Accelerating Diffusion Models in Particle Physics

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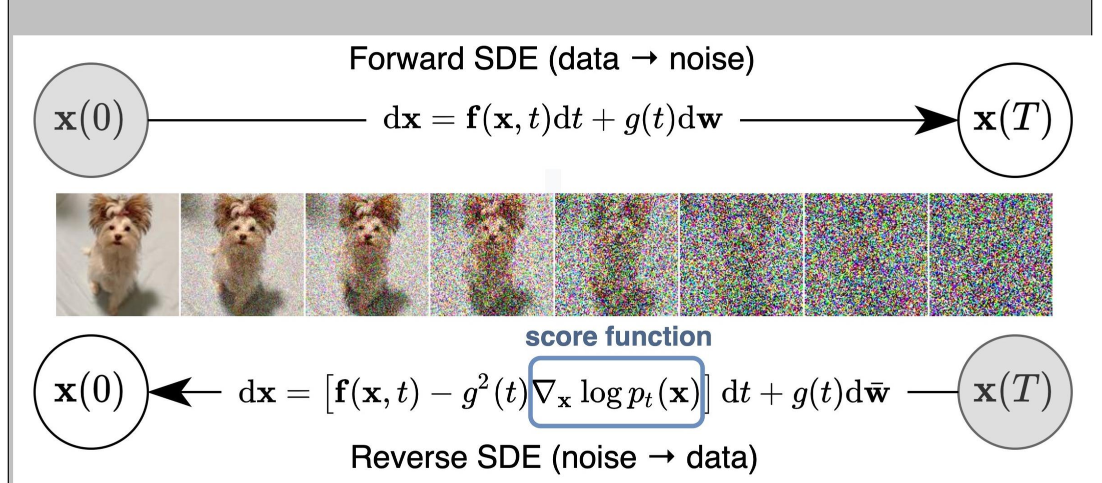
Abstract

Our research delves into the optimization of sampling techniques for particle physics datasets, emphasizing numerical methods and data analysis. Particle physics data present unique challenges, including continuous coordinates, stochastic dimensionality, and symmetries like permutation invariance. Traditional deep generative models designed for images may not directly apply to such datasets. To address these challenges, this study uses Fast Point Cloud Diffusion (FPCD), a novel neural network simulation. The primary objective is to accelerate diffusion models and improve sampling efficiency, measured by reduced sampling time and minimized Wasserstein Distances between generated and true data distributions.

Background

- The FPCD model estimates gradients of the log-likelihood with respect to data points (**score function**).
- FPCD uses the score function to guide a diffusion process for generating new samples that capture the underlying data distribution.
- Evaluation of sampling techniques involves using the **Wasserstein Distance (W1)** metric to quantify dissimilarity between generated and true data distributions.



- The denoising process in FPCD is stochastic[1], resulting in Stochastic Differential Equations (SDEs) that require solving.

Numerical Methods

- **ODE Solver:** The SDE yields a deterministic ordinary differential equation[2] (ODE) we solve using scipy **RK45** (Runge-Kutta) models:

$$\mathrm{d}\mathbf{z}_t = [f(\mathbf{z}_t, t) - \frac{1}{2}g^2(t)\nabla_z \log \hat{p}_\theta(\mathbf{z}_t)]\mathrm{d}t,$$

- **SDE Solver:** We implement a Euler-Maruyama solver (**EMSampler**) to solve the reverse SDE.

Research Question

How can sampling from particle physics datasets be optimized using the FPCD model with efficient numerical methods and minimized Wasserstein Distances?

Results & Analysis

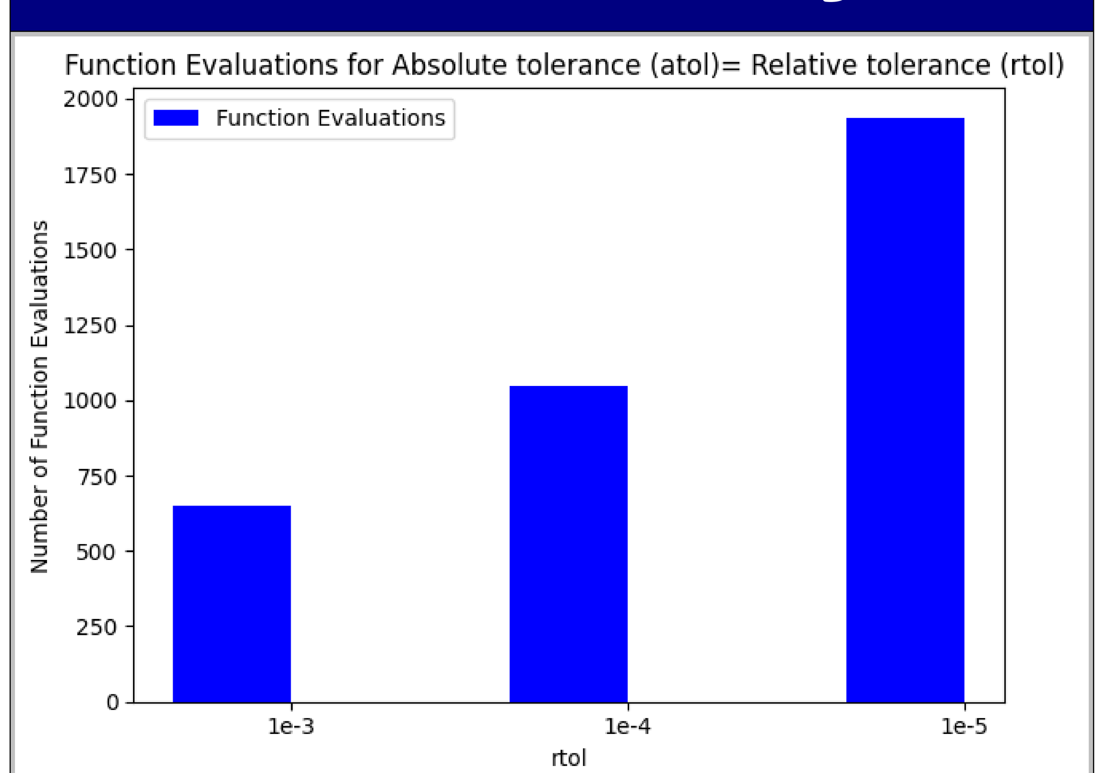


Figure 1. Number of function evaluations for different tolerance values in RK45 models

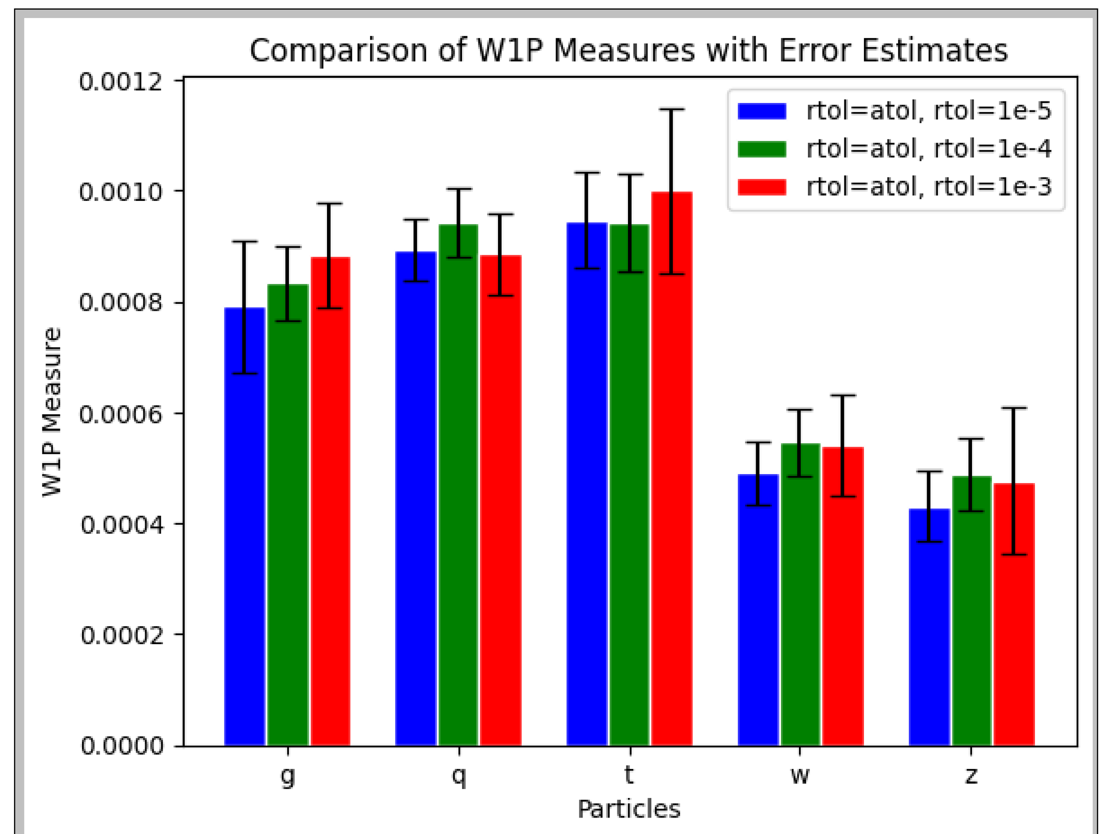


Figure 2 & 3. Comparison of W1 measure for particle momenta (W1P)

Result: RK45(atol=rtol=1e-3) samples **3 times faster than baseline,** RK45(atol=rtol=1e-5), without significant increase in W1P measures.

We then implement our EMSampler that samples 2 times faster than our RK45 benchmark with **300** function evaluations, **6 times** faster than baseline:

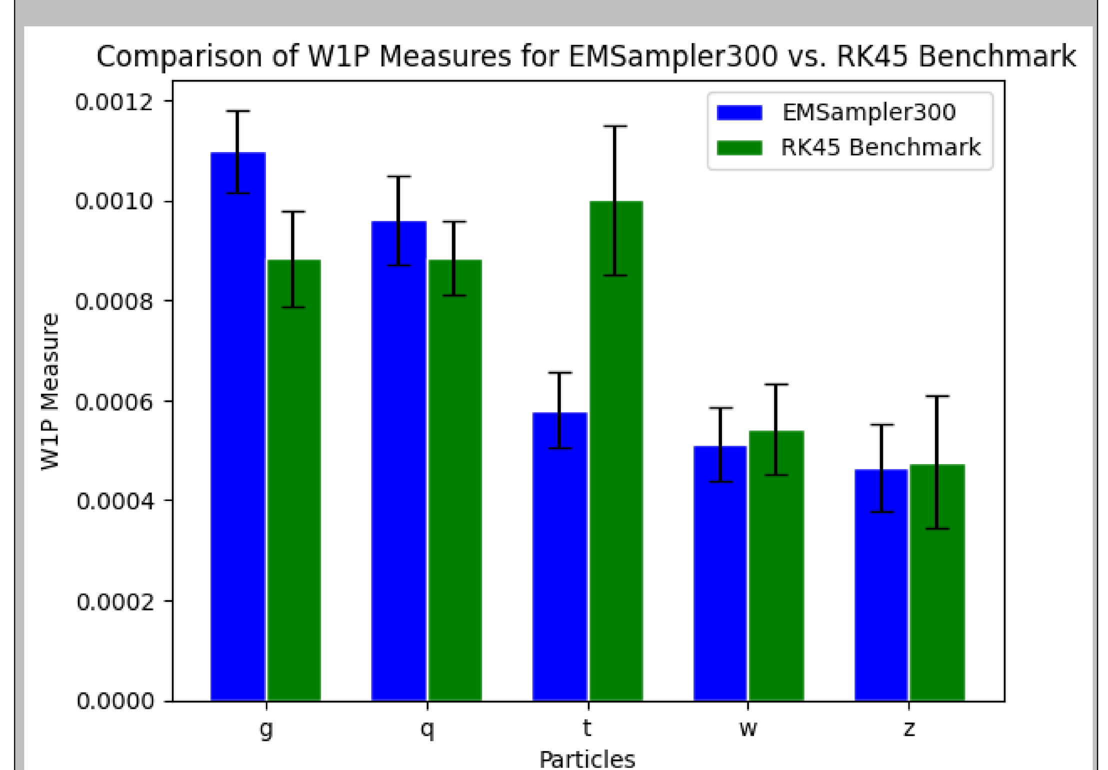


Figure 3

Since the increase in W1P measures is no longer trivial in this case, we employ **Predictor-Corrector** method in our SDE-Solver **0165EM250** to improve accuracy. This solver only uses **250** function evaluations, compared to **2000** for RK45.

0165EM250, without compromising average accuracy across 5 particle types in our datasets, samples **8x faster** than RK45 Benchmark.

Particle Type	Method with Minimal Average W_1 Metrics
g	0165EM250
q	0165EM250
t	RK45 Benchmark
w	0165EM250
z	RK45 Benchmark

Table 1: Method with Minimal Average W_1 Metrics for Each Metric

Conclusions

Employing SDE Solvers has better potential for optimization using FPCD compared to RK45's blackbox ODE Solvers as it leads to faster and more accurate sampling. Further research on corrections for our SDE Solver can lead to solving many large-scale issues in particle physics.

References

1. Song et al. 2020, *Score-Based Generative Modeling through Stochastic Differential Equations.*
2. Mikuni et al. 2023, *Fast Point Cloud Generation with Diffusion Models in High Energy Physics.*

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