Generative networks for particle physics

Lecture at QU Data Science Basics (Hamburg)
June 2021

Anja Butter

Paradigm shift

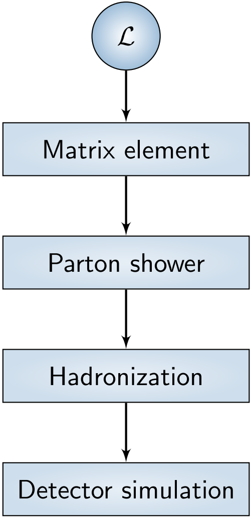
Given data $\rightarrow$ find label

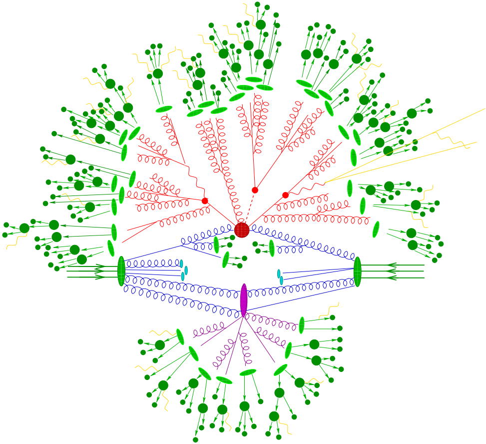
$\downarrow$

Given data $\rightarrow$ generate new data

What do we generate in high energy physics?

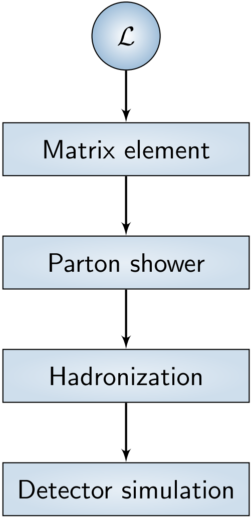
First principle based event generation

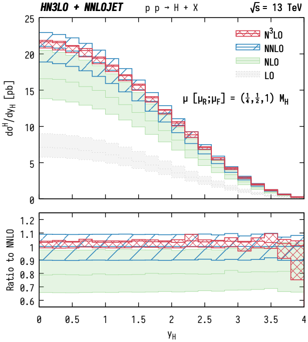




a sherpa artist

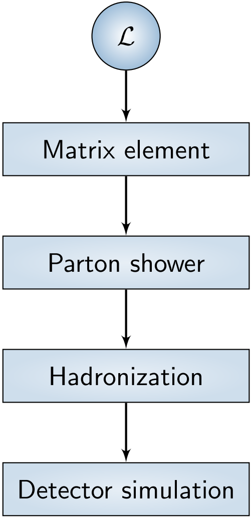
First principle based event generation

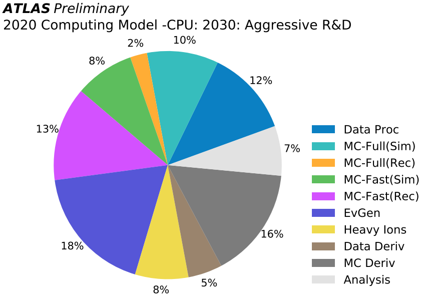




[1807.11501] Cieri, Chen, Gehrmann, Glover, Huss

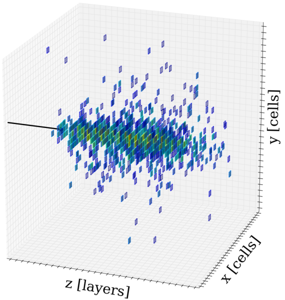
First principle based event generation

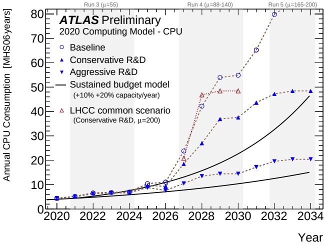




Fast detector simulations

- Important R&D potential
  NN evaluation $\times$100-1000
  faster than GEANT4





- Challenge:
  High-dimensional output
  $\leftarrow$ 30 $\times$ 30 $\times$ 30

Why do we need machine learning for data simulation?

precision
event generation

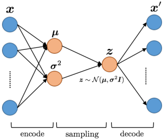
detailed
detector simulation

limited computing ressources

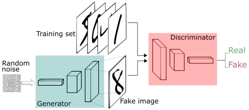
Speed → more events = higher order → Precision

Use NN to speed up simulations!

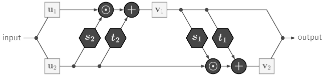
Neural network based generative networks



VAE

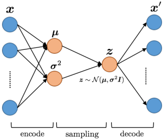


GAN



NF

Neural network based generative networks



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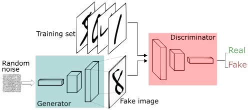
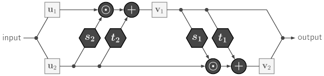


GAN

all kinds of hybrids



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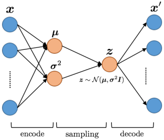
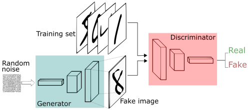


VAE



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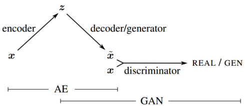
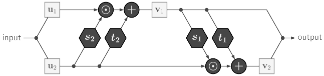
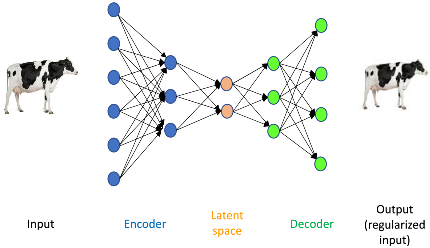


VAE-GAN



NF

From autoencoders to variational autoencoders



$$\text{AE: } \boldsymbol{x} \xrightarrow{\text{encoder}} \boldsymbol{z} \xrightarrow{\text{decoder}} \boldsymbol{x}' \qquad \mathcal{L}_{AE} = (\boldsymbol{x} - \boldsymbol{x}')^2$$

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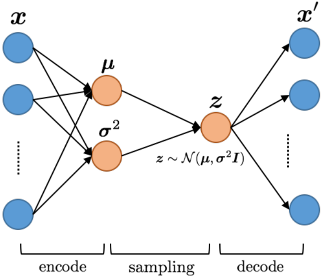

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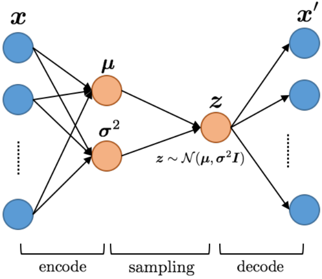

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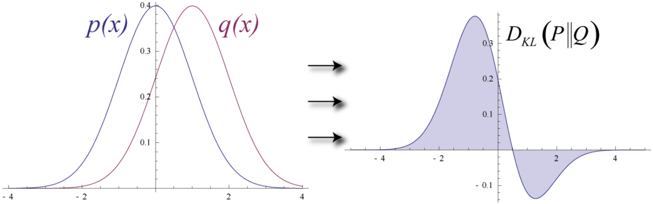
Loss enforces Gaussian latent space

$$\mathcal{L}_{VAE} = \mathcal{L}_{AE} + \beta \cdot \text{KL}(\mathcal{N}(\mu, \sigma) | \mathcal{N}(0, 1)) \qquad \leftarrow \text{similarity measure}$$

Interlude: KL Divergence

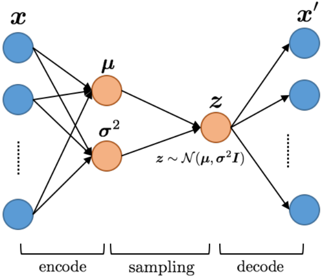
- Distance measure for probability distributions P and Q
- $D_{\mathrm{KL}}(P \parallel Q) = \int_{-\infty}^{\infty} p(x) \log\left(\frac{p(x)}{q(x)}\right)\, dx$



By Mundhenk at English Wikipedia, CC BY-SA 3.0

$$D_{\mathrm{KL}}(\mathcal{N}(\mu, \sigma) \parallel \mathcal{N}(0, 1)) = \frac{1}{2}(1 + \log(\sigma^2) - \mu^2 - \sigma^2)$$

From autoencoders to variational autoencoders



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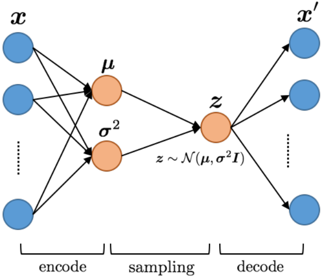

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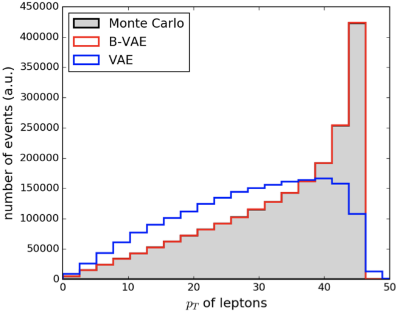
$$\begin{aligned} \mathcal{L}_{VAE} &= \mathcal{L}_{AE} + \beta \cdot \mathrm{KL}(\mathcal{N}(\mu, \sigma) | \mathcal{N}(0, 1)) \qquad \leftarrow \text{similarity measure} \\ &= \mathcal{L}_{AE} + \frac{\beta}{2} \sum_j 1 + \log(\sigma_j^2) - \mu_j^2 - \sigma_j^2 \end{aligned}$$

$e^+e^- \to Z \to l^+l^-$ with VAE

[1901.00875] S. Otten et al.

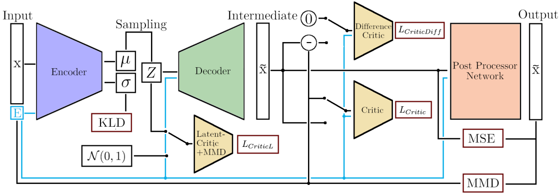


naive VAE fails to reproduce distributions

Why? $\to$ latent space not perfectly Gaussian
Fix: insert information buffer to sample from real latent distribution
$\to$ B-VAE shows excellent performance

Detector simulation with BIB-AE PP

Bounded-Information-Bottleneck autoencoder with post processing



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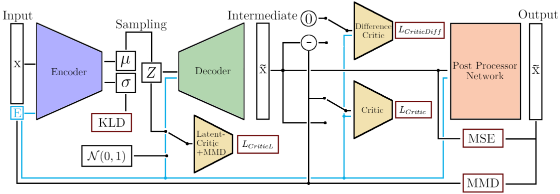
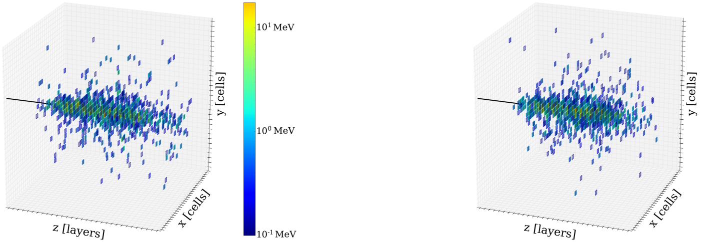
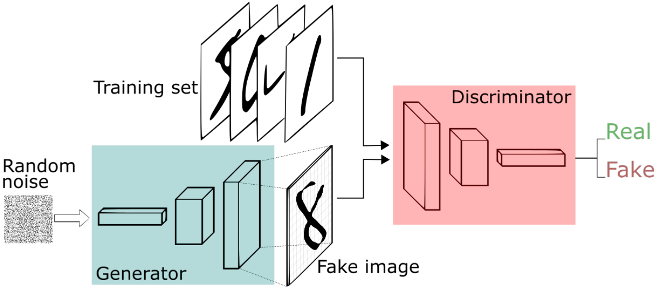


GEANT4

Simulation



Generative Adversarial Networks



Discriminator

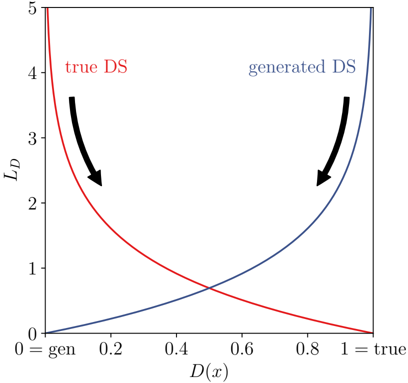
$$L_D = \langle -\log D(x) \rangle_{x \sim P_{Truth}} + \langle -\log(1 - D(x)) \rangle_{x \sim P_{Gen}}$$

Generator

$$L_G = \langle -\log D(x) \rangle_{x \sim P_{Gen}}$$

Training the Discriminator

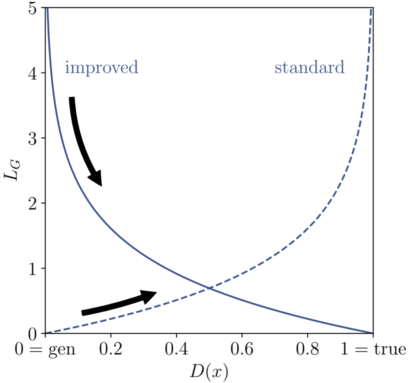
Discriminator loss



Minimize $\quad L_D = \big\langle -\log D(x) \big\rangle_{x\sim P_T} + \big\langle -\log(1 - D(x)) \big\rangle_{x\sim P_G}$

Training the Generator

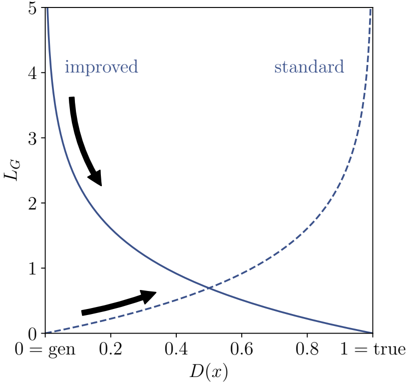
Generator loss



Maximize $\quad L_G = \big\langle -\log(1 - D(x)) \big\rangle_{x \sim P_G}$

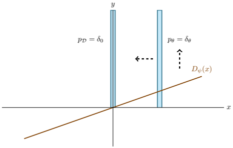
Training the Generator

Generator loss

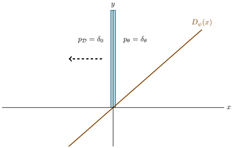


Minimize $\quad L_G = \big\langle -\log D(x) \big\rangle_{x\sim P_G}$

Regularization



(a) $t = t_0$



(b) $t = t_1$

[1801.04406]

Adding gradient penalty

$$\phi(x) = \log \frac{D(x)}{1 - D(x)} \qquad \Rightarrow \qquad \frac{\partial \phi}{\partial x} = \frac{1}{D(x)} \frac{1}{1 - D(x)} \frac{\partial D}{\partial x}$$

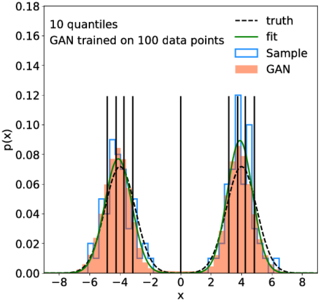
$$L_D \to L_D + \lambda_D \Big\langle \left(1 - D(x)\right)^2 |\nabla \phi|^2 \Big\rangle_{x \sim P_T} + \lambda_D \Big\langle D(x)^2 |\nabla \phi|^2 \Big\rangle_{x \sim P_G}$$

What is the statistical value of GANned events?[2008.06545]

- Camel function
- Sample vs. GAN vs. 5 param.-fit

Evaluation on quantiles:

$$\mathrm{MSE}^* = \sum_{j=1}^{N_\mathrm{quant}} \left(p_j - \frac{1}{N_\mathrm{quant}} \right)^2$$



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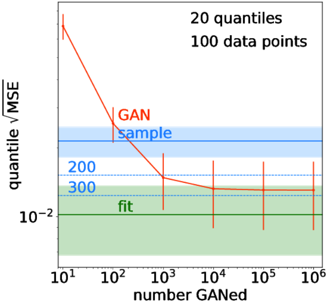


→ Amplification factor 2.5

$\boxed{\text{Sparser data} \rightarrow \text{bigger amplification}}$

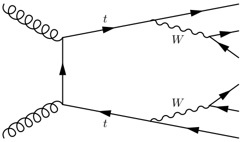
How to GAN LHC events

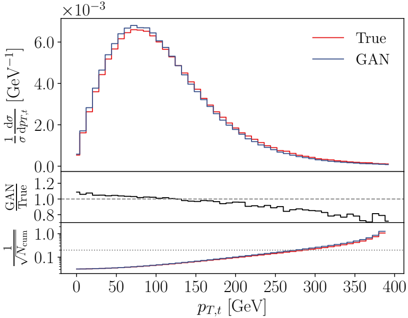
[1907.03764]

- $t\bar{t} \to 6$ quarks
- 18 dim output
  - external masses fixed
  - no momentum conservation

+ Flat observables ✓

– Systematic undershoot in tails





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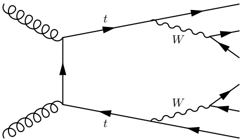
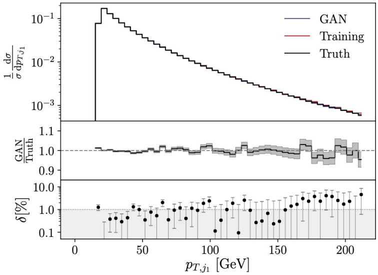


- $t\bar{t} \to 6$ quarks
- 18 dim output
  - external masses fixed
  - no momentum conservation
- + Flat observables ✓
- – Systematic undershoot in tails
  $\to$ improve network (symmetries, preprocessing, ...) ✓



unpublished

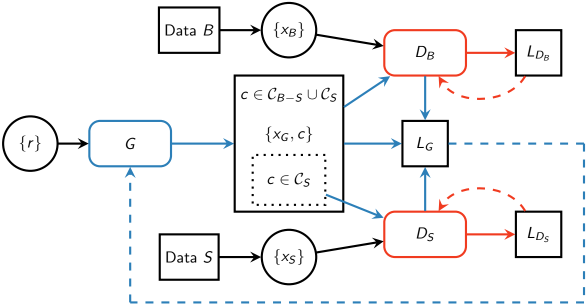
Generating the high-dim. difference of distributions

[1912.08824]

- Necessary to include negative events
- Beat bin-induced uncertainty

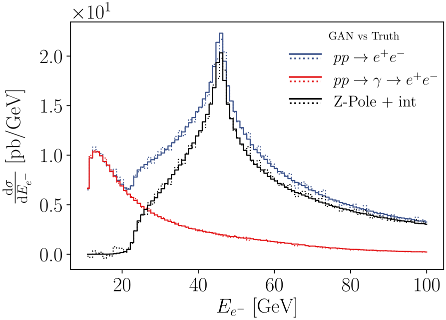
$$\Delta_{B-S} > \max(\Delta_B, \Delta_S)$$

- Applications:
  - Background subtraction, soft-collinear subtraction, ...



Generative background subtraction

- Training data:
  - $pp \to e^+e^-$
  - $pp \to \gamma \to e^+e^-$
- Generated events: Z-Pole + interference



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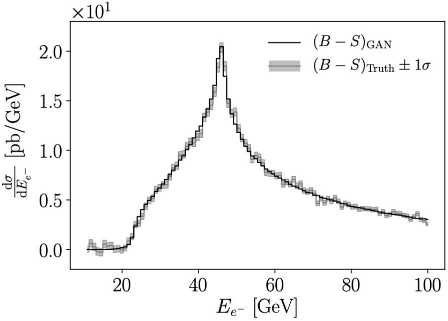
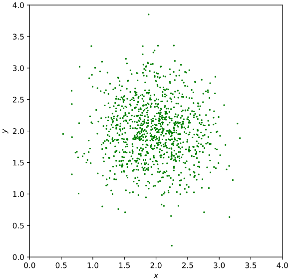
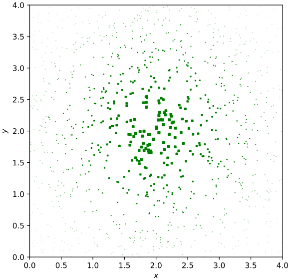


Information in distributions



Information in space distribution
(what we want)

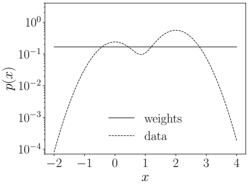
=



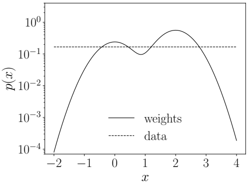
Information in weight
(what we have)

Training on weighted events

Information contained in distribution or event weights



Train on
weighted events



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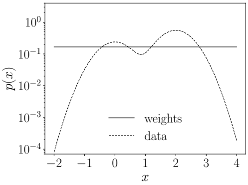
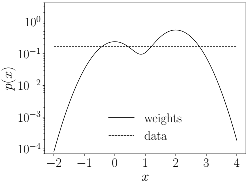
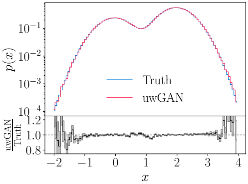
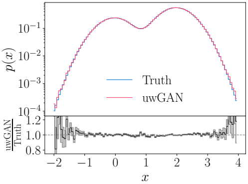




Train on
weighted events

Generate
unweighted events

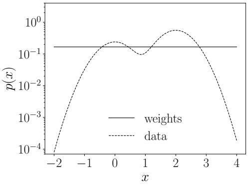


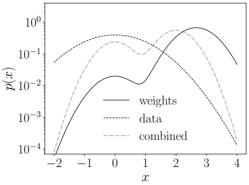


$$L_D = \Big\langle -w \log D(x) \Big\rangle_{x \sim P_{Truth}} + \Big\langle -\log(1 - D(x)) \Big\rangle_{x \sim P_{Gen}}$$

Training on weighted events

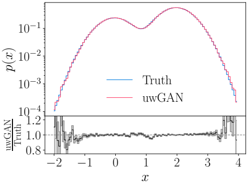
Information contained in distribution or event weights

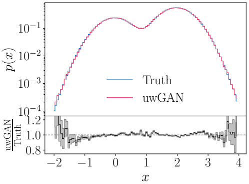




Train on
weighted events

Generate
unweighted events





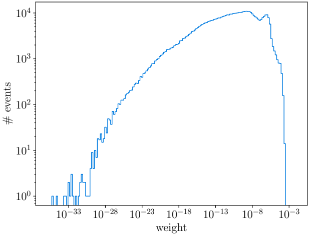
$$L_D = \Big\langle -w \log D(x) \Big\rangle_{x\sim P_{Truth}} + \Big\langle -\log(1-D(x)) \Big\rangle_{x\sim P_{Gen}}$$

The unweighting bottleneck

- High-multiplicity / higher-order $\rightarrow$ large variation of weights
  $\rightarrow$ unweighting efficiencies $< 1\%$

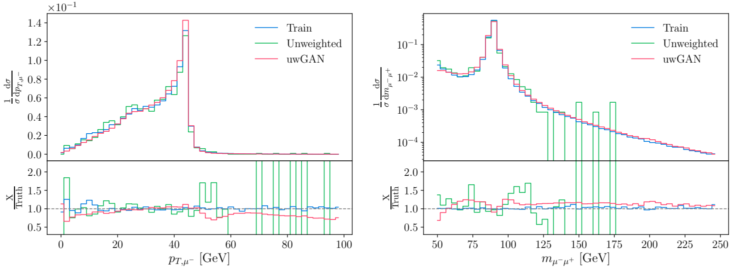
$\rightarrow$ Simulate conditions with naive Monte Carlo generator
ME by `Sherpa`, parton densities from `LHAPDF`, Rambo-on-diet

$pp \rightarrow \mu^+\mu^-$ with $m_{\mu\mu} > 50$ GeV



$\rightarrow$ unweighting efficieny 0.2%

uwGAN results

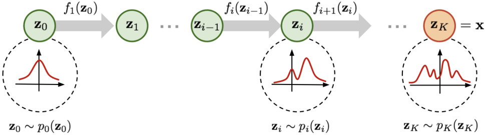


Populates high energy tails

Large amplification wrt. unweighted data!

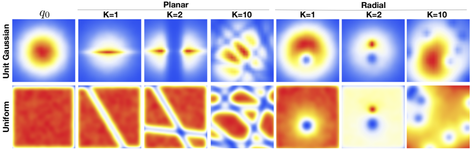
Normalizing flow

Transform input distribution into target distribution via invertible layers

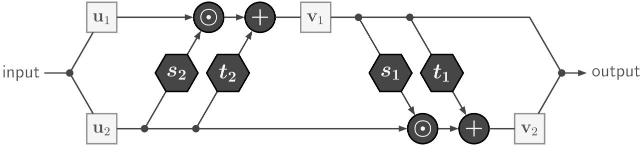


https://lilianweng.github.io/lil-log/2018/10/13/flow-based-deep-generative-models.html

- planar flow: $\boldsymbol{g}(\boldsymbol{x}) = \boldsymbol{x} + \boldsymbol{u}h(\boldsymbol{w}^T\boldsymbol{x} + b)$ [2015 Rezende, Mohamed]



Advanced coupling blocs



Features:
+ invertible
+ efficient evaluation in both directions
+ tractable Jacobian $(J(L_2(L_1)) = J(L_2) \cdot J(L_1))$

+ trainable on samples OR probability

Standard event generation in a nutshell

1. Generate phase space points

2. Calculate event weight

$$w_{event} = \boxed{f(x_1, Q^2) f(x_2, Q^2)} \times \boxed{\mathcal{M}(x_1, x_2, p_1, \ldots p_n)} \times \boxed{J(p_i(r))^{-1}}$$

3. Unweighting
$\rightarrow$ keep events if $w_{event}/w_{max} > r \in [0, 1]$
$\rightarrow$ optimal for $w \approx 1$

Standard event generation in a nutshell

Matrix element

$$w_{event} = \boxed{f(x_1, Q^2)f(x_2, Q^2)} \times \boxed{\mathcal{M}(x_1, x_2, p_1, \ldots p_n)} \times \boxed{J(p_i(r))^{-1}}$$

PDF

Phase space mapping

Find phase space mapping p_i such that $w \approx 1$

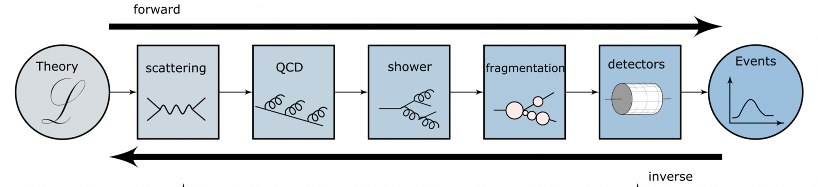
Training on samples

$$\text{events } \boldsymbol{x} \xleftrightarrow[\leftarrow \text{ generating } f^{-1}(\boldsymbol{z})]{\text{training } f(\boldsymbol{x})\rightarrow} \boldsymbol{z} \sim \mathcal{N}$$

How to formulate the loss?
$\rightarrow$ Maximize posterior over network parameters

$$\begin{aligned} L &= -\left\langle \log p(\theta|x) \right\rangle_{x\sim P_x} \\ &= -\left\langle \log p(x|\theta) \right\rangle_{x\sim P_x} - \log p(\theta) + \text{const. (Bayes' theorem)} \\ &= -\left\langle \log p(f(x)) + \log \left| \frac{\partial f(x)}{\partial x} \right| \right\rangle_{x\sim P_x} - \log p(\theta) + \text{const.} \\ &= -\left\langle -f(x)^2 + \log |J| \right\rangle_{x\sim P_x} - \log p(\theta) + \text{const.}\ . \end{aligned}$$

Can we invert the simulation chain?



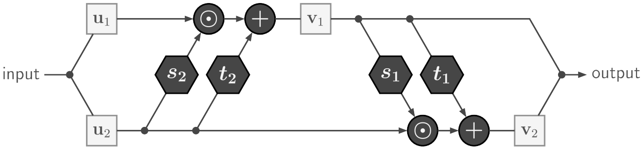
What we
want to know

What we
measure or simulate

wish list: ☐ multi-dimensional
☐ bin independent
☐ statistically well defined

Invertible networks

$$\left(x_{part}\right) \xleftrightarrow[\leftarrow \text{ unfolding:} \bar{g}]{\text{PYTHIA,DELPHES:} g \rightarrow} \left(x_{det}\right)$$



[1808.04730] L. Ardizzone, J. Kruse, S. Wirkert, D. Rahner, E. W. Pellegrini, R. S. Klessen, L. Maier-Hein, C. Rother, U. Köthe

+ Bijective mapping

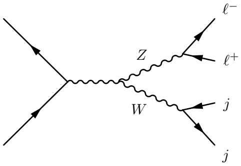
+ Tractable Jacobian

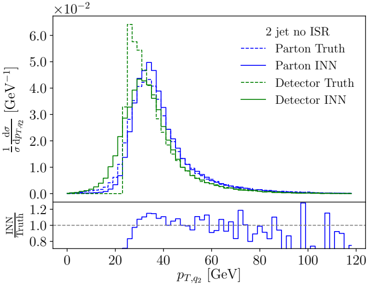
+ Fast evaluation in both directions

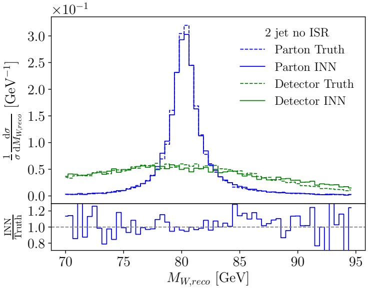
+ Arbitrary networks s and t

Inverting detector effects

- $pp \to ZW \to (ll)(jj)$
- Train: parton $\to$ detector
- Evaluate: parton $\leftarrow$ detector





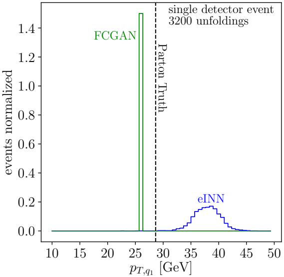


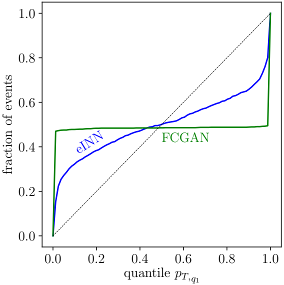
multi-dimensional ✓ bin independent ✓ statistically well defined ?

Including stochastical effects

$$\begin{pmatrix} x_p \\ r_p \end{pmatrix} \xleftrightarrow[\leftarrow \text{ unfolding:}\bar{g}]{\text{PYTHIA,DELPHES:}g\rightarrow} \begin{pmatrix} x_d \\ r_d \end{pmatrix}$$

Sample r_d for fixed detector event
How often is Truth included in distribution quantile?



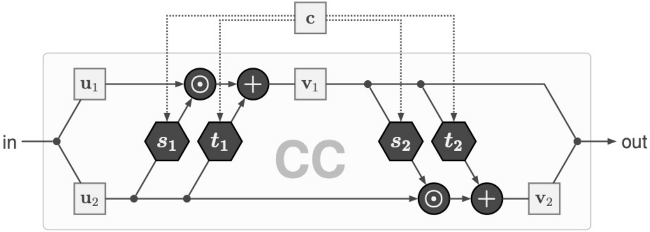


- Problem: arbitrary balance of many loss functions

Taking a different angle

Given an event x_d, what is the probability distribution at parton level?
$\rightarrow$ sample over r, condition on x_d

$$x_p \xleftrightarrow[\leftarrow \text{ unfolding: } \bar{g}(r, f(x_d))]{g(x_p, f(x_d))\rightarrow} r$$



Taking a different angle

Given an event x_d, what is the probability distribution at parton level?
$\rightarrow$ sample over r, condition on x_d

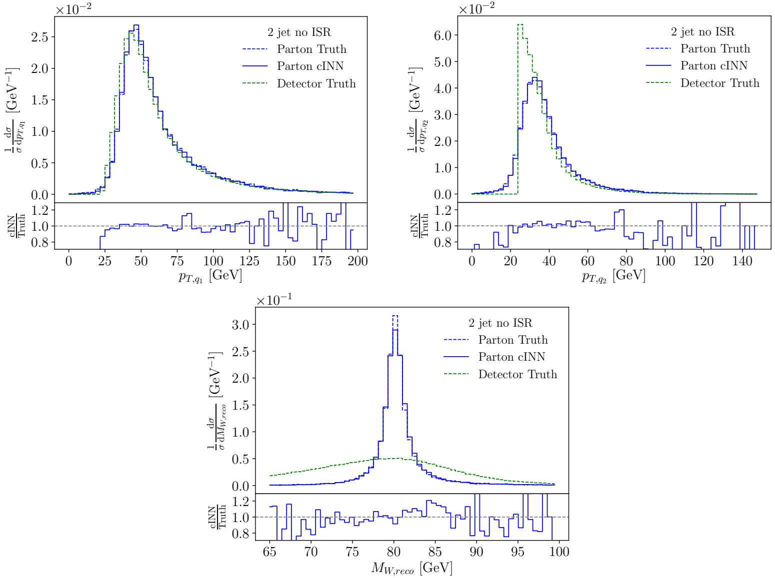
$$x_p \xleftrightarrow[\leftarrow \text{ unfolding: } \bar{g}(r, f(x_d))]{g(x_p, f(x_d)) \rightarrow} r$$

$\rightarrow$ Training: Maximize posterior over model parameters

$$\begin{aligned}
L &= -\left\langle \log p(\theta | x_p, x_d) \right\rangle_{x_p \sim P_p, x_d \sim P_d} \\
&= -\left\langle \log p(x_p | \theta, x_d) \right\rangle_{x_p \sim P_p, x_d \sim P_d} - \log p(\theta) + \text{const.} \quad \leftarrow \text{Bayes} \\
&= -\left\langle \log p(\bar{g}(x_p, x_d)) + \log \left| \frac{\partial \bar{g}(x_p, x_d)}{\partial x_p} \right| \right\rangle - \log p(\theta) \leftarrow \text{change of var} \\
&= \left\langle 0.5 ||\bar{g}(x_p, f(x_d))||_2^2 - \log |J| \right\rangle_{x_p \sim P_p, x_d \sim P_d} - \log p(\theta)
\end{aligned}$$

$\rightarrow$ Jacobian of bijective mapping

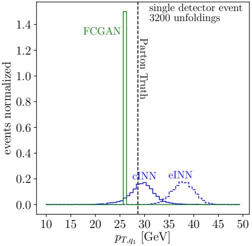
Cross check distributions

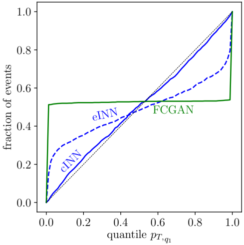


Condition INN on detector data [2006.06685]

$$x_p \underset{\leftarrow \text{ unfolding: } \bar{g}(r, f(x_d))}{\overset{g(x_p, f(x_d)) \rightarrow}{\longleftrightarrow}} r$$

$$\text{Minimizing } L = \left\langle 0.5 ||\bar{g}(x_p, f(x_d))||_2^2 - \log|J| \right\rangle_{x_p \sim P_p, x_d \sim P_d} - \log p(\theta)$$





multi-dimensional ✓ bin independent ✓ statistically well defined ✓

Summary

- Three types of generative models VAE, GAN, NF
- VAE: latent space encoding, KL loss can limit performance
- GAN: based on simple classifier, efficient training if stabilized
- NF: invertible, useable to train directly on probability

Now it's your turn