Dealing with Nuisance Parameters using Machine Learning in High Energy Physics: a Review

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In this work we discuss the impact of nuisance parameters on the effectiveness of machine learning in high-energy physics problems, and provide a review of techniques that may reduce or remove their effect in the search for optimal selection criteria and variable transformations. Nuisance parameters often limit the usefulness of supervised learning in physical analyses due to the degradation of model performances in real data and/or the reduction of their statistical reach. The approaches discussed include nuisance-parametrized models, modified or adversary losses, semi-supervised learning approaches and inference-aware techniques.

1. Introduction

Particle physics offers a variety of use cases for machine learning techniques. Of these, probably the most common is the use of supervised classification to construct low-dimensional event summaries, which are informative to carry out statistical inference for a given set of parameters of interest. The learned *summary statistics* –functions of the data that are informative on their relevant properties– can efficiently combine high-dimensional information from each event into one or a few variables which can be used as the basis of statistical inference. The informational source for this compression are simulated observations produced by a complex generative model; the latter reproduces the chain of physical processes occurring in subatomic collisions and the subsequent interaction of the produced final state particles with the detection elements.

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The fidelity of the event description provided by the simulation is usually limited, due to a variety of factors. These may include imperfections in the modelling of the physical processes employed by the simulation (such as the use of a leading order approximation for the hard scattering process), limited precision in the description of detector response (e.g. due to an imperfect knowledge of the relevant calibration constants), uncertainty in fundamental physics parameters liable to condition the observations (e.g. the mass of a decaying particle), or simply a consequence of the finiteness of the number of simulated observations in a given region of feature space. To account for these “known unknowns”, commonly referred to as nuisance parameters in Statistics literature, the model needs to be enlarged by the inclusion of corresponding variables which are not of direct relevance, yet have to be considered during inference in order to make calibrated statements about the parameters of interest.

Because simulated observations are also used in the construction of the likelihood function (or any other estimator employed for the extraction of the wanted information), nuisance parameters must be directly included in the statistical model. The introduced uncertainties result in the enlargement of confidence intervals on the parameters of interest, and are thus referred to as systematic uncertainties. This degradation is not exclusive of parameter estimation problems: nuisance parameters have also to be accounted for in hypothesis testing problems, such as when a test of the presence of a new physics signal is performed on data otherwise conforming to the Standard Model hypothesis. The effect of nuisances is then a reduction of the statistical power of the test. Hence, nuisance parameters are one of main factors limiting the precision and discovery reach of HEP analyses.

The mentioned hindrances also apply in the same manner to analyses which employ machine learning algorithms to reduce the dimensionality of the data: the effect of nuisance parameters has to be accounted for statistical inference based on summary statistics constructed from the output of those algorithms. Besides, training and performance evaluation for the learning task itself (e.g. classification or regression) is not well-defined when the simulated observations themselves depend on additional modelling parameters that are unknown. This Chapter focuses on issues arising from the application of machine learning techniques to problems where nuisance parameters are relevant, and the different approaches that have been proposed to overcome the resulting limitations.
1.1. Probabilistic Classification as Density Ratio Estimation

Before delving into the subject matter, it is important to review the relation between the learning tasks often performed in HEP data analysis and the statistical properties of the training data. As introduced earlier, machine-learning based data transformations in HEP are often based on probabilistic classification models trained with samples from computer simulations of the different processes. The simplest way to understand a probabilistic classifier is in terms of probability density ratios.

By training a probabilistic classification model to distinguish samples labelled by \( y = 1 \) (heretofore signal simulated samples) and \( y = 0 \) respectively (background simulated samples), e.g. a neural network optimising binary cross entropy (BCE), we are approximating the density ratio \( r(x) = p(x|y = 1)/p(x|y = 0) \) between the signal and background generating distributions \( p(x|y = 1), p(x|y = 0) \). For example, in the case of using BCE as a loss, the density ratio \( r(x) \) can be approximated using the classification output \( c(x) \) by virtue of the following relation:

\[
\frac{c(x)}{1 - c(x)} \approx \frac{p(y = 1|x)}{p(y = 0|x)} = \frac{p(x|y = 1)}{p(x|y = 0)} \frac{p(y = 1)}{p(y = 0)} = r(x) \frac{p(y = 1)}{p(y = 0)} \tag{1}
\]

where \( p(y = 1)/p(y = 0) \) is independent on \( x \), and can be simply estimated as the ratio between the total number of observations from each category in the training dataset. The previous approximation becomes an exact equality only for the best possible classifier, so-called Bayes optimal classifier, which is a function of the true and generally unknown density ratio between the generating distributions of training data. In practice, really good approximations can be obtained given enough data, flexible enough models, and a powerful learning rule. The previous relation is not unique of BCE-based probabilistic classification models, as it also holds for other approaches that minimise continuous relaxations of the zero-one loss and could be generalised for the multi-class case.

Viewing probabilistic classifiers as probabilistic density ratio estimators allows us to abstract away from the specific machine learning techniques used to construct the model (e.g. gradient boosting or neural networks trained by stochastic gradient descent), and also provides a clear theoretical definition for the best possible classifier, i.e. the one that optimally minimises the risk or generalisation error of a classification problem, as a simple function of the probability density ratios between the data-generating distributions. Furthermore, density ratios can also be easily linked with the statistical inference goals of data analysis and may effectively be used to
study the limitations of machine learning approaches.

We can also explore the previous formulation in the case when the generating distributions of data are not fully specified, but depend on additional unknown nuisance parameters $\theta$. A classifier distinguishing samples from the data-generating distributions $p(x|\theta, y = 1)$ and $p(x|\theta, y = 0)$ will still be approximating a function of the density ratio

$$r(x; \theta) = \frac{p(x|\theta, y = 1)}{p(x|\theta, y = 0)}$$

and hence will itself depend on the actual value of the parameters $\theta$. If we assume that the true value of the parameters is fixed but unknown (which is the typical setting used for frequentist inference in HEP), then the optimal classifier is not uniquely defined\(^a\). For example, a classifier trained using simulated data generated for specific parameters $\theta_s$ might not be optimal at classifying experimental data observations that correspond to the unknown parameter value $\theta_d$. This is the main issue with nuisance parameters from the perspective of the machine learning performance.

### 1.2. Nuisance Parameters in Statistical Inference

Another challenge with nuisance parameters, arguably the most relevant one, is the way they degrade our ability to extract useful information about our models of nature from experimental data when carrying out statistical inference in the form of hypothesis testing or interval estimation. This is not solely a problem for analyses based on machine learning approaches, as it also applies to analysis based on manual variable transformations. However, as will be discussed in detail in Sec.\(^a\) the presence of nuisance parameters can put into question the role of supervised learning models in the context of statistical inference, voiding them of the standard advantages that otherwise make them so apt for dimensional reduction in physical analyses.

The previous concerns are closely related with the misalignment between the goal of particle physics analyses—to infer information about our models of nature given the data—and the classification and regression objectives of supervised learning approaches. For example, for inference problems in mixture models where the mixture fraction is the only parameter of interest in the absence of nuisance parameters or for simple hypothesis testing, \(^a\)In a Bayesian setting, if the parameters are treated as random variables associated with a prior probability density distribution $\pi(\theta)$, then the optimal Bayes classifier can be uniquely defined, because parameter sampling from $\pi(\theta)$ can be considered part of the data generating procedure so the density ratio can be implicitly marginalised.
probabilistic classification models offer principled guarantees of optimality at the inference goal. In general terms, the supervised learning task can be considered a proxy objective to obtain low-dimensional data transformations that are still informative of the parameters of interest.

In this context, it is worth introducing the concept of summary statistic. For a set of $n$ experimental data independent and identically distributed (i.i.d.) observations or events $D = \{x_0, ..., x_n\}$, where each $x \in \mathcal{X} \subseteq \mathbb{R}^d$ is a $d$-dimensional representation of the event information at an arbitrary representational level (e.g. raw detector readout, physical objects or a subset of columnar variables), a summary statistic of the data $D$ is simply a function of the data that reduces the dimensionality. An infinite number of different summary statistics can be constructed for a given set of data, but we are generally only interested on those which are as low-dimensional as possible while preserving as much information relevant for the statistical inference goal of a given analysis. The low-dimensionality requirement is a consequence of the curse of dimensionality, due to $p(x|\theta)$ not being known analytically and having to be estimated from a finite number of simulated observations by non-parametric means.

Most of the work that reduces the dimensionality of the experimental data both in terms of reducing the number of events (e.g. trigger and event selection) or its representation (e.g. reconstruction, physics object selection, feature engineering, multivariate methods or histograms) can be viewed through the lenses of summary statistics (see Chapter 3 of [1]). Summary statistics in high-energy physics are often a composition of several transformations, yet for the purpose of machine learning models we are usually interested the final components of the type $s(D) = \{ s(x_i) | \forall x_i \in D \}$ that are the product of the event-wise application of a function

$$s(x) : \mathcal{X} \subseteq \mathbb{R}^d \rightarrow \mathcal{Y} \subseteq \mathbb{R}^b$$

reducing the dimensionality of each event from the original feature space $\mathcal{X} \subseteq \mathbb{R}^d$, which could be already a transformation of the detector readout or set of engineered features, to a new low-dimensional space $\mathcal{Y} \subseteq \mathbb{R}^b$.

Such transformation can be used to reduce the data dimensionality from $n \times d$ to $n \times b$. If $b$ is very small and because the observations are assumed i.i.d., we could use simulated observations to estimate the probability density $p(s(x)|\theta)$ by non-parametric means to carry out the inference goal. Most commonly, even simpler sample-wise statistics are instead constructed from $s(D)$ such as the number of observations for which $s(x)$ is within a given range (in so-called cut-and-count analyses) or simply a histogram of
For these simpler statistics, the simulations of each process adapted for different values of nuisance parameters are interpolated to build a likelihoods based on the product of Poisson terms.

A reduction of the dimensionality of the data is required to carry out inference in HEP problems, yet the choice of the transformation determines the inference reach of a given analyses. Choosing a summary statistic is not easy even in the absence of nuisance parameters, since naive choices of data transformation can very easily lead to a significant loss of useful information about the parameter of interest. Machine learning models, in particular probabilistic classification models trained to distinguish observations from different processes, are increasingly being used as an automated way to obtain summary statistic transformations. This is because the output of probabilistic classifiers approximates density ratios, and the latter are closely related with the optimal likelihood ratio test statistic for simple hypothesis testing and sufficient summary statistic in the case of parameter estimation for the problem of inference of mixture fractions in the absence of nuisance parameters.

It is of benefit for the ensuing discussion to succinctly recall how nuisance parameters can be “profiled away” from a likelihood function in the extraction of confidence intervals on parameters of interest; for a more general discussion of how the effect of nuisance parameters is accounted for in physics measurements see e.g. [2–4].

We consider the measurement of a physical quantity in statistical terms as a problem of parameter estimation, whose solution relies on the specification of a statistical model wherein those quantities appear as free parameters. Under the assumption that experimental data conform to the specified model, the measurement may be carried out by constructing suitable estimators for the parameters of interest, which here we formulate through the specification of a likelihood function. Letting $\theta$ identify the parameters of interest, $\alpha$ describe systematic uncertainties affecting the model, and $x_i$, $i = 1...N$ be the collected data, understood to be a set of N random i.i.d. variables, the joint probability density can be written as $p(x, \theta, \alpha)$. This enables, e.g., the construction of a likelihood function

$$L(\theta, \alpha) = \prod_{i=1}^{N} p(x_i, \theta, \alpha). \quad (4)$$

If nuisance parameters $\alpha$ were absent in the above formulation, one would proceed directly to construct estimators of the parameters of interest as

$$\hat{\theta} = \arg \max_{\theta} L(\theta). \quad (5)$$
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The dependence on $\alpha$ can be dealt with by first obtaining the profile of the likelihood function, $PL(\theta)$, by maximizing $L$ as a function of the nuisances,

$$PL(\theta) = \sup_\alpha L(\theta, \alpha),$$

and then proceeding as above. Uncertainties in the parameters of interest may then be extracted from the curvature of the profile likelihood at its maximum exactly as is done with $L$ in the general case [5, 6]. This “profile likelihood method” is conceptually simple and practical to implement if the likelihood is differentiable with respect to the parameters, but may meet with technical problems e.g. a slow convergence) as well as intractability for high dimensional $\alpha$. The same issues affect in general the main alternative solution, of Bayesian flavour, which consists in computing the marginalized likelihood $L_m(\theta)$ as

$$L_m(\theta) = \int L(\theta, \alpha)p(\alpha)d\alpha.$$ 

In both cases, a prior knowledge of the PDF of nuisance parameters $p(\alpha)$ is mandatory for a meaningful solution; any imprecision in $p(\alpha)$ will in general affect the parameter estimates with increases in bias and/or variance.

### 1.3. Toward Fully Sufficient Statistic Summaries

The reduction of statistical uncertainty on the estimate of parameters of interest is a common goal of machine learning applications in experimental HEP. A suitable summary statistic may be obtained by training a high-performance boosted decision tree or an artificial neural network on simulated sets of data. The summary enables the extraction of the highest possible amount of information on the unknown true values of the physical quantities under measurement, conditional to the validity of the underlying physics model used to generate the training samples, as well as of specific assumptions on the value of relevant nuisance parameters. The conditional clause is usually hard to get rid of, because of the complexity of the problems, their high dimensionality, the typically unknown PDF of nuisance parameters, and/or the effects those parameters have on the physical model. In statistical parlance, the obtained summary statistic cannot then be sufficient: being oblivious of a part of the feature space, it does not retain all the information contained in the data relevant to the parameter estimation task, and is therefore liable to be outperformed.

In particle physics practice a widely used implementation is the MINUIT package [7], which offers profile likelihood evaluation through the MIGRAD routine.
In spite of the ubiquity of the above stated problem, the word *optimization* is liberally perused when reporting physics analysis results, usually in connection with incremental advances over state-of-the-art of the employed techniques, for the common use case of classification performance in signal versus background discrimination problems. The classical justification for a claim that a chosen algorithm or architecture and its output (a classification score) be *optimal* for the measurement task at hand is based on examination of associated performance measures such as the integral of the Receiver Output Characteristic curve (see Chapter 1), or on background acceptance estimates at fixed purity (or vice versa). In the absence of nuisance parameters those figures of merit are generally effective as a proxy to classification performance, when their maximization closely tracks the theoretical minimum value of the statistical uncertainty on the intermediate physical parameter to which the classification algorithm is sensitive, such as, e.g., a signal fraction. Yet they are blind to the more general problem connected with the subsequent extraction of, say, the cross section of a physical reaction contributing to events labelled as signal, when uncertainties of non-stochastic nature are included.

A simple toy example may help pointing out the typical issues. Let us suppose that a dataset includes events originated from a signal process of interest \( S \), in addition to ones coming from a known background source \( B \). The typical output of a classifier trained to distinguish the event classes may be the one shown in Fig.1 (left), which we parametrized using exponential functions with normalized density functions in the \( x \in [0, 1] \) range:

\[
S(x) = \frac{e^x}{1 - e^{-1}}, \quad B(x) = \frac{\alpha e^{-\alpha x}}{1 - e^{-\alpha}}.
\]

Above, we have included a nuisance parameter \( \alpha \) in the definition of the background PDF. If we define the true positive rate (TPR) and false positive rate (FPR) of a selection criterion \( x > x^* \) as

\[
TPR(x^*) = \int_{x^*}^{1} S(x) \, dx = \frac{e-x^*}{e-1}, \quad FPR(x^*) = \int_{x^*}^{1} B(x) \, dx = \frac{\alpha e^{-\alpha x^*} - e^{-\alpha}}{1 - e^{-\alpha}},
\]

then with simple algebra we may derive the ROC curve as the functional dependence of TPR on FPR:

\[
TPR(FPR) = \frac{e^{-[-e^{-\alpha} + (1+e^{-\alpha})FPR]^{-1/\alpha}}}{e-1}
\]
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Fig. 1. A simple toy classification model. Left: the PDF of a signal process (red) is compared to the PDF of background for three values of the nuisance parameter, $\alpha = 1.0, 1.5, 2.0$; center: ROC curves corresponding to the three background distributions; right: values of the AMS figure of merit (see text for details) as a function of the selection cut value $x^*$. The location of maxima are shown by the corresponding arrows.

By examining the shape of ROC curves resulting from different values of the nuisance parameter $\alpha$ (see Fig. 1, center), one may verify the qualitative benefit of $B(x)$ densities peaking more sharply at $x = 0$, which correspond to larger values of $\alpha$. The performance of a classifier trained under a given hypothesis for the nuisance parameter (say, $\alpha = 1.5$) is then liable to be under- or overestimated if the value of $\alpha$ is uncertain; the choice of a critical region $x > x^*$ corresponding to a pre-defined FPR will similarly be affected, as will the resulting value of TPR.

In the given example the fraction of data selected in the critical region plays the role of our summary statistic, as we have assumed that it is the only input to a subsequent extraction of signal fraction. The fraction is of course affected by the unknown value of the nuisance parameter $\alpha$, yet its value alone does not retain information on it: the statistic is therefore not sufficient. A sufficient statistic in this example would be the whole distribution of the classifier output shown by the observed data; that choice however fails to reduce as desired the dimensionality of the input, so it is not an effective summary for the inference task.

To discuss how an optimal choice of $x^*$ based on the above densities may be influenced by the presence of the nuisance parameter $\alpha$, we may consider the figure of merit called approximate median significance (AMS) [8], already introduced in Chapter 1:

$$AMS = \sqrt{2 \cdot \left[ (N_s + N_b + N_r) \ln \left( 1 + \frac{N_s}{N_s + N_r} \right) - N_s \right]}.$$ 

The AMS is a robust predictor of the statistical significance of an excess of
observed events if a signal of mean rate $N_s$ contributes to a data sample assumed to be only composed of background events coming from a Poisson distribution of known mean $N_b$; the regularization term $N_r$ reduces the impact of Poisson fluctuations in low-event-counts situations, preventing divergent behaviour when $N_b$ gets too low. If we set, e.g., $N_r = 10$ and compute the AMS as a function of the selection cut $x^*$ for the three considered values of $\alpha$ of our toy model, and for a choice of $N_s = 20$, $N_b = 400$ in the data sample, we obtain the curves shown in the right panel of Fig.1. It can then be observed, as expected, that the value of $\alpha$ affects both the peak value of the figure of merit and the optimal value of $x^*$ which achieves it.

The above toy model exemplifies how not only do nuisance parameters have the power to modify the optimal working point of a ROC curve, but they also in general affect the overall classification performance, as well as the relative merit of different classifiers. For that reason, standard supervised classification techniques may not reach optimality unless they more broadly address the conditionality issue stated above, or prove to be decoupled from it.

From a statistical point of view, in real-life situations “all models are wrong”, hence strictly speaking sufficient statistics may not exist! However, in most experimental situations approximate sufficiency is achievable, provided that the relevant nuisance parameters are included in the model and considered in the construction of the statistic. A number of brilliant ideas have been recently proposed to achieve that goal, in some cases effectively exploiting methods developed in Computer Science to endow learning algorithms of domain adaptation capabilities –the flexibility to achieve good results on data coming from one domain when trained with data coming from a different one, such as e.g. the capability of driving a truck when trained to drive a car. In the context of point estimation in experimental particle physics, the different domains may involve a different relative importance of some of the features, or the absence of others, and are akin to the imperfections in the training model which are usually the culprit.

It must be noted here that a possible misalignment between the specification of the classification task and the true objective of the analysis should always be considered. In the given example we studied the AMS score as a robust proxy of the significance of an excess of signal events: such is a good choice when the objective of the analysts is the discovery of a yet hypothetical signal in the data. If, however their focus were rather the setting of the most stringent upper limit on the signal rate—a common situation when the a priori sensitivity of a search does not offer chances of a discovery—then the whole learning task and optimization criteria would have to be revised.
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The growing interest in the development of new techniques to reduce or remove the effect of nuisance parameters in physics inference, powered by the availability of new machine learning tools and larger computing resources, has brought the focus of experimentalists on the central problem of how to achieve a true end-to-end optimization of physics measurements, and highlighted the need to pay undivided attention to the expected total uncertainty on the parameters of interest already in the training phase of learning algorithms. Below we provide an overview of methods developed to address those issues, and discuss their merits, applicability, and potential extensions.

2. Nuisance-Parametrized Models

A direct way to account for the effect of nuisance parameters in the construction of a sufficient summary statistic is to include them in the physical model through a parametrization of their effect on the observable event features. This requires the injection of a priori knowledge of their PDF in the model, and may or may not be practical to implement depending on the problem.

In the simplest situations, as e.g. when the problem is low-dimensional, a fully analytical solution may be sought. An example is offered by the decorrelation of the "N-subjettiness ratio" variable $\tau_{21}$ \cite{9} designed in the context of searches for the two-body decay of boosted resonances to evidence the resulting sub-structure in the produced hadronic jets. The variable may be likened to a classification score as it possesses large discrimination power against QCD background jets, but a selection based on its value biases the distribution of reconstructed "soft-drop" mass successively used for inference, because of its dependence on jet $p_T$, which can be here seen as a nuisance variable. As shown in \cite{10}, an analytical parametrization of the dependence of $\tau_{21}$ on jet $p_T$ removes almost entirely the distortions in the mass spectrum. In the same context of boosted decay searches, similar results have been obtained for the observable $D_2$ \cite{11}.

In cases where experimental data are informative of the value of nuisance parameters, one may try to exploit that dependence in the construction of estimators for the parameters of interest. This situation was considered by Neal \cite{12}, who addressed the question of how the extraction of a sufficient summary for the signal fraction $\theta$ with a binary classifier is affected by unknown parameters $\alpha$, when these modify the PDF of signal $p_s(x, \alpha)$ and
background events \( p_b(x, \alpha) \). The likelihood for \( N \) observations \( x_i \),

\[
L(\theta, \alpha) = \prod_{i=1}^{N} \left[ \theta p_s(x_i, \alpha) + (1 - \theta) p_b(x_i, \alpha) \right], \tag{8}
\]

may be rewritten as

\[
L(\theta, \alpha) = \left[ \prod_{i=1}^{N} p_b(x_i, \alpha) \right] \cdot \prod_{i=1}^{N} \left[ \frac{\theta p_s(x_i, \alpha)}{p_b(x_i, \alpha)} + (1 - \theta) \right]. \tag{9}
\]

The first term in the right-hand side of the last expression is not a constant when nuisance parameters are present: factoring it out of the likelihood would therefore cause loss of information, since background events alone carry constraining power on the value of \( \alpha \). The usual classifier task of learning the ratio of signal and background PDFs \( p_s(x)/p_b(x) \) is then no longer sufficient to solve the problem as it would if no nuisances were present. The solution outlined in \cite{12} involves the construction of low-dimensional summaries for both the nuisance parameters \( \alpha \) and the observable event features \( x \), using e.g. a neural network. If good parametric models of the summaries can be constructed one may use them for inference, exploiting the informative power of the data themselves to constrain nuisance parameters. Approximate sufficiency can in principle be obtained with this recipe, if the parametrizations do not cause significant loss of information.

In other cases of HEP interest no prior knowledge of a nuisance parameter may be available, yet a parametrization of its effect on the observations successfully solves the issue. The classical example of this situation is the search for a new particle whose mass \( M_{\text{true}} \) is unknown, when signal events exhibit smooth variations in the momenta of the decay products as \( M_{\text{true}} \) changes. A classifier trained to distinguish the new particle from backgrounds using signal events simulated assuming a mass \( M_1 = M_{\text{true}} + \alpha \) will consequently suffer a progressive degradation in performance as \( |\alpha| \) increases. This was a common situation in early applications of binary classification to new particle searches, which focused on a mass range of particular interest, \( M_{\text{true}} \simeq M_1 \), and accepted the residual loss of power resulting for \( \alpha \neq 0 \). A more performant yet CPU-consuming solution \cite{13, 14} was to independently train a set of classifiers \( C_i \) using in turn data simulated assuming different mass values \( M_i \) for the unknown signal. This approach is still sub-optimal in a general sense, since it does not fully exploit available resources (the simulated data). Each classifier is oblivious

\[\text{d}\]A dependence of the particle branching fractions on \( M_{\text{true}} \) does not complicate matters if the resulting acceptance variations are known.
of the information processed by the other ones, as it only knows the precise mass hypothesis it corresponds to: in general, it is not possible to interpolate the results of different hypotheses.

A way to avoid the above shortcomings, first proposed in [15], is to parametrize the effect of the nuisance parameter in the construction of the classifier. This may be achieved by including the unknown value of $M_{true}$ within the set of features that describe simulated signal events; for background events an arbitrary mass value, or one chosen at random for each different training event, is correspondingly added. A suitable admixture of training data with signal events corresponding to different $M_i$ hypotheses spanning the range of interest may then be used in the learning phase.

The benefit of this procedure is that it yields a valid classification score $C_k$ even for events with mass values $M_k$ never seen during training. An interpolation of the scores resulting from different mass hypotheses is also possible; a smoother dependence can be expected if the classifier is a neural network rather than, e.g., a decision tree.

Regardless of the a priori choice of signal admixture employed in the training, the resulting inference cannot be considered Bayesian, as the choice only affects the power of the classifier.
The effectiveness of this strategy was demonstrated using a simple neural network architecture for the discrimination of a new particle $X$ decaying to top-antitop quark pairs from non-resonant $t\bar{t}$ backgrounds in proton-proton collision data reconstructed by the ATLAS detector as simulated by DELPHES. It was shown how for a given specific mass hypothesis $M$, a parameterized NN performed similarly to a non-parametrized NN trained with signal at the same mass, but it outperformed it for all other masses (red curve in Fig. 2), even when the non-parametrized NN was trained with an admixture of mass values (black curve).

The parametrization of the dependence of observable variables on the latent features of the underlying physical model—which include both interesting and nuisance parameters—has been more generally considered in the context of likelihood-free inference. The proposed algorithm performs a dimensionality reduction of the data through a parametrization that is monotonic with the likelihood ratio, allowing optimal inference via a calibration of the output of a binary classifier. We refer the reader to Sec. 5.2 for more detail on this approach.

3. Feature Decorrelation, Penalized Methods, and Adversary Losses

When a direct parametrization of the effect of nuisance parameters on the summary statistic used for classification proves ineffective or impractical to implement, there are several possible alternatives. In a few specific applications it proves sufficient to operate a suitable preprocessing of training data that reduces or removes the dependence of the classifier output on a variable sensitive to nuisance parameters. A second class of solutions aim to make the classifier score insensitive to variations in the value of nuisances by engineering a robust optimization objective for the classification task. Finally, a more radical approach is to change the overall architecture of the algorithm used in the search of the optimal solution, using adversarial techniques to find the best compromise between signal discrimination and impact of nuisances. Below we briefly discuss each of these approaches.

3.1. Mass Decorrelation

The intensive search for new physics carried out by the ATLAS and CMS experiments in final states dominated by QCD backgrounds fostered in the past decade the development of a number of imaginative new methods to
increase signal purity without modifying the shape of the distribution of reconstructed mass \( M_{\text{rec}} \) of the hypothetical new particle, which is commonly used at the end of the selection step to estimate or limit the signal contamination in the sample. Since the QCD background is complex to model reliably, a selection cut on the output of a well-trained classifier does not guarantee optimal inference on the presence of signal, because the background retained by the cut is usually biased toward displaying a "signal-like" mass distribution. In this situation \( M_{\text{rec}} \) is not in itself a nuisance parameter; however, the reduction of its discrimination power caused by the selection enhances the noxious effect of background normalization and shape uncertainties on the estimate of signal fraction. Further, a reshaping of the background distribution complicates the application of bump hunting techniques, e.g. by hindering the use of data-driven background estimates based on mass sidebands.

The most straightforward way to reduce the dependence of a classification score on \( M_{\text{rec}} \) (or any other specific observable of relevance for inference downstream of the selection) is called "planing" \([18, 19]\). A simple way to implement planing is to pre-select training samples for signal and background such that they have the same marginal PDF in the variable one aims to decorrelate, \( p_S(M_{\text{rec}})_{\text{sel}} = p_B(M_{\text{rec}})_{\text{sel}} \). As the above corresponds to making limited use of available training data, it proves more effective to weigh each event \( i \) by a mass-dependent value \( w(M_{\text{rec},i}) \) derived from the PDFs of the two training datasets, \( p_S(M_{\text{rec}})_{\text{train}} \) and \( p_B(M_{\text{rec}})_{\text{train}} \),

\[
  w(M_{\text{rec},i}) = \begin{cases} 
    1/p_S(M_{\text{rec},i})_{\text{train}}, & i \in S \\
    1/p_B(M_{\text{rec},i})_{\text{train}}, & i \in B
  \end{cases}
\]

Weights \( w(M_{\text{rec},i}) \) enter directly the calculation of the loss function (e.g. the binary cross-entropy) of the classifier in the training stage, but are not used for validation and testing. Planing has been shown to significantly reduce the dependence of classifier output on the planed variable in specific situations, and due to the simplicity of its implementation it may constitute a quite practical solution to the problem; however, its effectiveness is limited when other event features in one or both classes indirectly inform the classifier on the value of the planed variable, if the latter –as is often the case– carries discriminant power.

In the context of searches for new physics in boosted hadronic jets, a decorrelation of the output of a NN classifier from the mass of the boosted jet was instead achieved by feature preprocessing based on principal com-
ponent analysis [18]. The proposed method involved the PCA rotation and standardization of 17 employed NN inputs (a basis set of N-subjettiness variables $\tau_{N}^\beta$ proposed in [20]) from trained data suitably binned in jet mass. Besides avoiding the sculpting of the jet mass distribution of QCD background events, the resulting classifier was shown to be effective for signal discrimination also at signal masses for which it was not trained.

3.2. Modified Boosting and Penalized Loss Methods

As mentioned above, a decorrelation of the classifier output from a variable of interest $x$ may be difficult to obtain with data preprocessing techniques when other event features are informative of the value of $x$, especially if $x$ itself contains discriminant information.

The search for new low-mass resonances in Dalitz plots [21] or with amplitude analysis provides strong motivation to achieve uniformity of a classifier selection as a function of kinematical variables of interest, as systematic uncertainties may be greatly amplified by the unevenness of selection efficiency. The first algorithm explicitly targeting that use case is uBoost [22], which relies on boosted decision trees to improve signal purity. The method builds on the standard AdaBoost prescription [23] of increasing the weight of training events misclassified by the decision tree built in the previous iteration of the BDT sequence, augmenting it by modifying the weight of signal events depending on the disuniformity of the selection. If $w_{i}^{n-1}$ is the weight of event $i$ at boosting iteration $n - 1$, the new weight is computed as

$$w_{i}^{n} = c_{i}^{n}u_{i}^{n}w_{i}^{n-1}$$

where $c_{i}^{n} = exp(-\gamma_{i}p_{i}^{n-1})$ is the AdaBoost classification weight, with $\gamma_{i} = +1 \ (-1)$ for signal (background) events and where $p_{i}$ is the prediction of the previous decision tree in the series.

The uniformity weight $u_{i}^{n}$ is defined as the inverse of the density of signal in proximity of event $i$, and is computed with the k-nearest-neighbor algorithm; for background events $u_{i}$ is set to unity. Due to the need of considering many different values of signal efficiency in the construction of the final BDT score and to the use of kNN, the CPU cost of training with uBoost is higher than that of a regular BDT, but not prohibitive in practical applications. Tested on a Dalitz analysis, the method was shown to achieve the wanted uniformity with almost no loss in classification performance [22].

Following on the thread of uBoost, a number of interesting alternatives
to achieve uniform selection efficiency of a BDT classifier were introduced in [24], again targeting the use case of Dalitz plot analysis. E.g., the algorithm called kNNAdaBoost achieves the uniformity goal by modifying the AdaBoost weights to include information on the classification probability of k nearest neighbors to each event,

\[ w^n_i = w^{n-1}_i \exp \left[ -\gamma_i \sum_j a_{ij} p_j \right], \]

where the \( a_{ij} \) matrix collects information on the density of events of the same class around event \( i \), by setting \( a_{ij} = 1/k \) if \( j \) is among the k neighbours of \( i \) and \( = 0 \) otherwise. Other methods proposed in [24] involve the use of \( a_{ij} \) in the loss of the classifier, minimized with the use of gradient boosting. These techniques are shown to improve over uBoost by achieving better uniformity in specific use cases.

More recently, the issue of the decorrelation from variables of interest or, more generally, robustness to nuisance parameters has been addressed by using neural network classifiers, adding suitable regularizer terms to their loss function. An option discussed in [25] is to use for that purpose a measure of the extent to which two sets of features \( \vec{x}, \vec{y} \) are independent

The proposed measure is dubbed DisCo ("distance correlation") [25], a function of the considered features which can be constructed by first defining a distance covariance

\[ d\text{Cov}^2(X,Y) = \langle |X-X'| |Y-Y'| \rangle + \langle |X-X'| \rangle \langle |Y-Y'| \rangle - 2 \langle |X-X'| |Y-Y'\prime | \rangle - 2 \langle |X-X'| |Y-Y'' | \rangle \]

where \( |\cdot| \) is the Euclidean vector norm and \( (X,Y), (X',Y') \) and \( (X'',Y'') \) are i.i.d. pairs from the joint distribution of the two features. The distance correlation, defined as

\[ d\text{Corr}^2(X,Y) = \frac{d\text{Cov}^2(X,Y)}{d\text{Cov}(X,Y) d\text{Cov}(Y,Y)} \]

is then bound between 0 and 1, and is null only if \( x \) and \( y \) are fully independent. \( d\text{Corr}^2(X,Y) \) is differentiable and can be computed from data samples; its value can be profitably added as a penalty term to the loss of the classifier, once multiplied by a positive hyperparameter \( \lambda \) controlling its strength. The multiplier allows to gain control over the acceptable amount of interdependence of \( x \) and \( y \) achieved by a minimization of the penalized loss. In the single-dimensional application considered in [25] DisCo

\[ ^\dagger \text{In their work Kasieczka and Shih discuss the classical single-dimensional case when } x = M_{rec} \text{ is the mass of a searched particle and } y = c \text{ the output of the classifier itself, but the extension to multi-dimensional problems is straightforward.} \]
proves competitive or advantageous over, *e.g.*, adversarial setups (see below) or other methods; further studies are needed to gauge its performance in more complex situations.

A similar approach is taken [26] in a study more explicitly aiming at a reduction of the dependence of classifier score from nuisance parameters $\alpha$. In the proposed technique the $n$-bin histogrammed distribution of classifier output $f(x)$ from input features $x$ is first made differentiable with the use of a Gaussian smoothing,

$$N_k(f(x)) = \sum_b G_k(f(x))$$

where $k$ runs on the bins and $b$ runs on the training events in a batch. The usual loss $L_0$ of the classifier can then be penalized by a term derived from the difference in smoothed bin counts of the original output $f(x)$ and its nuisance-varied value $f(x + \alpha)$,

$$L(\lambda) = L_0 + \lambda \frac{1}{n} \sum_k \left( \frac{N_k(f(x)) - N_k(f(x + \alpha))}{N_k(f(x))} \right)^2.$$ 

The modified loss effectively decouples the classifier output from the value of $\alpha$, both in a synthetic example and in the benchmark problem of $H \rightarrow \tau\tau$ discrimination proposed in the ATLAS kaggle challenge [27], where the tau lepton momentum scale is considered as the nuisance parameter.

### 3.3. Adversarial Setups

The construction of an adversarial setup where two independent neural networks are pitched one against the other in the search for the optimal working point in a constrained classification problem may be considered an extension, if not the logical next step, of the penalized loss methods discussed above. In fact, the global loss function is still the combination of two parts, one of which is the usual classification loss (*e.g.* a BCE term) and the other is a penalization contributed by the adversary, usually modulated by a regularization multiplier $\lambda$. The difference is that adversarial architectures create a conceptual symmetry between the classification task aiming at a signal-background separation and the discrimination of different values of a nuisance parameter, putting the two minimization problems on equal footing.

The above idea was investigated in Computer Science research with the goal of achieving domain adaptation of discriminative classifiers [28, 29] much before the first proposals of application to HEP problems were put
forth. The general problem addressed by those seminal works arises when training and test data are not drawn from the same distribution. This is common when the two sets come from different domains (a source and a target one) or, more to relevance for HEP, when training data are simulated by an imperfect model of real (test) data. It was shown that robust classification can be achieved in such situations if one can find a suitable representation of the data which is maximally insensitive to their source. An adversarial neural network is thus tasked to learn such a representation while competing with one that tries to achieve maximal separation of labeled classes of training data [30].

The first proposal of adversarial neural networks to achieve robustness to systematic uncertainties in HEP problems was the one of Louppe, Kagan and Cranmer [31], who showed the feasibility of using adversarial techniques to make the classification score \( f(X; \theta_f) \) a "pivotal quantity" in the statistical sense [32], i.e. one whose distribution is independent on the value of nuisance parameters \( z \); above, \( \theta_f \) are the parameters of the classifier, and \( X \) denote the data. If one further denotes as \( r \) the adversary, with parameters \( \theta_r \), whose task is to discern values of \( z \) from the output value \( f(X, \theta_f) \) of the classifier, the loss functions of the two networks may be succinctly written \( L_f(\theta_f) \) and \( L_r(\theta_f, \theta_r) \), and a simultaneous training can be carried out by using the value function

\[
E(\theta_f, \theta_r) = L_f(\theta_f) - L_r(\theta_f, \theta_r) \tag{10}
\]

which can be optimized by the minimax solution

\[
\hat{\theta}_f, \hat{\theta}_r = \arg\min_{\theta_f} \max_{\theta_r} E(\theta_f, \theta_r).
\]

Convergence to the optimal solution cannot be guaranteed if the nuisance parameters shape the decision boundary directly. In that case a hyperparameter \( \lambda \) multiplying the adversary loss \( L_r \) may be introduced in Eq. (10), and a search for approximate optimality must be performed. To exemplify their method, Louppe et al. consider both a synthetic example and a HEP use case when the nuisance parameter \( Z \) is categorical, describing the absence \( (Z = 0) \) or presence \( (Z = 1) \) of pile-up in LHC collisions data. In the latter case they show (see Fig.3) how an effective compromise between the classification and the pivotal tasks may be found by a tuning of \( \lambda \).

The application of the above technique to the discrimination of the decay of boosted heavy particles in a situation where background systematics
Fig. 3. AMS score as a function of classifier score for a binary classification task, for different values of the hyperparameter $\lambda$ modulating the loss penalization, and for the case when no nuisance parameter is present. For $\lambda = 10$ an advantageous tradeoff of classification accuracy and robustness to the nuisance is obtained at high classification scores. Reprinted with permission from [31].

affect the inferential step downstream of the NN-based selection was considered in [33]. In their work, authors showed how the relevant utility function in the problem—the significance of a resonant signal in the data, once systematics were accounted for—was indeed maximized by an adversarially trained classifier, despite its slight degradation of separation power with respect to a non-adversarial classifier.

A further comparison of the effectiveness of the adversarial training proposed in [31] to alternatives based on data augmentation and tangent propagation, for the goal of optimizing classification in presence of nuisance parameters, was produced in [34]. The considered HEP problem was the one of $H \rightarrow \tau \tau$ discrimination from backgrounds proposed by the Higgs Kaggle Challenge [27], where an uncertainty on the $\tau$ lepton energy scale was introduced and propagated to the input features of signal and back-
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Besides a baseline, non-systematics-aware neural network classifier, they employed in their comparison a data augmentation method based on training datasets constructed so as to appropriately sample the relevant range of values of the nuisance parameter. Finally, the tangent propagation method consisted in modeling nuisance parameters as coherent geometric transforms of the event features, operated by differentiable functions; a regularization of the model was provided through the derivative of the classifier score on the nuisance parameter value, as introduced by [35]. The comparison showed that adversarial learning had a minor advantage over data augmentation, although further work was deemed necessary to achieve more conclusive results on the matter. Tangent propagation was instead shown to be unsuccessful on the specific problem considered, due to large uncertainties introduced in the geometrical transformation caused by the large class overlap in the feature space.

We conclude this survey of applications of adversarial techniques to constrain the effect of nuisance parameters with a mention of two very recent studies. The first, by Blance, Spannowsky and Waite [36], examines adversarial classification as a preliminary step to the use of autoencoders for unsupervised classification, to verify their effectiveness in reducing the dependence of the autoencoder task on systematic uncertainties. They apply this idea to the search of resonances decaying to semileptonic $t\bar{t}$ final states, showing promising independence of the resulting classification task on the considered smearings of the input models. A second interesting recent study [37] attacks the problem of theoretical uncertainties with adversarial networks. As uncertain theory parameters affect the data in a coherent way, they can be controlled more effectively than experimental ones in machine learning applications. The authors consider the case of searches for new physics in events with a Higgs boson and a high-momentum jet, where renormalization and factorization scale variations heavily affect the predictions of standard model backgrounds, making traditional discrimination methods unreliable. Sensitivity to new physics can be retained by an adversarial technique which ensures robustness to theoretical scale uncertainties, with however smaller, and more realistic, discrimination power.

Overall, the adversarial methods discussed in this section prove effective to achieve approximate independence of the classification from the value of selected input features. In general, however, there is no guarantee that the resulting equilibrium point between the two competing tasks be optimal for the final goal of the analysis in which they are embedded. For this reason, the hyperparameter $\lambda$ governing the tradeoff between the two losses
must be optimized independently. More direct ways to strive for a complete optimization of classification in physics measurements and searches are examined in Sec. 5.

4. Semi-Supervised Approaches

In Sec. 1 nuisance parameters were introduced as additional parameters that account for the limitations of the description of the data and have to be accounted for making accurate statistical statements. Given that most machine learning models in HEP are usually trained using simulated observations, the resulting models could only aspire to be optimal at the task at hand, typically classification or regression, for the specific configuration of nuisance parameters used for data generation. The previous sections discussed some solutions to ameliorate this problem, such as parametrizing the model or decorrelating its output using additional loss terms. In this section we review alternative approaches that are based on using actual experimental data to complement or instead of simulated samples in the model training procedure, focusing on how these techniques could help to deal with nuisance parameters.

Experimental data are the source of information used to test hypothesis or estimate parameters given a model. Models are usually based on detailed simulations of the underlying physical processes and the detector response, providing in general a fairly good but not perfect description of the data. Oftentimes, experimental data from well-known processes are also used to cross-check the accuracy of the description by the model and to estimate correction factors and associated uncertainties as necessary. These calibration procedures, which also constitute statistical inference analyses on their own right, provide a mechanism to improve possible mismodelling issues and obtain data-based estimates for nuisance parameter constraints. While general calibrations are typically performed experiment-wide, more detailed calibrations are often carried out for specific analysis scenarios to improve their precision and discovery reach, for example using an independent subset of data that is expected to be well-modelled to further correct or constrain known unknowns at the inference stage. In some cases, yet arguably not often in analyses that use machine learning to reduce the dimensionality of their summary statistics, known properties of experimental data allow to use a well-understood subset to model one of the mixture components.

The interrelation between experimental data and the generative model
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and its parameters in HEP is thus more involved that the ideal depiction in statistical books. When training supervised machine learning models using simulated data, the expected performance at the objective task in experimental data would benefit from training and validation datasets that are well-calibrated and correspond to the best estimates of the parameters of interest. Leaving aside issues with whether the supervised learning task is a good proxy of the analysis inference goal when nuisance parameters are important, which we discuss in Sec. 5, we review here methodologies that use experimental data during training to close the gap between the performance at the inference task between real and simulated data.

Many of the efforts to achieve such goal in HEP are based on innovations from weak supervision and semi-supervised learning, that focus on the problem of learning useful models from partial, non-standard or noisy label information. In this context, when considering a classification task, simulated observations can be considered as fully labelled data that provide a possibly imperfect description, while real data observations can be thought as unlabelled or very sparsely labelled mixtures from different classes. For example, Dery et al. [38] proposed an approach based on learning from label proportions (LLP), where instead of a label per observation a neural network is trained only based on the class proportions for a given set are known in average using a custom loss. They validate the method on a quark versus gluon tagging example problem and find that it can be used to obtain a similar performance to that of a fully supervised classifier, while being more robust to simulation mismodelling of the input variables.

One of the potential advantages of approaches based on learning from label proportions (and weak supervision more generally) is that in principle they could be extended to train the classifier directly using real data. However, the previous approach based on LLP requires at least knowledge of the label proportions in the mixed samples, which might not be known at training time. To address this limitation, Metodiev et al. [39] proposed a new paradigm referred to as classification without labels (CWoLA), where the classifier is trained to distinguish between two mixed sample with different (and possibly unknown) component fractions. This also simplifies the previous approach because it is based on standard classification loss, where the label is not the observation class but an identifier of the mixed

8For completeness, we note that even when the machine learning model is not trained with the most accurate description of the data, it is still possible to make calibrated statistical statements, as long as known unknowns are properly accounted for in the statistical model used for inference procedure,
sample it belongs to, as depicted in Fig. 4. The authors prove that the optimal binary classifier (in the Bayes sense) for distinguishing samples from each of the mixed samples is a simple function of the density ratio between the components. Furthermore, they demonstrate that CWoLA as well as LLP work similarly to a fully supervised classifier on pure samples, using practical examples such as a quark/gluon discrimination problem.

![Mixed Sample 1 and Mixed Sample 2](image)

**Fig. 4.** An illustration of the CWoLa framework. Figure and description by the authors of CWoLa [39] and licensed under CC BY 4.0.

While CWoLA has a wider range of applicability than vanilla LLP, it also requires two (possibly smaller) mixed test data samples with known fractions to establish operating points. After its introduction, two other studies have applied variations of CWoLa to sample use cases. Cohen et al. [40] applied weakly supervised neural networks to the new-physics search of gluino production using fast simulation samples, and also demonstrated that weak supervision can perform similarly to full supervision and that it is robust to certain types of mismodelling. Further work by Komiske et al. [41] has also demonstrated that weak supervision approaches scale well to problems with high-dimensional inputs and larger models, by successfully applying LLP and CWoLa to the quark/gluon discrimination problem directly using a convolutional network model applied directly to jet images.

Nevertheless, probably the main advantage of weak supervision techniques such as LLP and CWoLa it is that in principle they could allow
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the use of real data during the training procedure. The use of experimental data for training with this family of techniques has not been demonstrated in HEP practice so far. In the best case scenario, a weakly supervised classifier trained with data could be used to extract the optimal classifier (in the Bayes sense) between each of the mixture components (e.g. signal and background). The output of this classifier could then be used to select or construct a summary statistic to carry out the inference goal of the analysis, yet most likely the model would have to be constructed using simulated observations that are subjected to the effect of nuisance parameters. Hence a potentially Bayes-optimal weakly supervised classifier would then suffer the same pitfalls of any other classifier in relation with the analysis inference goal, as we discuss below, in Sec. 5. Furthermore, if experimental data are used during training, then the model might be overfitted to the particular statistical fluctuations of the dataset, so an experimental data splitting scheme, or the use experimental data from an independent subset, might be needed to avoid biased estimations. If the data representing different mixture fractions are taken from different control regions, the previous caveat could be avoided but then the density of the components for each of the mixed samples is not the same, so that the basic theoretical assumption of CWoLA or LLP does not hold. In conclusion, while weak supervision could be useful to build classifiers that might benefit the model classification performance, due to their being more robust to certain types of mismodelling, existing practical approaches do not fully address the issue of dealing with nuisance parameters.

5. Inference-Aware Approaches

The approaches discussed so far use diverse methodologies in order to overcome situations where the generative model is not perfectly known and thus the performance of the supervised learning task considered (typically classification) might be degraded once it is applied on real data. However, recent work has shown that some of the innovations in the field of machine learning are flexible enough so as to be re-purposed to deal more closely with the statistical inference objective of HEP analyses.

The solutions discussed in this section thus move away from the overall goal of optimising models to become performant at proxy supervised learning tasks such as classification, and attempt to frame the problem directly as one of statistical inference. This change of paradigm is often referred to as likelihood-free or simulation-based inference, and is a rapidly evolving
line of research, with applications within particle physics as well as in other scientific domains that heavily rely on complex generative models, such as epidemiology or cosmology.

For a broader overview of the techniques proposed to deal with this problem and their role in particle physics we refer to other general reviews [42]. In this section we instead focus on how some of these inference-aware approaches could be useful to deal with nuisance parameters in the context of particle physics. Given that most of these solutions already cast the problem in the form of statistical inference on a set of parameters given the data, it is not surprising that nuisance parameters could be incorporated or dealt with in a principled way for many of these methods.

5.1. Why are classification and regression not enough?

Before delving into these new techniques, it is worth considering the limitations of classification and regression as proxy supervised tasks from the point of view of statistical inference. For simplicity, let us consider the paradigmatic problem of inference about the mixture coefficient in a two-component mixture model, which can be thought of as the basis for both cross section measurements and new physics searches:

$$p(x|\mu, \theta) = (1 - \mu)p_b(x|\theta) + \mu p_s(x|\theta)$$

(11)

where $\mu$ is a parameter corresponding to the signal mixture fraction, $x$ is the event feature space and $\theta$ are other parameters which the component distribution functions might depend on. For the problems of relevance for machine learning techniques, we may assume that the component probability density functions for signal $p_s(x|\theta)$ and background $p_b(x|\theta)$ are not known parametrically, yet we have access to random samples from a simulator that is able to model them implicitly.

The relation between the density ratio approximations from Eq. (1) and the typical problems of inference in HEP (i.e. measurements and searches) can be studied using two different statistical constructions: likelihood ratios or summary statistics. Both approaches lead to equivalent conclusions regarding the limitations of classification as a means of obtaining useful transformations for statistical inference in the presence of nuisance parameters, but they are both relevant because they imply ways of framing the problem which map very well to different families of new techniques built to address this issue which we discuss later in this section.

Let us start with likelihood ratios, which can be generally defined for a set of $n$ data observations $D = \{x_0, \ldots, x_n\}$ between two simple hypotheses...
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\[ H_0 \text{ and } H_1 \text{ as:} \]

\[ \Lambda(D; H_0, H_1) = \frac{p(D|H_0)}{p(D|H_1)} = \prod_{x \in D} \frac{p(x|H_0)}{p(x|H_1)} \quad (12) \]

where the last expansion requires independence between observations, and where we note that the quantity \( p(x|H_0)/p(x|H_1) \) is a density ratio and could be approximated as discussed before by training a probabilistic classifier to distinguish samples generated under each hypothesis. From the Neyman-Pearson lemma \[43\], we know the likelihood ratio is the most powerful test statistic to distinguish the two simple hypotheses \( H_0 \) and \( H_1 \) at a given significance level \( \alpha = P(\Lambda(D; H_0, H_1) \leq t_{\text{cut}}) \), for any threshold \( t_{\text{cut}} \).

Going back to problems where hypotheses have a mixture structure like the one discussed in Eq. (11) and differ in their mixture composition, this would mean training a classifier between samples generated from \( p(x|\mu, \theta) \) for the specific mixture fractions \( \mu_0 \) and \( \mu_1 \) that characterise each of the hypotheses \( p(x|H_0) = p(x|\mu_0, \theta) \) and \( p(x|H_1) = p(x|\mu_1, \theta) \), which would become rapidly cumbersome if we are dealing with multiple tests for a set of different \( \mu_0 \) and \( \mu_1 \) values. Luckily, each factor in the likelihood ratio from Eq. (12) can be expressed in the following manner:

\[ \frac{p(x|H_0)}{p(x|H_1)} = (1 - \mu_0) p_b(x|\theta) + \mu_0 p_s(x|\theta) \]

\[ (1 - \mu_1) p_b(x|\theta) + \mu_1 p_s(x|\theta) \quad (13) \]

so for a given pair \( \mu_0 \) and \( \mu_1 \) the density ratio between hypotheses factor in the likelihood ratio is a bijective function of the ratio \( p_s(x|\theta)/p_b(x|\theta) \).

That quantity can be approximated by training a probabilistic classifier to distinguish signal and background simulated samples, which is computationally more efficient and easier to interpret intuitively than directly the ratio \( p(x|H_0)/p(x|H_1) \) mentioned earlier.

A likelihood ratio approximation can thus be obtained in the case of two simple two-component mixture hypotheses that only differ in the mixture fractions by plugging the output of a probabilistic classifier \( c(x) \) trained to distinguish signal and background observations in Eq. (14) with the corresponding values of \( \mu_0 \) and \( \mu_1 \) in Eq. (12). Oftentimes, that is not necessary because the classifier output directly contains all the relevant information about the ratio approximation so it can be used directly as a summary for inference with the help of histograms or non-parametric density estimation techniques, with the added advantage that is typically a \([0, 1]\) bounded variable and thus easy to interpret. It is worth mentioning that the relation...
between the likelihood ratio and the component density ratios can also be useful in the multi-component setting, where the likelihood ratio factor can be expressed in terms of the density ratios that can be obtained for pairwise component classification problems [17].

Within this framework, the usefulness of probabilistic classifiers that distinguish signal and background observations is that they can be used to approximate the likelihood ratio, which is the most powerful summary statistic for two simple hypothesis that differ only on the mixture fraction parameters. If the hypotheses are not fully specified, i.e. they depend on additional parameters (the dependence with the mixture fractions can be factored out as discussed before), the likelihood ratio as defined in Eq. (12) also depends on these parameters. The Neyman-Pearson lemma does not hold when parameters are varied nor for composite generalisations such as the profile likelihood ratio. Hence, when nuisance parameters are important, a fixed probabilistic classifier, even if optimal in the Bayes sense, is not guaranteed to provide a transformation that is optimal for inference in any statistically meaningful way.

An alternative formulation of the limitations of classification for statistical inference is based on the sufficiency conditions required for summary statistics, according to the Fisher-Neyman factorisation criterion. A summary statistic for a set of i.i.d. observations \(D = \{x_0, ..., x_n\}\) is sufficient with respect to a statistical model and a set of parameters \(\theta\) if and only the generating probability distribution function of the data \(p(x|\theta)\) can be factorised as follows:

\[
p(x|\theta) = q(x)r(s(x)|\theta)
\]  

(15)

where \(q(x)\) is a non-negative function that does not depend on the parameters and \(r(x)\) is also a non-negative function for which the dependence on the parameters \(x\) is a function of the summary statistic \(s(x)\). Such a sufficient statistic contains all the information in the observed sample useful to compute any estimate on the model parameters, and no complementary statistic can add any additional information about \(\theta\) contained in the set of observations.

A trivial sufficient summary statistic according to the previous definition is the identity function \(s(x) = x\), yet typically we are only interested in summaries that reduce the original data dimensionality. If \(p(x|\theta)\) is not known in closed form, as is often the case in HEP analyses, the general task of finding a sufficient summary statistic that reduces the dimensionality cannot be tackled directly by analytic means. An exception to this can be
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easily shown in the case of a mixture model where the mixture fraction \( \mu \) is the only parameter. By both dividing and multiplying by the mixture distribution function from Eq. (11) we easily obtain:

\[
p(x|\mu, \theta) = p_b(x|\theta) \left( 1 - \mu + \mu \frac{p_s(x|\theta)}{p_b(x|\theta)} \right)
\]

(16)

from which we can already prove that the density ratio \( s_s/b(x) = p_s(x|\theta)/p_b(x|\theta) \) (or alternatively its inverse) is a sufficient summary statistic for the mixture coefficient parameter, according to the Fisher-Neyman factorisation criterion from Eq. (15). This quantity could be efficiently approximated by considering the problem of probabilistic classification between signal and background as discussed in Eq. (1). Because any bijective function of a sufficient summary statistic is also a sufficient summary statistic, the conditional probability from the conditional output of a balanced classifier

\[
c(x) = s_s/(s+b)(x) = \frac{p_s(x|\theta)}{p_s(x|\theta) + p_b(x|\theta)}
\]

(17)

can be used directly as a summary instead of \( s_s/b(x) \), with the additional advantage that it is bounded between zero and one, a fact that greatly simplifies visualisation and calibration.

From this perspective, the utility of signal versus background classification to obtain an approximately sufficient summary statistic with respect to the mixture model and mixture fraction \( \mu \) is evident. However, if the statistical model depends on additional nuisance parameters, even Bayes optimal probabilistic classification does not provide any sufficient guarantees, so useful information which can be used to constrain the parameters of interest might be lost if a low-dimensional classification-based summary statistic is used in place of the original data \( x \).

Above we have reviewed from a statistical perspective the limitations of signal versus background classification models when the goal is inference in the presence of nuisance parameters. In practice, classifiers can be trained for the most probable likely value of the nuisance parameters and their effect can be adequately accounted during calibration, yet the resulting inference will be degraded even if the classification is optimal. Alternative uses of classification and regression models such as particle identification and momentum or energy regression can be understood as approximations of a subset of relevant latent variables \( z \) of the generative model. This information could be then be used to complement the reconstruction output.
for each object and design better hand-crafted or classification-based summary statistics, so at the end the final goal is inference, and the previously mentioned shortcomings still apply.

5.2. Generalising the likelihood ratio trick

The first known attempts to study the relation between statistical inference in HEP with nuisance parameters and probabilistic classifiers date to Neal [12]. In his seminal paper, in addition of making explicit the problem of not being able to compute the data generating likelihood in closed form and clarifying the useful relation between likelihood ratios and probabilistic classifiers discussed in the previous subsection, he also acknowledges the limitations of this approach in the presence of nuisance parameters and suggests a few possible candidate solutions.

To ameliorate the problems of losing useful information when reducing the dimensionality of the data with summary statistics, a few variations over classical signal versus background classification trained with the best estimation of the nuisance parameters are proposed. The first proposal foresees the training of a single robust classifier by combining simulated observations of signal and background generated with different nuisance parameters, for example drawn from their prior or from a reasonable distribution, to constrain the nuisance parameters $\pi(\theta)$.

The drawbacks of such marginal classifier are similar to the concerns on models trained for the most likely values of the nuisance parameters: it might not be possible to accurately classify without knowing $\theta$, and even when that is possible the usefulness of the resulting score will be degraded when calibrated statistical inference is carried out. To address these concerns, the author suggests a generalisation based on training a single classifier $t$ considering both the observations $x$ and the nuisance parameters $\theta$ as input. The resulting model would be a nuisance-parametrized signal versus background classifier, thus an early precedent for some of the approaches discussed below. In order to use these parametrized classifiers on real data, for which the correct values of $\theta$ are not known, Neal argues that an additional per-event regression model for $\theta$ could be trained on simulated observations.

The ideas developed by Neal [12] were not applied in practice until they were generalised and extended by Cranmer et al. [17]. The authors of that cited work identify the same problem regarding the use of discriminative classifiers to approximate likelihood ratios with nuisance parameters and
introduce a generic framework for inference using calibrated parametrized classifiers referred to as CARL. In their more general formulation, they propose using a doubly parametrized classifier to approximate the likelihood ratio for all possible pairs of relevant parameters \( \theta_0 \) and \( \theta_1 \) of a generative model \( p(x|\theta) \) as follows:

\[
\hat{r}(x; \theta_0, \theta_1) \approx \frac{p(x|\theta_0)}{p(x|\theta_1)} \tag{18}
\]

where the classifier output \( \hat{r}(x; \theta_0, \theta_1) \) has a specific dependence on the parameter vectors \( \theta_0 \) and \( \theta_1 \) and the approximation becomes an equality only for a Bayes optimal classifier for each combination. In order to train such classifier in a data-efficient manner, they suggest using smooth models such as neural networks and a single learning stage based on a large dataset where each observation correspond to an instantiation of the parameters \( \theta_0 \) and \( \theta_1 \) drawn from a reasonable prior distribution \( \pi(\theta) \) and where \( x \) is drawn from the generative model using those parameters.

Given a flexible enough model and enough training data, the procedure described above could be used to learn a good approximation of the quantity in Eq. (18). For problems where the underlying structure is a mixture model, Cranmer et al. also point out that is possible to obtain the quantity \( \hat{r}(x; \theta_0, \theta_1) \) based on the parametrized output for each pairwise component classification problem which are simpler learning tasks. Because in practice the approximation cannot be assumed to be exact, the authors also propose to have a second stage where generative model samples are used again to calibrate the for all the relevant values of the parameters and set of diagnostic procedures. They successfully apply this methodology to a set of example problems and discuss it potential usefulness in the context of HEP analysis.

It is worth noting that the component of the vector parameters in \( \theta \) in CARL could include both nuisance parameters and parameters of interests in the same manner. The nuisance parameters could also be incorporated in the calibration and profiled away at the inference stage. Hence, with the caveats associated with a more involved training procedure and parametric calibration procedure, this technique presents the first principled and general solution for dealing with parameters when using machine learning techniques in the context of HEP inference.
5.3. Learning more efficiently from the simulator

As mentioned earlier, one of the caveats of the general applicability of CARL is that the training and calibration procedure may potentially require a large amount of simulated data to approximate accurately the likelihood ratio \( r(x; \theta_0, \theta_1) \) for all relevant \( \theta_0 \) and \( \theta_1 \) when the dimension of \( \theta \). This practical limitation motivated Brehmer and the original authors of CARL to develop a family of methods [44–46] to estimate the likelihood ratio and other useful quantities for inference in a more data-efficient manner, by augmenting training data with information from the simulator. The source for that information from the simulation comes from the properties and structure of the data generating process:

\[
p(x|\theta) = \int p(x, z|\theta)dz
\]  

which are characterised by the the joint distribution function \( p(x, z|\theta)dz \) where \( z \) are all the latent variables of each observation. In high-energy physics event generation, the joint probability distribution can be factorised in a series of conditional factors matching the various simulation steps and their dependencies:

\[
p(x, z|\theta) = p(x|z_d)p(z_d|z_s)p(z_s|z_p)\sum_{j=0}^{K-1} p(z_i = j|\theta_{th})p(z_p|\theta_{th}, z_i = j)
\]

where \( p(z_i = j|\theta) \) is the probability of a given type of process \( j \) occurring, \( p(z_p|\theta, z_i = j) \) is the conditional probability density of a given set of parton-level four-momenta particles for a given process, \( p(z_s|z_p) \) is the conditional density of a given parton-shower outcome, \( p(z_d|z_s) \) is the conditional density of a set of detector interactions and readout noise and \( p(x|z_d) \) is the conditional density of a given detector readout. Note that all the factors could depend on additional nuisance parameters; here only the theoretical parameters \( \theta_{th} \) are made explicit for notational simplicity because they are normally the parameters of interest. Also note that the last factor gives rise to the mixture structure mentioned in the last subsection. While \( p(x|\theta) \) and ratios of that quantity are typically intractable, the authors suitably remark that the joint likelihood ratio

\[
r(x, z|\theta_0, \theta_1) = \frac{p(x, z|\theta_0)}{p(x, z|\theta_1)}
\]

and the joint score

\[
t(x, z|\theta_0) = \nabla_{\theta} \log p(x, z|\theta)|_{\theta_0}
\]
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can often be obtained exactly for a given simulated observation due to its factorised structure. They propose two regression losses $L_r$ and $L_b$ for each of the previous quantities, which may be used to obtain an approximation of the likelihood ratio $r(x|\theta_0, \theta_1)$ and the score $t(x|\theta_0)$ by empirical risk minimisation with various machine learning models such as neural networks. Based on these loss functions, Brehmer et al. develop a family of new methods as well as extensions of CARL to more efficiently approximate the parametrized likelihood ratio $r(x|\theta_0, \theta_1)$ and demonstrate their effectiveness in a few example problems. Another practical innovation developed by the authors, applicable to all the new parametrized likelihood ratio estimators and also to CARL, is that the parameters of the reference hypothesis in $\theta_1$ in Eq. (18) can be kept fixed at an arbitrary value, thus simplifying the learning task significantly. Building upon this work, Stoye and the previous authors [47] also developed two new methods that can incorporate the joint likelihood ratio and the joint score to a loss function based on the cross entropy, which reduces the variance during the learning tasks further improving sample efficiency for obtaining accurate likelihood ratio approximations.

In addition to the efficient techniques for parametrized likelihood ratio estimation discussed above, Brehmer et al. [44–46] also propose a new class of methods referred to as SALLY using the regressed score approximation $\hat{t}(x|\theta_{\text{ref}})$ at a single reference parameter point $\theta_{\text{ref}}$ to construct a summary statistic. The score $t(x|\theta_{\text{ref}})$, whose dimensionality is the same as that of the parameter vector $\theta$, is a sufficient statistic in the neighborhood of $\theta_{\text{ref}}$, so it is a very useful transformation. Because the dimensionality might still be high in cases with a large number of parameters, they propose alternatively to use a one-dimensional projection (i.e. SALLINO) in the direction of parameter variation as alternative lower-dimensional statistic. In the same work, the authors also experiment with augmenting conditional neural density estimators, such as density network or normalised flows, with a joint score regression loss function. A calibrated estimation of the likelihood $\hat{p}(x|\theta)$ can be used as basis for any statistical inference task but its accurate approximation is challenging with a finite data samples with many recent advances coming from the field of machine learning.

Similarly to CARL, all these improved techniques for the estimation of likelihood ratios, likelihood scores or the conditional likelihood itself make no distinction between the the statistical parameters in the model. Hence, nuisance parameters can be incorporated in the vector of parameters $\theta$, accounted for like any another parameter in the calibration, and profiled
away at the inference stage. The challenge for their direct application in HEP, particularly for the methods that use augmented data from the simulator, is to approximate or model the effect of all relevant nuisance parameters in the joint likelihood ratio and score. In a recent publication, Brehmer et al. [48] presented a software library to simplify the application of these techniques to LHC measurements and included the effect of nuisance parameters from scale and parton distribution function choices by varying the weights associated to each simulated observations.

5.4. Inference-aware summary statistics

The previous techniques, with the exception of Sally (and Sallino for a fixed projection) are based directly on calibrated likelihood ratios or likelihood approximations so they are at their core a different form of inference from what is typically done in HEP: they are designed to tackle the inference problem directly, rather than to construct summary statistics. Such a strong paradigm change can be very advantageous but also poses some challenges for its adoption. In recent years, another complementary family of inference-aware techniques has been proposed, whose objective is the construction of machine-learning based summary statistics that are better aligned with the statistical inference goal of HEP analysis, including nuisance parameters. Once constructed, these summary statistics can be used in place of simplified physical summaries or signal background classification outputs.

A generic technique in this category, which has direct applicability to HEP analyses, is Inferno [49]. In that work, authors demonstrate how non-linear summary statistics can be constructed by minimising inference-motivated losses via stochastic gradient descent specific for the analysis goal. For example, for an analysis focusing on the measuring of a physical quantity such a cross section, the proposed approach can be used to minimise directly as a loss an approximation of the expected uncertainty on the parameter of interest, fully accounting for the effect of relevant nuisance parameters.

In Inferno and other similar approaches discussed later, the parameters of a neural network are optimised by stochastic gradient descent within an automatic differentiation framework, where the considered loss function accounts for the details of the statistical model as well as the expected effect of nuisance parameters. An graphical depiction of this technique is included in Fig. 5. The left-most block refers to sampling a differentiable
simulator or approximating the effect of the parameters $\theta$ over existing simulated observations, including relevant nuisance parameters. These observations go through a neural network that depends on a set of parameters $\phi$ (second block from the left) and then a histogram-like summary statistics is constructed from the neural network output (third block from the left). Still within the automatic differentiation framework, a synthetic likelihood (e.g. product of Poisson counts for a histogram-like summary statistic) is constructed. A final inference-aware loss, for example an approximation of the expected uncertainty for the parameters of interest accounting for nuisance parameters, can then be constructed based on the inverse Hessian matrix and used to optimise the neural network parameters.

Once the summary statistic transformation has been learned with the procedure described above, it can be used, e.g. using an argmax operator instead of a softmax to compute the summary statistic if the approximation of Fig. 5 is used, to carry out statistical inference with the with usual procedures and tools. The main challenge of using this approach in HEP analyses is that the effect of nuisance parameters has to be included in the auto-differentiation framework, for example by transforming the input features (e.g. momenta and energy calibration uncertainties), by interpolating simulated observation weights (e.g. theoretical and parton distribution function uncertainties) or by considering the interpolation between histogram counts as a last resource. If those challenges can be overcome, this method provides an alternative to perform dimensionality reduction using directly an approximation of the inference objective of a given analysis, even in the presence of nuisance parameters, in contrast with a transformation based on probabilis-

Fig. 5. Learning inference-aware summary statistics. Figure by the authors of inferno [49] and licensed under CC BY 4.0.
tic classification or a physics-motivated feature. The authors demonstrate the effectiveness of this technique in a multi-dimensional synthetic example with up to 3 nuisance parameters, where the inference-aware summary statistics outperform even optimal classification-based summaries.

A technique with a similar reach, but that was developed instead for tackling likelihood-free inference problems in astrophysical observations, was presented by Charnock et al. [50]. In their work, authors present an approach to train an information-maximising neural network (IMNN) by constructing a loss function based on a Fisher matrix determinant for Gaussian likelihoods, approximated from the covariance matrix of simulated data. While the authors do not consider the problem of nuisance parameters specifically, Alsing et al. [51] develop a useful transformation that can be applied to implicitly marginalise the summary statistics resulting from IMNN or score $t(x|\theta) = \nabla_\theta \log p(x|\theta)$ approximations (e.g. SALLY from the previous subsection).

More recently, there has also been some recent work building upon the ideas behind INFERNO that attempt to simplify its application to high-energy physics analysis or extend its functionality. For example, Wunch et al. [52] suggest using a differentiable transformation of a neural network with a single node to construct a Poisson count likelihood instead of a softmax as the basis for the inference-aware loss. Similarly to what was observed for INFERNO, the authors demonstrate the usefulness of an inference-aware construction in a synthetic example, and also using an extension of the Higgs ML benchmark including nuisance parameters. Following a different path, the authors of NEOS [53] use a technique referred to as fixed-point differentiation to compute gradients of the profile likelihood, thus avoiding the Hessian inverse approximation, and to directly minimise the expected upper limits $CL_s$. Both Wunch et al. and the authors of NEOS restrict the modelling of the effect of nuisance parameters to histogram interpolation.

In addition to the mentioned approaches, it is worth noting other alternatives with a more limited range of applicability but that could be useful for certain use cases. Elwood et al. [54] propose using the expected significance approximation formula for a single bin count experiment, optionally including the effect of a single source of systematic uncertainty directly as a loss of a neural network. For a different type of models, Xia [55] develop a variation of boosted decision tree training referred to as QBDT which targets directly the statistical significance, and which can also include the effect of nuisance parameters in its approximation. In both cases, authors demonstrate with practical examples that the significance optimising algorithms
outperform their classification counterparts.

6. Outlook

The reduction of the effect of systematic uncertainties in parameter estimation is a crucial problem in particle physics. In the past, the problem was attacked by striving for redundancy of the measurement apparatus, robustness of the detection techniques, and the use of analysis methods aiming for inter-calibration, cross-validation, and leveraging as much as possible control datasets and measurements. In the machine learning era, automated methods have become available to handle many of the effects that imprecise knowledge of latent features of the data bear on physics measurement. While already a conspicuous arsenal of techniques has been amassed, no catch-all procedure has emerged yet, so insight is still required to discern the salient features of the problem to be solved and the appropriate method to deploy. The most promising avenues for a general procedure of handling nuisance parameters are those described in Sec. 5 where the optimization objectives are more directly linked to the inference goal.

Acknowledgements

The authors would like to thank Johann Brehmer for some discussions about the techniques included in MadMiner and how they can deal with nuisance parameters.
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