**Title**
Generative Models for Particle Clouds and Anomaly Detection



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**Publication Date**
2024

UNIVERSITY OF CALIFORNIA SAN DIEGO

# Generative Models for Particle Clouds and Anomaly Detection

A thesis submitted in partial satisfaction of the
requirements for the degree Master of Science

in

Computer Science

by

Steven Adam Tsan

Committee in charge:

Professor Javier Duarte, Chair
Professor Hao Su, Co-Chair
Professor Jingbo Shang

2024

The Thesis of Steven Adam Tsan is approved, and it is acceptable in quality and form for publication on microfilm and electronically.

University of California San Diego

2024

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ACKNOWLEDGEMENTS

I would like to acknowledge my advisor Professor Javier Duarte for their support as the chair of my committee and in supporting my research. I would also like to acknowledge Raghav Kansal, PhD candidate, for offering mentorship for my research.

Chapter 1 in full was published in [62] at the 2021 Machine Learning for Physical Sciences Workshop at the Conference on Neural Information Processing Systems. The thesis author is the first author of this paper. An earlier version of this publication is also included as a section in [34], published in the 2021 Reports on Progress in Physics Journal.

ABSTRACT OF THE THESIS

Generative Models for Particle Clouds and Anomaly Detection

by

Steven Adam Tsan

Master of Science in Computer Science

University of California San Diego, 2024

Professor Javier Duarte, Chair
Professor Hao Su, Co-Chair

In high energy physics (HEP), there has been persistent interest in leveraging generative machine learning to model the structure of jets: the collection of particles generated from particle collisions. Being able to model the distribution of jet data enables downstream tasks such as anomaly detection, improving our search methodologies for rare and new physics. Traditionally, jet modeling has been performed on 2D jet-image representations; however, extending 3D point clouds to jet data has led to the much more natural "particle cloud" representation, where jets are modeled as a set of particles in momentum-space [31]. In this thesis, I present two such generative machine learning methods for modeling jets by their particle cloud representations,

one using a graph-based autoencoder model and one using diffusion models.

# Introduction

One of the primary motivations behind the development of the CERN Large Hadron Collider (LHC) was to search for new physics that may explain experimental observations left unaddressed by the standard model (SM) and expand our understanding of phenomena such as gravity and dark matter. The search for beyond the SM (BSM) physics has had limited success at the LHC possibly because current methods rely too heavily on hypothesized BSM signatures that may not reflect the true nature of the new physics. To address this, there has been a growing interest in employing unsupervised machine learning models that can search for new physics independent of underlying signature assumptions.

In Chapter 1 we will explore a design of autoencoders for the aforementioned purpose. Autoencoders have useful applications in high energy physics in anomaly detection, particularly for jets—collimated showers of particles produced in collisions such as those at the CERN Large Hadron Collider. We explore the use of graph-based autoencoders, which operate on jets in their "particle cloud" representations and can leverage the interdependencies among the particles within a jet, for such tasks. Additionally, we develop a differentiable approximation to the energy mover's distance via a graph neural network, which may subsequently be used as a reconstruction loss function for autoencoders.

In Chapter 2 we will explore the use of diffusion models for particle cloud generation. Diffusion models have gained significant traction as one of the most powerful generative models available, and current work indicates they may also have potential for anomaly detection based on their ability to be used for likelihood estimation [61]. However, diffusion models have traditionally suffered from slow inference speeds; accordingly, this thesis will explore techniques for fast diffusion models such as Point Straight Flow [66] and progressive distillation [55] for particle cloud generation.

# Chapter 1

# Particle Graph Autoencoders and Differentiable, Learned Energy Mover's Distance

## 1.1 Introduction

One of the primary motivations behind the development of the CERN Large Hadron Collider (LHC) was to search for new physics that may explain experimental observations left unaddressed by the standard model (SM) and expand our understanding of phenomena such as gravity and dark matter. The search for beyond the SM (BSM) physics has had limited success at the LHC possibly because current methods rely too heavily on hypothesized BSM signatures that may not reflect the true nature of the new physics. To address this, there has been a growing interest in employing unsupervised machine learning (ML) models that can search for new physics independent of underlying signature assumptions. For example, autoencoders, ML models that learn to map data down to a compressed encoding of its most salient features and then reverse such encodings back to their original form, have been employed for unsupervised anomaly detection [3, 14, 15, 23, 34, 44]. Autoencoders learn to accurately reconstruct data similar to what is seen during its training; however, anomalous signals rare or absent in the training data may not be accurately reconstructed—a property that can be used to detect them.

We propose particle graph autoencoders (PGAEs) based on graph neural networks

(GNNs) [20, 56] for unsupervised detection of new physics in multijet final states at the LHC. By embedding particle jet showers as a graph, GNNs are able to exploit particle-to-particle relationships to efficiently encode and reconstruct particle-level information within jets. We posit that this can improve the capacity of autoencoders to learn a compressed representation of a jet and consequently help identify anomalous BSM multijet signal events from LHC data. We also develop and validate a differentiable, learned approximation to an important distance metric, the energy mover's distance [35], using a GNN, dubbed EMD-GNN, which has the potential to be used as both a loss function to train a PGAE as well as a metric by which to judge how anomalous a jet is.

## 1.2 Related Work

**Autoencoders in HEP**

A number of different autoencoder models have been studied for application in searching for new physics at the LHC [14, 15, 23, 44]. One major drawback of many of these studies is the use of vector- or image-based representations of HEP data, which aren't well-suited to the sparsity and irregular geometry typical data produced at the LHC. We propose instead to use the more natural set-based "particle cloud" [50] representation for particles in a jet, which is inherently sparse and agnostic to the underlying geometry, and operate on this representation using GNNs.

**Graph networks**

GNNs are powerful, expressive networks that can operate on particle clouds and respect permutation invariance (for graph-level outputs) and covariance (for edge- and node-level outputs) [10]. Due to this they have been steadily gaining prominence in HEP [56]. Notable examples include the dynamic graph convolutional neural network (DGCNN) [65], which has been used for calorimetry in a high-granularity calorimeter [30] and jet identification [50], as well as the interaction network [6] and its generalization to "graph networks" [5], which have been used for jet identification [45,46] and particle tracking [18,30]. Other network architectures, GravNet and GarNet, have been studied for calorimetry [28,49].

GNNs for anomaly detection in HEP have not yet been fully explored. However, recent work [3] develops an autoencoder-based strategy to facilitate anomaly detection for boosted jets, using a symmetric decoder that simultaneously reconstructs edge features and node features. Latent-space discriminators are used isolate W bosons, top quarks, and exotic hadronically-decaying exotic scalar bosons from QCD multijet background. This work expands on that by performing a realistic resonance search using the PGAE model.

### 1.2.1 Reconstruction loss functions

Since the inputs and outputs are sets, a reconstruction loss needs to address the assignment problem, i.e. find a one-to-one correspondence between the two sets of nodes. For a permutation-equivariant model, such as the presently considered GNN, the mean-squared error (MSE) is a standard choice because the order is preserved between the inputs and outputs. The Chamfer loss [4, 22, 67] is permutation invariant, but has been found to be suboptimal [34]. Finally, the energy mover's distance (EMD) [35], related to the Earth mover's distance [25, 47, 54], is a desirable loss, which quantifies the difference between jets through optimal transport as the minimum "work" required to rearrange one jet into another by movements of transverse momentum between the particles in each jet. Finding the EMD is a linear program [47], the exact solution to which is not efficiently differentiable, which limits its use directly as a loss function for training with backpropagation. Thus, instead we develop a GNN-based approximation of the EMD, "EMD-GNN", which may be used in the future as a differentiable loss function. Others have studied alternative approximations to the Earth or energy mover's distance to improve computability [13, 17, 21].

## 1.3 Network Architectures

### PGAE

In the PGAE model, we represent input jets as fully-connected graphs where each constituent particle is represented as a node, and with edges between each pair of nodes. When encoding and decoding, the graph structure of the data remains the same, but the node features, initially the particle's three-momentum $p = (p_x, p_y, p_z)$, have their dimensionality reduced during the encoding phase. We note the model can be expanded to consider additional particle-level information, such as particle type, electromagnetic charge, and pileup probability weight [7]. For the encoder and decoder, we use the edge convolution layer from Ref. [65], which performs message passing along the edges and aggregation of messages at the nodes of the graphs.

The PGAE model is constructed using the PyTorch Geometric library [24]. The node features inputted to the encoder are first processed by a batch normalization layer [29]. The encoder itself is a single DGCNN layer, built from a fully connected neural network $\phi_{\mathrm{e}}$ with layers of sizes $(32, 32, 2)$ and rectified linear activation unit (ReLU) activation functions [1]. The network takes in as input $(p_i, p_j - p_i)$, where $p_i$ $(p_j)$ is the three-momentum for particle $i$ $(j)$ and $i \neq j$. The final layer produces a two-dimensional message vector from each pair of distinct particles. These message vectors are aggregated (using a mean function) for each receiving particle using

$$h_i = \frac{1}{|\mathcal{N}(i)|} \sum_{j \in \mathcal{N}(i)} \phi_{\mathrm{e}}(p_i, p_j - p_i)\,, \tag{1.1}$$

where $\mathcal{N}(i)$ is the neighborhood of particles connected to the $i$-th particle, which corresponds to all other particles in this case. This summed message $\vec{h}_i$ is the bottleneck or encoded representation for the $i$-th particle. The decoder is also a DGCNN layer, containing a network $\phi_{\mathrm{d}}$ with layers of sizes $(32, 32, 3)$ and ReLU activation functions after all but the final layer. The input is a 3-dimensional vector representing $(h_i, h_j - h_i)$ and the output is intended to reconstruct each particle's momentum. We note that the architecture itself is covariant under permutations of the input particles and applicable to variable-size jets.

### EMD-GNN

The input to the EMD network is a pair of jets, represented in a single graph in a similar format to the PGAE's input, but with an extra binary channel per node to differentiate which jet it belongs to: $+1$ ($-1$) for the first (second) jet.

The EMD network itself is a GNN that utilizes three DGCNN layers, each one using two-layered fully connected networks with ReLU activations and batch normalization. For each DGCNN layer the graph structure is dynamically recomputed with edges directed to each node from its 16-nearest-neighbors in feature space. A softplus activation is applied to the final output.

To ensure a symmetric distance metric, the network is inputted both permutations of the input jets and the predicted EMD value is the average of the network outputs. We also utilize a symmetric loss function consisting of the MSE between the predicted and true EMD value, plus the MSE between the predicted EMDs for the two inputs.

## 1.4 Experiments

### Datasets

The dataset [33] comes from the LHC Olympics (LHCO) 2020 challenge and consists of a collection of simulated particle collisions divided up across three "black boxes" (BB) and one background QCD dijet events sample, each with one million particle collision events. Two of the black boxes (1 and 3) were injected with anomalous signals, while one (2) had no anomalous signals injected. In addition, we also use a R&D dataset from the LHCO [32], which has similar QCD events plus an additional 100,000 injected signal events with labels[1].

For input to the PGAE, we process the events using pyjet [51] to cluster $R = 1$ anti-$k_{\mathrm{T}}$ jets [11, 12], selecting only the leading two jets by transverse momentum per event, and then representing each jet as a vector of its constituents' three-momenta $p = (p_x, p_y, p_z)$, with array format $(N_{\text{particles}}, 3)$. We also require each jet to have $p_{\mathrm{T}} > 200\,\mathrm{GeV}$. We train the autoencoders on the processed background dataset, and then evaluate them on the black boxes. For the EMD-

[1] Both datasets have been released under the CC-BY 4.0 license.

GNN, we use the same LHCO background data for training, but represent each particle in a jet by its relative $(p_{\mathrm{T}}, \eta, \phi)$, forming all possible unique pairs of jets from 1,000 total events. The true EMD value is computed with the EnergyFlow library [35], which bases its computation on the Python Optimal Transport library [25]. The dataset is randomly partitioned into training (80%), validation (10%), and testing samples (10%).

**PGAE+MSE Results**

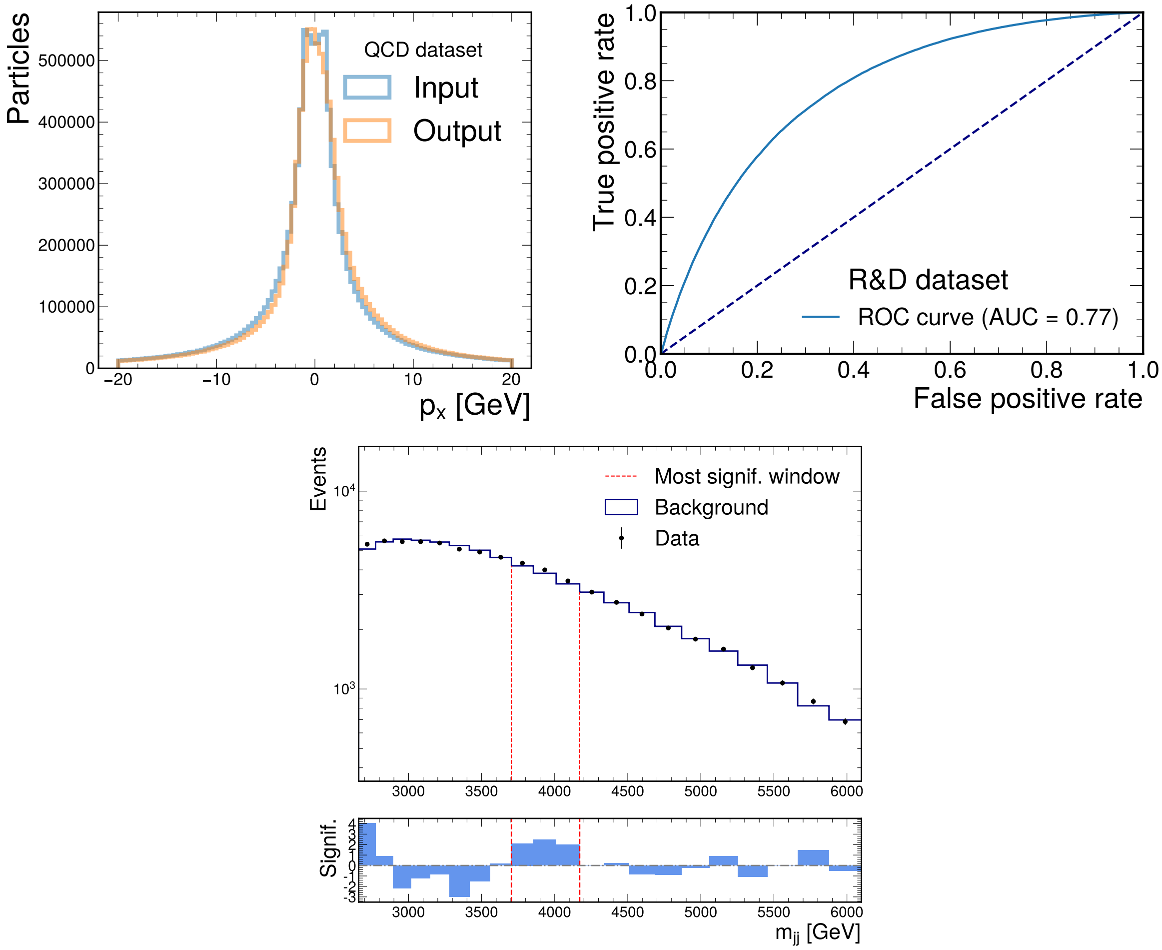


**Figure 1.1.** Comparison of input and reconstructed distributions of a sample particle feature $p_x$ (top left) for the models trained with PGAE, evaluated on a test set. ROC curve on the R&D dataset for the PGAE model (top right), and the result of a resonance search using the dijet invariant mass performed on BB 1 (bottom). For the search on BB 1, outlier jets have a reconstruction loss in the top 30% and outlier events are required to have two outlier jets.

Training details for both the PGAE and EMD networks can be found in App. 1.6.

Figure 1.1 (left) shows a comparison of input and reconstructed features for the models trained with PGAE evaluated on a test set. We see that the PGAE trained using a MSE loss performs well at reconstructing particles features. Although the model does not perfectly reconstruct the (double) peak in the center of the feature distributions, for the purpose of anomaly detection, this may not be a problem as long as non-outliers are reconstructed well enough that they have a lower reconstruction loss compared to actual outliers.

For anomaly detection we first study our algorithm on the R&D dataset. As the truth information is provided, we construct a receiver operating characteristic (ROC) curve to determine the effectiveness of the PGAE to identify a signal ($\mathrm{W}' \to \mathrm{XY}$, $\mathrm{X} \to \mathrm{qq}$, and $\mathrm{Y} \to \mathrm{qq}$ with $m_{\mathrm{W}'} = 3.5\,\mathrm{TeV}$, $m_{\mathrm{X}} = 500\,\mathrm{GeV}$, and $m_{\mathrm{Y}} = 100\,\mathrm{GeV}$) that it did not observe during training. As seen in Fig. 1.1 (center), the PGAE is capable of correctly identifying anomalies.

To evaluate the model's performance on unlabeled data, we perform a resonance search in the dijet invariant mass $m_{\mathrm{jj}}$, computed from the two leading jets per event, using a variable-width mass binning [57] in the range from 2659 GeV to 6099 GeV. We perform this dijet resonance search in BB 1, which contains a resonant dijet signal at $m_{\mathrm{jj}} \approx 3.8\,\mathrm{TeV}$. We require both of the jets to be "outliers," which we define as having a reconstruction loss exceeding a threshold corresponding to the 70% quantile of the loss distribution on the evaluation dataset. We note that because our algorithm is jet-focused, it is straightforward to generalize this search to multijet events. To predict the background in the signal-enriched outlier region, we use the shape of the data in the background-enriched nonoutlier region. We perform a maximum-likelihood fit to the ratio of the nonoutlier-to-outlier dijet mass distribution with a fourth-order polynomial to derive a transfer factor (TF) and take the nonoutlier data distribution weighted by the TF as an estimate of the expected background in the outlier region. To derive the observed significance with the simplified background prediction, we use the bump hunter (BH) algorithm [16, 63] to look for resonances in windows spanning two to five bins. With the MSE model in BB 1, we identify a possible resonance around 3.7 TeV with a global significance of $2.8\,\sigma$, which is consistent with the injected dijet resonance mass.

**Comparison to other LHCO Contributions**

Many algorithms proposed for the 2020 LHCO [34] performed similar evaluations on the R&D and BB 1 dataset. Bump hunting in latent space [8] implemented a VAE that incorporates an invariant mass embedding in its latent space. This method obtained an AUC of 0.915 for an event-level discriminant on the R&D dataset. Another algorithm combined a generative adversarial network (GAN) based autoencoder (AE) with the BH algorithm and achieved an AUC of about 0.90 on the R&D dataset. They also performed a dijet resonance search on BB 1, estimating a signal in the 3000–3600 GeV range. Another contribution used regularized likelihoods with manifold-learning flows [9] to construct an anomaly score, which achieved an AUC of 0.7882 for their best performing model. Tag N' Train [2] achieved an AUC of 0.918 on the full R&D dataset, and detected a dijet resonance in BB 1 around 3800 GeV with a local significance of $4\,\sigma$. The deep ensemble anomaly detection method obtained an AUC of 0.96 using boosted decision trees, though we note that they performed semisupervised training on the R&D dataset compared to our fully unsupervised training.

In comparison to our application of the PGAE, many of the other LHCO proposals achieved a higher AUC on the R&D dataset. However, because our discriminant is per jet, the discriminant values from multiple jets may be combined to achieve a better event-level discrimination. Moreover, many of the analysis methodologies are independent of the anomaly detection algorithm itself, thus are complementary to and can be integrated with our PGAE approach.

**EMD-GNN Performance**

As shown in Fig. 1.2, the EMD-GNN can learn to approximate the EMD between real jets with a very high degree of accuracy, with a $-0.003\%$ relative difference between the predicted and true EMD on average, and a standard deviation of 1.6%. This indicates the potential to use this architecture to define a differentiable loss function for particle graph reconstruction.

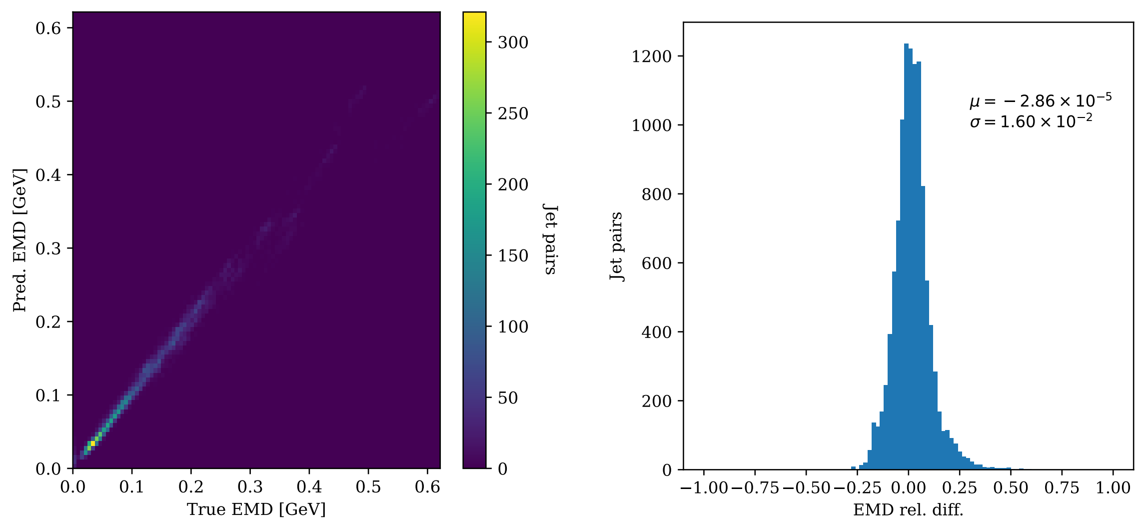


**Figure 1.2.** Correlation between EMD-GNN's EMD prediction and the true EMD (left) and relative difference between corresponding true and predicted EMD (right) for the testing dataset composed of random pairs of jets.

## 1.5 Summary

We demonstrated that particle graph autoencoders (PGAEs) are effective at reconstruction of QCD background jets and, by extension, anomaly detection of anomalous jet signals. Good discrimination between background and signal jets was observed on the LHC Olympics (LHCO) R&D dataset, which provides labels. Moreover, using this algorithm, a dijet resonance was identified in the correct mass range in the LHCO Black Box 1 dataset with a global significance of $2.8\,\sigma$. Additionally, we show that a graph neural network (GNN) can be used to approximate the energy mover's distance (EMD) and therefore potentially be used as a differentiable, permutation-invariant loss function. Future work will investigate optimizing the PGAE with the EMD-GNN as its loss function.

### Broader Impact

Our PGAE demonstrates the potential of unsupervised anomaly detection through particle graph representations of jets. As jet representations shift towards this particle cloud based format, permutation invariant loss functions such as the EMD become increasingly important. However approximations of EMD are known for their extremely large time complexity, as such, our EMD-GNN serves as an effective and differentiable alternative for approximating EMD. In general, GNNs are becoming increasingly prevalent in many fields, including areas in which they may have harmful impacts on human welfare, to which this work may potentially contribute.

## 1.6 PGAE+MSE and EMD-GNN Training

For training the PGAE, we use a batch size of 256, early stopping with a patience of 10 epochs, and an initial learning rate of 0.01. Additionally we employ a learning rate scheduler that lowers the learning rate by a factor of 0.1 after every 4 epochs where the validation loss does not improve, with the minimum learning rate set by this process being $10^{-6}$. We use MSE as the loss in our experiments with the PGAE.

To train the EMD-GNN, we use the same training hyperparameters as the PGAE except for the batch size, which we set to 128. Both models were trained on Nvidia GTX 1080Ti GPUs. The PGAE model requires about 5 days to train, and the EMD-GNN model takes about 20 hours.


## 1.7 Acknowledgements

Chapter 1 in full was published in [62] at the 2021 Machine Learning for Physical Sciences Workshop at the Conference on Neural Information Processing Systems. The thesis author is the first author of this paper. An earlier version of this publication is also included as a section in [34], published in the 2021 Reports on Progress in Physics Journal.

# Chapter 2

# Diffusion Models for 3D Particle Cloud Generation

## 2.1 Introduction

Diffusion models have emerged as a powerful generative model rivaling GANs in image [19] and point cloud [41] tasks. While early diffusion model designs [19, 27, 41] were hampered by their considerably slow sampling process, recent methodologies have vastly sped up the sampling speeds [40, 55, 60, 66]. Large amount of data collection and high computation costs dissuade the usage of slow models for simulating particle data in the field of HEP. Therefore, this chapter will discuss fast sampling diffusion models for particle cloud generation.

## 2.2 Background

### Diffusion Models

Diffusion models are a class of generative models that learn how to generate samples by iteratively denoising an initial Gaussian noise. The Denoising Diffusion Probabilistic Model (DDPM) model originates from [58] and was popularized by [27], which showed that it had good results on 2D image synthesis tasks. [19] introduced a wide range of optimizations such that the DDPM model could rival state-of-the-art GANs on image synthesis. Advances such as Latent Diffusion Models (LDMs) [52], which perform diffusion over the latent space of samples passed through an autoencoder, have both sped up training diffusion models and vastly improved their results in tasks such as shape completion and image synthesis. Beyond 2D datasets, DDPMs have also seen impressive results for 3D generative tasks such as 3D point cloud generation [41, 68] and text-to-3D synthesis [48]. These papers have largely tackled tasks on dense data like image and shape datasets, where convolutional neural networks (CNNs) like UNet [53], which underlies most diffusion models as the denoising neural network [19, 27, 52], are highly effective. However, particle clouds are a sparse data representation where any jet can only be represented by a finite set of particles generated from a particle collision [31], making traditional CNN-based diffusion models less effective [26]. Recent papers tackling diffusion models for particle cloud generation have opted for using attention [64] based architectures [36, 43].

**Fast Diffusion Models**

Diffusion models generate samples by mapping noisy samples at arbitrary noise-levels to lower noise-levels. Starting from pure Gaussian noise, samples would therefore be generated by sequential mappings to increasingly lower noise-levels. Achieving high quality samples from diffusion models require a long iterative sampling procedure, often taking 1000 steps or more when the denoising begins from pure Gaussian noise [19, 27]. Progressive distillation for diffusion models [55] was proposed in order to reduce the many sampling steps required for high quality samples to only a few steps. Using a "parent" diffusion model that has learned to denoise across many noise-levels, progressive distillation [55] will teach a "student" model to learn to denoise at every other noise-level in the sequence that the "parent" model has learned the mappings for, effectively halving the number of steps needed to generate a sample. This student can then be distilled into yet another student model using the same pattern. Repeating this training pattern can create a model that can perform the diffusion model's sampling process in just a few steps. However, every time the model is distilled the quality of generated samples will degrade.

While progressive distillation was able to generate high quality samples in only a few steps, single-step sampling severely underperformed [55]. [66] proposed Point Straight Flows

(PSF), a modification to diffusion modeling that generates high quality samples in just a single step by also utilizing model distillation. PSF trains a diffusion model and then performs several steps inspired by rectified flows (reflow), a technique to simplify the transport trajectory in normalizing flow models [38, 39]. Reflow [39] enables the PSF model to be distilled down without the large quality degradation in the samples seen with progressive distillation [55], though generating samples through a few steps would still outperform one step. Consistency models [60] are another proposed model that can sample with one step and is also based on distilling down a diffusion model. But whereas progressive distillation taught a student model the mappings at discrete noise-levels from a parent model, consistency models learn the mapping over the continuous range of a trained diffusion model's generation trajectory formed by an ODE [59]. This chapter will focus on the efficacy of PSF for fast particle cloud generation.

## 2.3 Methodology

**Dataset**

We train the model described in Fig. 2.1 using the gluon particle cloud dataset provided by [31]. The dataset is a collection of particle clouds with a dimensionality of [N, 30, 3], where N is the number of jets in the dataset, 30 is the maximum number of particles in a jet, and the 3 is the particle features: the relative 3-momentum ($\eta^{rel}$, $\phi^{rel}$, $p_T^{rel}$).

**Model Architecture**

As seen in Fig. 2.1, our model is composed of a linear layer with embedding dimension of 64, followed by 8 attention blocks using the GAPT model from [31, 37], then 2 more linear layers with 64 and 3 embedding dimensions. The very first linear layer embeds the features of the particle cloud $x$. The output of this linear layer is then added to a random amount of noise at noise-level $t$, set by a sinusoidal embedding as is performed in [19]. The noised input is then passed through the remaining series of attention blocks and linear layers, generating an output with the same dimension as the original particle cloud.

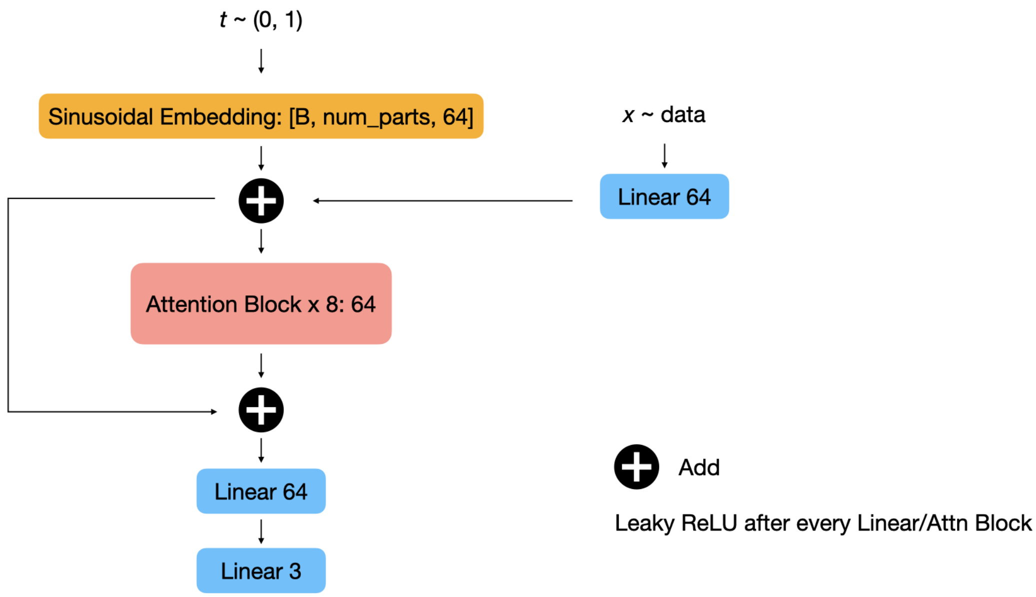


**Figure 2.1.** The diffusion model is an attention model architecture trained on particle clouds $x$ modified with varying noise-levels $t$. $x$ comes with information on each particles relative 3-momentum $(\eta^{rel}, \phi^{rel}, p_T^{rel})$.

### Training and Sampling

Alternative models are trained using the progressive distillation [55] methodology and PSF methodology [66]. For progressive distillation, an initial diffusion model using the velocity prediction setting described in [55] is trained to denoise samples over a the continuous noise-level interval $t \in (0, 1)$. This initial model is then distilled using progressive distillation, starting with a distillation down to 512 discrete noise-levels. The PSF model uses the same architecture as the progressive distillation model but the training is as formulated in Algorithm 1 of [66]. All training procedures use early stopping with a patience of 15 to determine how long to train. Sampling from the progressive distillation model uses the DDIM sampling method [55, 59], whereas sampling from the PSF model is performed by Euler's method exactly as described in [66].

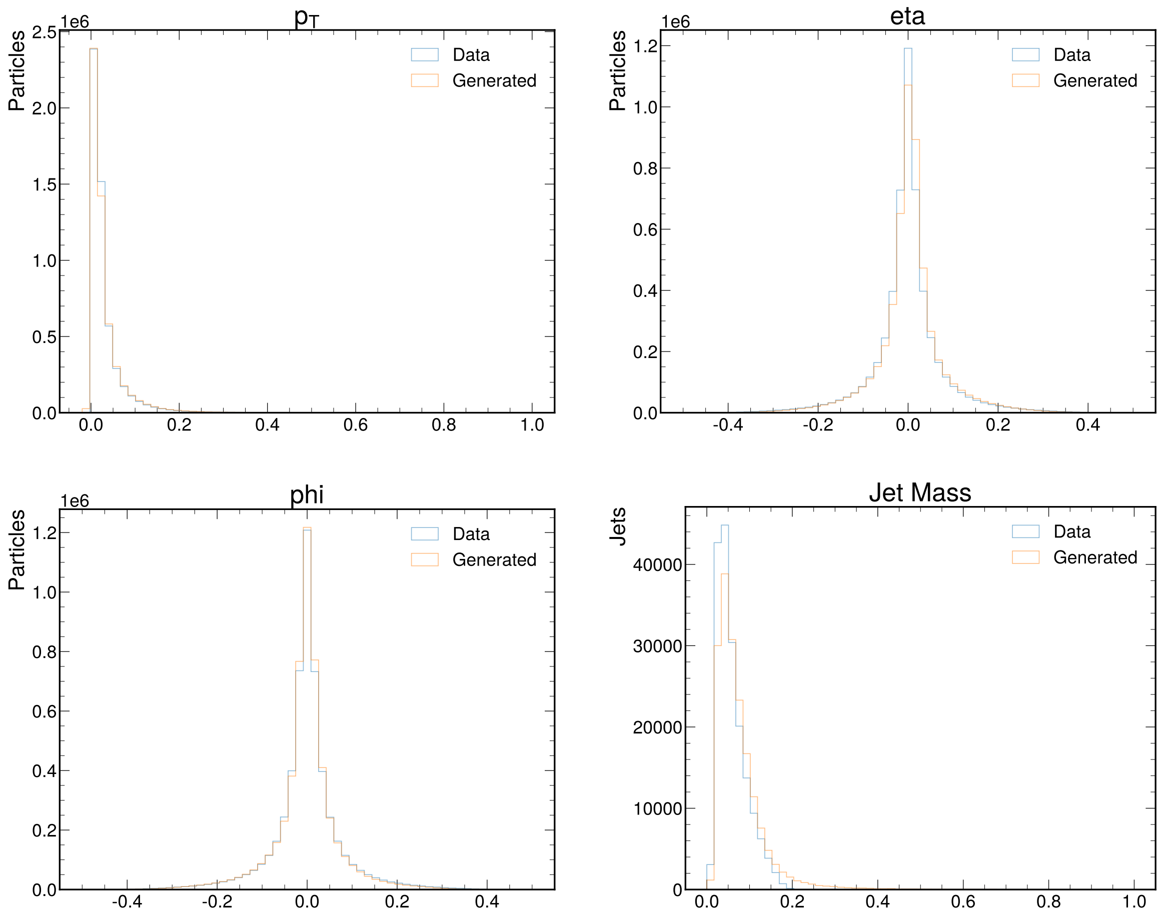


**Figure 2.2.** Progressive Distillation: Feature distributions of the gluon particles compared between real gluons and generated gluons from the initial diffusion model used for progressive distillation. Samples are generated using 1024 DDIM steps. Jet mass is calculated from the particle features.

## 2.4 Experiments

To evaluate the models, samples are generated for models trained with both aforementioned methodologies. The distribution of features for the generated samples are then compared to the distributions for the original gluons dataset the model was trained on. 177252 particle clouds padded up to 30 particles per cloud are generated for each comparison (equalling the amount in the original dataset, and the padding used for training). For the progressive distillation model, we notice that the quality of the samples significantly degrade as we decrease the number

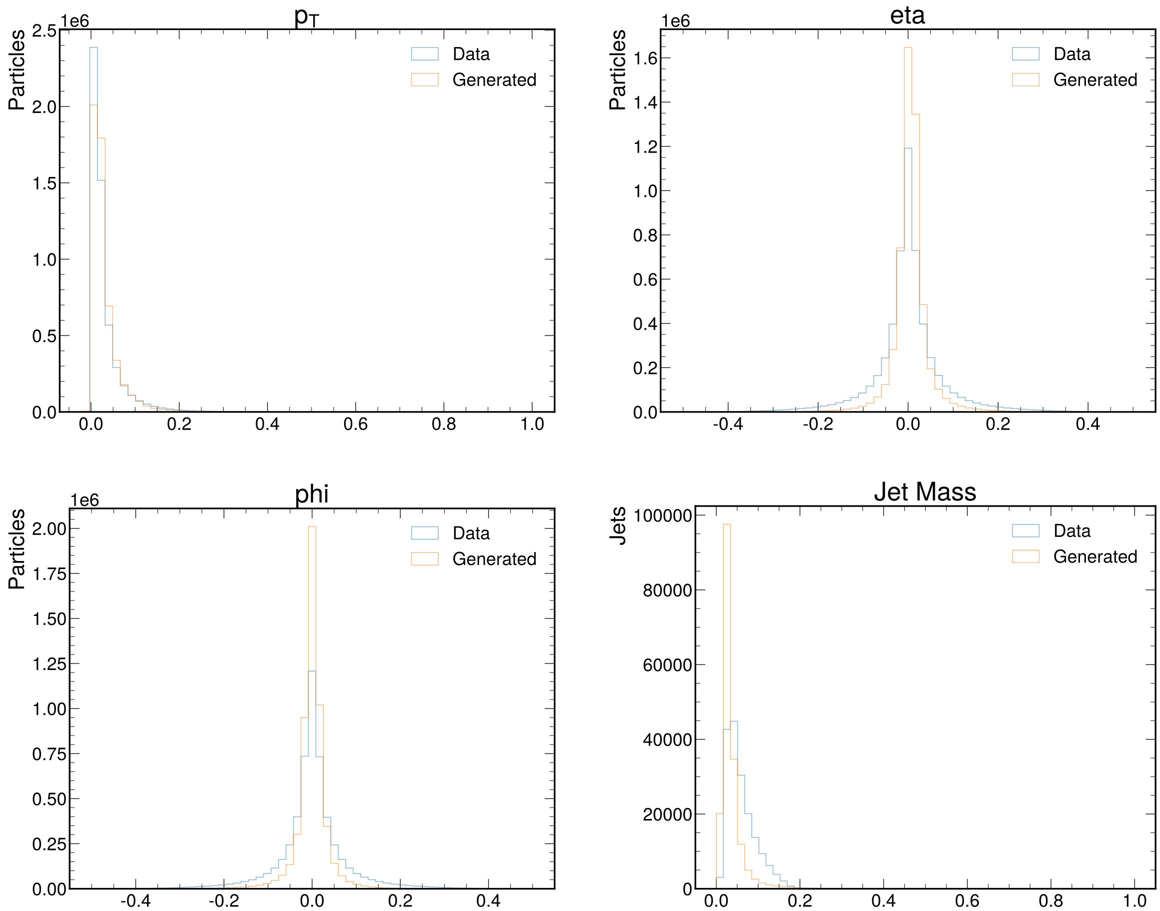


**Figure 2.3.** Progressive Distillation: Feature distributions of the gluon particles compared between real gluons and generated gluons from the progressively distilled diffusion model for 32 sampling steps. Jet mass is calculated from the particle features. We can see severe degradation in sample quality compared to the base model sampled in Fig. 2.2. Further distillation causes significantly worse sample quality.

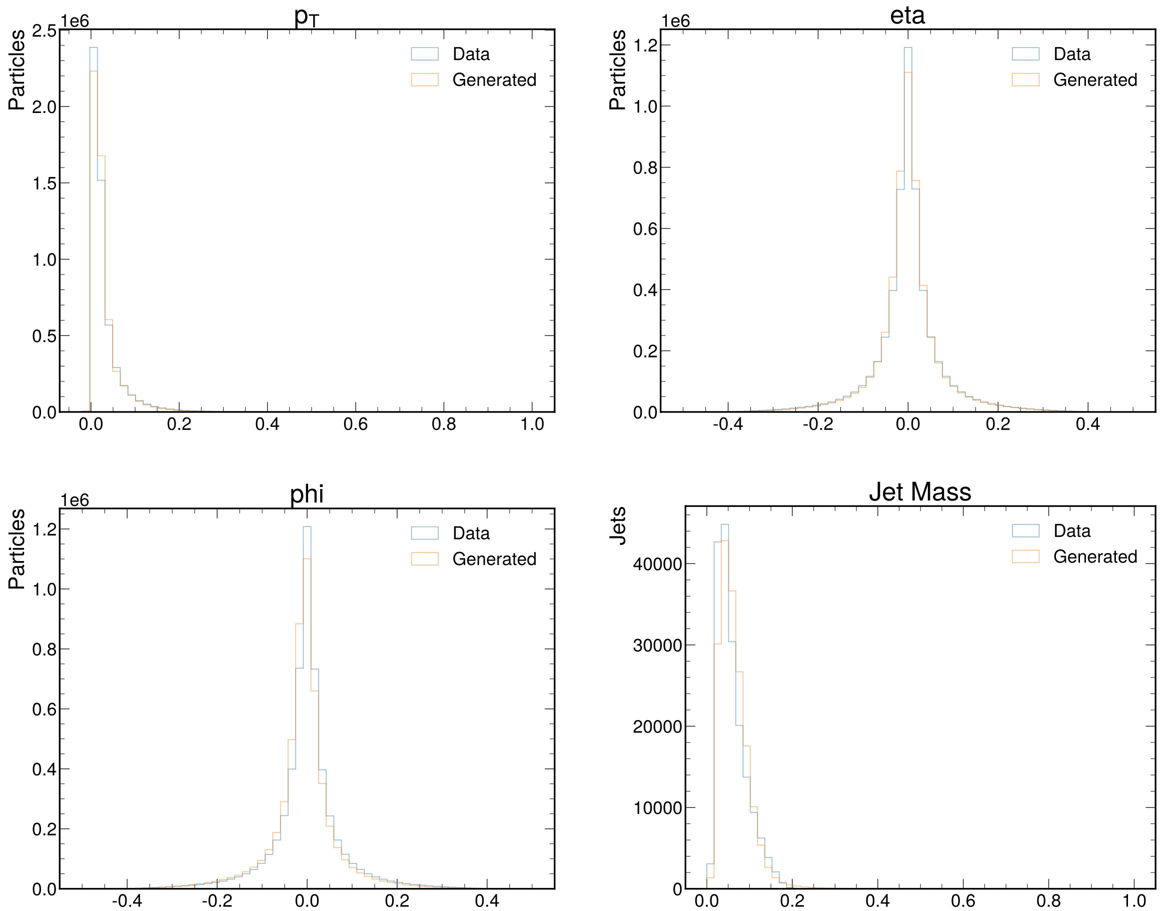


**Figure 2.4.** PSF: Feature distributions of the gluon particles compared between real gluons and generated gluons from the initial diffusion model used for PSF before reflow and distillation. Jet mass is calculated from the particle features.

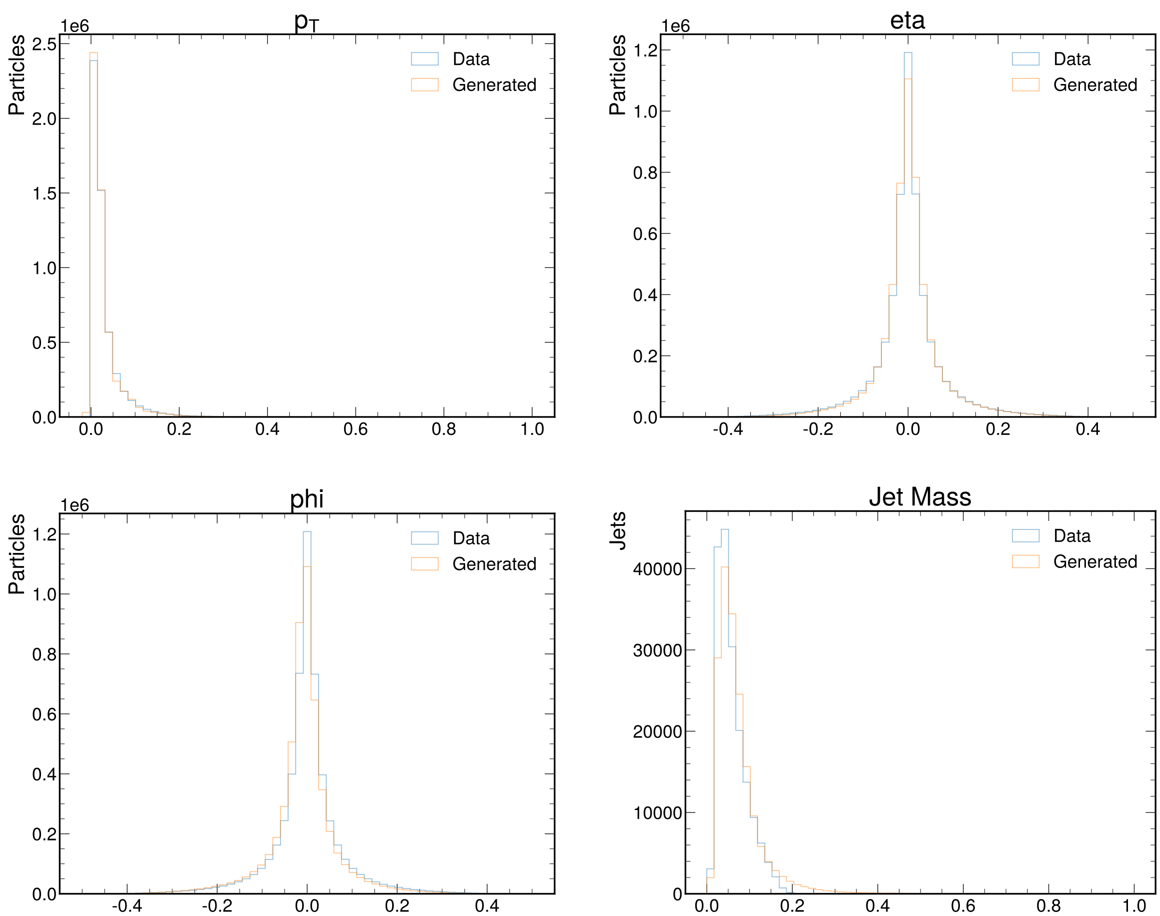


**Figure 2.5.** PSF: Feature distributions of the gluon particles compared between real gluons and generated gluons using single-step sampling from the PSF model. Very little discernable degradation in sample quality compared to the undistilled model in Fig. 2.4.

of sampling steps as seen at 32 steps in Fig. 2.3. PSF on the other hand demonstrates significantly improved performance over progressive distillation, even at just a single-step as seen in Fig. 2.5. Even compared to the undistilled diffusion model used for PSF seen in Fig. 2.4, the distilled PSF model still holds up in sample quality with very little noticeable loss in sample quality.

## 2.5 Conclusion

In this chapter we present distilled diffusion models as an effective way of generating particle clouds without the massive speed detriment evident in undistilled diffusion models. While there will be some loss in sample quality with distillation techniques, it is possible to signficantly reduce this sample quality reduction while still maintaining a significant speed up as evidenced by the PSF methodology. Anomaly detection using diffusion models in HEP has also recently been explored in another work [42] using a diffusion model formulated by a variance preserving SDE [61]. Further testing the potency of diffusion models for anomaly detection and exploring the effects of faster diffusion models like PSF on the current anomaly detection methodology may be worth studying.

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