

Modern Machine Learning and Particle Physics Phenomenology at the LHC

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Abstract

Modern machine learning is driving a paradigm shift in particle physics phenomenology at the Large Hadron Collider. This short review examines the transformative role of machine learning across the entire theoretical prediction pipeline, from parton-level calculations to full simulations. We discuss applications to scattering amplitude computations, phase space integration, Parton Distribution Function determination, and parameter extraction. Some critical frontiers for the field including uncertainty quantification, the role of symmetries, and interpretability are highlighted.

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1 Introduction

The discovery of the Higgs boson at the LHC in 2012 inaugurated a new era in high-energy physics, opening the exploration of the new Yukawa force and confronting persistent puzzles that the Standard Model (SM) cannot explain, including dark matter, neutrino masses, matter-antimatter asymmetry, and the nature of gravity. The LHC is rapidly evolving into a precision machine, able to measure small deviations from SM predictions. This precision programme demands rigorous methodologies to interpret the extremely accurate and highly correlated experimental data and the increasingly complex theoretical predictions.

Particle physics phenomenology serves as the bridge between experimental observations and theoretical models, connecting what is measured at colliders to our fundamental understanding of Nature. In Bayesian terms, we seek the probability of a given theory given experimental data. At the LHC, however, the likelihood itself is extraordinarily complex, requiring a *divide-and-conquer* approach across multiple stages of the theoretical computations, from a given Lagrangian – whether the SM one or the one of some beyond-SM (BSM) scenarios.

From this starting point, predictions flow through several distinct levels: parton-level calculations involving scattering amplitudes, phase space integration, and Parton Distribution Functions (PDFs); particle-level simulations including QCD and QED radiation through parton

showers, fragmentation, and hadronisation; and finally detector-level modeling encompassing detector simulation, event reconstruction, and selection criteria.

Machine Learning (ML) is revolutionising every component of this intricate chain. The HEP ML living review [1] documents the breadth of this transformation. This short review starts with an attempt in Sect. 2 to provide an overview of some selected applications where ML provides unique advantages, focussing on the ingredients entering parton level predictions. In Sect. 3 we provide a brief sketch on some applications that enable to go beyond parton level, and simulate the full event. Finally, before concluding, in Sect. 4 we highlight some of the most compelling challenges in the field.

2 Machine Learning for Parton-Level Predictions

A differential cross section at the parton level at the LHC can be expressed as the product of squared scattering amplitudes, n -particle phase space, and PDFs characterising the proton's subnuclear structure. In this section we provide some examples that show how ML enables to extend, improve, simplify and speed up the determination of the main ingredients that enter any parton-level theoretical predictions at the LHC, namely the calculation of scattering amplitudes (Sect. 2.1), the phase space integration (Sect. 2.2) and the PDFs (Sect. 2.3). Finally in Sect. 2.4 we will quickly discuss parameter determination from parton level predictions. The list of applications mentioned here is certainly far from complete, and it is subject to the author's knowledge and unavoidable bias. Nevertheless we hope it gives an idea of the great power of machine learning in tackling the problems that we face as particle physicists.

2.1 Scattering Amplitude Calculations

Computing scattering amplitudes, particularly at higher multiplicities and loop orders, represents one of the most computationally intensive tasks in theoretical physics. Machine learning offers a natural solution through regression problems that exploit neural network (NN) flexibility to accelerate the computation of amplitudes. The approach trains ML regressors, often NNs or ensembles of NNs, on pre-computed "true" amplitudes evaluated at numerous phase space points. These trained networks then predict amplitudes accurately and rapidly for new phase space configurations.

Recent applications span processes from simple two-to-two scattering to complex multi-particle final states, with NNs demonstrating performance superior to traditional numerical simulations for higher-multiplicity processes [2–12]. For ML surrogates to generate reliable higher-order predictions, they must achieve precision reflecting underlying theoretical accuracy. Comprehensive uncertainty estimation becomes crucial for using these surrogates in actual simulations. Several complementary approaches address this challenge. Heteroscedastic losses incorporate unknown uncertainties directly into the loss function, learning them through deterministic networks. Bayesian neural networks on the other hand provide natural uncertainty quantification through posterior distributions over network parameters. Repulsive ensembles offer an alternative framework for tracking both statistical and systematic uncertainties. Benchmarking studies compare these methods' performance in representative amplitude calculations, see for example Refs. [13–15].

Beyond amplitude evaluation itself, ML techniques can be used to enhance the computation of multi-loop integrals that appear at next-to-leading-order (NLO) and higher order corrections. These integrals typically contain integrable singularities on the real axis, necessitating contour deformation into the complex plane. NN-assisted algorithms based on normalising flows significantly amplify the precision of standard contour deformation methods [16]. Alternative approaches employ NNs to solve numerically the differential equations satisfied by

Feynman integrals, offering complementary strategies for multi-loop calculations [17, 18].

A somewhat different and exciting direction is to use ML to simplify algebraic expressions. Integration of scattering amplitudes generates mathematical functions lacking classical simplification algorithms, such as for example generalised polylogarithms. In [19] reinforcement learning is used by treating known identities as moves in a game, training agents to apply these transformations. Alternatively transformer networks are used to translate complicated expressions into simplified forms, essentially performing symbolic manipulation through learned patterns. Similar techniques using transformers and contrastive learning simplify spinor-helicity representations of scattering amplitudes [20]. In the context of planar $N=4$ Super Yang-Mills theory, a further ML application appears quite exciting, as transformer models are used to predict coefficients at loop order L using only small subsets of related coefficients from loop order $L - 1$, demonstrating genuine pattern recognition across loop levels [21, 22].

2.2 Phase Space Integration

Another critical computational bottleneck in the computation of parton-level cross sections is the efficient integration of squared amplitudes over the phase space. The challenge lies in importance sampling and multi-channel techniques whose efficiency depends on variable transformations and channel selection. The traditional VEGAS [23] algorithm implements adaptive importance sampling by fitting bins with equal probability and varying width. While computationally cheap, VEGAS neglects correlations between variables and struggles with multimodal functions when peaks misalign with coordinate axes.

Bijjective normalising flows provide a powerful ML-based alternative. These architectures put together invertible, learnable transformations with exact likelihood evaluation through change-of-variables formulas. By redistributing input random variables through learned mappings, normalising flows adapt naturally to complex integrand structures. Applications to phase space integration demonstrate substantial improvements over traditional approaches, see for example [24–30]. The MadNIS framework [31–33] exemplifies the practical integration of ML tools with established tools, as it combines the standard automated event generator MadGraph [34] with two NN components: a channel-weight network encoding local multi-channel weights, and an invertible network implementing normalising flows that function efficiently in both forward and inverse directions. This hybrid approach achieves in some cases a strong improvement in both accuracy and efficiency compared to standard methods, while maintaining compatibility with existing computational workflows.

2.3 Parton Distribution Functions

PDFs encode the probability that a parton carries a given momentum fraction of its parent proton. These universal, non-perturbative objects cannot be computed from first principles and must be extracted from experimental data [35, 36]. The PDF fitting problem constitutes an infinite-dimensional inverse problem [37]: given a finite set of discrete experimental measurements, determine n_{flac} continuous functions of x with proper uncertainty estimate. The NNPDF collaboration pioneered a NN approach to this challenge [38], using NNs as flexible functional parametrisation that did not introduce parametrisation bias that might affect traditional polynomial parametrisations. The NNPDF4.0 methodology is the modern version of the initial NNPDF idea and it employs a single deep neural network with hyperparameters optimized through K -fold cross-validation procedures [39, 40]. Approximately five thousand parton-level data points from electron-proton, electron-nucleon, proton-antiproton, and proton-proton experiments are used to extract eight PDFs. Uncertainty estimation follows Monte Carlo error propagation principles through bootstrap sampling [41]. The procedure generates pseudo-data replicas by adding random fluctuations to experimental measurements

according to their multivariate normal distributions with experimental covariance matrices. For each replica, training with validation-based stopping yields optimal parameter values. Repeating this process provides importance sampling of the posterior distribution in PDF space, projecting from data-space sampling. This deep learning-based methodology yields smaller uncertainties in data regions while maintaining conservative extrapolation uncertainties [42]. The NNPDF4.0 public code [43] enables testing and reproducibility, with methodology rigorously scrutinised through statistical closure tests [44]. Another ML application in the context of NNPDF is the use of generative adversarial networks providing compressed PDF representations with fewer replicas matching full ensemble accuracy [45, 46]. The techniques can now be tested in a fully automated and flexible PDF regression framework Colibri [47], in which the NN parametrisation and the bootstrap uncertainty estimate can be tested against other models and Bayesian error propagation, assessing the reliability of ML approaches for this foundational task.

2.4 Parameter determination

Another key challenge at the LHC is the precise and robust determination of SM and BSM parameters from LHC data. Determining which measurements provide optimal sensitivity to specific parameters, and selecting observables and binnings, challenges human two-dimensional intuition in high-dimensional parameter spaces. ML tools naturally "see" in arbitrarily high dimensions, identifying optimal variables and binning. Neural simulation-based inference exemplifies this capability [48, 49].

Among the many applications that could be mentioned, an interesting one is the application of such techniques to the determination of the Wilson coefficients of the SM effective field theory (SMEFT). The SMEFT provides a model-independent framework for parametrising deviations from SM predictions through Wilson coefficients multiplying higher-dimensional operators [50]. As experimental precision and theoretical accuracy improve, identifying patterns of small deviations – corresponding to non-zero Wilson coefficients – would allow to extract hints on the underlying new physics model. In [51] unbinned parton-level likelihoods are generated and for each point of the phase space the SMEFT is compared to the SM, by training NN to approximate likelihood ratios. These trained classifiers compute signal strengths and enable inference about Wilson coefficients directly from unbinned, multidimensional data. Related methodologies include parametrised classifiers for SMEFT [52–55], tree-boosting approaches for learning EFT likelihoods [56], and techniques for designing optimal observables through deep learning [57, 58]. Recent ATLAS analyses employ these methods for measuring off-shell Higgs boson couplings to Z bosons [59, 60], demonstrating practical deployment in experimental measurements.

Further developments related to the determination of SMEFT coefficients have to do with simultaneous fits of these parameters and PDFs using deep NNs [61, 62], recognising the interplay and accounting for correlations between these quantities [63].

3 Beyond Parton Level: End-to-End Simulations

In this section we briefly mention some of the numerous applications of ML to go beyond parton level, to a full simulation. Traditional Monte Carlo event generation proceeds sequentially through parton shower, hadronisation, detector simulation, and particle reconstruction stages. Each step introduces approximations and computational costs. End-to-end machine learning surrogates for fast event simulation learn multiple stages simultaneously, potentially improving both speed and robustness, see [64] for a comprehensive review.

Early approaches employed generative adversarial networks and variational autoencoders for calorimeter shower simulation and jet generation [65–70]. While demonstrating proof-of-concept, these methods faced challenges with training stability and mode coverage. Normalising flows improved both speed and efficiency through their tractable likelihood evaluation and stable training dynamics [71–74]. Recent diffusion models and transformer architectures achieve a very high level of precision in generating realistic detector-level events [75–77]. Importantly, conditional generative adversarial networks and transformer architectures enable inversion of the simulation chain, mapping from detector-level observations back to parton-level configurations. This, combined with uncertainty quantification through Bayesian NNs and classifier-based methods, provides end-to-end error control across the simulation pipeline [78]. An alternative approach, optimal transport-based unfolding and simulation (OTUS), employs probabilistic autoencoders to learn bidirectional mappings between parton and reconstruction levels without requiring paired event samples. This framework has the potential to handle both simulation and unfolding, learning both directions simultaneously [79].

Something that is worth mentioning in this context is the matrix element method (MEM), building full likelihoods using matrix elements from theory combined with transfer functions describing detector response. This approach allows direct inference of fundamental theory parameters from reconstructed events. Modern implementations employ normalising flows with transformers for transfer functions, classifier networks for acceptance probabilities, and generative networks for efficient Monte Carlo sampling, while incorporating direct theory input for parton-level event generation. This integration of traditional theoretical calculations with ML components exemplifies the synergy between established methods and modern tools [80,81]. However, while traditional analyses from reconstructed events to parton level necessarily lose information through binning and hand-crafted observable selection. Access to full likelihoods would enable unbinned, multivariate analyses with optimal information extraction. While the full likelihood remains intractable in realistic settings, combining ML components for detector modeling with theoretical inputs for parton-level calculations approximates this ideal, enabling more powerful inference than conventional approaches.

4 Frontiers: Uncertainty, Symmetry, and Interpretability

In this section, we summarise what we believe are the most exciting and relevant frontiers at the interface of ML and theoretical particle physics, namely uncertainty quantification, the encoding of theoretical constraints and symmetries in the ML models and interpretability.

As ML is used across all steps of the pipeline to build theoretical predictions, it is paramount to ensure that ML tools provide robust results with comprehensive uncertainty quantification. High-energy physics possesses unique potential to advance from deterministic ML to probabilistic frameworks, given the rigorous uncertainty treatment and statistical methodologies used in the field. Multiple approaches to uncertainty quantification have emerged across different contexts: bootstrap sampling for PDF uncertainties, heteroscedastic losses for amplitude regression, Bayesian neural networks for posterior distributions, repulsive ensembles for diverse predictions, and posterior sampling for generative models. Understanding relationships between these methods, benchmarking their performance, analysing prior dependence, and developing appropriate statistical tests represents crucial ongoing work. The transition from deterministic outputs to probabilistic predictions fundamentally changes how ML integrates with fundamental physics. Rather than single point predictions, probabilistic models provide full distributions over possible outcomes, naturally incorporating both aleatoric uncertainty from irreducible stochasticity and epistemic uncertainty from limited training data or model capacity.

The second frontier has to do with smart inductive bias. Physics laws fundamentally respect symmetries, such as Lorentz invariance, gauge symmetry, and other transformation properties defining quantum field theories. Incorporating known symmetries directly into ML architectures provides powerful inductive biases that improve generalisation, efficiency, and physical consistency. As an example Lorentz-equivariant transformers encode Lorentz symmetry into network architecture to provide appropriate latent representations of phase space points [82–85]. Applications span amplitude regression, event classification, and generation, demonstrating that symmetry-aware architectures consistently outperform symmetry-agnostic alternatives while guaranteeing physically consistent behavior.

Beyond incorporating known symmetries, ML offers exciting potential for discovering symmetries in data. Detecting previously unknown symmetries would signify fundamental principles manifesting as physical laws and selection rules. Classifiers and symmetry generative adversarial networks explore deep learning approaches to symmetry discovery, with applications ranging from identifying approximate symmetries in complex systems to uncovering hidden patterns in HEP data [86–88].

Finally, the third frontier is interpretability. As physicists we seek understanding, striving for simplicity and unity in natural laws. While numerical simulations and black-box predictions suffice for some applications, particularly when comprehensive uncertainty quantification provides statistical rigor, analytical understanding offers distinct advantages including superior extrapolation and conceptual clarity. Symbolic regression bridges machine learning and analytical formulas, learning complex functions from high-dimensional data while expressing results in closed form. There is an increasing number of Applications to HEP [89–95], most using evolutionary algorithms that evaluate and optimize symbolic expressions such as PySR [96]. The resulting formulas provide both computational efficiency and physical insight unavailable from purely numerical approaches. Complementary directions investigate understanding deep neural networks themselves using principles from quantum field theory or cosmological dynamics, see for example [97–99]. These theoretical frameworks for analysing neural network behavior may reveal why certain architectures succeed and guide future development.

5 Conclusion

A revolution in LHC physics through modern machine learning is ongoing. Contemporary ML tools, combining regression, classification, generation, and conditional generation, benefit every stage of theoretical predictions at the LHC. The exceptional quality and quantity of high-energy physics data, with careful control of systematic uncertainties and correlations, provides labeled and well-characterised datasets that make particle physics an ideal testing ground for ML methodologies. Critical frontiers for future development include comprehensive uncertainty quantification across all applications. The synergy between traditional theoretical methods and modern ML tools promises continued rapid progress. By maintaining physics rigour while embracing computational advances, the field strives toward the ultimate goal: extracting maximal information from collider data to reveal nature’s fundamental principles. As Alan Turing observed, "We can only see a short distance ahead, but we can see plenty there that needs to be done." The landscape of ML applications in particle physics phenomenology presents abundant opportunities for meaningful contributions that will shape the future of high-energy physics at the LHC and beyond.

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