# DijetGAN: A Generative-Adversarial Network Approach for the Simulation of QCD Dijet Events at the LHC

# Riccardo Di Sipio, Michele Faucci Giannelli, Sana Ketabchi Haghighat, <u>Serena Palazzo</u>

3rd Machine Learning Workshop

April 15-18, 2019





#### Introduction

## **Motivations:**

- G→ In the next years experiments at the LHC need to cope to a substantial 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:

- <sup>9→</sup> In this context **Machine Learning** techniques are considered.
- $\hookrightarrow$  A Generative Adversial Network (GAN) is used to simulate the production of particle pairs in *pp* collisions at LHC.
- $\hookrightarrow$  This approach is applied to dijet events production:
  - In the SM precision measurements and searches for physics beyond the SM is one of most common background source.

Paper draft on arXiv and submitted to JHEP: • arXiv 1903.02433

#### Monte Carlo Simulation @ the LHC

 $\hookrightarrow$  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.
- PYTHIA8 and HERWIG7 to simulate the parton shower process.
- GEANT4 to simulate the detector response.

## Limitations:

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

## **Current solution:**

 $\hookrightarrow$  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.

- ↔ At the LHC, pp collisions result in interaction of quarks and gluons referred to as partons.
- ↔ Parton scattering processes via strong interaction result in most of the cases in two outgoing partons producing parton showers that hadronize into cluster called jets.
- ↔ Parton scattering processes with a pair of jets in the final state are called **dijet** events.



#### **Events generation:**

- $\hookrightarrow$  A sample of 2 milion dijet events has been used.
  - Generated using MADGRAPH5 and PYTHIA8 samples.

#### **Detector response:**

- ⊕ DELPHES3 Fast Simulation with setting that reproduce the ATLAS detector geometry.
- $\hookrightarrow$  An average of 25 additional soft QCD *pp* collisions were overlaid to reproduce more realistic data-taking conditions.

#### **Object Reconstruction:**

- $\hookrightarrow$  Objects ( $e^-$ ,  $\mu$ ,  $E_T^{miss}$ , jets) are reconstructed using DELPHES3 algorithm before and after the detector simulations:
  - Particle and reconstruction levels, respectively.
- $\hookrightarrow$  Jets were reconstructed using the anti- $k_T$  algorithm as implemented n FastJet with a distance parameter R=1.0.

#### Selection:

- ↔ Applied a cut on the scalar sum of  $p_T$  of the outgoing partons (H<sub>T</sub> > 500 GeV) to increase the number of events with  $p_T$  > 250 GeV.
- $\hookrightarrow \sim$  1.5 million of events passed this selection at particle level and about 800,000 at reco level.
- $\hookrightarrow$  These events were used to train the network.

GANs are generative models that try to learn the model to generate the 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 Generator from the real data.



- ↔ The overall architecture of the network is composed of two main blocks: a Generator (G) and a Discriminator (D), based on convolutional layers.
- $\hookrightarrow$  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 Keras with TENSORFLOW v1.12 back-end <sup>\*</sup>.
  - Input features are scaled in the range [-1,1] and pre-processed using SCIKIT-LEARN libraries.

## Network architecture (2/2)



- $\hookrightarrow$  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*<sub>T</sub>, η and *m* of the leading jet
    - $p_T$ ,  $\eta \phi$  and m of the 2nd-leading jet.
- $\hookrightarrow$  The **Discriminator** is trained with MC events.
- $\hookrightarrow$  Achieved significant improvement by using the intrinsic  $\phi$  symmetry of dijet events  $\rightarrow \phi$  of the leading jet set to 0.
- $\hookrightarrow$  All events were used twice by switching  $\eta$  sign ( $\eta$ -flip).
  - For the event generation η randomly flipped to remove any not physical effects.
- $\rightarrow$  100K iterations with mini-batches of 32 events each.
- $\hookrightarrow$  1 hour to complete the training on a GPU NVIDIA Quadro P6000.

- G→ Once satisfactory performances have been reached, no further parameter optimisation was carried on.

## Loss Function settings:

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

## **Optimizer setting:**

 $\hookrightarrow$  for both Discriminator and Generator the optimizer is *Adam* with learning rate Ir = 10<sup>-5</sup>,  $\beta_1 = 0.5$  and  $\beta_2 = 0.9$ 

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

#### Loss functions



- ↔ The stationary state between generator and discriminator (Nash equilibrium) is reached after few thousands epochs.
- $\rightarrow$  This is true for both particle and reco levels.

#### **Discriminator accuracy**



- ↔ Weights of generator model are saved during the training every 5000 epochs and used to generate events.
  - $\bullet~\sim$  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.
- $\hookrightarrow$  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  $p_T$ ,  $\eta$ , m
  - Sub Leading large R-jet  $p_T$ ,  $\eta$ , m
  - Dijet system  $p_T$ ,  $\eta$ , m

## Results



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

- $\hookrightarrow$  Performed further investigations in regions of the phase spaces with low cross-section  $\rightarrow$  kinematic region of particularly interest for searches of physics BSM.
- $\hookrightarrow$  Fit the MC with this 4p analytic function:  $f(x) = \frac{p_0(1-x)^{p_1}}{x^{(p^2+p_3)ogx}}$ ,  $x = m_{jj}/\sqrt{s}$
- $\hookrightarrow$  Trained GAN with ~ 40K events with  $m_{jj} > 1.5$  TeV. Then used the trained model to generate 10 million events (sample » of MC).



- $\hookrightarrow$  The fit in the region between 3 and 10 TeV can predict the shape of the MC distribution with a  $\chi^2/\text{NDF} = 1.04$ .
- $\hookrightarrow$  The sample generated with the GAN shows an agreement of  $\chi^2/\text{NDF}=$  1.29.

## Further investigations (2/2)



- 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 (172.5 GeV) in the MC simulation.
- When *b*-quarks are produced at an angle where only *W* bosons are found, a second peak is expected around *W* boson mass ( $\sim$  80 GeV).

 $\hookrightarrow$  The figure shows that the GAN can learn these physics processes.

- A Generative Adversial Network approach for the simulation of QCD dijet events at the LHC has been presented.
- ↔ This novel approach is an 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.
- $\hookrightarrow$  Results show that the GAN can reproduced simulated events with very high accuracy.

BACKUP

#### Backup

# GANs functions (1/2)

#### Generator

 $z \to \mathsf{Noise} \; \mathsf{vector}$ 

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

## Discriminator

 $\begin{array}{l} x \rightarrow \text{training sample} \\ D(x) \rightarrow \text{Generator's output for } x_{real} \\ D(G(z)) \rightarrow \text{Discriminator's output} \\ \text{for } x_{fake} \end{array}$ 

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

## Loss functions

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

$$\begin{array}{l} D_{loss_{real}} = \log(\mathsf{D}(\mathsf{x})) \\ D_{loss_{fake}} = \log(1\text{-}\mathsf{D}(\mathsf{G}(\mathsf{z})) \\ D_{loss} = D_{loss_{real}} + D_{loss_{fake}} = \\ \log(\mathsf{D}(\mathsf{x})) + \log(1\text{-}\mathsf{D}(\mathsf{G}(\mathsf{z})) \end{array}$$

## **GANs** functions (2/2)

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

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

- $\hookrightarrow x \sim p_{data}$  probability density function of trainig sample generated using MC method.
- $\rightarrow z \sim p_{fake}$  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<sub>fake</sub> ~ p<sub>data</sub>.

#### Training GANs process

#### Training steps:

- $\hookrightarrow$  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.