On the Evaluation of Generative Models in High Energy Physics

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There has been a recent explosion in research into machine-learning-based generative modeling to tackle computational challenges for simulations in high energy physics (HEP). In order to use such alternative simulators in practice, we need well defined metrics to compare different generative models and evaluate their discrepancy from the true distributions. We present the first systematic review and investigation into evaluation metrics and their sensitivity to failure modes of generative models, using the framework of two-sample goodness-of-fit testing, and their relevance and viability for HEP. Inspired by previous work in both physics and computer vision, we propose two new metrics, the Fréchet and kernel physics distances (FPD and KPD), and perform a variety of experiments measuring their performance on simple Gaussian-distributed, and simulated high energy jet datasets. We find FPD, in particular, to be the most sensitive metric to all alternative jet distributions tested and recommend its adoption, along with the KPD and Wasserstein distances between individual feature distributions, for evaluating generative models in HEP. We finally demonstrate the efficacy of these proposed metrics in evaluating and comparing a novel attention-based generative adversarial particle transformer to the state-of-the-art message-passing generative adversarial network jet simulation model.

I. INTRODUCTION

In high energy physics (HEP), accurate simulations are critical for precision measurements and searches such as those performed at the CERN Large Hadron Collider (LHC). These are traditionally performed using Monte Carlo (MC) event generators, detailed modeling of particles’ propagation and interaction through detectors (typically with the GEANT4 [1] package), and reconstruction algorithms to unfold detector measurements back to particles and high-level objects such as jets. While these methods have been highly successful for the physics goals of the LHC, scaling up to the simulation challenges of the upcoming high-luminosity phase of the LHC (HL-LHC) [2] necessitates significant advancements in speed and resource requirements [3–5], while maintaining the quality of current simulations.

To tackle this problem, a plethora of techniques for fast simulation of calorimeter showers and jets have been developed and explored in the last few years, particularly using generative modeling techniques in machine learning (ML) [6–22]. Reviews of these approaches can be found in Refs. [23, 24]. For an experimental collaboration to apply one of these techniques in real data analyses, however, they require methods to objectively compare the performance of different simulation techniques and extensively validate the produced simulations. This calls for the study and adoption of standard quantitative evaluation metrics for generative modeling in HEP.

Recently, several metrics have been proposed to address this challenge. However, to our knowledge, there has been no systematic investigation of their sensitivity to expected failure modes of generative models, and their relevance to validation and feasibility for broad adoption in HEP. To this end, we study the performance of proposed metrics from HEP and computer vision. Inspired by both domains, we develop two novel metrics we call the Fréchet and kernel physics distances (FPD and KPD, respectively), and find them to collectively have excellent sensitivity to all tested data mismodeling, and to satisfy practical requirements for evaluation and comparison of generative models in HEP. We conclude our experiments by recommending the adoption of FPD and KPD, along with quantifying differences in individual feature distributions using the Wasserstein 1-Distance, and demonstrate their use in evaluating a novel attention-based generative adversarial particle transformer, or GAPT.

This paper is structured as follows. In Section II we define our criteria for evaluation metrics in HEP and review existing metrics. We present results on the performance of these metrics on Gaussian-distributed synthetic toy data and simulated high energy jets in Sections III and IV respectively. Based on these experiments, we provide our recommendations and concretely illustrate their application by evaluating and comparing GAPT to the current state-of-the-art (SOTA) MPGAN [17] model in
Section V. Finally, we conclude in Section VI.

II. EVALUATION METRICS FOR GENERATIVE MODELS

In evaluating generative models, we aim to quantify the difference between the real and generated data distributions \( p_{\text{real}}(x) \) and \( p_{\text{gen}}(x) \) respectively, where data samples \( x \in \mathbb{R}^d \) are typically high dimensional. Lacking tractable analytic distributions in general, this can be viewed as a form of two-sample goodness-of-fit (GOF) testing of the hypothesis \( p_{\text{real}}(x) = p_{\text{gen}}(x) \) using real and generated samples, \( \{x_{\text{real}}\} \) and \( \{x_{\text{gen}}\} \), drawn from their respective distributions. As illustrated in Ref. [25], in general, there is no “best” GOF test with power against all alternative hypotheses. Instead, we aim for a set of tests that collectively have power against the relevant alternatives we expect, and are practically most appropriate. In this section, we first outline the criteria we require of our evaluation metrics in Section II A, then review and discuss the suitability of possible metrics in Section II B, and end in Section II C with a discussion on the features to use in comparing such high dimensional distributions, motivating FPD and KPD.

A. Criteria for Evaluation Metrics in HEP

Typical failure modes in ML generative models such as normalizing flows and auto-regressive models include a lack of sharpness and smearing of low-level features, while generative adversarial networks (GANs) often suffer from “mode collapse”, where they fail to capture the entire real distribution, only generating samples similar to a particular subset. Therefore, with regard to the performance of generative models, we require first and foremost that the tests be sensitive to both the quality and the diversity of the generated samples. It is critical that these tests be multivariate as well, particularly when measuring the performance of conditional models, which learn conditional distributions given input features such as those of the incoming particle into a calorimeter or originating parton of a jet, and which will be necessary for applications to LHC simulations [26]. Multivariate tests are required in order to capture the correlations between different features, including those on which such a model is conditioned. Finally, it is desirable for the test’s results to be interpretable to ensure trust in the simulations.

To facilitate a fair, objective comparison between generative models, we also require the tests to be reproducible — i.e., repeating the test on a fixed set of samples should produce the same result — and standardizable across different datasets, such that the same test can be used for multiple classes and data structures (e.g., both images and point clouds for calorimeter showers or jets). It is also desirable for the test to be reasonably efficient in terms of speed and computational resources, to minimize the burden on researchers evaluating their models.

B. Evaluation Metrics

Having outlined criteria for our metrics, we now discuss possible metrics and their merits and limitations. The traditional method for evaluating simulations in HEP, is to compare physical feature distributions using one-dimensional (1D) histograms. This allows valuable, interpretable insight into the physics performance of these simulators, and can be quantified by measures such as the binned chi-squared (\( \chi^2 \)) test or the unbinned Wasserstein \( p \)-distance (\( W_p \)). However, it is intractable to extend this approach to multiple distributions simultaneously as it falls victim to the curse of dimensionality — the number of bins and samples required to retain a reasonable granularity in our estimation of the multidimensional distribution grows exponentially with the number of dimensions. Therefore, while valuable, this method is restricted to evaluating single features, losing sensitivity to correlations and conditional distributions.

1. Integral Probability Metrics and \( f \)-Divergences

To extend to multivariate distributions, we first review measures of differences between probability distributions. The two prevalent classes of discrepancy measures are integral probability metrics (IPMs) [27], defined as

\[
D_F(p_{\text{real}}, p_{\text{gen}}) = \sup_{f \in \mathcal{F}} |E_{x \sim p_{\text{real}}} f(x) - E_{y \sim p_{\text{gen}}} f(y)|, \tag{1}
\]

and \( f \)-divergences, defined as

\[
D_f(p_{\text{gen}}, p_{\text{real}}) = \int p_{\text{real}}(x) f(\frac{p_{\text{real}}(x)}{p_{\text{gen}}(x)}) \, dx. \tag{2}
\]

IPMs include popular measures such as \( W_1 \), maximum mean discrepancy (MMD) [28], and energy distance [29], while measures such as the Kullback–Leibler (KL) [30], Jenson–Shannon (JS) [31, 32], and Pearson \( \chi^2 \) [33] divergences are all forms of \( f \)-divergences. These two, almost mutually exclusive\(^1\), classes each have unique, interesting properties.

IPMs measure differences in distributions by finding a “witness” function, \( f \) in Eq. (1), out of a certain class of functions \( \mathcal{F} \), which maximizes the absolute difference in its expected value over the two distributions. Crucially, IPMs are metrics, with measures such \( W_1 \) and MMD able to metrize the weak convergence of probability measures [35, 36], and provide a powerful and intuitive quantitative measure of distance between distributions. On

\(^1\) The total variation distance is the only non-trivial discrepancy measure that is both an IPM and an \( f \)-divergence [34].
the other hand, in general, \( f \)-divergences do not take the metric space into account, and instead measure pointwise differences in probability mass \([37]\). This allows for coordinate invariance and convenient information-theoretic interpretations. \( f \)-divergences can thus be powerful measures of discrepancies, with the \( \chi^2 \) GOF test and related variants \([38–40]\) ubiquitous in HEP. However, as they are not generally metrics, we argue that IPMs are more appropriate for comparing generative models and their respective learnt distributions.

Additionally, on the practical side, finite-sample estimation of \( f \)-divergences such as the KL and the Pearson \( \chi^2 \) divergences is intractable in high dimensions, generally requiring partitioning in feature space, which suffers from the curse of dimensionality as described above. References \([34, 41]\) demonstrate more rigorously the efficacy of finite-sample estimation of IPMs, in comparison to the difficulty of estimating \( f \)-divergences.

2. **IPMs as Evaluation Metrics**

Having argued in their favor, we discuss specific IPMs and related measures, and their viability as evaluation metrics. The most famous is the Wasserstein distance \([42, 43]\), for which \( \mathcal{F} \) in Eq. (1) is the set of all \( K \)-Lipschitz functions (where \( K \) is any positive constant), and intuitively is the optimal cost of transporting the probability mass of one distribution to another. This metric is sensitive to both quality and diversity of the generated distributions, however, its finite-sample estimator is the optimum of a linear program, which, while tractable in 1D, is biased with very poor convergence in high dimensions \([44]\). We demonstrate these characteristics empirically in Sections III and IV.

A related pseudometric\(^2\) is the Fréchet, or \( W_2 \), distance between Gaussian distributions fitted to the features of interest, which we generically call the Fréchet Gaussian Distance (FGD). A form of this known as the Fréchet Inception Distance (FID) \([45]\), using the activations of the Inception v3 convolutional neural network (CNN) model \([46]\) on samples of real and generated images as its features, is currently the standard metric for evaluation in computer vision. The FID has been shown to be sensitive to both quality and mode collapse in generative models, and is extremely efficient to compute, however, has the drawback of assuming Gaussian distributions for its features. While finite sample estimates of the FGD are biased \([47]\), Ref. \([48]\) introduces an effectively unbiased estimator \( \text{FGD}_\infty \), obtained by extrapolating from multiple finite sample estimates to the infinite sample value.

The final IPM we discuss is the maximum mean discrepancy (MMD) \([49]\), for which \( \mathcal{F} \) is the unit ball in a reproducing kernel Hilbert space (RKHS) for a chosen kernel \( k(x, y) \). Intuitively, it is the distance between the mean embeddings of the two distributions in the RKHS, and it has been demonstrated to be a powerful two-sample test \([28, 50]\). However, generally high sensitivity requires tuning the kernel based on the two sets of samples. For example, the traditional choice is a Gaussian RBF kernel, where kernel bandwidth is typically chosen based on the statistics of the two samples \([28]\). While such a kernel has the advantage of being characteristic, i.e. it produces an injective embedding \([51]\), to maintain a standard and reproducible metric, we experiment instead with fixed polynomial kernels of different orders. These kernels allow access to high order moments of the distributions and have been proposed in computer vision as an alternative to FID, termed kernel Inception distance (KID) \([47]\). MMD has unbiased estimators \([28]\), which have shown to converge quickly even in high dimensions \([47]\).

3. **Manifold Estimation**

Another form of evaluation metrics recently popularized in computer vision involves estimating the underlying manifold of the real and generated samples. While theoretically and computationally challenging, such metrics are very intuitive and allow us to disentangle the aspects of quality and diversity of the generated samples, which can be valuable in diagnosing individual failure modes of generative models. The most popular metrics are “precision” and “recall” as defined in Ref. \([52]\). For these, manifolds are first estimated as the union of spheres centred on each sample with radii equal to the distance to the \( k \)-th-nearest-neighbor. Rather intuitively, precision is defined as the number of generated points which lie within the real manifold, and recall as the number of real within the generated manifold. Alternatives, named diversity and coverage, are proposed in Ref. \([53]\) with a similar approach, but which use only the real manifold, and take into account the density of the spheres rather than just their union. We study the efficacy of both pairs of metrics for our problem in Sections III and IV.

4. **Classifier-Based Metrics**

Finally, an alternative class of GOF tests proposed in Refs. \([54–56]\), and most relevantly in Ref. \([18]\) and the Fast Calorimeter Simulation Challenge \([57]\) to evaluate simulated calorimeter showers, are based on binary classifiers trained between real and generated data. These tests have been posited to have sensitivity to both quality and diversity, however, have significant practical and conceptual drawbacks in terms of understanding and comparing generative models.

\(^2\) This is a pseudometric because distinct distributions can have a distance of 0 if they have the same means and covariances.
First, deep neural networks (DNNs) are widely considered uninterpretable black boxes [58], hence it is difficult to discern which features of the generated data the network is identifying as discrepant or compatible. Second, the performance of DNNs is highly dependent on both the architecture and dataset, and it is unclear how to specify a standard architecture sensitive to all possible discrepancies for all datasets. Furthermore, training of DNNs is typically stochastic, minimizing a complex loss function with several potential local minima, and slow, hence it is neither reproducible nor efficient.

In terms of GOF testing, evaluating the performance of an individual generative model requires a more careful understanding of the null distribution of the test statistic than is proposed in Refs. [18, 57], such as by using a permutation test as suggested in Refs. [54, 56]. However, even if such a test was performed for each model, which would itself be practically burdensome, it would remain difficult to fairly compare models, as, since different classifiers are trained for each model, this means comparing values of entirely different test statistics. Despite these flaws, we perform a classifier-based test in Section IV and find that, perhaps surprisingly, it is insensitive to a large class of failures typical of ML generative models.

C. Feature Selection

We end this section by discussing which features to select for evaluation. Generally, for data such as calorimeter showers and jets, individual samples \( \mathbf{x} \in \mathbb{R}^d \) are extremely high dimensional, with showers and jets containing up to \( \mathcal{O}(1000) \) s of hits and particles respectively, each with its own set of features. Apart from the practical challenges of comparing distributions in this \( d \)-dimensional case, often this full set of low-level features are not the most relevant for our downstream use case.

This is an issue in computer vision as well, where images are similarly high dimensional, and comparing directly the low-level, high-dimensional feature space of pixels is not practical or meaningful. Instead, the current solution is to derive salient, high-level features from the penultimate layer of a pre-trained SOTA classifier.

This approach is necessary for images, for which it is difficult to define such meaningful numerical features by hand. It can also be used in HEP as in Ref. [17], which proposed the Fréchet ParticleNet Distance (FPND), using the ParticleNet [59] jet classifier to derive its features. However, one key insight and study of this work is that this may be unnecessary for HEP applications, as we have already developed a variety of meaningful, hand-engineered features such as jet observables [60–62] and shower-shape variables [63, 64]. Using these instead may lead to a more efficient, more easily standardized, and interpretable test. We experiment with both types of features in Section IV.

III. EXPERIMENTS ON GAUSSIAN-DISTRIBUTED DATA

As a first test and filtering of the many metrics discussed, we evaluate their performance on simple 2D (mixture of) Gaussian-distributed datasets. We describe the specific metrics tested in Section III A, the distributions we evaluate in Section III B, and experimental results in Section III C.

A. Metrics

We test several metrics discussed in Section II, with implementation details provided below. Values are measured for different numbers of test samples, using the mean of 5 measurements each and their standard deviation as the error, for all metrics but \( \text{FGD}_{\infty} \) and MMD.

1. Wasserstein distance is estimated by solving the linear program described in, for example, Ref. [65], using the Python Optimal Transport library [66].

2. \( \text{FGD}_{\infty} \) is calculated by using 200 measurements of FGD between a minimum batch size of 5000 and varying maximum batch size. A linear fit is performed of the FGD as a function of the reciprocal of the batch size, and \( \text{FGD}_{\infty} \) is defined to be the \( y \)-intercept. It thus corresponds to the infinite batch size limit. The error is taken to be the standard error of the intercept. Each of the 200 points is measured 10 times and the average is used for the linear fit. This closely follows the recommendation of Ref. [48], except we find it necessary to use a significantly higher number of points and measurements of FGD to obtain accurate estimates of the intercept and, importantly, the error.

3. MMD is calculated using the unbiased quadratic time estimator defined in Ref. [28]. We test 3rd (as in KID) and 4th order polynomial kernels. We find MMD measurements to be extremely sensitive to outlier sets of samples, hence we use the median of 10 measurements each per sample size as our estimates, and half the difference between the 16th and 84th percentile as the error. We find empirically that this interval has 74% coverage of the true value when testing on the true distribution.

4. Precision and recall [52], and

5. Density and coverage [53] are both calculated using the recommendations of their respective authors, apart from the maximum batch size, which we vary.
B. Distributions

We use a 2D Gaussian with 0 means and covariance matrix $\Sigma = \begin{pmatrix} 1 & 0.25 \\ 0.25 & 1 \end{pmatrix}$ as the true distribution. We test the sensitivity of the above metrics to the following distortions, shown in Figure 1.

1. A large shift in $x$ (1 standard deviation $\sigma$);
2. A small shift in $x$ ($0.1 \sigma$);
3. Removing the covariance between the parameters — this tests the sensitivity of each metric to correlations;
4. Multiplying the (co)variances by 10 — tests sensitivity to quality;
5. Dividing (co)variances by 10 — tests sensitivity to diversity; and, finally,
6 & 7. Two mixtures of two Gaussian distributions with the same combined means, variances, and covariances as the truth — this tests sensitivity to the shape of the distribution.

C. Results

1. Bias

We first discuss the performance of each metric in distinguishing between two sets of samples from the truth distribution in Figure 2, effectively estimating the null distributions of each test statistic. A fourth-order polynomial kernel for MMD is shown as it proved most sensitive. We see that indeed FGD$_\infty$ and MMD are effectively unbiased, while the values of others depend on the sample size. This is a significant drawback; even if the same number of samples are specified for each metric to mitigate the effect of the bias, as discussed in Ref. [48], in general there is no guarantee that the level of bias for a given sample size is the same across different distributions. One possible solution is to use a sufficiently large number of samples to ensure convergence within a certain percentage of the true value. However, from a practical standpoint, the Wasserstein distance quickly becomes computationally intractable beyond $O(1000)$ samples, before which, as we see in Figure 2, it does not converge even for a two-dimensional distribution. Similarly, density and coverage require a large number of samples for convergence, which is impractical given their $O(n^2)$ scaling, while precision and recall suffer from the same scaling but converge faster.

2. Sensitivity

Table I lists the means and errors of each metric per dataset for the largest sample size tested for each. A similar plot to Figure 2 for each alternative distribution can be found in Appendix A. The scores most discrepant per distribution with the truth values of the respective metric are highlighted in bold. This is conceptually equivalent to
 assuming a Gaussian null (truth) distribution\(^3\), and highlighting the test statistic producing a central value with the highest p-value per alternative distribution. We can infer several properties of each metric from these measurements.

Focusing first on the holistic metrics (Wasserstein, FGD\(_\infty\), and MMD), we find that each converges to \(\approx 0\) on the truth distribution, indicating their estimators are consistent. We can evaluate the sensitivity to each alternative distribution by considering the difference in scores versus the truth scores. With the notable exception of FGD\(_\infty\) on the mixtures of two Gaussian distributions, we observe that all three metrics find the alternatives to be significantly discrepant from the true distribution, where significant is defined as the central value of the distribution score being two standard deviations away from the truth score. This is equivalent to again assuming a Gaussian null distribution and requiring a p-value on the alternative distribution to be \(\leq 0.05\).

As expected, despite the clear difference in the shapes of the mixtures compared to the truth, since FGD\(_\infty\) only

\(^3\) We note that this is not necessarily the case, particularly for the Wasserstein distance, which has a biased estimator. However, this is not a significant limitation because, as can be seen in Table 1, there is rarely a significant overlap between the null and alternative distributions which would require an understanding of the shape of the former.
has access to up to the second-order moments of the distributions, it is not sensitive to such shape distortions. We also note that a fourth-order polynomial kernel, as opposed to the third-order kernel proposed for KID, is required for MMD to be sensitive to the mixtures of Gaussian distributions, as shown in Appendix A. FGD$_\infty$ is, however, generally the most sensitive to other alternative distributions.

Finally, we note that precision and recall are clearly sensitive to the two distributions designed to reduce quality and diversity respectively, while not sensitive to others. This indicates that they are valuable for diagnosing these individual failure modes but not for a rigorous evaluation or comparison. Density and coverage are also sensitive to these distributions, but their relationship to quality and diversity is less clear. For example, the coverage of the second mixture of two Gaussian distributions is higher for the true distribution, whereas the inverse should be true in terms of diversity. Similarly, the coverage is lower with the covariances multiplied by 10, when in fact the diversity should remain unchanged. We therefore conclude that precision and recall are the more meaningful metrics to disentangle quality and diversity, and use those going forward.

IV. EXPERIMENTS ON JET DATA

We next test the performance of the Wasserstein distance, FGD$_\infty$, MMD, precision, and recall on a realistic high energy physics dataset comprised of high momentum gluon jets. As discussed in Section II C, we test all metrics on two sets of features per jet: 1) physically meaningful high-level features, and 2) features derived from a pre-trained classifier. We choose a set of 36 energy flow polynomials (EFPs) [62] (all EFPs of degree less than five) for the former, as they form a complete basis for all infrared- and collinear- (IRC-) safe observables. The classifier features are derived from the activations of the penultimate layer of the SOTA ParticleNet [59] classifier, as described in Ref. [17]. Finally, we test the binary classifier metric as in Refs. [18, 57] using both ParticleNet directly on the low-level jet features and a two-layer fully connected network (FCN) on the high-level EFPs. We describe the dataset and tested distortions in Section IV A, and experimental results in Section IV B.

A. Dataset

As our true distribution we use simulated gluon jets of $\approx$1 TeV transverse momentum ($p_T$) from the JetNet dataset [67], using the associated JetNet library [68]. Details of the simulation and representation of the dataset can be found in Ref. [17]. To obtain alternative distributions we distort the dataset in several ways typical of the mismodeling we observe in ML generative models: lower feature resolution, systematic shifts in the features, and inability to capture the full distribution.

We perform both distribution-level distortions, by re-weighting the samples in jet mass to produce a mass distribution that is 1) smeared, 2) smeared and shifted higher, and 3) missing the tail of the distribution, as well as direct particle-level distortions, by 4) smearing all three $\phi$ and $\eta$, and 5) $p_T^\text{rel}$ features, smearing the 5) $p_T^\text{rel}$ and 6) $\eta$ individually, and 7) shifting the $p_T^\text{rel}$ higher. The effects of the distortions on the relative jet mass are shown in Figure 3.

B. Results

Table II shows the central values and errors for each metric, as defined in Section III A, with the scores most discrepant with the truth distribution highlighted in bold. The first row shows the Wasserstein distance between only the 1D jet mass distributions ($W_1^\text{J}$) as introduced in Ref. [17], as a test of the power and limitations of considering only 1D histograms. Using the same metric of significance as in Section III C, we see that in fact $W_1^\text{J}$ is quite sensitive to most distortions, but misses subtle changes such as particle $p_T^\text{rel}$ smearing. Additionally, even with up to 50,000 samples, it is unable to converge to the true value. Nevertheless, it proves to be a valuable metric that can be used for focused evaluation of specific physical features, in conjunction with aggregate metrics.

The next five rows show values for metrics which use EFPs as their features. We find that, perhaps surprisingly, FGD$_\infty$ is the most sensitive to all distortions, and the only one which finds all alternative distributions to be significantly discrepant from the truth. The Wasserstein distance is not sensitive to many distortions for the sample sizes tested. The MMD is successful, failing only in identifying the particle $p_T^\text{rel}$ smearing, but not as sensitive as FGD$_\infty$. It also is clear that precision and recall have difficulty discerning the quality and diversity of distributions in high dimensional feature spaces, which is perhaps expected considering the difficulty of manifold estimation in such a space.

An extremely similar conclusion is reached when considering the metrics using ParticleNet activations, with FGD$_\infty$ again the highest performing. Broadly, ParticleNet activations allow the metric to distinguish particle-level distortions slightly better, and vice versa for distribution-level distortions, although overall the sensitivities are quite similar. We posit that including a subset of lower-level particle features in addition to EFPs could improve sensitivity to particle-level distortions, a study of which we leave to future work.

Finally, the last two rows provide the AUC values for a ParticleNet classifier trained on the particle low-level features (LLF), and an FCN trained on high-level features (HLF). We find that while both appear to be able to distinguish well the samples with particle-level distortions, they have no sensitivity to the distribution level
distortions.

In conclusion, we find from these experiments that $\text{FGD}_\infty$ is in fact the most sensitive metric to all distortions tested. Additionally, applying it on hand-engineered physical features — Fréchet physics distance (FPD) in short — is not only practically beneficial, in terms of ease of standardisation and interpretability, but also results in similar, if not better, performance to using ParticleNet activations. Despite the Gaussian assumption, it is clear that access to the first order moments of the distribution is sufficient for it to have high power against the relevant alternative distributions we expect from generative models. Hence, we propose FPD as a novel efficient, interpretable, and highly sensitive met-

| Metric                        | Truth | Smereared | Shifted | Removing tail | Particle features smeared | Particle $\eta^{rel}$ smeared | Particle $p_T^{rel}$ smeared | Particle $p_T^{rel}$ shifted |
|-------------------------------|-------|-----------|---------|---------------|---------------------------|------------------------------|-----------------------------|-------------------------------|
| $W_1^M \times 10^3$           | 0.28 ± 0.05 | 2.1 ± 0.2 | 6.0 ± 0.3 | 0.6 ± 0.2     | 1.7 ± 0.2                  | 0.9 ± 0.3                    | 0.5 ± 0.2                    | 5.8 ± 0.2                     |
| Wasserstein EFP               | 0.02 ± 0.01 | 0.09 ± 0.05 | 0.10 ± 0.02 | 0.016 ± 0.007 | 0.19 ± 0.08                | 0.03 ± 0.01                  | 0.03 ± 0.02                  | 0.06 ± 0.02                   |
| FGD$\infty$ EFP $\times 10^3$ | 0.01 ± 0.02 | 21.5 ± 0.3 | 26.8 ± 0.3 | 2.31 ± 0.07   | 23.4 ± 0.3                 | 3.59 ± 0.09                  | 2.29 ± 0.05                  | 28.9 ± 0.2                    |
| MMD EFP $\times 10^3$         | -0.006 ± 0.005 | 0.17 ± 0.06 | 0.9 ± 0.1 | 0.03 ± 0.02   | 0.35 ± 0.09                | 0.08 ± 0.05                  | 0.01 ± 0.02                  | 1.8 ± 0.1                     |
| Precision EFP                 | 0.9 ± 0.1   | 0.94 ± 0.04 | 0.97 ± 0.005 | 0.88 ± 0.08 | 0.7 ± 0.1                  | 0.94 ± 0.06                  | 0.7 ± 0.1                    | 0.79 ± 0.09                   |
| Recall EFP                    | 0.9 ± 0.1   | 0.88 ± 0.07 | 0.97 ± 0.01 | 0.92 ± 0.06   | 0.83 ± 0.05                | 0.92 ± 0.07                  | 0.8 ± 0.1                    | 0.8 ± 0.1                     |
| Wasserstein PN                | 1.65 ± 0.06 | 1.7 ± 0.1 | 2.4 ± 0.4 | 1.71 ± 0.08 | 4.5 ± 0.1                  | 1.79 ± 0.05                  | 4.0 ± 0.4                    | 7.6 ± 0.2                     |
| FGD$\infty$ PN $\times 10^3$  | 0.8 ± 0.7   | 40.2 ± 2  | 193 ± 9  | 5.0 ± 0.9    | 1250 ± 10                  | 20 ± 1                       | 1230 ± 10                    | 3640 ± 10                     |
| MMD PN $\times 10^3$          | -2 ± 2      | 4 ± 8    | 80 ± 10  | -1 ± 4       | 500 ± 100                  | 3 ± 2                        | 560 ± 60                     | 1100 ± 40                     |
| Precision PN                  | 0.68 ± 0.07 | 0.64 ± 0.04 | 0.71 ± 0.06 | 0.73 ± 0.03 | 0.09 ± 0.04                | 0.75 ± 0.08                  | 0.08 ± 0.04                  | 0.39 ± 0.08                   |
| Recall PN                     | 0.70 ± 0.05 | 0.61 ± 0.04 | 0.61 ± 0.08 | 0.73 ± 0.06 | 0.014 ± 0.009              | 0.7 ± 0.1                    | 0.01 ± 0.01                  | 0.57 ± 0.09                   |

TABLE II. Values and errors of metrics, as defined in Sections III A and IV B, for each jet distribution, for the largest sample size tested. EFP and PN refer to metrics using EFPs and ParticleNet activations as their input features, respectively. The scores most discrepant with the truth per distribution are highlighted in bold.
FIG. 4. Correlations between FPD and FPND, KPD, and $W_1^M$ on 400 separate batches of 50,000 GAPT generated jets.

FIG. 4. Correlations between FPD and FPND, KPD, and $W_1^M$ on 400 separate batches of 50,000 GAPT generated jets.

ric for evaluating generative models in HEP. However, MMD on hand-engineered features, or kernel physics distance (KPD), and $W_1$ scores between individual feature distributions also provide valuable information, and as demonstrated in Sec. III, can cover alternative distributions than FPD does not have power against.

V. DEMONSTRATION ON MPGAN VERSUS GAPT

We now provide a practical demonstration of the efficacy of our proposed metrics in evaluating two high performing generative models: the message-passing GAN (MPGAN) and the new generative adversarial particle transformer (GAPT), on the same gluon jet dataset described in Section IV. We describe the models in detail in Section VA, and discuss experimental results in V B.

A. MPGAN and GAPT

MPGAN is a graph-based GAN using a message-passing framework for the generator and discriminator networks, which is the current SOTA in simulating particle clouds — jets represented as point clouds in momentum space. We use the same architecture and pre-trained models provided by Ref. [17] to generate gluon jets from the JetNet dataset.

We also introduce GAPT, a new GAN for particle cloud data which employs self attention instead of message passing in the two networks. It is based on the generative adversarial set transformer (GAST) architecture [69], which makes use of set transformer [70] blocks to aggregate information across all points and update their features. It maintains the key inductive biases which makes MPGAN successful — permutation symmetry-respecting operations, and fully connected interaction between nodes during generation to learn high-level global features, but with a significant improvement in speed (Table III), and promising avenues to scale the architecture linearly in the number of nodes using induced self-attention blocks [70] and conditional generation [69]. The code for both models is available in Ref. [71]. Further training and implementation details can be found in Appendix B.

Because of the similarity in architectures of MPGAN and GAST, both visually and using the 1D $W_1$ physics-based metrics discussed in Ref. [17], it is difficult to discern which is more performant. Hence, this makes an effective test bench for our proposed FPD, KPD and $W_1$ metrics.

B. Results

Figure 4 shows correlation plots between FPD and FPND, KPD, and $W_1^M$ on 400 separate batches of 50,000 GAPT generated jets. While there is some correlation between each metric, it is quite weak, particularly at low values of each, indicating that these metrics are complementary in understanding different aspects of the model’s performance. We posit as well that FPD and FPND would be more strongly correlated were the former to use a subset of lower-level particle features as well, a study of which we leave to future work.

Histograms of sample feature distributions and FPD, KPD, and $W_1^M$ scores from the best performing MPGAN, as provided by Ref. [17], and GAPT, based on FPD, models are shown in Figure 5 and Table III respectively. For completeness, Table III also shows measurements of the inference time per jet for each model, measured on an NVIDIA RTX A6000 GPU. It is extremely difficult to either distinguish between the performance of the two models or draw a conclusion for their viability as alternative simulators based only on visual inspection of the histograms or even the 1D $W_1^M$ scores. However, FPD and KPD both provide crucial information in this regard, clearly indicating that MPGAN significantly outperforms GAPT, but its samples remain discrepant from the true
distribution. Finally, we note that despite the suboptimal performance, GAPT provides the benefits of speed and scalability.

VI. CONCLUSION

We have discussed several potential evaluation metrics for generative models in high energy physics (HEP), using the framework of two-sample goodness of fit (GOF) testing between real and simulated data. Inspired by validation of simulations in both physics and machine learning, we introduce two new metrics, the Fréchet and kernel physics distances (FPD and KPD, respectively), which employ hand-engineered physical features, to compare and evaluate alternative simulators. Practically, these metrics are efficient, reproducible, easily standardized, and, being multivariate, can be naturally extended to conditional generation.

We performed a variety of experiments using the proposed metrics on toy Gaussian-distributed and high energy jet data. We illustrated as well the power of these metrics to discern between two state-of-the-art machine learning (ML) models for simulating jets: the message-passing generative adversarial network (MPGAN) and our newly developed generative adversarial particle transformer (GAPT), which is significantly faster. We find that FPD is extremely sensitive to expected distortions from ML generative models, and collectively, FPD, KPD and the Wasserstein 1-distance ($W_1$) between individual feature distributions, should successfully cover all relevant alternative generated distributions. Hence, we recommend the adoption of these metrics in HEP for evaluating generative models. Future work may explore the specific set of physical features for jets, calorimeter showers, and beyond, to use for FPD and KPD.

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for the kernel physics distance. Hence, we recommend a fourth-order kernel Gaussian. Hence, we recommend a fourth-order kernel in computer vision, is not sufficient to discern the mixtures of Gaussian distributions from the single Gaussian. We recommend a fourth-order kernel for the kernel physics distance.

Appendix A: Further Discussion on Gaussian Dataset Experiments

Figures 6 and 7 show measurements of each metric on each distribution discussed in Section III, as well as Fréchet Gaussian distance (FGD) and maximum mean discrepancy (MMD) with a third-order polynomial kernel for varying sample sizes. We can see from these plots that indeed, as discussed in Refs. [47, 48] FGD is biased, but the solution from Ref. [48] of extrapolating to infinite sample size (FGD$_\infty$) largely solves this issue. We also note that, perhaps surprisingly, a third-order polynomial kernel, as used for the kernel Inception distance (KID) [47] in computer vision, is not sufficient to discern the mixtures of Gaussian distributions from the single Gaussian. Hence, we recommend a fourth-order kernel for the kernel physics distance.

Appendix B: Neural Network Implementation and Training Details

1. Binary Classifiers

In Section IV, we use the ParticleNet [59] graph neural network (GNN) model and a simple dense fully-connected neural network (FCN) as binary classifiers on low-level particle and high-level features, respectively, for evaluating true and distorted jet distributions. We use the same architecture and hyperparameters for ParticleNet as described in Ref. [59]. We use two hidden layers of 128 neurons each with LeakyReLU activations, with negative slope coefficient 0.2, after all but the final layer, which uses a sigmoid activation function. We follow the same training scheme as in Ref. [59], with a 70%/30% training/validation split on the dataset, and report in Table II the highest AUC achieved by each model on the validation dataset.

2. GAPT

The generative adversarial particle transformer (GAPT) is based on the generative adversarial set transformer (GAST) model [69]. The generator and discriminator networks are composed of permutation-invariant multilead self-attention blocks (SAB) as defined in Ref. [70]. We use four and two SAB blocks in the generator and discriminator respectively. Each SAB block uses 8 attention heads, and a 128-dimensional embedding space for each of the query, key, and value vectors. It also contains a one-layer feed-forward neural network (FFN) after each attention step, which maintains the 128-dimensional embedding for node features, and applies a LeakyReLU activations, with negative slope coefficient 0.2. Residual connections to the pre-SAB node features are used after both the attention step and FFN. After the final SAB block, a tanh activation is applied to the generator, whereas in the discriminator, the results are first pooled using a pooling by multihead attention (PMA) block [70], followed by a fully connected layer and sigmoid activation.

For training, we use the mean squared error loss function, as in the LSGAN [72], and the RMSProp optimizer with a two time-scale update rule [45], using a learning rate of $3 \times 10^{-4}$ and $10^{-4}$ for the discriminator and generator respectively. Dropout, with probability 0.5, is used to regularise the discriminator. We train for 2000 epochs and select the model with the lowest Fréchet physics distance.
FIG. 6. Scores of each metric on Gaussian-distributed datasets as described in Section III.
FIG. 7. Scores of each metric on Gaussian-distributed datasets as described in Section III.