the impact of different uncertainties on the outcome of the network. We test the behavior of different neural networks with uncertainty estimation, including Bayesian neural networks and repulsive ensembles.

Presenter: ELMER, Nina

Session Classification: Social

Contribution ID: **81**

Type: **not specified**

Poster 2

Presenter: LANGFORD, Jonathon Mark (Imperial College (GB))

Session Classification: Social

Contribution ID: **82**

Type: **not specified**

Poster 3

Presenter: LANGFORD, Jonathon Mark (Imperial College (GB))

Session Classification: Social

Contribution ID: 83

Type: **Poster**

Generative models: their evaluation and their limitations

I will present and discuss several proposed metrics, based on integral probability measures, for the evaluation of generative models (and, more generally, for the comparison of different generators). Some of the metrics are particularly efficient to be computed in parallel, and show good performances. I will first compare the metrics on toy multivariate/multimodal distributions, and then focus on HEP examples from the JetNet jet dataset. I will discuss the power of the tests and their implementation in TensorFlow2, taking the opportunity to discuss, more generally, the limitations in the usage of generative models in HEP.

Presenter: GROSSI, Samuele (Università degli studi di Genova & INFN sezione di Genova)

Session Classification: Social

Contribution ID: 84

Type: **Poster**

Limits to classification performance by relating Kullback-Leibler divergence to Cohen's Kappa

The performance of machine learning classification algorithms are evaluated by estimating metrics, often from the confusion matrix, using training data and cross-validation. However, these do not prove that the best possible performance has been achieved. Fundamental limits to error rates can be estimated using information distance measures. To this end, the confusion matrix has been formulated to comply with the Chernoff-Stein Lemma. This links the error rates to the Kullback-Leibler divergences between the probability density functions describing the two classes. This leads to a key result that relates Cohen's Kappa to the Resistor Average Distance which is the parallel resistor combination of the two Kullback-Leibler divergences. The Resistor Average Distance has units of bits and is estimated from the same training data used by the classification algorithm, using kNN estimates of the Kullback-Leibler divergences. The classification algorithm gives the confusion matrix and Kappa. Theory and methods are discussed in detail and then applied to Monte Carlo data and real datasets. Four very different real datasets - Breast Cancer, Coronary Heart Disease, Bankruptcy, and Particle Identification - are analysed, with both continuous and discrete values, and their classification performance compared to the expected theoretical limit. In all cases this analysis shows that the algorithms could not have performed any better due to the underlying probability density functions for the two classes. Important lessons are learnt on how to predict the performance of algorithms for imbalanced data. Preprint available at [arXiv:2403.01571](https://arxiv.org/abs/2403.01571).

Presenter: WATTS, Stephen

Session Classification: Social

Contribution ID: 85

Type: **Poster**

Precision-Machine Learning for the Matrix Element Method

The matrix element method is the LHC inference method of choice for limited statistics, as it allows for optimal use of available information. We present a dedicated machine learning framework, based on efficient phase-space integration, a learned acceptance and transfer function. It is based on a choice of INN and diffusion networks, and a transformer to solve jet combinatorics. We showcase this setup for the CP-phase of the top Yukawa coupling in associated Higgs and single-top production.

Presenter: HUETSCH, Nathan (Heidelberg University, ITP Heidelberg)

Session Classification: Social

Contribution ID: 86

Type: **Poster**

Graph neural networks on the test bench in HEP applications

Data analyses in the high-energy particle physics (HEP) community more and more often exploit advanced multivariate methods to separate signal from background processes. In this talk, a maximally unbiased, in-depth comparison of the graph neural network (GNN) architecture, which is of increasing popularity in the HEP community, with the already well-established technology of fully connected feed-forward deep neural networks (DNNs) is presented. When it comes to choosing a suitable machine-learning model, it is not a priori clear, what model this should be to benefit from inherent properties of the task. Also, the design of a fair and unbiased benchmark is non-trivial. This GNN vs. DNN comparison is insightful in terms of the details it reveals as to which aspects of GNNs are superior to DNNs - and which are not. The study is performed on a typical data set of a complex challenge recently faced at the Large Hadron Collider: the classification of events with top quark-antiquark pairs with additional heavy flavour jets originating from gluon splittings, Z or Higgs bosons.

The study is documented in the paper “A Case Study of Sending Graph Neural Networks Back to the Test Bench for Applications in High-Energy Particle Physics” published in *Computing and Software for Big Science*, <https://doi.org/10.1007/s41781-024-00122-3>.

Presenter: PFEFFER, Emanuel Lorenz (KIT - Karlsruhe Institute of Technology (DE))

Session Classification: Social

Contribution ID: 87

Type: **Poster**

The Landscape of Unfolding with Machine Learning

Recent innovations from machine learning allow for data unfolding, without binning and including correlations across many dimensions. We describe a set of known, upgraded, and new methods for ML-based unfolding. The performance of these approaches are evaluated on the same two datasets. We find that all techniques are capable of accurately reproducing the particle-level spectra across complex observables. Given that these approaches are conceptually diverse, they offer an exciting toolkit for a new class of measurements that can probe the Standard Model with an unprecedented level of detail and may enable sensitivity to new phenomena.

Presenter: MARIÑO VILLADAMIGO, Javier (Institut für Theoretische Physik - University of Heidelberg)

Session Classification: Social

Contribution ID: **88**Type: **Poster**

Interpolated Likelihoods for Fast Reinterpretations

We present a method to accelerate Effective Field Theory reinterpretations using interpolated likelihoods. By employing Radial Basis Functions for interpolation and Gaussian Processes to strategically select interpolation points, we show that we can reduce the computational burden while maintaining accuracy. We apply this in the context of the Combined Higgs Boson measurement at CMS, a complex statistical model with many thousands of parameters requiring large computing power to evaluate.

Presenter: RUNTING, Tom (Imperial College (GB))

Session Classification: Social

Contribution ID: **89**Type: **Poster**

How to Unfold Top Decays

Many physics analyses at the LHC rely on algorithms to remove detector effect, commonly known as unfolding. Whereas classical methods only work with binned, one-dimensional data, Machine Learning promises to overcome both problems. Using a generative unfolding pipeline, we show how it can be build into an existing LHC analysis, designed to measure the top mass. We discuss the model-dependence of our algorithm, i.e. the bias of our measurement towards the top mass used in simulation and propose a method to reliably achieve unbiased results.

Presenter: PALACIOS SCHWEITZER, Sofia (ITP, University Heidelberg)

Session Classification: Social

Contribution ID: 90

Type: **Poster**

Efficient machine learning for statistical hypothesis testing

Traditional statistical methods are often not adequate to perform inclusive and signal-agnostic searches at modern collider experiments delivering large amounts of multivariate data. Machine learning provides a set of tools to enhance analyses in large scale regimes, but the adoption of these methodologies comes with new challenges, such as the lack of efficiency and robustness, and potential hidden biases. In this talk, I will discuss these aspects in the context of a recent proposal for a likelihood-ratio-based goodness-of-fit test powered by large-scale implementations of kernel methods, nonparametric learning models that can approximate any continuous function given enough data.

Presenter: Dr LETIZIA, Marco

Session Classification: Social

Contribution ID: 91

Type: **Poster**

Integrating Explainable AI in Modern High-Energy Physics (the MUCCA Project)

The Multi-disciplinary Use Cases for Convergent new Approaches to AI explainability (MUCCA) project is pioneering efforts to enhance the transparency and interpretability of AI algorithms in complex scientific endeavours. The presented study focuses on the role of Explainable AI (xAI) in the domain of high-energy physics (HEP). Approaches based on Machine Learning (ML) methodologies, from classical boosted decision trees to Graph Neural Nets, are considered to search for new physics models.

A set of use-cases are exploited to highlight the potential of ML, based on studies performed on the ATLAS experiment at the Large Hadron Collider (LHC). Results demonstrate there can be significant enhancements in sensitivity when using ML approaches, affirming the effectiveness of these tools in exploring a broad range of phase space and new physics models that traditional searches may not reach. Maintaining this balance is critical for consistent result interpretation and scientific rigour. The studies performed so far and presented in this talk emphasise this crucial balance in HEP between state-of-the-art ML techniques and transparency achievable through xAI.

Presenter: CARMIGNANI, Joseph (University of Liverpool (GB))

Session Classification: Social

Contribution ID: 92

Type: **Poster**

Integrating Energy Flow Networks with Jet Substructure Observables for Enhanced Jet Quenching Studies

The phenomena of Jet Quenching, a key signature of the Quark-Gluon Plasma (QGP) formed in Heavy-Ion (HI) collisions, provides a window of insight into the properties of this primordial liquid. In this study, we rigorously evaluate the discriminating power of Energy Flow Networks (EFNs), enhanced with substructure observables, in distinguishing between jets stemming from proton-proton (pp) and jets stemming from HI collisions. This work is yet another step towards separating significantly quenched jets from relatively unmodified ones on a per-jet basis, which would enable increasingly more precise measurements of QGP properties. We have analyzed simple Energy Flow Networks (EFNs) and subsequently augmented them with global features such as N-Subjettiness observables and Energy Flow Polynomials (EFPs). Our primary objective is to gauge the power of these approaches in the context of Jet Quenching. Initial evaluations using Linear Discriminant Analysis (LDA) set a performance baseline, which is further enhanced through simple Deep Neural Networks (DNNs), capable of capturing non-linear relations in the data. Integrating EFPs and N-Subjettiness observables into EFNs results in the most performant model over this task, achieving state-of-the-art ROC AUC values of approximately 0.84, a very considerable value given that both medium response and underlying event contamination effects are taken into account.

Presenter: A. GONÇALVES, João (LIP - IST)

Session Classification: Social

Contribution ID: 93

Type: **Poster**

Proximal Nested Sampling with Data-Driven AI Priors

Bayesian model selection provides a powerful framework for objectively comparing models directly from observed data, without reference to ground truth data. However, Bayesian model selection requires the computation of the marginal likelihood (model evidence), which is computationally challenging, prohibiting its use in many high-dimensional Bayesian inverse problems. With Bayesian imaging applications in mind, we introduce the proximal nested sampling methodology to objectively compare alternative Bayesian imaging models for applications that use images to inform decisions under uncertainty. The methodology is based on nested sampling, a Monte Carlo approach specialised for model comparison, and exploits proximal Markov chain Monte Carlo techniques to scale efficiently to large problems and to tackle models that are log-concave and not necessarily smooth (e.g., involving l1 or total-variation priors). Taking one step further, we show how proximal nested sampling can be extended using Tweedie's formula to support data-driven priors, such as deep neural networks learned from training data. We demonstrate our method by carrying out Bayesian model comparison between data-driven and hand-crafted priors in imaging applications like radio-interferometric image reconstruction.

Presenter: ALDRIDGE, Henry (UCL)

Session Classification: Social

Contribution ID: 94

Type: **Poster**

Generative models of astrophysical fields with scattering transforms on the sphere

Scattering transforms are a new type of summary statistics recently developed for the study of highly non-Gaussian processes, which have been shown to be very promising for astrophysical studies. In particular, they allow one to build generative models of complex non-linear fields from a limited amount of data, and have also been used as the basis of new statistical component separation algorithms. In the context of upcoming cosmological surveys, such as LiteBIRD for the cosmic microwave background polarization or Rubin-LSST and Euclid for study of the large scale structures of the Universe, the extension of these tools to spherical data is necessary. We develop scattering transforms on the sphere and focus on the construction of maximum-entropy generative models of several astrophysical fields. We construct, from a single target field, generative models of homogeneous astrophysical and cosmological fields, whose samples are quantitatively compared to the target fields using common statistics (power spectrum, pixel probability density function and Minkowski functionals). Our sampled fields agree well with the target fields, both statistically and visually. These generative models therefore open up a wide range of new applications for future astrophysical and cosmological studies; particularly those for which very little simulated data is available. We make our code available to the community so that this work can be easily reproduced and developed further.

Primary author: PRICE, Matthew (Mullard Space Science Laboratory, University College London)

Presenter: PRICE, Matthew (Mullard Space Science Laboratory, University College London)

Session Classification: Social

Contribution ID: 95

Type: **Poster**

Advanced techniques for Simulation Based Inference in collider physics

We present an application of Simulation-Based Inference (SBI) in collider physics, aiming to constrain anomalous interactions beyond the Standard Model (SM). This is achieved by leveraging Neural Networks to learn otherwise intractable likelihood ratios. We explore methods to incorporate the underlying physics structure into the likelihood estimation process. Specifically, we compare two approaches: morphing-aware likelihood estimation and derivative learning. Furthermore, we illustrate how uncertainty-aware networks can be employed to compare the performance of these methods. Additionally, we demonstrate two new techniques for enhancing the accuracy and reliability of the network training. First, we introduce a new way to treat the outliers in the target reconstruction-level distributions by repeated smearing and modifying their parton-level weights accordingly (dubbed fractional smearing). Second, we utilise Lorentz-equivariant network architectures to exploit the symmetry structure inherent in the underlying particle physics amplitudes.

Presenter: DE CRESCENZO, Giovanni (University of Heidelberg)

Session Classification: Social

Contribution ID: 96

Type: **Poster**

SBI for wide field weak lensing

The standard approach to inference from cosmic large-scale structure data employs summary statistics that are compared to analytic models in a Gaussian likelihood with pre-computed covariance. To overcome many of the idealising assumptions that go into this type of explicit likelihood inference, and to take advantage of the high-fidelity wide field data that Euclid and LSST will provide, we can employ simulation-based inference (SBI). In previous work we have demonstrated the power of SBI in the context of performing a full re-analysis of the KiDS-1000 survey (MvWK & KL 2024) whilst modelling anisotropic observational systematics with forward simulations that significantly impact the outcome of the inference and must be included in the analysis of Euclid and LSST data. We further report on the effects of different levels of Gaussianity imposed on the inference. Our current work explores the use of wavelet summary statistics to construct higher order summary statistics directly from the field without any machine learning. This method thus does not suffer from many of the problems that are associated with using neural methods whilst being fast and capable of extracting large amounts of information. We present here an outlook of how we can tackle the task of SBI applied to upcoming wide field weak lensing surveys.

Presenter: LIN, Kiyam

Session Classification: Social

Contribution ID: 97

Type: **Poster**

Exhaustive Symbolic Regression: Learning Astrophysics directly from Data

A key challenge in the field of AI is to make machine-assisted discovery interpretable, enabling it not only to uncover correlations but also to improve our physical understanding of the world. A nascent branch of machine learning – Symbolic Regression (SR) – aims to discover the optimal functional representations of datasets, producing perfectly interpretable outputs (equations) by construction. SR is traditionally done using a “genetic algorithm” which stochastically selects trial functions by analogy with natural selection; I will describe the more ambitious approach of exhaustively searching and evaluating function space.

Coupled to an information-theoretic model selection principle based on minimum description length, our algorithm “Exhaustive Symbolic Regression” (ESR) is guaranteed to find the simple functions that optimally balance accuracy with simplicity on a dataset. This gives it broad application across science. I will detail the method, its relation to Bayesian statistics and an optional language model-based prior on functions designed to enhance their physicality. Then I will use ESR to quantify the extent to which state-of-the-art astrophysical theories – FLRW cosmology, General Relativity and Inflation – are implied by the current data.

Presenter: DESMOND, Harry (University of Portsmouth)

Session Classification: Social

Contribution ID: 98

Type: **Poster**

Usage of weakly correlated observables for nuisance parameter fits

Precision measurements at the Large Hadron Collider (LHC), such as the measurement of the top quark mass, are essential for advancing our understanding of fundamental particle physics. Profile likelihood fits have become the standard method to extract physical quantities and parameters from the measurements. These fits incorporate nuisance parameters to include systematic uncertainties. The results depend critically on the selection of observables. Including multiple observables from the measurements is beneficial for precision, as it helps to restrict the nuisance parameters, leading to more reliable fits. Usually, the used observables are assumed to be independent; however, including more observables can introduce correlations that complicate the analysis, as these correlations violate the assumption of independence. At the current precision of the top quark mass measurement, introducing more observables with minor correlations might already lead to a significant distortion of the results of the profile likelihood fit. This project aims to investigate the threshold of correlation at which the accuracy of likelihood fits begins to degrade. We utilize the realistically correlated reconstructed top and W mass, applying an uncorrelated single event likelihood fit for the analysis. To assess the accuracy of our fits, we calculate the pull for the nuisance parameters alongside the top quark mass distribution. Subsequently, we will explore machine learning techniques, such as normalizing flows, that take correlations into account instead of avoiding them.

Presenter: STIETZ, Lars (Hamburg University of Technology (DE))

Session Classification: Social

Contribution ID: 99

Type: **Poster**

Accounting for Selection Effects in Supernova Cosmology with Simulation-Based Inference and Hierarchical Bayesian Modelling

Type Ia supernovae (SNe Ia) are thermonuclear exploding stars that can be used to put constraints on the nature of our universe. One challenge with population analyses of SNe Ia is Malmquist bias, where we preferentially observe the brighter SNe due to limitations of our telescopes. If untreated, this bias can propagate through to our posteriors on cosmological parameters. In this work, we develop a novel technique of using a normalising flow to learn the non-analytical likelihood of observing a SN Ia for a given survey from simulations, that is independent of any cosmological model. The learnt likelihood is then used in a hierarchical Bayesian model with Hamiltonian Monte Carlo sampling to put constraints on different sets of cosmological parameters conditioned on the observed data. The technique is verified on toy model simulations finding excellent agreement with analytically-derived posteriors to within . We conclude by discussing plans to show the generalisation of our flexible method to real survey selection effects where analytical solutions are intractable.

Presenter: BOYD, Benjamin (University of Cambridge)

Session Classification: Social

Contribution ID: 100

Type: **Poster**

COMoving Computer Acceleration (COCA): Correcting Emulation Errors for Trustworthy N-Body Simulations

Neural networks are increasingly used to emulate complex simulations due to their speed and efficiency. Unfortunately, many ML algorithms, including (deep) neural networks, lack interpretability. If machines predict something humans do not understand, how can we check (and trust) the results? Even if we could identify potential mistakes, current methods lack effective mechanisms to correct them, limiting the reliability of these emulators. To address these issues, we introduce COMoving Computer Acceleration (COCA), a novel hybrid framework that integrates machine learning with traditional N-body simulators. COCA solves the correct physical equations of motion within an emulated frame of reference, inherently correcting any prediction errors. Our framework significantly reduces emulation errors in particle trajectories but also requires far fewer force evaluations compared to conventional simulations. This method effectively addresses the critical challenges of interpretability and accuracy in cosmological applications of machine learning, ensuring both speed and trustworthiness in complex simulations.

Presenter: BARTLETT, Deaglan (Institut d'Astrophysique de Paris)

Session Classification: Social

Contribution ID: 101

Type: **Poster**

Application of Machine Learning Based Top Quark and \bar{X} Jet Tagging to Hadronic Four-Top Final States Induced by SM as well as BSM Processes

The aim of this work is to solve the problem of hadronic jet substructure recognition using classical subjettiness variables available in the parameterized detector simulation package, Delphes. Jets produced in simulated proton-proton collisions are identified as either originating from the decay of a top quark or a W boson and are used to reconstruct the mass of a hypothetical scalar resonance decaying into a pair of top quarks in events where a total of four top quarks are produced. We compare a simple cut-based tagging method for the stacked histograms of a mixture of the Standard Model and new physics processes with a multi-layer perceptron classifier and a gradient boosting classifier. Due to the sufficient amount of data, we applied various undersampling techniques to the training sets. Our findings demonstrate that gradient boosting methods provide better results than the other tested approaches.

Presenter: MACHALOVÁ, Monika

Session Classification: Social

Contribution ID: **102**Type: **Poster**

Emulation of Cosmological Observables under Model Misspecification in the Era of Petascale Cosmology

The modeling of cosmological observables becomes increasingly complex and we need to rely on computationally costly computer models for scalable inference. I will present a current project on advancing current emulation efforts to include functional input like selection functions into the emulation. In particular I will highlight opportunities to include Machine Learning models into the emulator design and discuss the impact of model misspecification error on emulation and inference. I will summarize the basic problem and present prior work and proposals to mitigate the issue.

Presenter: RAU, Markus Michael

Session Classification: Social

Contribution ID: **103**Type: **Poster**

Amplitude interpolation with equivariant neural networks

We present a detailed comparison of multiple interpolation methods to characterize the amplitude distribution of several Higgs boson production modes at the LHC. Apart from standard interpolation techniques, we develop a new approach based on the use of the Lorentz Geometric Algebra Transformer (L-GATr). L-GATr is an equivariant neural network that is able to encode Lorentz and permutation equivariant operations into a transformer architecture. Thanks to its symmetry awareness and the attention mechanism, we are able to obtain excellent results for the interpolation at tree-level and one-loop, specially at the low sample limit.

Presenter: BRESÓ PLA, Víctor (University of Heidelberg)

Session Classification: Social

Contribution ID: 104

Type: **Poster**

Non-standard boundary behaviour arising in binary mixture problems

Consider a binary mixture model of the form $\mu = \alpha \phi + (1 - \alpha) \psi$, where ϕ is standard normal and ψ is a completely specified heavy-tailed distribution with the same support. Gaussianity of μ reflects a reduction of the raw data to a set of pivotal test statistics at each site (e.g. an energy level in a particle physics context). For a sample of independent and identically distributed values X_1, \dots, X_n , the maximum likelihood estimator $\hat{\alpha}$ is asymptotically normal provided that α is an interior point. This paper investigates the large-sample behaviour for boundary points, which is entirely different and strikingly asymmetric for $\alpha = 0$ and $\alpha = 1$. On the right boundary, well known results on boundary parameter problems are recovered, giving

. On the left boundary (which corresponds to no new physics) $\hat{\alpha} \sim \alpha + \frac{1}{n} \log \frac{1 - \alpha}{\alpha}$, where \log indexes the domain of attraction of the density ratio when $\alpha = 0$. For $\alpha = 1$, which is the most important case in practice, the tail behaviour of ψ governs the properties of the maximum likelihood estimator and related statistics. Most notably, conditional on the event $\{X_n > 0\}$, the likelihood ratio statistic has a conditional null limit distribution that is not the usual $N(0, 1)$. In the talk I will omit technical details and focus on the conceptual points with a view to ascertaining whether the formulation is reasonable in a particle physics context.

This is joint work with Peter McCullagh and Daniel Xiang at the University of Chicago.

Presenter: BATTEY, Heather (Imperial College London)

Session Classification: Social

Contribution ID: 105

Type: **Poster**

Accelerating High-Dimensional Cosmological Inference with COSMOPOWER

A new generation of astronomical surveys, such as the recently launched European Space Agency's Euclid mission, will soon deliver exquisite datasets with unparalleled amounts of cosmological information, poised to change our understanding of the Universe. However, analysing these datasets presents unprecedented statistical challenges. Multiple systematic effects need to be carefully accounted for, which would otherwise lead to incorrect physical interpretations. Efficiently navigating the large, complex parameter spaces required for robust systematics modelling is critical to ensuring that the anticipated increase in precision translates into equally enhanced accuracy in the final cosmological measurements.

My software COSMOPOWER tackles this challenge by training neural networks to emulate the computationally intensive calculation of cosmological power spectra. The emulation produces orders-of-magnitude acceleration in the inference pipeline. COSMOPOWER also enables the creation of fully-differentiable pipelines to leverage gradient-based sampling methods, which scale efficiently to high-dimensional parameter spaces. The acceleration provided by COSMOPOWER has led major international collaborations (e.g. Euclid, KiDS, ACT, Simons Observatory), working on both large-scale structure and Cosmic Microwave Background data, to adopt this software in their cosmological inference pipelines.

In this talk, I will showcase how recent advancements in COSMOPOWER pave the way for a new paradigm in cosmological inference, allowing for comprehensive Bayesian analyses—including both parameter estimation and model selection—to be conducted in a fraction of the time required by traditional methods, and extracting more information from the data than the traditional approach based on two-point statistics. The framework not only accelerates the inference process but also improves our ability to accurately model the underlying physics, especially for beyond-standard models, making it a critical tool for the future of cosmological research.

Presenter: SPURIO MANCINI, Alessio (Department of Physics, Royal Holloway, University of London)

Session Classification: Social

Contribution ID: 106

Type: **Poster**

Learning Optimal and Interpretable Summary Statistics of Galaxy Catalogs with SBI

How much cosmological information can we reliably extract from existing and upcoming large-scale structure observations? Many summary statistics fall short in describing the non-Gaussian nature of the late-time Universe and modelling uncertainties from baryonic physics. Using simulation based inference (SBI) with automatic data-compression from graph neural networks, we learn optimal summary statistics for galaxy catalogs in the context of cosmological parameter estimation. By construction these summaries do not require the ability to write down an explicit likelihood. We demonstrate that they can be used for efficient parameter inference, outperforming existing (ML) methods for the same parameter estimation. These summary statistics offer a new avenue for analyzing different simulation models for baryonic physics with respect to their relevance for the resulting cosmological features. The learned summary statistics are low-dimensional, feature the underlying simulation parameters, and are similar across different network architectures. To link our models, we identify the relevant scales associated to our summary statistics (e.g. in the range of modes between) and we are able to match the summary statistics to underlying simulation parameters across various simulation models. Furthermore, we compare different baryonic feedback models in latent space and find differences in the flexibility of their parametrizations.

Presenter: LEHMAN, Kai (LMU Munich)

Session Classification: Social

Contribution ID: **107**Type: **Poster**

Bayesian evidence estimation with normalizing flows

Using , an improved Bayesian evidence (and its numerical uncertainty) estimation method based on normalizing flows, we estimate the Bayes factor in favor of gravitational wave overtones in the ringdown of the first detection. We find good agreement with nested sampling. Provided representative samples from the target posterior are available, our method is more robust to posterior distributions with sharp features, especially in higher dimensions. I propose a metric to evaluate the flow training completion using the latent space map of the posterior samples. Finally, I introduce a nested flow technique for improved density estimation.

Presenter: SRINIVASAN, Rahul

Session Classification: Social

Contribution ID: **108**Type: **Poster**

lsbi: linear simulation based inference

Simulation-based inference is undergoing a renaissance in statistics and machine learning. With several packages implementing the state-of-the-art in expressive AI [mackelab/sbi] [undark-lab/swyft], it is now being effectively applied to a wide range of problems in the physical sciences, biology, and beyond.

Given the rapid pace of AI/ML, there is little expectation that the implementations of the future will resemble these current first generation neural network-based approaches. This talk will present a new framework for simulation-based inference, linear simulation-based inference (lsbi), which abstracts the core principles of SBI from the specific details of machine learning, implementing a plug-and-play framework of linear and mixture models.

lsbi has several use-cases:

1. It is pedagogically helpful to separate out the general principles of SBI from the specific details of neural networks (particularly for ML skeptics).
2. It is practically useful for producing expressive examples with known ground truths.
3. It is pragmatically useful, since in many cases, lsbi is competitive with neural approaches in terms of accuracy, whilst being faster and more interpretable.

An evolving code-driven PyPI/conda research package is available at:
<https://github.com/handley-lab/lsbi>

Presenter: Dr HANDLEY, William

Session Classification: Social

Contribution ID: **109**Type: **Poster**

Noise injection node regularization for robust learning

We introduce Noise Injection Node Regularization (NINR), a method that injects structured noise into Deep Neural Networks (DNNs) during the training stage, resulting in an emergent regularizing effect. We present both theoretical and empirical evidence demonstrating substantial improvements in robustness against various test data perturbations for feed-forward DNNs trained under NINR. The novelty of our approach lies in the interplay between adaptive noise injection and initialization conditions, such that noise becomes the dominant driver of dynamics at the start of training. Since this method simply requires the addition of external nodes without altering the existing network structure or optimization algorithms, it can be easily incorporated into many standard problem specifications. We observe improved stability against a range of data perturbations, including domain shifts, with the most dramatic improvement occurring for unstructured noise, where our technique outperforms existing methods such as Dropout or L2 regularization in some cases. Additionally, we show that desirable generalization properties on clean data are generally maintained. This method is well-suited for many physical scenarios where robust predictions are critical to neural network performance. Currently, we are employing this method to improve networks' ability to discriminate between prompt and non-prompt photons in highly noisy processes in the most recent simulations of the ATLAS detector.

Presenter: LEVI, Noam (Tel Aviv University)

Session Classification: Social

Contribution ID: **110**

Type: **Poster**

Poster 1

Primary Field of Research

Presenter: DAS, Indranil (Imperial College London (GB))

Session Classification: Social

Contribution ID: 111

Type: **Contributed Talk**

Lorentz-Equivariant Geometric Algebra Transformers for High-Energy Physics

Tuesday 10 September 2024 10:00 (30 minutes)

Extracting scientific understanding from particle-physics experiments requires solving diverse learning problems with high precision and good data efficiency. We propose the Lorentz Geometric Algebra Transformer (L-GATr), a new multi-purpose architecture for high-energy physics. L-GATr represents high-energy data in a geometric algebra over four-dimensional space-time and is equivariant under Lorentz transformations, the symmetry group of relativistic kinematics. At the same time, the architecture is a Transformer, which makes it versatile and scalable to large systems. L-GATr is first demonstrated on regression and classification tasks from particle physics. We then construct the first Lorentz-equivariant generative model: a continuous normalizing flow based on an L-GATr network, trained with Riemannian flow matching. Across our experiments, L-GATr is on par with or outperforms strong domain-specific baselines.

Presenter: SPINNER, Jonas**Session Classification:** Talks

Contribution ID: 112

Type: **Contributed Talk**

Improved Weak Lensing Photometric Redshift Calibration via StratLearn and Hierarchical Modeling

Wednesday 11 September 2024 10:10 (25 minutes)

Discrepancies between cosmological parameter estimates from cosmic shear surveys and from recent Planck cosmic microwave background measurements challenge the ability of the highly successful Λ CDM model to describe the nature of the Universe. To rule out systematic biases in cosmic shear survey analyses, accurate redshift calibration within tomographic bins is key. In this work, we improve photo- z calibration via Bayesian hierarchical modeling of full galaxy photo- z conditional densities, by employing StratLearn, a recently developed statistical methodology, which accounts for systematic differences in the distribution of the spectroscopic training/source set and the photometric target set. Using realistic simulations that were designed to resemble the KiDS+VIKING-450 dataset, we show that StratLearn-estimated conditional densities improve the galaxy tomographic bin assignment, and that our StratLearn-Bayesian framework leads to nearly unbiased estimates of the target population means. This leads to a factor of ~ 2 improvement upon often used and state-of-the-art photo- z calibration methods. Our approach delivers a maximum bias per tomographic bin of $\Delta\langle z \rangle = 0.0095 \pm 0.0089$, with an average absolute bias of 0.0052 ± 0.0067 across the five tomographic bins.

Presenter: AUTENRIETH, Maximilian (Imperial College London)

Session Classification: Talks

Contribution ID: 113

Type: **Contributed Talk**

Anomaly aware machine learning for dark matter direct detection at the DARWIN experiment

Tuesday 10 September 2024 17:10 (25 minutes)

This talk presents a novel approach to dark matter direct detection using anomaly-aware machine learning techniques in the DARWIN next-generation dark matter direct detection experiment. I will introduce a semi-supervised deep learning pipeline that falls under the umbrella of generalized Simulation-Based Inference (SBI), an approach that allows one to effectively learn likelihoods straight from simulated data, without the need for complex functional dependence on systematics or nuisance parameters. I also present an inference procedure to detect non-background physics utilizing an anomaly function derived from the loss functions of the semi-supervised architecture. The pipeline's performance is evaluated using pseudo-data sets in a sensitivity forecasting task, and the results suggest that it offers improved sensitivity over traditional methods.

Presenter: SCAFFIDI, Andre Joshua**Session Classification:** Talks

Contribution ID: 114

Type: **not specified**

Extending Unfolding Methods With Machine Learning

Wednesday 11 September 2024 11:45 (45 minutes)

Correcting experimental measurements for detector effects, or unfolding, is a standard technique used at the LHC to report multi-differential cross section measurements. These techniques rely on binned data and are limited to low dimensional observables. In this talk, I will cover recent ideas to extend standard methods of unfolding using machine learning, enabling the measurements of unbinned and high-dimensional differential cross sections. These include methods using classifiers as approximators to the likelihood ratio, generative models, and high dimensional interpolation techniques.

Primary Field of Research

Primary author: MIKUNI, Vinicius (LBL)

Presenter: MIKUNI, Vinicius (LBL)

Session Classification: Talks

Contribution ID: 115

Type: **not specified**

The statistics of deep generative models for the LHC

Wednesday 11 September 2024 15:15 (45 minutes)

In recent years, deep generative models (DGMs) have become essential for various steps in the LHC simulation and analysis chain. While there are many types of DGMs, no Swiss-army-knife architecture exists that can effectively handle speed, precision, and control simultaneously. In this talk, I will explore different DGMs, outline their strengths and weaknesses, and illustrate typical applications in high-energy physics. Moreover, I will introduce several methods to quantify and enhance model quality, including Bayesian neural networks for uncertainty estimation, the classifier test to identify failure modes, and reweighting using the DCTR approach. Lastly, to spark further discussion, I will discuss the *amplification methods for addressing the question, “How many more events can a DGM generate?”

Presenter: WINTERHALDER, Ramon (UCLouvain)

Session Classification: Talks

Contribution ID: 116

Type: **Contributed Talk**

Development of systematic-aware neural network trainings for binned-likelihood-analyses at the LHC

Wednesday 11 September 2024 17:40 (25 minutes)

We demonstrate a neural network training, capable of accounting for the effects of systematic variations of the utilized data model in the training process and describe its extension towards neural network multiclass classification. We show the importance of adjusting backpropagation to be able to handle derivatives of histogram bins during training and add an interpretation of the optimization process itself, highlighting the differences between the systematic aware and conventional training strategies. Trainings for binary and multiclass classification with seven output classes are performed, based on a comprehensive data model with 86 nontrivial shape-altering systematic variations, as used for a previous measurement. The neural network output functions are used to infer the signal strengths for inclusive Higgs boson production, as well as for Higgs boson production via gluon-fusion (rggH) and vector boson fusion (rqqH). With respect to a conventional training, based on cross-entropy, we observe improvements of 12 and 16 %, for the sensitivity in rggH and rqqH, respectively.

Presenter: MONSCH, Artur (KIT - Karlsruhe Institute of Technology (DE))

Session Classification: Talks

Contribution ID: 117

Type: **Poster**

Uncertainty-aware machine learning for the LHC

Tuesday 10 September 2024 18:00 (1 minute)

Estimating uncertainties is a fundamental aspect in every physics problem, no measurements or calculations comes without uncertainties. Hence it is crucial to consider the effect of training a neural network to problems in physics. I will present our work on amplitude regression, using loop amplitudes from LHC processes, as an example to examine the impact of different uncertainties on the outcome of the network. We test the behavior of different neural networks with uncertainty estimation, including Bayesian neural networks and repulsive ensembles.

Presenter: ELMER, Nina**Session Classification:** Social

Contribution ID: **118**Type: **Poster**

Generative models: their evaluation and their limitations

Tuesday 10 September 2024 18:01 (1 minute)

I will present and discuss several proposed metrics, based on integral probability measures, for the evaluation of generative models (and, more generally, for the comparison of different generators). Some of the metrics are particularly efficient to be computed in parallel, and show good performances. I will first compare the metrics on toy multivariate/multimodal distributions, and then focus on HEP examples from the JetNet jet dataset. I will discuss the power of the tests and their implementation in TensorFlow2, making the opportunity to discuss, more generally, the limitations in the usage of generative models in HEP.

Presenter: GROSSI, Samuele (Università degli studi di Genova & INFN sezione di Genova)

Session Classification: Social

Contribution ID: 119

Type: **Poster**

Limits to classification performance by relating Kullback-Leibler divergence to Cohen's Kappa

Tuesday 10 September 2024 18:02 (1 minute)

The performance of machine learning classification algorithms are evaluated by estimating metrics, often from the confusion matrix, using training data and cross-validation. However, these do not prove that the best possible performance has been achieved. Fundamental limits to error rates can be estimated using information distance measures. To this end, the confusion matrix has been formulated to comply with the Chernoff-Stein Lemma. This links the error rates to the Kullback-Leibler divergences between the probability density functions describing the two classes. This leads to a key result that relates Cohen's Kappa to the Resistor Average Distance which is the parallel resistor combination of the two Kullback-Leibler divergences. The Resistor Average Distance has units of bits and is estimated from the same training data used by the classification algorithm, using kNN estimates of the Kullback-Leibler divergences. The classification algorithm gives the confusion matrix and Kappa. Theory and methods are discussed in detail and then applied to Monte Carlo data and real datasets. Four very different real datasets - Breast Cancer, Coronary Heart Disease, Bankruptcy, and Particle Identification - are analysed, with both continuous and discrete values, and their classification performance compared to the expected theoretical limit. In all cases this analysis shows that the algorithms could not have performed any better due to the underlying probability density functions for the two classes. Important lessons are learnt on how to predict the performance of algorithms for imbalanced data. Preprint available at [arXiv:2403.01571](https://arxiv.org/abs/2403.01571).

Presenter: WATTS, Stephen**Session Classification:** Social

Contribution ID: 120

Type: **not specified**

Graph neural networks on the test bench in HEP applications

Tuesday 10 September 2024 18:03 (1 minute)

Data analyses in the high-energy particle physics (HEP) community more and more often exploit advanced multivariate methods to separate signal from background processes. In this talk, a maximally unbiased, in-depth comparison of the graph neural network (GNN) architecture, which is of increasing popularity in the HEP community, with the already well-established technology of fully connected feed-forward deep neural networks (DNNs) is presented. When it comes to choosing a suitable machine-learning model, it is not a priori clear, what model this should be to benefit from inherent properties of the task. Also, the design of a fair and unbiased benchmark is non-trivial. This GNN vs. DNN comparison is insightful in terms of the details it reveals as to which aspects of GNNs are superior to DNNs - and which are not. The study is performed on a typical data set of a complex challenge recently faced at the Large Hadron Collider: the classification of events with top quark-antiquark pairs with additional heavy flavour jets originating from gluon splittings, Z or Higgs bosons.

The study is documented in the paper “A Case Study of Sending Graph Neural Networks Back to the Test Bench for Applications in High-Energy Particle Physics” published in *Computing and Software for Big Science*, <https://doi.org/10.1007/s41781-024-00122-3>.

Presenter: PFEFFER, Emanuel Lorenz (KIT - Karlsruhe Institute of Technology (DE))

Session Classification: Social

Contribution ID: 121

Type: **Poster**

The Landscape of Unfolding with Machine Learning

Recent innovations from machine learning allow for data unfolding, without binning and including correlations across many dimensions. We describe a set of known, upgraded, and new methods for ML-based unfolding. The performance of these approaches are evaluated on the same two datasets. We find that all techniques are capable of accurately reproducing the particle-level spectra across complex observables. Given that these approaches are conceptually diverse, they offer an exciting toolkit for a new class of measurements that can probe the Standard Model with an unprecedented level of detail and may enable sensitivity to new phenomena.

Presenter: MARIÑO VILLADAMIGO, Javier (Institut für Theoretische Physik - University of Heidelberg)

Session Classification: Social

Contribution ID: 122

Type: **Poster**

Interpolated Likelihoods for Fast Reinterpretations

Tuesday 10 September 2024 18:04 (1 minute)

We present a method to accelerate Effective Field Theory reinterpretations using interpolated likelihoods. By employing Radial Basis Functions for interpolation and Gaussian Processes to strategically select interpolation points, we show that we can reduce the computational burden while maintaining accuracy. We apply this in the context of the Combined Higgs Boson measurement at CMS, a complex statistical model with many thousands of parameters requiring large computing power to evaluate.

Presenter: RUNTING, Tom (Imperial College (GB))

Session Classification: Social

Contribution ID: 123

Type: **Poster**

Efficient machine learning for statistical hypothesis testing

Tuesday 10 September 2024 18:05 (1 minute)

Traditional statistical methods are often not adequate to perform inclusive and signal-agnostic searches at modern collider experiments delivering large amounts of multivariate data. Machine learning provides a set of tools to enhance analyses in large scale regimes, but the adoption of these methodologies comes with new challenges, such as the lack of efficiency and robustness, and potential hidden biases. In this talk, I will discuss these aspects in the context of a recent proposal for a likelihood-ratio-based goodness-of-fit test powered by large-scale implementations of kernel methods, nonparametric learning models that can approximate any continuous function given enough data.

Presenter: Dr LETIZIA, Marco

Session Classification: Social

Contribution ID: 124

Type: **Poster**

Integrating Explainable AI in Data Analyses of ATLAS Experiment at CERN

Tuesday 10 September 2024 18:06 (1 minute)

“The Multi-disciplinary Use Cases for Convergent Approaches to AI Explainability (MUCCA) project is pioneering efforts to enhance the transparency and interpretability of AI algorithms in complex scientific fields. This study focuses on the application of Explainable AI (XAI) in high-energy physics (HEP), utilising a range of machine learning (ML) methodologies, from classical boosted decision trees to Graph Neural Networks (GNNs), to explore new physics models.

Our work leverages case studies from the ATLAS experiment at the Large Hadron Collider (LHC) to demonstrate the potential of ML in improving sensitivity to new physics. Notably, GNNs outperformed traditional Convolutional Neural Networks (CNNs), with the DarkJetGraphs code achieving a 2-5% improvement in detection accuracy and twice the background rejection efficiency. These findings affirm the value of GNNs in extending the search space for new physics models that conventional methods may not adequately capture. Balancing the use of cutting-edge ML with transparency and interpretability through XAI techniques is critical to ensuring both scientific rigor and robust result interpretation.

The presented research highlights this balance, with further developments in XAI techniques, including Kappa pruning and differentiable programming, proved to further enhance performance. A full publication of these methods and results is anticipated in Autumn 2024.

Primary Field of Research

Presenter: CARMIGNANI, Joseph (University of Liverpool (GB))

Session Classification: Social

Contribution ID: 125

Type: **Poster**

Proximal Nested Sampling with Data-Driven AI Priors

Tuesday 10 September 2024 18:07 (1 minute)

Bayesian model selection provides a powerful framework for objectively comparing models directly from observed data, without reference to ground truth data. However, Bayesian model selection requires the computation of the marginal likelihood (model evidence), which is computationally challenging, prohibiting its use in many high-dimensional Bayesian inverse problems. With Bayesian imaging applications in mind, we introduce the proximal nested sampling methodology to objectively compare alternative Bayesian imaging models for applications that use images to inform decisions under uncertainty. The methodology is based on nested sampling, a Monte Carlo approach specialised for model comparison, and exploits proximal Markov chain Monte Carlo techniques to scale efficiently to large problems and to tackle models that are log-concave and not necessarily smooth (e.g., involving l_1 or total-variation priors). Taking one step further, we show how proximal nested sampling can be extended using Tweedie's formula to support data-driven priors, such as deep neural networks learned from training data. We demonstrate our method by carrying out Bayesian model comparison between data-driven and hand-crafted priors in imaging applications like radio-interferometric image reconstruction. Based on arXiv:2106.03646 and arXiv:2307.00056

Presenter: ALDRIDGE, Henry (UCL)**Session Classification:** Social

Contribution ID: 126

Type: **Poster**

Generative models of astrophysical fields with scattering transforms on the sphere

Tuesday 10 September 2024 18:08 (1 minute)

Scattering transforms are a new type of summary statistics recently developed for the study of highly non-Gaussian processes, which have been shown to be very promising for astrophysical studies. In particular, they allow one to build generative models of complex non-linear fields from a limited amount of data, and have also been used as the basis of new statistical component separation algorithms. In the context of upcoming cosmological surveys, such as LiteBIRD for the cosmic microwave background polarization or Rubin-LSST and Euclid for study of the large scale structures of the Universe, the extension of these tools to spherical data is necessary. We develop scattering transforms on the sphere and focus on the construction of maximum-entropy generative models of several astrophysical fields. We construct, from a single target field, generative models of homogeneous astrophysical and cosmological fields, whose samples are quantitatively compared to the target fields using common statistics (power spectrum, pixel probability density function and Minkowski functionals). Our sampled fields agree well with the target fields, both statistically and visually. These generative models therefore open up a wide range of new applications for future astrophysical and cosmological studies; particularly those for which very little simulated data is available. We make our code available to the community so that this work can be easily reproduced and developed further.

Presenter: PRICE, Matt**Session Classification:** Social

Contribution ID: 127

Type: **Poster**

Advanced techniques for Simulation Based Inference in collider physics

Tuesday 10 September 2024 18:09 (1 minute)

We present an application of Simulation-Based Inference (SBI) in collider physics, aiming to constrain anomalous interactions beyond the Standard Model (SM). This is achieved by leveraging Neural Networks to learn otherwise intractable likelihood ratios. We explore methods to incorporate the underlying physics structure into the likelihood estimation process. Specifically, we compare two approaches: morphing-aware likelihood estimation and derivative learning. Furthermore, we illustrate how uncertainty-aware networks can be employed to compare the performance of these methods. Additionally, we demonstrate two new techniques for enhancing the accuracy and reliability of the network training. First, we introduce a new way to treat the outliers in the target reconstruction-level distributions by repeated smearing and modifying their parton-level weights accordingly (dubbed fractional smearing). Second, we utilise Lorentz-equivariant network architectures to exploit the symmetry structure inherent in the underlying particle physics amplitudes.

Presenter: DE CRESCENZO, Giovanni (University of Heidelberg)

Session Classification: Social

Contribution ID: 128

Type: **Poster**

SBI for wide field weak lensing

Tuesday 10 September 2024 18:10 (1 minute)

The standard approach to inference from cosmic large-scale structure data employs summary statistics that are compared to analytic models in a Gaussian likelihood with pre-computed covariance. To overcome many of the idealising assumptions that go into this type of explicit likelihood inference, and to take advantage of the high-fidelity wide field data that Euclid and LSST will provide, we can employ simulation-based inference (SBI). In previous work we have demonstrated the power of SBI in the context of performing a full re-analysis of the KiDS-1000 survey (MvWK & KL 2024) whilst modelling anisotropic observational systematics with forward simulations that significantly impact the outcome of the inference and must be included in the analysis of Euclid and LSST data. We further report on the effects of different levels of Gaussianity imposed on the inference. Our current work explores the use of wavelet summary statistics to construct higher order summary statistics directly from the field without any machine learning. This method thus does not suffer from many of the problems that are associated with using neural methods whilst being fast and capable of extracting large amounts of information. We present here an outlook of how we can tackle the task of SBI applied to upcoming wide field weak lensing surveys.

Presenter: LIN, Kiyam**Session Classification:** Social

Contribution ID: 129

Type: **Poster**

Exhaustive Symbolic Regression: Learning Astrophysics directly from Data

Tuesday 10 September 2024 18:11 (1 minute)

A key challenge in the field of AI is to make machine-assisted discovery interpretable, enabling it not only to uncover correlations but also to improve our physical understanding of the world. A nascent branch of machine learning –Symbolic Regression (SR) –aims to discover the optimal functional representations of datasets, producing perfectly interpretable outputs (equations) by construction.

SR is traditionally done using a “genetic algorithm” which stochastically selects trial functions by analogy with natural selection; I will describe the more ambitious approach of exhaustively searching and evaluating function space.

Coupled to an information-theoretic model selection principle based on minimum description length, our algorithm “Exhaustive Symbolic Regression”(ESR) is guaranteed to find the simple functions that optimally balance accuracy with simplicity on a dataset. This gives it broad application across science. I will detail the method, its relation to Bayesian statistics and an optional language model-based prior on functions designed to enhance their physicality. Then I will use ESR to quantify the extent to which state-of-the-art astrophysical theories –FLRW cosmology, General Relativity and Inflation –are implied by the current data.

Presenter: DESMOND, Harry (University of Portsmouth)

Session Classification: Social

Contribution ID: 130

Type: **Poster**

Usage of weakly correlated observables for nuisance parameter fits

Tuesday 10 September 2024 18:12 (1 minute)

Precision measurements at the Large Hadron Collider (LHC), such as the measurement of the top quark mass, are essential for advancing our understanding of fundamental particle physics. Profile likelihood fits have become the standard method to extract physical quantities and parameters from the measurements. These fits incorporate nuisance parameters to include systematic uncertainties. The results depend critically on the selection of observables. Including multiple observables from the measurements is beneficial for precision, as it helps to restrict the nuisance parameters, leading to more reliable fits. Usually, the used observables are assumed to be independent; however, including more observables can introduce correlations that complicate the analysis, as these correlations violate the assumption of independence. At the current precision of the top quark mass measurement, introducing more observables with minor correlations might already lead to a significant distortion of the results of the profile likelihood fit. This project aims to investigate the threshold of correlation at which the accuracy of likelihood fits begins to degrade. We utilize the realistically correlated reconstructed top and W mass, applying an uncorrelated single event likelihood fit for the analysis. To assess the accuracy of our fits, we calculate the pull for the nuisance parameters alongside the top quark mass distribution. Subsequently, we will explore machine learning techniques, such as normalizing flows, that take correlations into account instead of avoiding them.

Presenter: STIETZ, Lars (Hamburg University of Technology (DE))

Session Classification: Social

Contribution ID: 131

Type: **Poster**

Accounting for Selection Effects in Supernova Cosmology with Simulation-Based Inference and Hierarchical Bayesian Modelling

Tuesday 10 September 2024 18:13 (1 minute)

Type Ia supernovae (SNe Ia) are thermonuclear exploding stars that can be used to put constraints on the nature of our universe. One challenge with population analyses of SNe Ia is Malmquist bias, where we preferentially observe the brighter SNe due to limitations of our telescopes. If untreated, this bias can propagate through to our posteriors on cosmological parameters. In this work, we develop a novel technique of using a normalising flow to learn the non-analytical likelihood of observing a SN Ia for a given survey from simulations, that is independent of any cosmological model. The learnt likelihood is then used in a hierarchical Bayesian model with Hamiltonian Monte Carlo sampling to put constraints on different sets of cosmological parameters conditioned on the observed data. The technique is verified on toy model simulations finding excellent agreement with analytically-derived posteriors to within 1σ . We conclude by discussing plans to show the generalisation of our flexible method to real survey selection effects where analytical solutions are intractable.

Presenter: BOYD, Benjamin (University of Cambridge)

Session Classification: Social

Contribution ID: 132

Type: **Poster**

COMoving Computer Acceleration (COCA): Correcting Emulation Errors for Trustworthy N-Body Simulations

Tuesday 10 September 2024 18:14 (1 minute)

Neural networks are increasingly used to emulate complex simulations due to their speed and efficiency. Unfortunately, many ML algorithms, including (deep) neural networks, lack interpretability. If machines predict something humans do not understand, how can we check (and trust) the results? Even if we could identify potential mistakes, current methods lack effective mechanisms to correct them, limiting the reliability of these emulators. To address these issues, we introduce COMoving Computer Acceleration (COCA), a novel hybrid framework that integrates machine learning with traditional N-body simulators. COCA solves the correct physical equations of motion within an emulated frame of reference, inherently correcting any prediction errors. Our framework significantly reduces emulation errors in particle trajectories but also requires far fewer force evaluations compared to conventional simulations. This method effectively addresses the critical challenges of interpretability and accuracy in cosmological applications of machine learning, ensuring both speed and trustworthiness in complex simulations.

Presenter: BARTLETT, Deaglan (Institut d'Astrophysique de Paris)

Session Classification: Social

Contribution ID: 133

Type: **Poster**

Application of Machine Learning Based Top Quark and Jet Tagging to Hadronic Four-Top Final States Induced by SM as well as BSM Processes

Tuesday 10 September 2024 18:15 (1 minute)

The aim of this work is to solve the problem of hadronic jet substructure recognition using classical subjetness variables available in the parameterized detector simulation package, Delphes. Jets produced in simulated proton-proton collisions are identified as either originating from the decay of a top quark or a W boson and are used to reconstruct the mass of a hypothetical scalar resonance decaying into a pair of top quarks in events where a total of four top quarks are produced. We compare a simple cut-based tagging method for the stacked histograms of a mixture of the Standard Model and new physics processes with a multi-layer perceptron classifier and a gradient boosting classifier. Due to the sufficient amount of data, we applied various undersampling techniques to the training sets. Our findings demonstrate that gradient boosting methods provide better results than the other tested approaches.

Presenter: MACHALOVÁ, Monika**Session Classification:** Social

Contribution ID: 134

Type: **Poster**

Accelerating High-Dimensional Cosmological Inference with COSMOPOWER

Tuesday 10 September 2024 18:16 (1 minute)

A new generation of astronomical surveys, such as the recently launched European Space Agency's Euclid mission, will soon deliver exquisite datasets with unparalleled amounts of cosmological information, poised to change our understanding of the Universe. However, analysing these datasets presents unprecedented statistical challenges. Multiple systematic effects need to be carefully accounted for, which would otherwise lead to incorrect physical interpretations. Efficiently navigating the large, complex parameter spaces required for robust systematics modelling is critical to ensuring that the anticipated increase in precision translates into equally enhanced accuracy in the final cosmological measurements.

My software COSMOPOWER tackles this challenge by training neural networks to emulate the computationally intensive calculation of cosmological power spectra. The emulation produces orders-of-magnitude acceleration in the inference pipeline. COSMOPOWER also enables the creation of fully-differentiable pipelines to leverage gradient-based sampling methods, which scale efficiently to high-dimensional parameter spaces. The acceleration provided by COSMOPOWER has led major international collaborations (e.g. Euclid, KiDS, ACT, Simons Observatory), working on both large-scale structure and Cosmic Microwave Background data, to adopt this software in their cosmological inference pipelines.

In this poster, I will showcase how recent advancements in COSMOPOWER pave the way for a new paradigm in cosmological inference, allowing for comprehensive Bayesian analyses—including both parameter estimation and model selection—to be conducted in a fraction of the time required by traditional methods, and extracting more information from the data than the traditional approach based on two-point statistics. The framework not only accelerates the inference process but also improves our ability to accurately model the underlying physics, especially for beyond-standard models, making it a critical tool for the future of cosmological research.

Presenter: SPURIO MANCINI, Alessio (Royal Holloway, University of London)

Session Classification: Social

Contribution ID: 135

Type: **Poster**

Learning Optimal and Interpretable Summary Statistics of Galaxy Catalogs with SBI

Tuesday 10 September 2024 18:17 (1 minute)

How much cosmological information can we reliably extract from existing and upcoming large-scale structure observations? Many summary statistics fall short in describing the non-Gaussian nature of the late-time Universe and modelling uncertainties from baryonic physics. Using simulation based inference (SBI) with automatic data-compression from graph neural networks, we learn optimal summary statistics for galaxy catalogs in the context of cosmological parameter estimation. By construction these summaries do not require the ability to write down an explicit likelihood. We demonstrate that they can be used for efficient parameter inference, outperforming existing (ML) methods for the same parameter estimation. These summary statistics offer a new avenue for analyzing different simulation models for baryonic physics with respect to their relevance for the resulting cosmological features. The learned summary statistics are low-dimensional, feature the underlying simulation parameters, and are similar across different network architectures. To link our models, we identify the relevant scales associated to our summary statistics (e.g. in the range of modes between $k = 5 - 30 h/M \text{ pc}$) and we are able to match the summary statistics to underlying simulation parameters across various simulation models. Furthermore, we compare different baryonic feedback models in latent space and find differences in the flexibility of their parametrizations.

Presenter: LEHMAN, Kai (LMU Munich)**Session Classification:** Social

Contribution ID: 136

Type: **Poster**

Bayesian evidence estimation with normalizing flows

Using floZ, an improved Bayesian evidence (and its numerical uncertainty) estimation method based on normalizing flows, we estimate the Bayes factor in favor of gravitational wave overtones in the ringdown of the first detection. We find good agreement with nested sampling. Provided representative samples from the target posterior are available, our method is more robust to posterior distributions with sharp features, especially in higher dimensions. I propose a metric to evaluate the flow training completion using the latent space map of the posterior samples. Finally, I introduce a nested flow technique for improved density estimation.

Presenter: SRINIVASAN, Rahul

Session Classification: Social

Contribution ID: 137

Type: **Poster**

Noise injection node regularization for robust learning

Tuesday 10 September 2024 18:19 (1 minute)

We introduce Noise Injection Node Regularization (NINR), a method that injects structured noise into Deep Neural Networks (DNNs) during the training stage, resulting in an emergent regularizing effect. We present both theoretical and empirical evidence demonstrating substantial improvements in robustness against various test data perturbations for feed-forward DNNs trained under NINR. The novelty of our approach lies in the interplay between adaptive noise injection and initialization conditions, such that noise becomes the dominant driver of dynamics at the start of training. Since this method simply requires the addition of external nodes without altering the existing network structure or optimization algorithms, it can be easily incorporated into many standard problem specifications. We observe improved stability against a range of data perturbations, including domain shifts, with the most dramatic improvement occurring for unstructured noise, where our technique outperforms existing methods such as Dropout or L2 regularization in some cases. Additionally, we show that desirable generalization properties on clean data are generally maintained. This method is well-suited for many physical scenarios where robust predictions are critical to neural network performance. Currently, we are employing this method to improve networks' ability to discriminate between prompt and non-prompt photons in highly noisy processes in the most recent simulations of the ATLAS detector.

Presenter: LEVI, Noam (Tel Aviv University)

Session Classification: Social

Contribution ID: 138

Type: **Poster**

Modeling Smooth Backgrounds at Collider Experiments With Log Gaussian Cox Processes

Tuesday 10 September 2024 18:20 (1 minute)

Background modeling is one of the critical elements of searches for new physics at experiments at the Large Hadron Collider. In many searches, backgrounds are modeled using analytic functional forms. Finding an acceptable function can be complicated, inefficient and time-consuming. This poster presents a novel approach to estimating the underlying PDF of a 1D dataset of samples using Log Gaussian Cox Processes (LGCP). Using LGCP allows inferring a posterior distribution for the PDF, and unlike a Gaussian Process fit, it does not require binning the dataset. Markov Chain Monte Carlo (MCMC) is used to optimize the LGCP fit. The final result is a fit model which is highly flexible, does not rely on an analytic fit assumption, and carries uncertainty bands.

Presenter: FRID, Yuval Yitzhak (Tel Aviv University (IL))

Session Classification: Social

Contribution ID: 139

Type: **Poster**

Modeling Smooth Backgrounds at Collider Experiments With Log Gaussian Cox Processes

Background modeling is one of the critical elements of searches for new physics at experiments at the Large Hadron Collider. In many searches, backgrounds are modeled using analytic functional forms. Finding an acceptable function can be complicated, inefficient and time-consuming. This poster presents a novel approach to estimating the underlying PDF of a 1D dataset of samples using Log Gaussian Cox Processes (LGCP). Using LGCP allows inferring a posterior distribution for the PDF, and unlike a Gaussian Process fit, it does not require binning the dataset. Markov Chain Monte Carlo (MCMC) is used to optimize the LCGP fit. The final result is a fit model which is highly flexible, does not rely on an analytic fit assumption, and carries uncertainty bands.

Primary Field of Research

Primary author: FRID, Yuval Yitzhak (Tel Aviv University (IL))

Presenter: FRID, Yuval Yitzhak (Tel Aviv University (IL))

Contribution ID: 140

Type: **Poster**

Noise injection node regularization for robust learning

We introduce Noise Injection Node Regularization (NINR), a method that injects structured noise into Deep Neural Networks (DNNs) during the training stage, resulting in an emergent regularizing effect. We present both theoretical and empirical evidence demonstrating substantial improvements in robustness against various test data perturbations for feed-forward DNNs trained under NINR. The novelty of our approach lies in the interplay between adaptive noise injection and initialization conditions, such that noise becomes the dominant driver of dynamics at the start of training. Since this method simply requires the addition of external nodes without altering the existing network structure or optimization algorithms, it can be easily incorporated into many standard problem specifications. We observe improved stability against a range of data perturbations, including domain shifts, with the most dramatic improvement occurring for unstructured noise, where our technique outperforms existing methods such as Dropout or L2 regularization in some cases. Additionally, we show that desirable generalization properties on clean data are generally maintained. This method is well-suited for many physical scenarios where robust predictions are critical to neural network performance. Currently, we are employing this method to improve networks' ability to discriminate between prompt and non-prompt photons in highly noisy processes in the most recent simulations of the ATLAS detector.

Primary Field of Research

Primary author: LEVI, Noam (Tel Aviv University)

Presenter: LEVI, Noam (Tel Aviv University)

Contribution ID: 141

Type: **not specified**

Generative Unfolding

Wednesday 11 September 2024 14:00 (25 minutes)

Looking for a way modern machine learning transforms LHC physics, unfolding has for a long time been one of our goal, and only modern networks allow us to do this meaningfully. It does not only make analyses with a wide range of theory hypotheses more efficient, it also allows the LHC collaborations to publish their data. I will show how generative networks can be used for this purpose, directly learning conditional probabilities in complete analogy to a forward simulations. I will then illustrate the power of this method using a challenging CMS case study.

Primary Field of Research

Presenter: PLEHN, Tilman (Heidelberg University)

Session Classification: Talks

Contribution ID: 142

Type: **Contributed Talk**

Fairness Methods in Particle Physics Event Classification

Wednesday 11 September 2024 16:30 (25 minutes)

In social sciences, fairness in Machine Learning (ML) comprises the attempt to correct or eliminate algorithmic bias of gender, ethnicity, or sexual orientation from ML models. Many high-energy physics (HEP) analyses that search for a resonant decay of a particle employ mass-decorrelated event classifiers, as the particle mass is often used to perform the final signal extraction fit. These classifiers are designed to maintain fairness with respect to the mass, which is accomplished primarily by retaining mass-correlated information during training.

Our studies present a first proof-of-concept for systematically applying, testing and comparing fairness methods for ML-based event classifiers in HEP analyses. We explore techniques that mitigate mass correlation during and after training. Through simulations and a case studies, we demonstrate the effectiveness of these methods in maintaining fairness while preserving the classifier performance.

Presenter: RIEGER, Oliver (Nikhef National institute for subatomic physics (NL))

Session Classification: Talks

Contribution ID: 143

Type: **Contributed Talk**

Feldman-Cousins' ML Cousin

Tuesday 10 September 2024 17:35 (25 minutes)

The statistical treatment of sterile neutrino searches suffers from the fact that Wilks' theorem, a beneficial simplifying assumption, does not hold across all regions of parameter space. The alternative, the Feldman-Cousins algorithm, suffers from expensive computational run times that prohibit its application into many-experiment global fits. This contribution introduces a deep learning-based method (which does not assume Wilks' theorem) that can fit electron (anti)neutrino disappearance experiments in a tractable amount of time. Though this procedure's utility for sterile neutrino searches are presented here, it will be useful for a variety of particle physics analyses.

Presenter: VILLARREAL, Joshua**Session Classification:** Talks

Contribution ID: 144

Type: **Poster**

Precision Machine Learning for the Matrix Element Method

Tuesday 10 September 2024 18:21 (1 minute)

The matrix element method is the LHC inference method of choice for limited statistics, as it allows for optimal use of available information. We present a dedicated machine learning framework, based on efficient phase-space integration, a learned acceptance and transfer function. It is based on a choice of INN and diffusion networks, and a transformer to solve jet combinatorics. We showcase this setup for the CP-phase of the top Yukawa coupling in associated Higgs and single-top production.

Primary Field of Research

Primary author: HUETSCH, Nathan (Heidelberg)

Co-author: PLEHN, Tilman (Heidelberg University)

Presenters: HUETSCH, Nathan (Heidelberg); PLEHN, Tilman (Heidelberg University)

Session Classification: Social

Contribution ID: 145

Type: **not specified**

The Landscape of Unfolding with Machine Learning

Tuesday 10 September 2024 18:22 (1 minute)

Recent innovations from machine learning allow for data unfolding, without binning and including correlations across many dimensions. We describe a set of known, upgraded, and new methods for ML-based unfolding. The performance of these approaches are evaluated on the same two datasets. We find that all techniques are capable of accurately reproducing the particle-level spectra across complex observables. Given that these approaches are conceptually diverse, they offer an exciting toolkit for a new class of measurements that can probe the Standard Model with an unprecedented level of detail and may enable sensitivity to new phenomena

Primary Field of Research

Primary author: MARINO, Xavier (Heidelberg)

Co-author: PLEHN, Tilman (Heidelberg University)

Presenters: PLEHN, Tilman (Heidelberg University); MARINO, Xavier (Heidelberg)

Session Classification: Social

Contribution ID: 146

Type: **Poster**

How to Unfold Top Decays

Tuesday 10 September 2024 18:18 (1 minute)

Many physics analyses at the LHC rely on algorithms to remove detector effect, commonly known as unfolding. Whereas classical methods only work with binned, one-dimensional data, Machine Learning promises to overcome both problems. Using a generative unfolding pipeline, we show how it can be build into an existing LHC analysis, designed to measure the top mass. We discuss the model-dependence of our algorithm, i.e. the bias of our measurement towards the top mass used in simulation and propose a method to reliably achieve unbiased results.

Primary Field of Research

Primary author: PALACIOS SCHWEITZER, Sofia (Heidelberg)

Co-author: PLEHN, Tilman (Heidelberg University)

Presenters: PALACIOS SCHWEITZER, Sofia (Heidelberg); PLEHN, Tilman (Heidelberg University)

Session Classification: Social

Contribution ID: 147

Type: **not specified**

Welcome

Monday 9 September 2024 13:45 (15 minutes)

Presenter: LYONS, Louis (Imperial College (GB))

Session Classification: Introductory talks. These optional talks are aimed at people who feel that they would like more background introductory material, before the next 3 days' talks.