DijetGAN: A Generative-Adversarial Network approach for the simulation of QCD dijet events at the LHC

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Introduction

Motivations:

- In the next years experiments at the LHC need to cope to a huge increase of data.
- At the same time, the strategy to produce accurate and statistically large samples of simulated *pp* collisions will be facing both technological limitations and new opportunities.

New approach:

- In this context **Machine Learning** techniques are considered.
- A Generative Adversial Network (GAN) is used to simulate the production of particle pairs in *pp* collisions at LHC.
- This approach is applied to dijet events production:
  - In the Standard Model precision measurements and searches for physics beyond the SM is one of most common background source.

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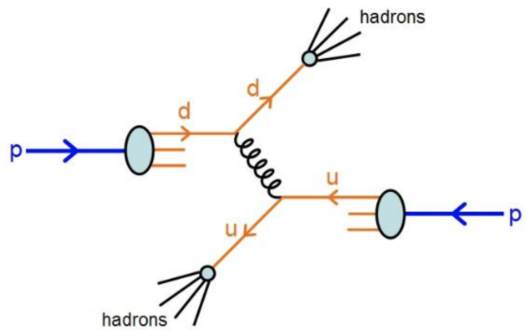
Physics of QCD dijet events

- At the LHC, *pp* collisions result in interaction of quarks and gluons (*partons*).
- Parton scattering processes via strong interaction result in most of the cases in 2 outgoing partons producing parton showers that hadronize into cluster called **jets**.
- $2 \rightarrow 2$ scattering processes with a pair of jets in the final state are called **dijet** events.
- The simulation of these events is performed by **Monte Carlo generators**.



Monte Carlo Simulation @ the LHC

- Both the ATLAS and CMS experiments at the LHC rely on:
  - Event generators such as MadGraph5, Powheg-Box and aMC@NLO to simulate the hard scattering process.
  - Event generators such as Pythia8 and Herwig7 to simulate the parton shower process.
  - Geant4 to simulate the detector response.

Limitations:

- Several minutes to simulate a single event:
  - Huge computational footprint with $O(10^9)$ events, both in terms of CPU usage and disk space.

Current solution:

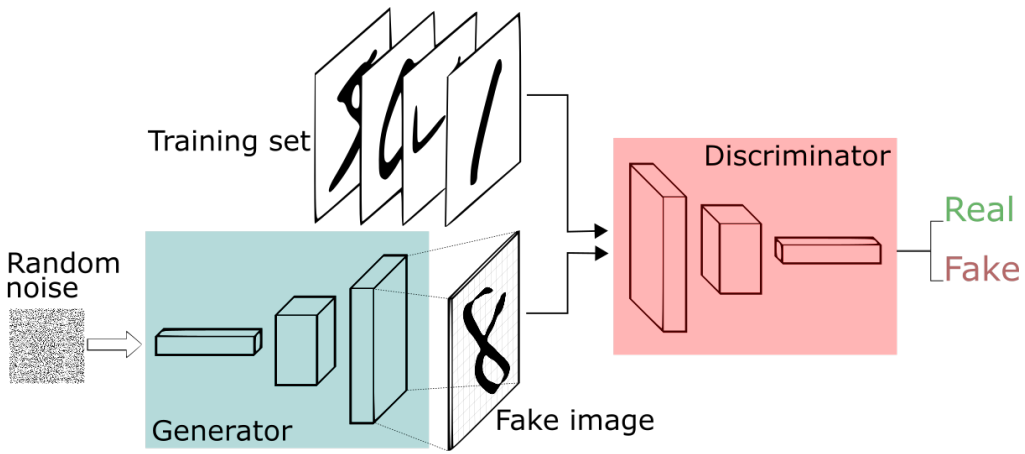
- Experiments rely on simpler but less accurate generators.

Providing a solution to extend the simulated events to the requirements of the LHC experiments will significantly enhance a wide range of measurements.

Generative Adversial Networks (GANs)

GANs are generative models that try to learn to generate an input distribution as realistically as possible.

- A GAN is an unsupervised learning technique and consists of two neural networks:
  - A generative model **Generator** (G) generates new data points from some random uniform distribution.
  - A discriminative model **Discriminator** (D) identifies fake data produced by the Generator from the real data.



Real Monte Carlo training sample

Events generation:

- A sample of 10 million dijet events has been used ($\sim 0.5 fb^{-1}$).
  - Generated using MadGraph5 and Pythia8 samples.

Detector response:

- Delphes3 Fast Simulation with setting that reproduce the ATLAS detector geometry.
- An average of 25 additional soft QCD *pp* collisions were overlaid to reproduce more realistic data-taking conditions.

Object definition and selection

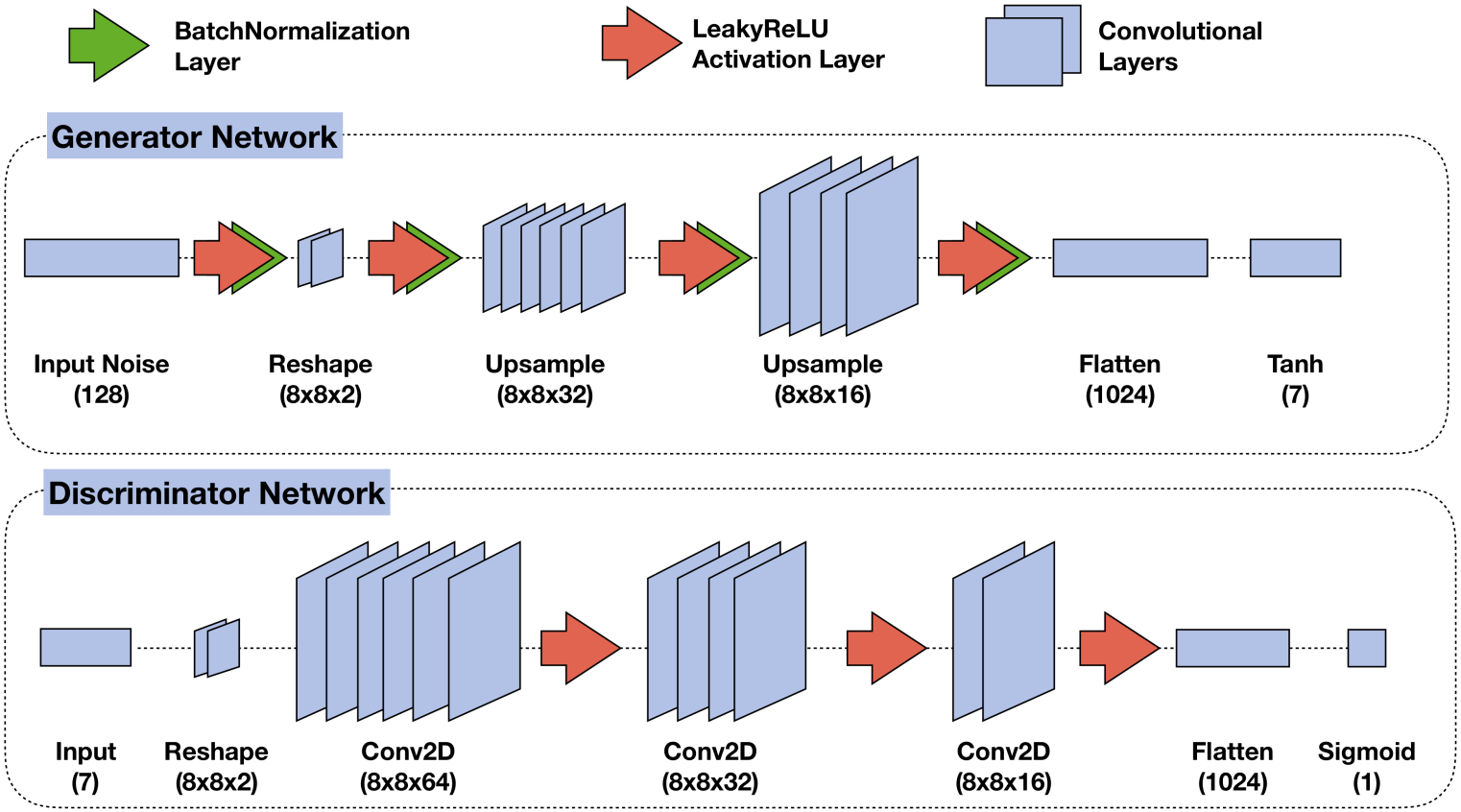
Object Reconstruction:

- Objects (e^-, μ, $E_{\mathrm{T}}^{\mathrm{miss}}$, jets) are reconstructed using DELPHES3 algorithm before and after the detector simulations:
  - Particle and reconstruction levels, respectively.
- Jets were reconstructed using the anti-k_{T} algorithm as implemented in FastJet with a distance parameter R=1.0, $p_{\mathrm{T}} > 250$ GeV.

Selection:

- Applied a cut on the scalar sum of p_{T} of the outgoing partons ($H_T >$ 500 GeV) to increase the number of events with $p_{\mathrm{T}} > 250$ GeV.
- $\sim$ 7.5 million of generated events (particle level) and about 4.5 million after detector simulation (reco level).
- These events were used to train the network.

Network architecture (1/2)



↬ Other architectures tries (fully connected, RNNs). The CNNs yielded best results due to their superior ability to learn complex pattern.

Network architecture (2/2)

- The overall architecture of the network is composed of two main blocks: a Generator (G) and a Discriminator (D), based on convolutional layers.
- All layers have LeakyReLU activation functions except the last layer of both G and D.
  - The last layer of G has a *tanh* activation function.
  - The last layer of D has a *sigmoid* activation function.
- The network is implemented and trained using KERAS v2.2.4 with TENSORFLOW v1.12 back-end.
  - Input features are scaled in the range [-1,1] and pre-processed using SCIKIT-LEARN and PANDAS libraries.

Pre-processing

- Dijet events have a number of intrinsic symmetries.
- Symmetries are hard to learn just by throwing events in the network.

Pre-processing

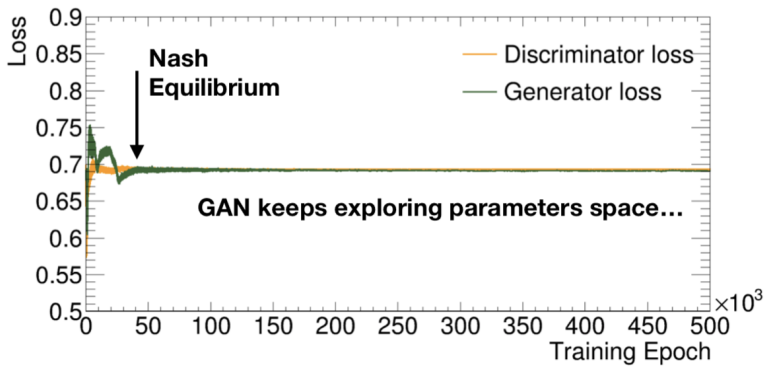
- Achieved significant improvement by using the intrinsic ϕ symmetry of dijet events $\rightarrow$ ϕ of the leading jet set to 0.
- All events were used twice by switching η sign (η-flip).
  - For the event generation η randomly flipped to remove any not physical effects.

$$[(p_{\mathrm{T}}^1,\ \eta^1,\ \phi^1, m^1)] \Rightarrow [(p_{\mathrm{T}}^1,\ \eta^1, m^1)]$$

$$[(p_{\mathrm{T}}^2,\ \eta^2,\ \phi^2, m^2)] \Rightarrow [(p_{\mathrm{T}}^2,\ \eta^2,\ \phi^2, m^2)]$$

Training process

- The **Generator** takes as input random noise:
  - It transforms a vector of 128 random numbers from a uniform distribution in the [0,1] range, into a vector of 7 elements that represent:
    - p_T, η and m of the leading jet
    - p_T, η ϕ and m of the 2nd-leading jet.
- The **Discriminator** is trained with MC events.
- Training is a minmax game.
  - Stabilization of the loss function.
  - No natural way to choose the best epoch.
    - Take the one with the lowest χ^2.



- 100K epochs with mini-batches of 32 events each.
- 100K epochs/1 hour on a GPU NVIDIA Quadro P6000.

Network parameters optimization

- Several parameters of the model have been optimised.
- Once satisfactory performances have been reached, no further parameter optimisation was carried on.

Loss Function settings:

- Generator $\rightarrow$ Mean squared error.
- Discriminator $\rightarrow$ Binary cross-entropy.

Optimizer setting:

- for both Discriminator and Generator the optimizer is *Adam* with learning rate lr $= 10^{-5}$, $\beta_1 = 0.5$ and $\beta_2 = 0.9$

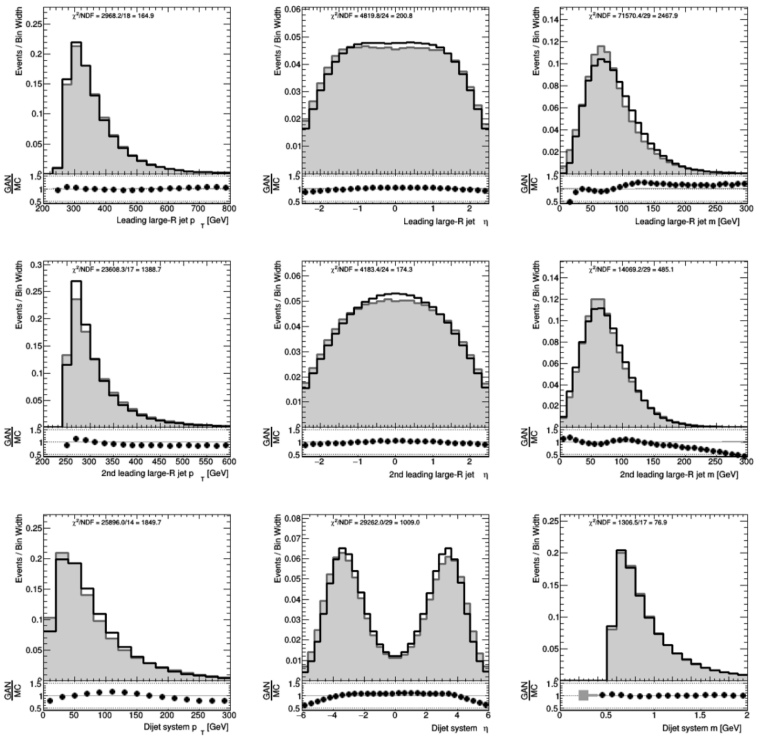
These parameters gave the best results among many values and configuration tested.

Event Generation

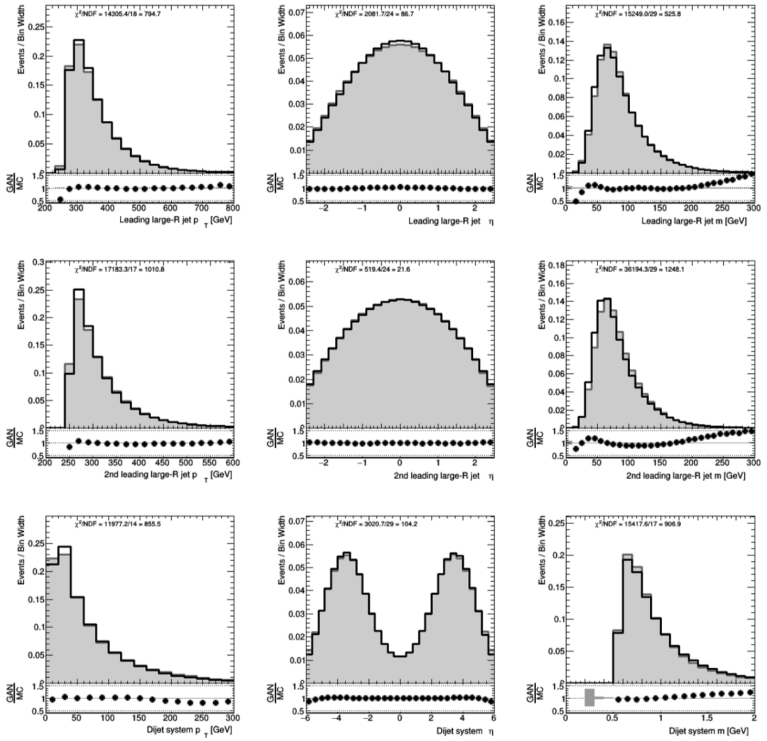
- Weights of generator model are saved during the training every 5000 epochs and used to generate events.
  - $\sim$ 80 s to generate 1 million events.
  - Events are filtered by applying the same cut that are applied to the real dataset:
    - both jets with $p_T > 250$ GeV.
- These events are used to fill the histograms.
- The comparison between the GAN output and the MC production is done for the following kinematic variables:
  - Leading large R-jet p_T, η, m
  - Sub Leading large R-jet p_T, η, m
  - Dijet system p_T, η, m

Results

Reco Level

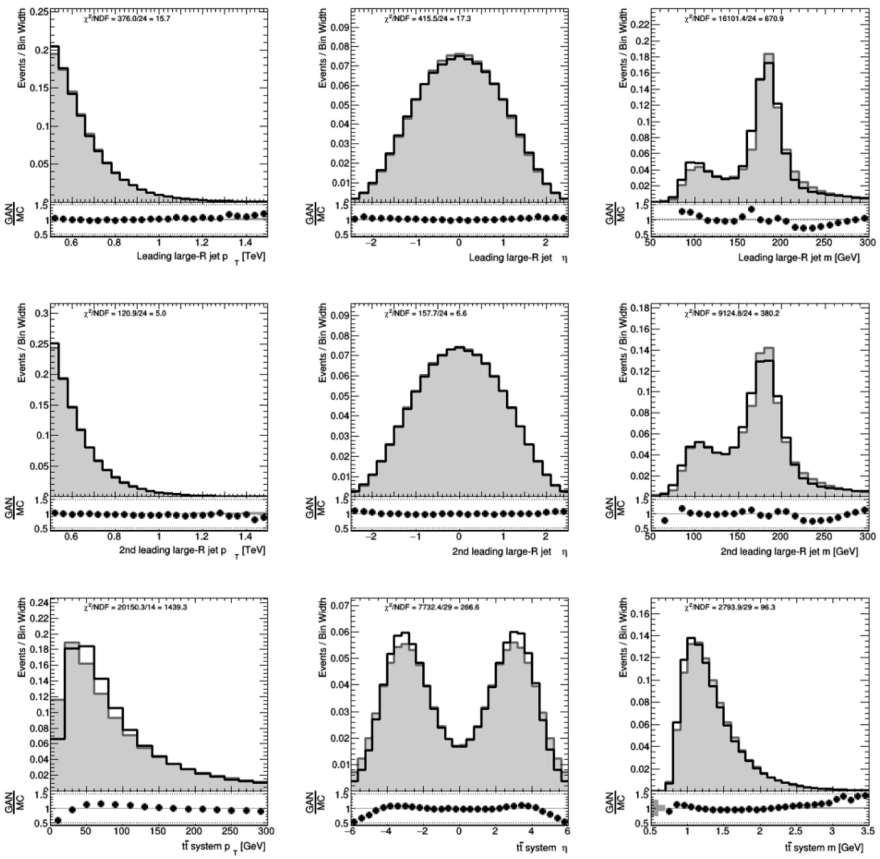


Particle Level

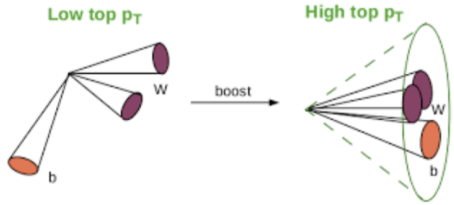


- Comparison of leading jets and dijet system kinematis as they appear at the iteration that yields the best agreement in terms of overall χ^2.
- Satisfactory level of agreement over a large range of kinematic regimes.

Results - Boosted top quarks



↬ **The GAN can learn these physics processes!**



↬ Trained GAN on a sample of top quark pairs decaying in the all hadronic channel ($t\bar{t} \rightarrow WbW\bar{b} \rightarrow bq\bar{q}'\bar{b}q\bar{q}'$)

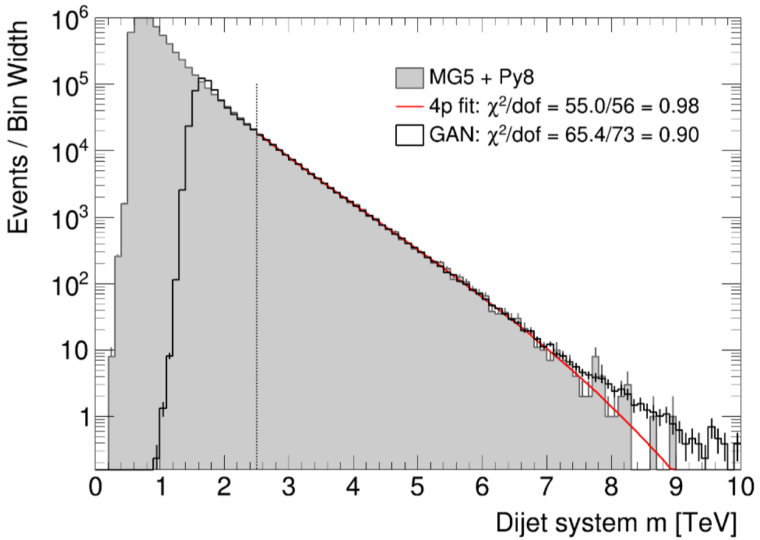
↬ Both jets at particle level are required to have $p_T > 350$ GeV and $m < 500$ GeV.

↬ In this phase space region the jet mass is expected to have a peak around the top mass ~ 173 GeV in the MC simulation (fully boosted).

↬ When b-quarks are produced at an angle where only W bosons are found, a second peak is expected around the W boson mass ~ 80 GeV (semi-boosted).

Results - Extrapolation

- Performed further investigations in regions of the phase spaces with low cross-section $\rightarrow$ kinematic region of particularly interest for searches of physics BSM.
- Fit the MC with this 4p analytic function: $f(x) = \frac{p_0(1-x)^{p_1}}{x^{(p2+p3 log x)}}$, $x = m_{jj}/\sqrt{s}$
- Trained GAN with $\sim$ 150K events with $m_{jj} > 1.5$ TeV. Then used the trained model to generate 1 million events (sample » of MC).



- The fit in the region between 2.5 and 10 TeV can predict the shape of the MC distribution with a $\chi^2/\text{NDF} = 0.98$.
- The sample generated with the GAN shows a comparable agreement.

Conclusions

- Increasing of Machine Learning application in HEP.
- A Generative Adversial Network approach for the simulation of QCD dijet events at the LHC has been presented.
  - Novel attractive solution to reduce CPU usage and disk space to generate and simulate events.
  - Very promising approach that will allow to improve the quality of MC production at the LHC.
- Results show that the GAN can reproduced simulated events with very high accuracy.
- It is important to exploit intrinsic symmetries to make the model learn better.
- GANs is not a minimisation problem, picking up the best epoch is not trivial (lowest χ^2).
- Generic method $\rightarrow$ possible extension and application to other processes.

Thanks for your attention!

BACKUP

GANs functions (1/2)

Generator

z $\rightarrow$ Noise vector

G(z) $\rightarrow$ Generator's output for x_{fake}

Discriminator

x $\rightarrow$ training sample

D(x) $\rightarrow$ Generator's output for x_{real}

D(G(z)) $\rightarrow$ Discriminator's output for x_{fake}

Generator G	Discriminator D
D(G(z)) $\rightarrow$ should be maximized	D(x) $\rightarrow$ should be maximized D(G(z)) $\rightarrow$ should be minimized

Loss functions

G_{loss} = log(1-D(G(z)) or -log(D(G(z))

$D_{loss_{real}}$ = log(D(x))

$D_{loss_{fake}}$ = log(1-D(G(z))

D_{loss} = $D_{loss_{real}}$ + $D_{loss_{fake}}$ = log(D(x)) + log(1-D(G(z))

GANs functions (2/2)

- Discriminator and Generator play a two player min-max game.

$$\begin{aligned}\min_G \max_D L(G,D) &= \mathbb{E}_{x\sim p_{data}(x)}\left[\log D(x)\right] + \mathbb{E}_{z\sim p_z(z)}\left[\log\left(1-D(G(z))\right)\right] \\ &= \mathbb{E}_{x\sim p_{data}(x)}\left[\log D(x)\right] + \mathbb{E}_{x\sim p_{fake}}(x)\left[\log\left(1-D(x)\right)\right]\end{aligned}$$

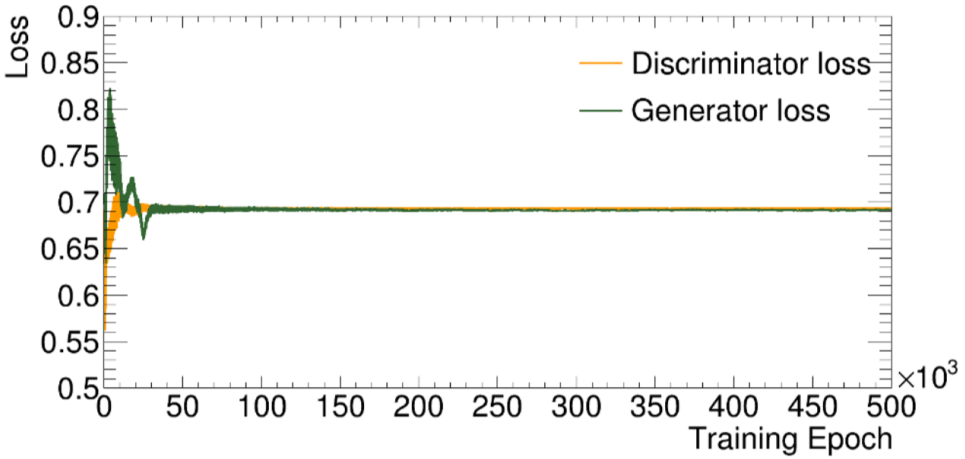
- $x \sim p_{data}$ probability density function of trainig sample generated using MC method.
- $z \sim p_{fake}$ probability density function of input noise.
- The Nash equilibrium (min-max game) is reached when D is unable to distinguish fake examples from real data.
  - Hence the generator has been trained to be a good approximator of the data pdf, i.e. $p_{fake} \sim p_{data}$.

Training GANs process

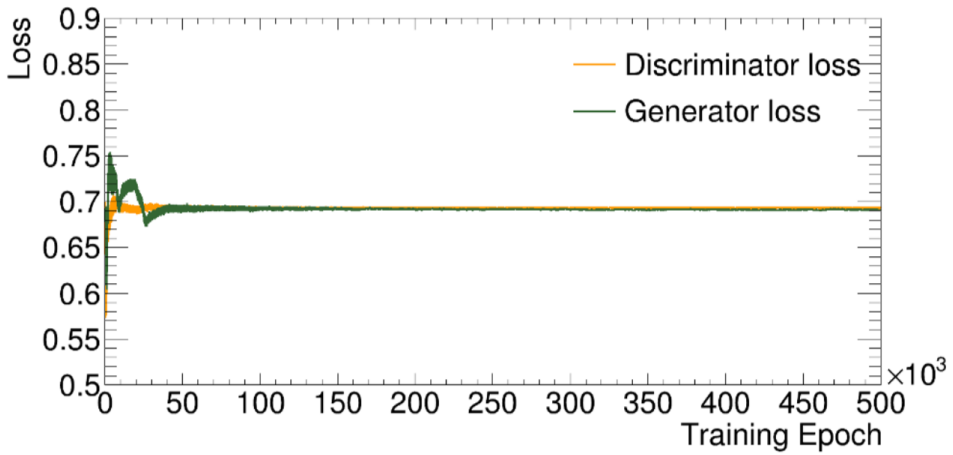
Training steps:

- The main idea is to train 2 different networks to compete with each other with two different objectives:
  1. The Generator G tries to fool the discriminator D into believing that the input sent by G is real.
  2. The Discriminator D identifies that the input is fake
  3. Then, the Generator G learns to produce similar type of training data inputs.
  4. This process, called **Adversial Training**, is repeated for a while or until Nash equilibrium is found.

Loss functions



↬ Reco Level



↬ Particle Level

↬ The stationary state between generator and discriminator (Nash equilibrium) is reached after few thousands epochs.