A Machine Learning Perspective on Hadronization Modeling with MLHAD

PIKIMO 15

Based on SciPost Phys. 14, 027 (2023), and 2311.XXXXX

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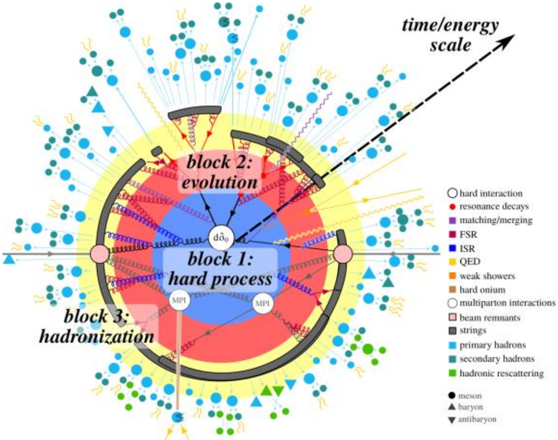
In collaboration with:
C. Bierlich, P. Ilten, T. Menzo, S. Mrenna, M. Szewc, M.K. Wilkinson, and J. Zupan

Motivation

Simulating Collision



➔ **Hard process:**
initial high-energy interaction

➔ **Evolution:**
parton shower

} *perturbative*

➔ **Hadronization:**
combine quarks and gluons

} *non -perturbative*

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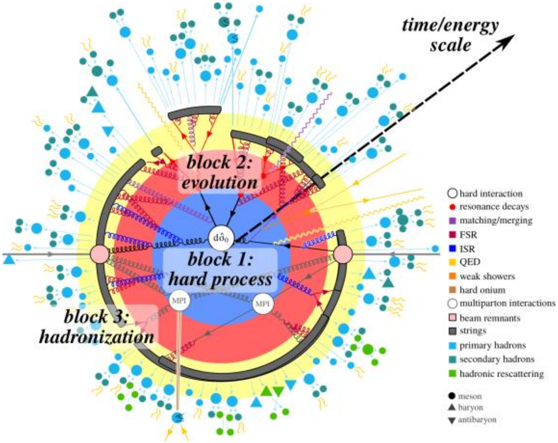


- **Hard process:**
  initial high-energy interaction
- **Evolution:**
  parton shower

perturbative

- **Hadronization**:
  combine quarks and gluons

non

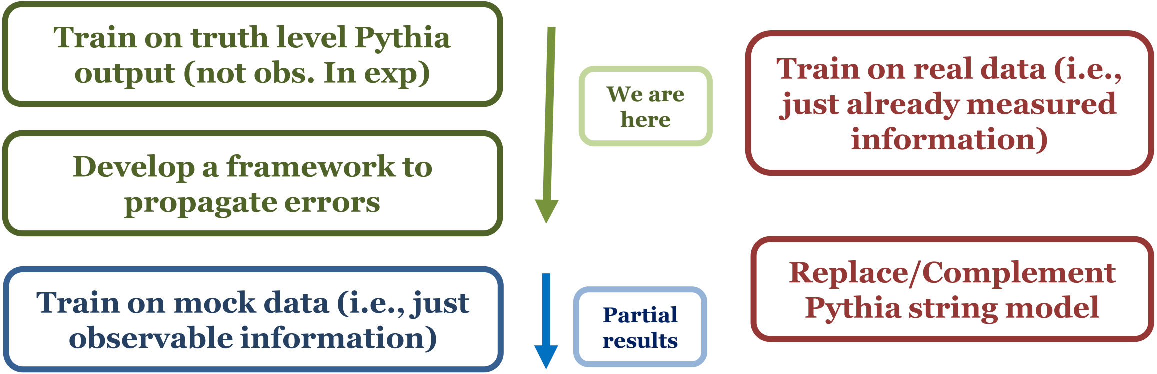
Use ML!

ve

MLHAD

Big Picture

A series of progressive steps needs to be done before practically useful in Pythia simulations



Train on truth level Pythia output (not obs. In exp)

Develop a framework to propagate errors

Train on mock data (i.e., just observable information)

We are here

Partial results

Train on real data (i.e., just already measured information)

Replace/Complement Pythia string model

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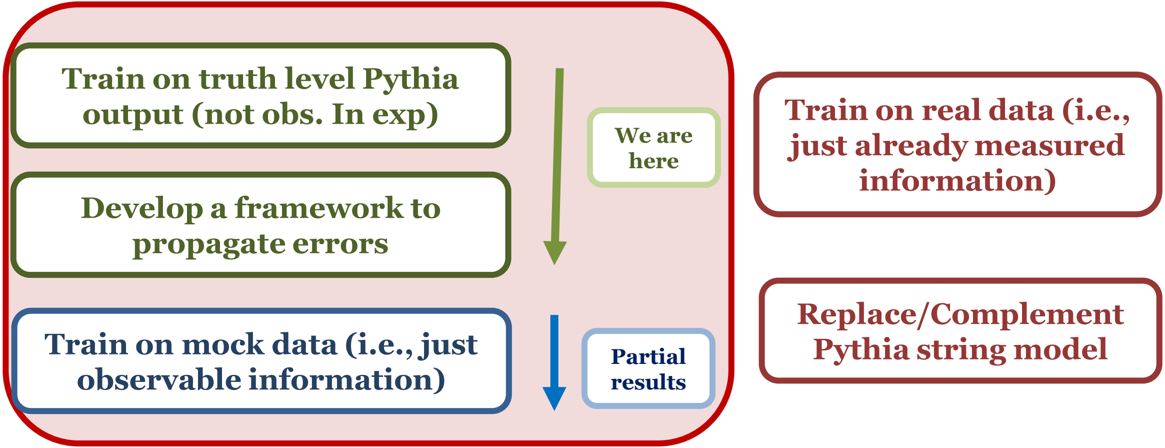

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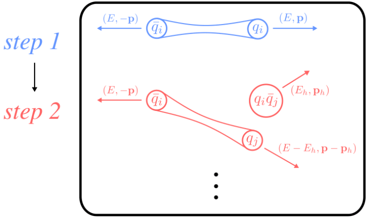
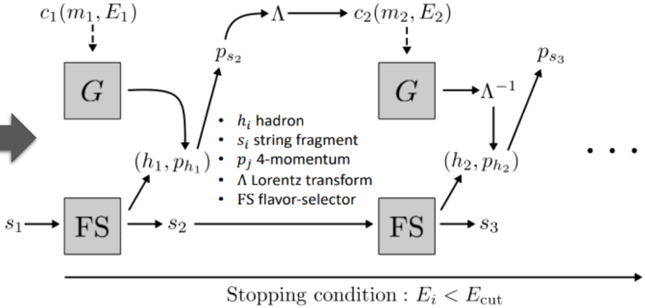
MLHAD Pipeline





- h_i hadron
- s_i string fragment
- p_j 4-momentum
- Λ Lorentz transform
- FS flavor-selector

Stopping condition : $E_i < E_{\text{cut}}$

We need a generative model!

Sample hadron kinematics:
Train on $\{\boldsymbol{p_z},\boldsymbol{p_T}\}$

Emission of different Mesons:
Condition on mass $(\boldsymbol{m})$ and energy $(\boldsymbol{E})$

Why Machine Learning?

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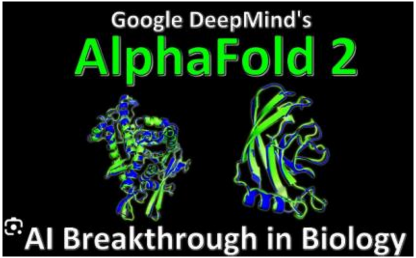

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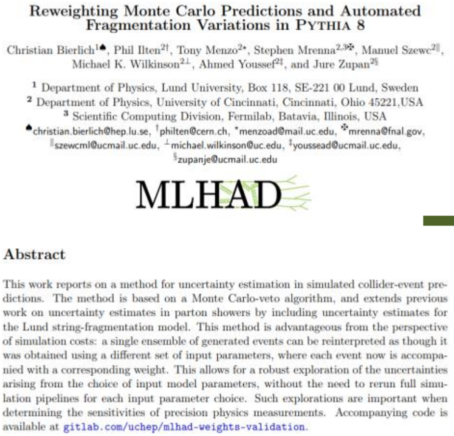

Reweighting Monte Carlo Predictions and Automated Fragmentation Variations in PYTHIA 8

Christian Bierlich[1♠], Phil Ilten[2†], Tony Menzo[2*], Stephen Mrenna[2,3✠], Manuel Szewc[2‖], Michael K. Wilkinson[2⊥], Ahmed Youssef[2‡], and Jure Zupan[2§]

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[2] Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221,USA
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MLHAD

Abstract

This work reports on a method for uncertainty estimation in simulated collider-event predictions. The method is based on a Monte Carlo-veto algorithm, and extends previous work on uncertainty estimates in parton showers by including uncertainty estimates for the Lund string-fragmentation model. This method is advantageous from the perspective of simulation costs: a single ensemble of generated events can be reinterpreted as though it was obtained using a different set of input parameters, where each event now is accompanied with a corresponding weight. This allows for a robust exploration of the uncertainties arising from the choice of input model parameters, without the need to rerun full simulation pipelines for each input parameter choice. Such explorations are important when determining the sensitivities of precision physics measurements. Accompanying code is available at gitlab.com/uchep/mlhad-weights-validation.

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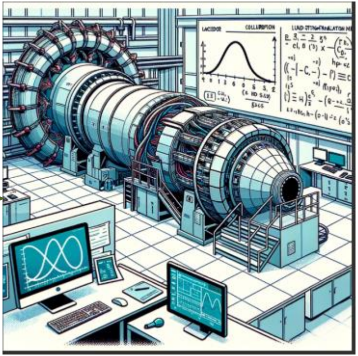
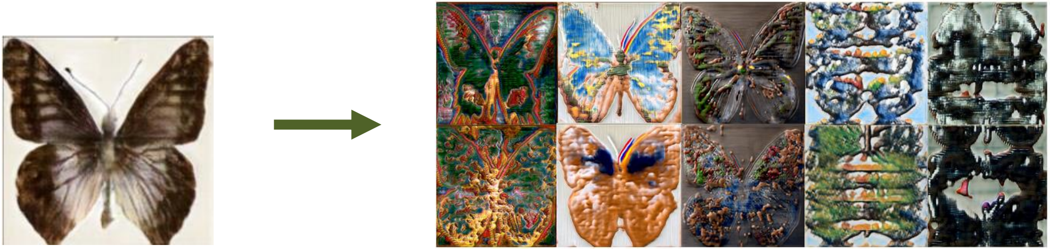


Why Machine Learning?

Hacking Generative Models with Differentiable Network Bending

NeurIPS, ML for Creativity and Design workshp

G. Aldeghery, A Rogalska, A. Youssef, E. Iofinova



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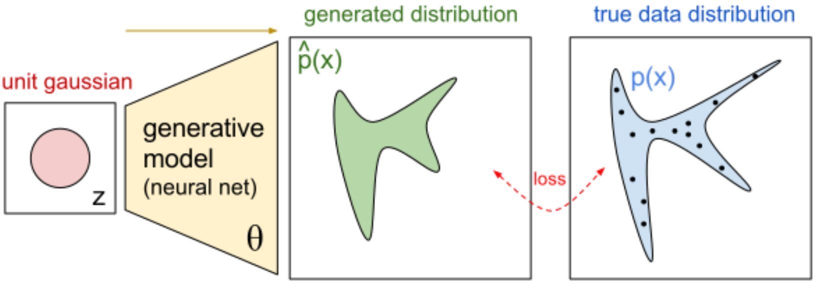
How is this useful for us?

Generative Models

https://openai.com/research/generative-models



Source: generative models

$\Longrightarrow$ Task: Learn the probability distribution $p(x)$ of the data

Which generative model should we choose?

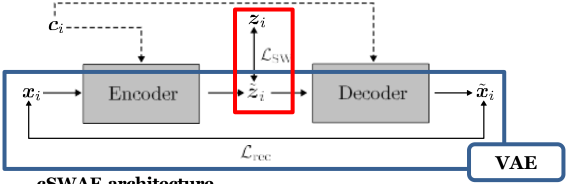
Is it able to learn **complex distributions**?

Do we have access to the **exact probability distribution**?

Generative Models

SciPost Phys. 14, 027 (2023)

Conditional Sliced Wasserstein (SW) Autoencoder (cSWAE)



cSWAE architecture
(Architecture used in SciPost Phys. 14, 027 (2023))

SW distance enables learning any sampleable latent distribution

⇒ **Can learn complex distributions!**

Decoder "just" generates samples

⇒ **No access to the probability distribution**

Generative Models

[SciPost Phys. 14, 027 (2023)](https://scipost.org)

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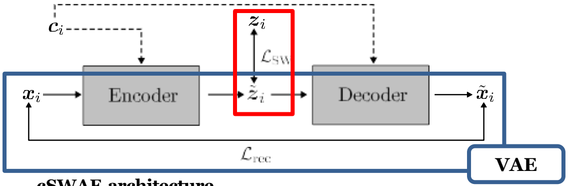

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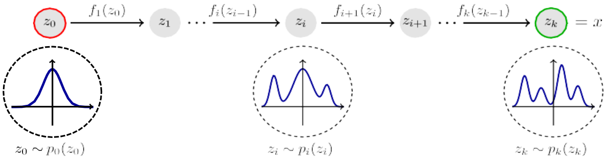
Normalizing Flows (NF)



hHps://github.com/janosh/awesome-normalizing-flows

$$p_k(z_k) = p_0(z_0)\prod_{i=1}^{K}\left|\det\left(\frac{\partial f_i(z_{i-1})}{\partial z_{i-1}}\right)\right|^{-1}$$

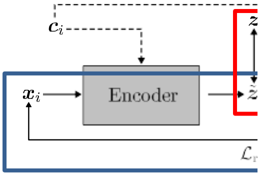
⇒ **Can learn complex distributions!**

⇒ **Access to the exact probability distribution**

Generative Models

SciPost Phys. 14, 027 (2023)

Conditional Sliced Wasse



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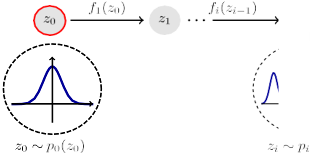

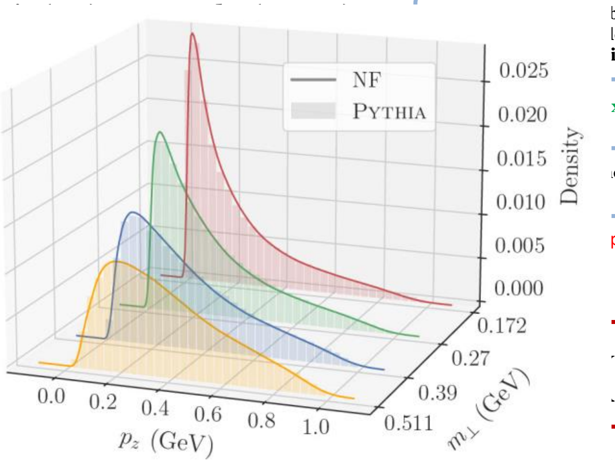

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x distributions!

erates

probability distribution

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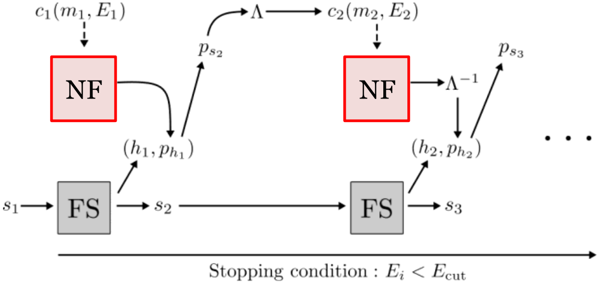
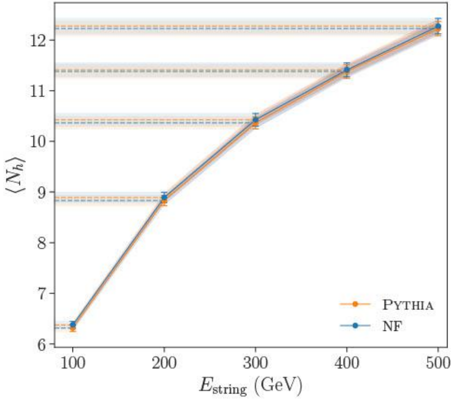
hHps://github.com/janosh/awesome-normalizing-flows

Back to Physics

Implement NF in the fragmentation chain to obtain physical observables





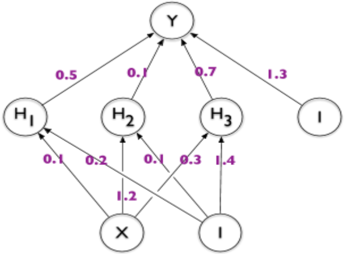
$\Rightarrow$ *Multiplicity obtained by MLHad agrees with Pythia!*

Uncertainty Quantification

Uncertainty estimation is crucial for event generator predictions!

Statistical (and Training) Uncertainties

„Classical“ Neural Networks



Weights have a fixed value
→ Weight values are updated in each epoch

(Image source: The very Basics of Bayesian Neural Networks)

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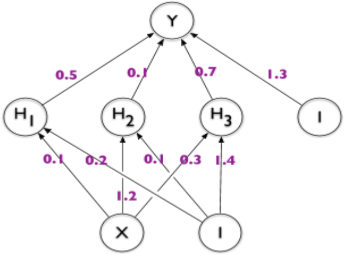

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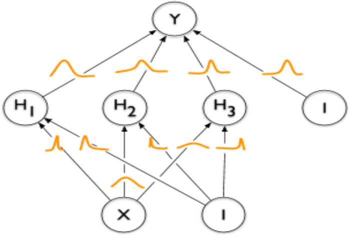
Bayesian Neural Networks (BNN)



Weights are sampled from a distribution
→ Distribution parameter are updated in each epoch

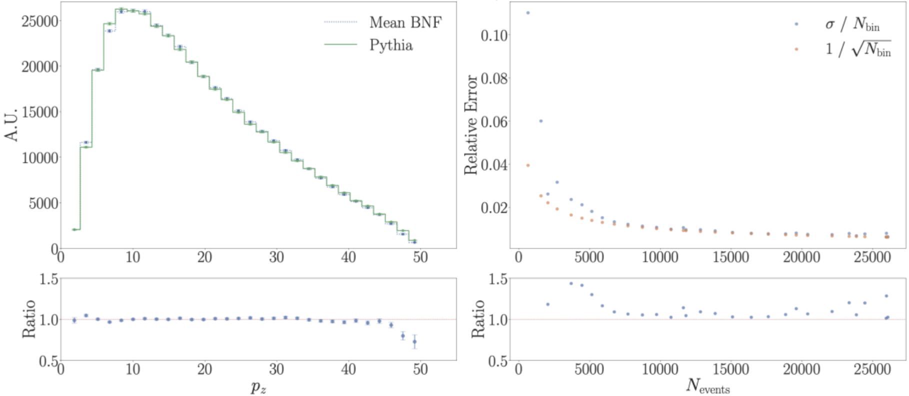
→ **BNN are easy to implement: Add additional loss function for weight distribution**

→ **Capture statistical and training uncertainties**

(Image source: The very Basics of Bayesian Neural Networks)

Bayesian NF Results

*Preliminary



Pythia Sample: One sample with errors corresponding to $\sqrt{N_{bin}}$

Mean BNF: 5×10^5 samples with errors corresponding to the standard deviation

BNF capture the statistical and training uncertainties

Bayesian NF Results

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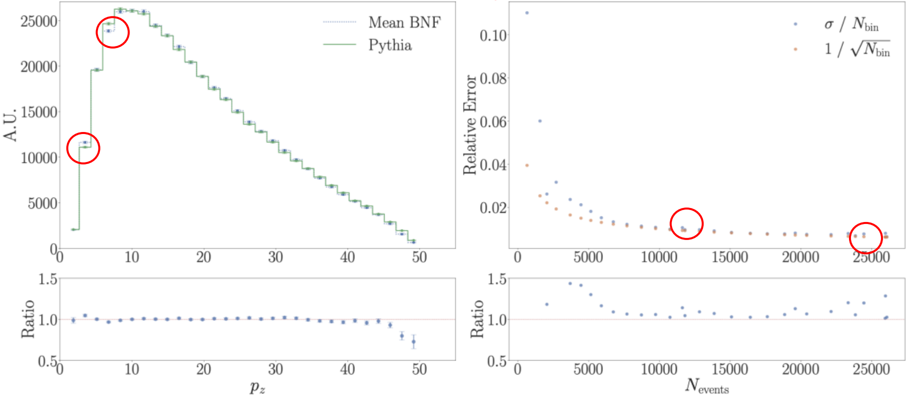

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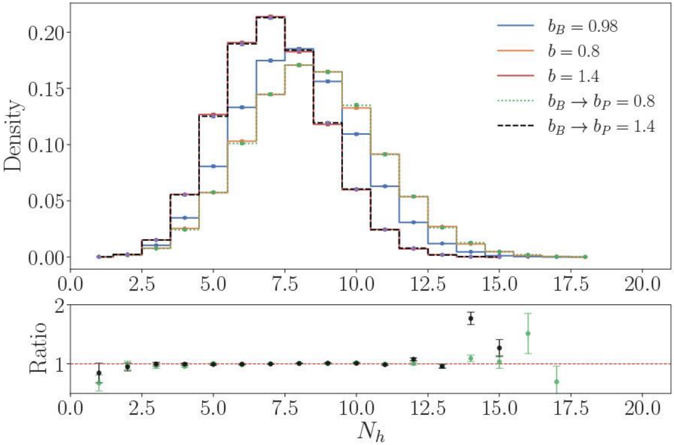
Reweighting with NFs

*Preliminary



b is a free parameter in the Lund function used in Pythia: StringZ:bLund

Train nominal NF conditioned on different b
→ Get likelihood

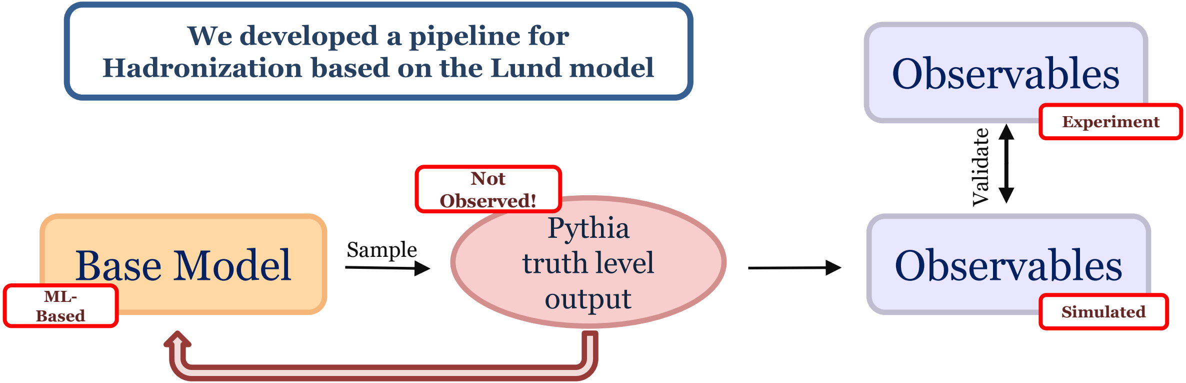
→ Reweight nominal output using ratio of likelihoods:

$$w = \prod_i \frac{p^{(i)}_{nom}(z)}{p^{(i)}_{pert}(z)}$$

Further Directions

MLhadPipeline

We developed a pipeline for Hadronization based on the Lund model



Observables

Experiment

Validate

Not Observed!

Base Model

ML-Based

Sample

Pythia truth level output

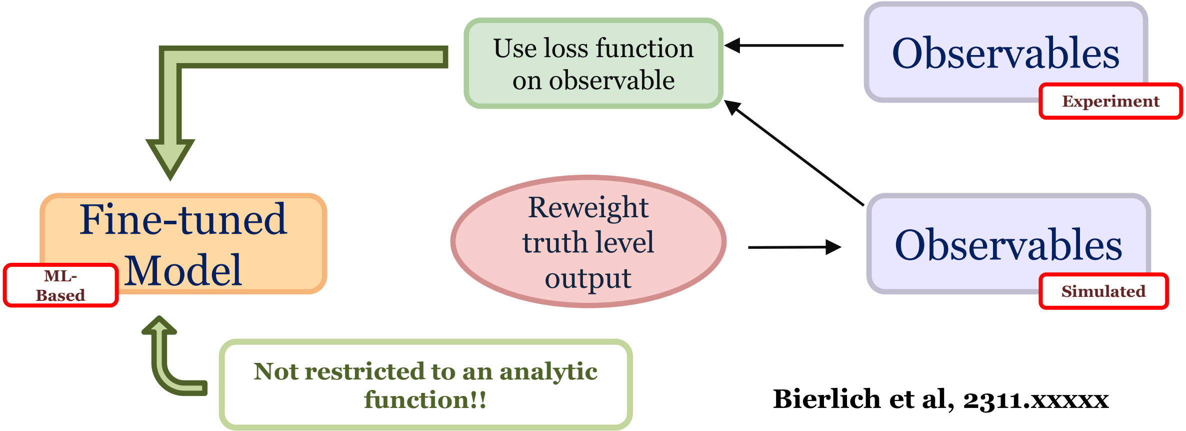
Observables

Simulated

First Step:
Train on **“pseudo” data**
from Pythia

Further Directions

MLhadPipeline



Use loss function on observable

Observables

Experiment

Fine-tuned Model

ML-Based

Reweight truth level output

Observables

Simulated

Not restricted to an analytic function!!

Bierlich et al, 2311.xxxxx

Conclusion and Outlook

- First MLHAD pipeline based on cSWAE was published in SciPost Phys. 14, 027 (2023)
- NFs overcome the limitations of cSWAE - can emit in principle any meson and have access to pdf
- NFs allow us to reweight events and capture uncertainties

Work in progress

- Finalize normalizing flows architecture (include model uncertainty)
- PYTHIA reweighting (Release as part of Pythia)
- Flavor Selector
- Performing training on physically accessible observables to train MLHAD on **experimental data**

Backup

Motivation

When is a hadronization model successful?

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➡ **The performance is judged by their description of experimental measurements!**

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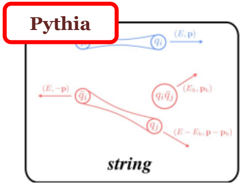
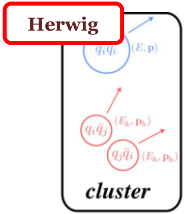
Pythia



Herwig



Phenomenological Models (String, Cluster) are currently state of art and are overall very successful, however:

➡ comparison of data from proton-proton and ion-ion collision with Pythia

➡ discrepancies at the level of O(20%) to O(50%) N. Fischer and T. Sj¨ostrand, JHEP 01, 140 (2017), 1610.09818.

➡ recovering collective effects can be challenging, for instance, heavy baryon production at high event multiplicities Alice Collaboration, arXiv: 1807.11321

➡ no efficient estimation of Uncertainties

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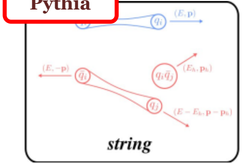
Pythia



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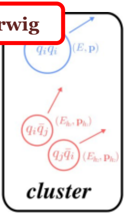

Both models have a discrepancy in describing experimental measurements!

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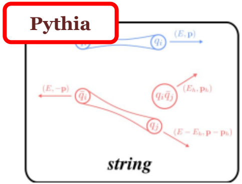

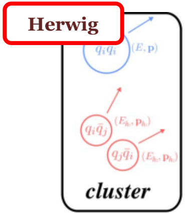

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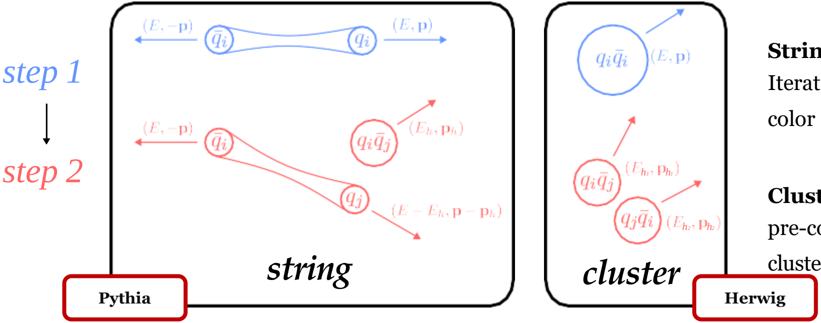
We need an innovative approach!

Both models have a discrepancy in describing experimental measurements!

Hadronization Models

Two primary hadronization models are used



String model:
Iteratively split parton connected by QCD color strings with linear potential

Cluster model:
pre-confine partons into proto-clusters, then split by two-body decays

MLhad: Ilten, Menzo,Youssef, Zupan, 2203.04983, https://gitlab.com/uchep/mlhad

HadML: (Chan, Ghosh,) Ju, (Kania), Nachman, (Sangli,) Siodmok, 2203.12660, 2305.17169

Uncertainty Quantification

Uncertainty estimation is crucial for event generator predictions!

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- **Hard matrix element**
- **Parton shower**

Efficient solutions exist!

perturbative calculations depend on choices of scale, values of gauge and other couplings, particle masses, and nonperturbative inputs

Giele et al, [Phys. Rev. D84, 054003 (2011)]

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- **Hadronization**

Efficient solution has remained elusive!

Standard procedure: perform repeated simulations with different sets of values for the model parameters

→ **Computationally very expensive!**

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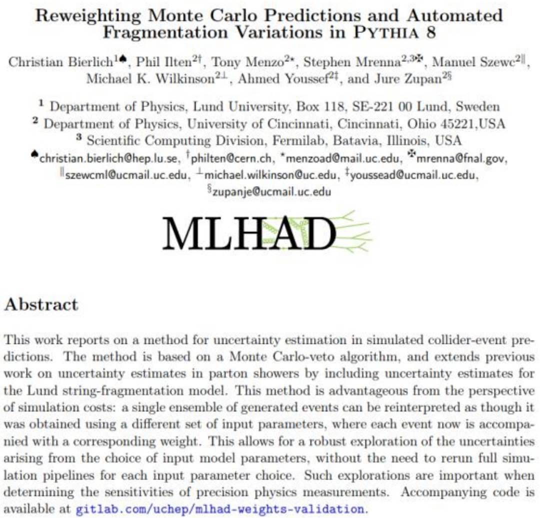
Need a more efficient way!

Reweighting Hadronized Pythia Events

Small Detour:
No ML, only Had



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[2] Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221,USA
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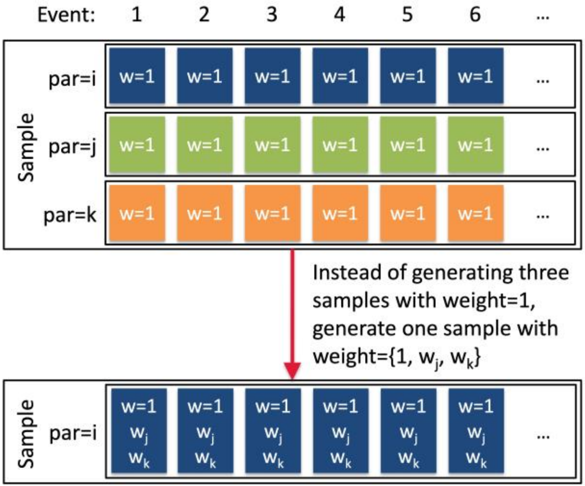
Reweighting Hadronized Pythia Events

- **Event generation is time consuming**
  - **We want to reweight events without regenerating**
- **Use a modified veto algorithm**
  - **New event weights for different hadronization param are book kept**

We calculate event weights for different hadronization options in a single event generation!



Sample

Event:	1	2	3	4	5	6	...
par=i	w=1	w=1	w=1	w=1	w=1	w=1	...
par=j	w=1	w=1	w=1	w=1	w=1	w=1	...
par=k	w=1	w=1	w=1	w=1	w=1	w=1	...

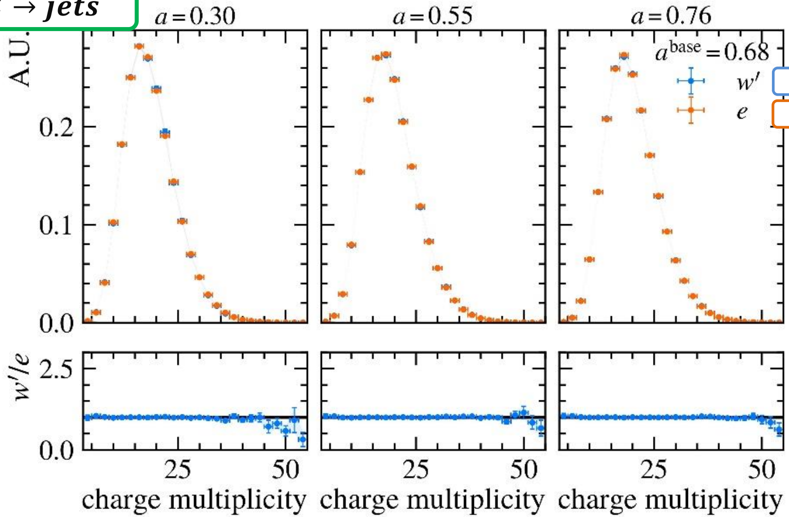
Instead of generating three samples with weight=1, generate one sample with weight={1, w_j, w_k}

Sample

par=i	w=1 w_j w_k	w=1 w_j w_k	w=1 w_j w_k	w=1 w_j w_k	w=1 w_j w_k	w=1 w_j w_k	...

Reweighting Hadronized Pythia Events

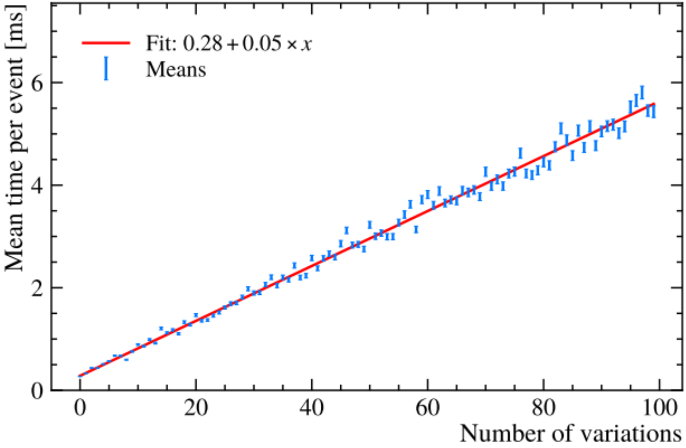
$e^+e^- \to Z \to jets$



reweighted

exact calc.

Reweighting Hadronized Pythia Events



- Generate 100 samples with different variations of aLund

- Each sample has 1000 events

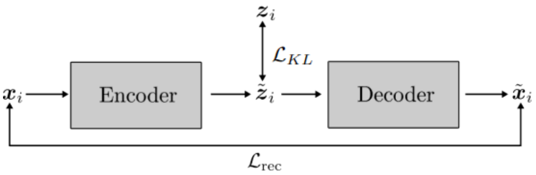
- Cost per additional parameter variation is around 0.05 ms

- We have a speed up by a factor ~3

Generative Models

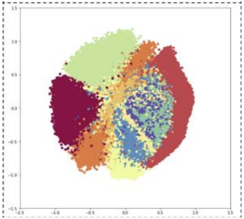
Variational Autoencoder (VAE)

Kingma et al, arXiv:1312.6114



Vanilla VAE

KL-divergence limits the latent space to a simple analytic distribution



VAE latent space
arXiv: 1804.01947

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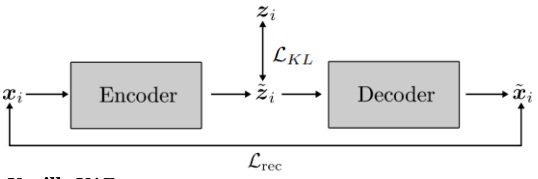

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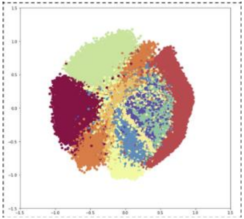

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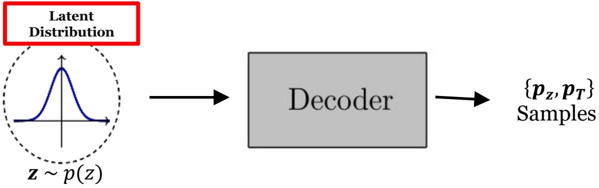
Inference



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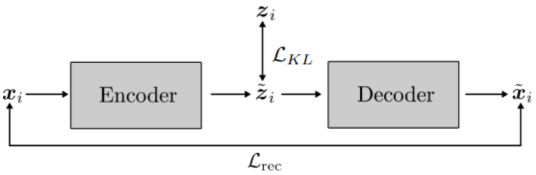

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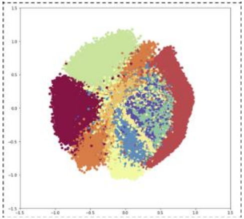

VAE latent space
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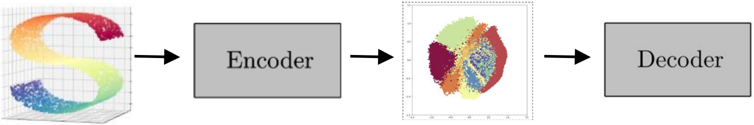
Complex input data

Simple latent space



⇒ **Complex distribution are hard to learn!**

Generative Models

Variational Autoencoder (VAE)

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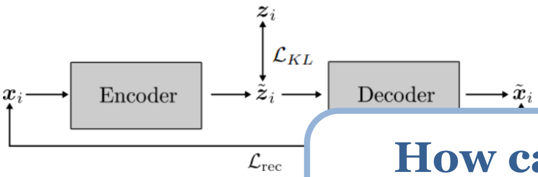

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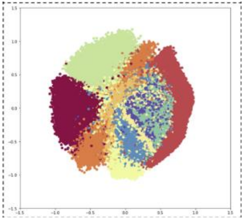
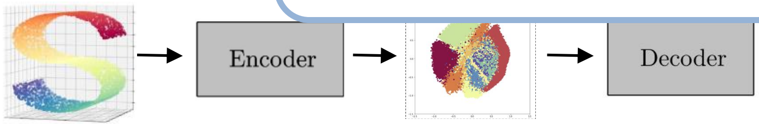


VAE latent space
arXiv: 1804.01947

How can we make VAEs learn more complex distribution?

Complex input data



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Generative Models

Use Sliced Wasserstein Distance as latent loss function!

Generative Models

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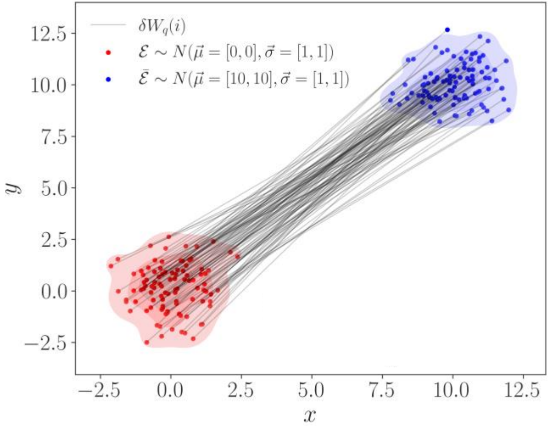
Wasserstein distance (WD)

$$W_q(\mathcal{E},\bar{\mathcal{E}}) = \left[\min_{\{f_{ij}\geq 0\}} \sum_{i=1}^{N}\sum_{j=1}^{\bar{N}} f_{ij}\left(\hat{d}_{ij}\right)^q\right]^{1/q}$$



Generative Models

Use Sliced Wasserstein Distance as latent loss function!

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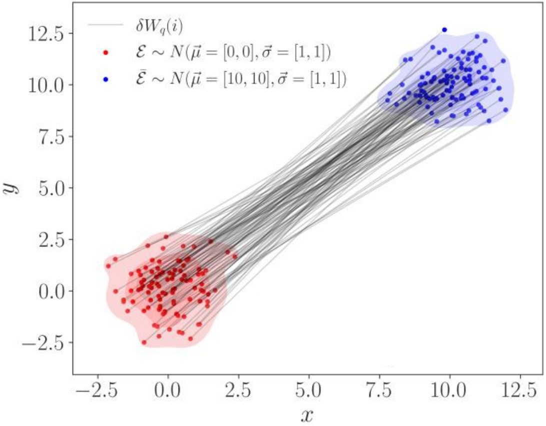
Sliced Wasserstein distance

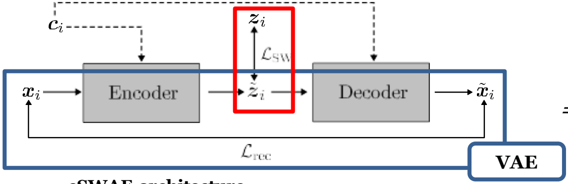
- ➡ Projects high dimensional data into one dimensional “slices”
- ➡ WD in 1D has a closed form solution
  - ➡ Sorted Difference of the two samples



Generative Models

[SciPost Phys. 14, 027 (2023)](https://scipost.org/SciPostPhys.14.027) **Conditional Sliced Wasserstein (SW) Autoencoder (cSWAE)**

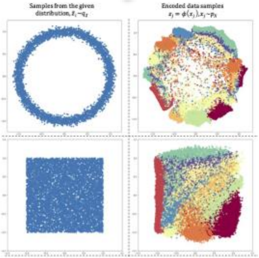
Restricted to Pion emissions



cSWAE architecture
(Architecture used in [SciPost Phys. 14, 027 (2023)](https://scipost.org/SciPostPhys.14.027))

SW distance enables learning any sampleable latent distribution

⇒ **Can learn complex distributions!**



SWAE latent space
(arXiv: 1804.01947)

Generative Models

SciPost Phys. 14, 027 (2023)

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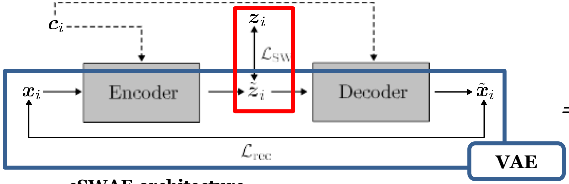

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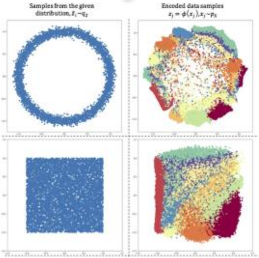

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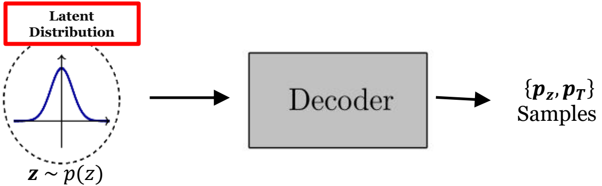
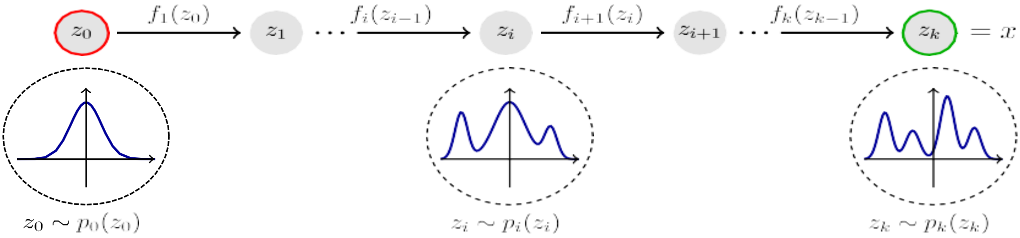


Decoder "just" generates samples

⇒ **No access to the probability distribution**

Normalizing Flows


$z_0 \xrightarrow{f_1(z_0)} z_1 \cdots \xrightarrow{f_i(z_{i-1})} z_i \xrightarrow{f_{i+1}(z_i)} z_{i+1} \cdots \xrightarrow{f_k(z_{k-1})} z_k = x$
$z_0 \sim p_0(z_0)$
$z_i \sim p_i(z_i)$
$z_k \sim p_k(z_k)$

Zo- random vector sampled from a Gaussian $p_0(z_0)$

Fi – invertible NN that transforms $p_0(z_0)$ to $p_i(z_i)$ by change of variables

Complex target distribution $p_k(z_k)$ is learned

⇒ **Can learn complex distributions!**

Exact probability distribution is obtained by change of variables

$$p_k(z_k) = p_0(z_0) \prod_{i=1}^{K} \left|\det\left(\frac{\partial f_i(z_{i-1})}{\partial z_{i-1}}\right)\right|^{-1}$$

hHps://github.com/janosh/awesome-normalizing-flows

⇒**Access to the exact probability distribution**

Removed pion emission restriction

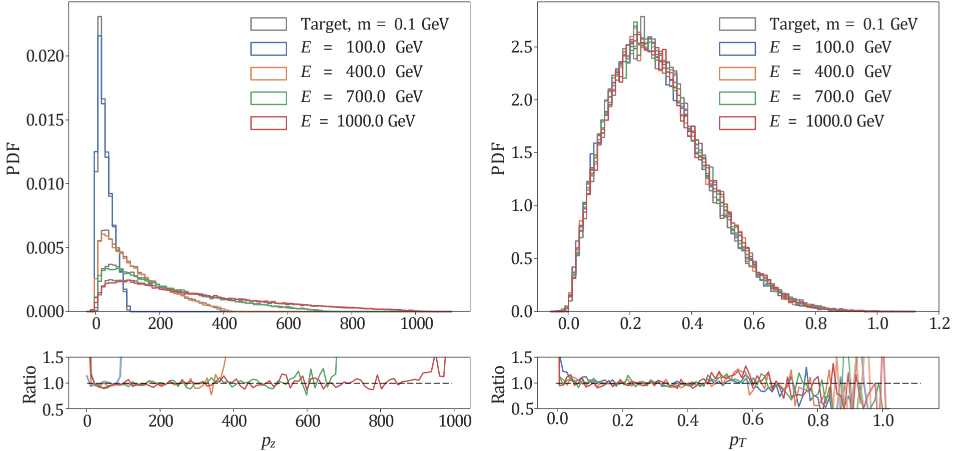
Further Directions

- **Propagation of errors**
  - **ML architecture with Bayesian Normalizing Flows (presented in part)**
- **Train on observables only**
  - **Two part reweighter (not part of the talk)**
  - **Train on global observables with Fine tuning (results not shown in this talk)**
- **To train on experimental data**
  - **Want fast evaluation of parameter dependency**
  - **Use reweighting method**
  - **First implementation in Pythia for Lund string model (to be released soon in Pythia)**

Back up

Training Results cNF

*Preliminary


Target, m = 0.1 GeV
E = 100.0 GeV
E = 400.0 GeV
E = 700.0 GeV
E = 1000.0 GeV
PDF
Ratio
p_z
Target, m = 0.1 GeV
E = 100.0 GeV
E = 400.0 GeV
E = 700.0 GeV
E = 1000.0 GeV
PDF
Ratio
p_T