INSTITUTE FOR COLLIDER PARTICLE PHYSICS
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An Alternative to Monte Carlo Generators via Deep Generative Models

Replacing a standard Monte Carlo simulation.

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ATLAS EXPERIMENT

Overview

- Brief History
- Introduction
- GANs
- GANs architecture
- GAN applications in HEP
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- Results
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Brief History

- A branch of Deep Learning: first attempts in 1940s
- Pioneered by Ian Goodfellow. et al. in 2014
- Rapidly adopted
  - Goodfellow: @Google - 2015, @OpenAI - 2016, @Apple - 2019
  - Some applications
    - produce anime characters, convert scripts into animations, image character arithmetic, text-to-image synthesis, image-to-image translation, etc.

TITLE	CITED BY	YEAR
Generative adversarial nets I Goodfellow, J Pouget-Abadie, M Mirza, B Xu, D Warde-Farley, S Ozair, ... Advances in neural information processing systems, 2672-2680	11650	2014

Introduction

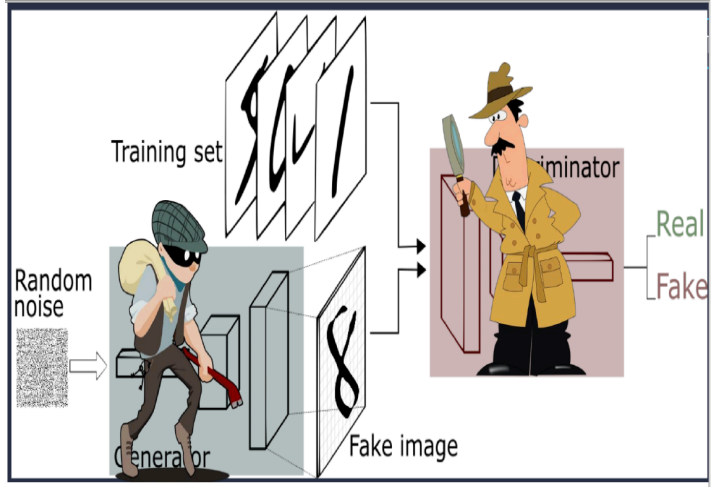
- Two kinds of machine learning models:
  - generative and discriminative models
- The fundamental difference between two models lies in the underlying probability inference structure,
  - discriminative models learn P(Y|X): the conditional relationship between the target variable Y and features X (limitations: Can't model P(X); thus, cannot sample from P(X))
  - generative models aim for a complete probabilistic description of the dataset. Their goal is to develop the joint probability distribution P(X, Y), either directly or by computing P(Y | X) and P(X) and then inferring the conditional probabilities required
  - to classify newer data. Can model P(X), thus can generate new images, solve the curse of dimensionality, etc.

- Some types of Generative models:
  - Auto-Encoder (**AE**) = non-linear PCA
    - vanilla Feed Forward AE
    - convolutional AE
    - variation AE (Break through Research, uses the concept of Reconstruction)
    - Probability & Directed Probabilistic Graphical Model (DPGM)
  - sequence models
  - Generative Adversarial Networks (**GANs**)
    - Vanilla GAN
    - Wasserstein-GAN (wGAN), Conditional GAN (cGAN), CycleGAN, etc.

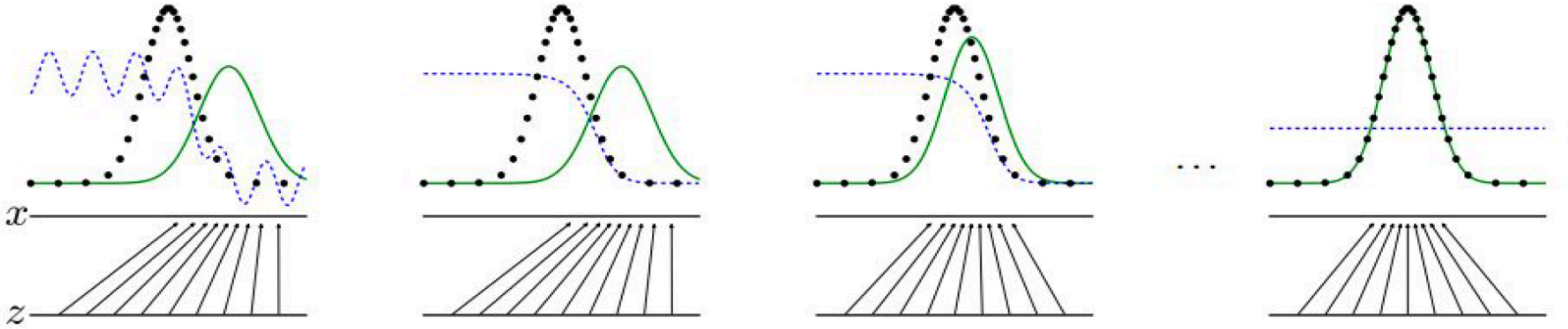
“Generative Adversarial Networks is the most interesting idea in the last 10 years in Machine Learning”

Yann LeCun, VP & Chief AI Scientist at Facebook & Professor at NYU (2016)

Generative Adversarial Nets (GANs)



- Idea: pit two deep subnets against each other
  - creating an adversarial "game" between Generator (G) & Discriminator (D)
  - G: generates fake samples from noise, tries to fool the D
  - D: tries to distinguish between real and fake samples
  - G & D train against each other repeatedly until we get a better Generator and Discriminator, i.e. until there's some type of a Nash equilibrium (which may not happen)
- GANs use a minimax structure that uses the **loss function** constructed to minimize the **Jensen-Shannon divergence** between the distribution of the real data and the distribution of the generated data



(GAN) Architecture

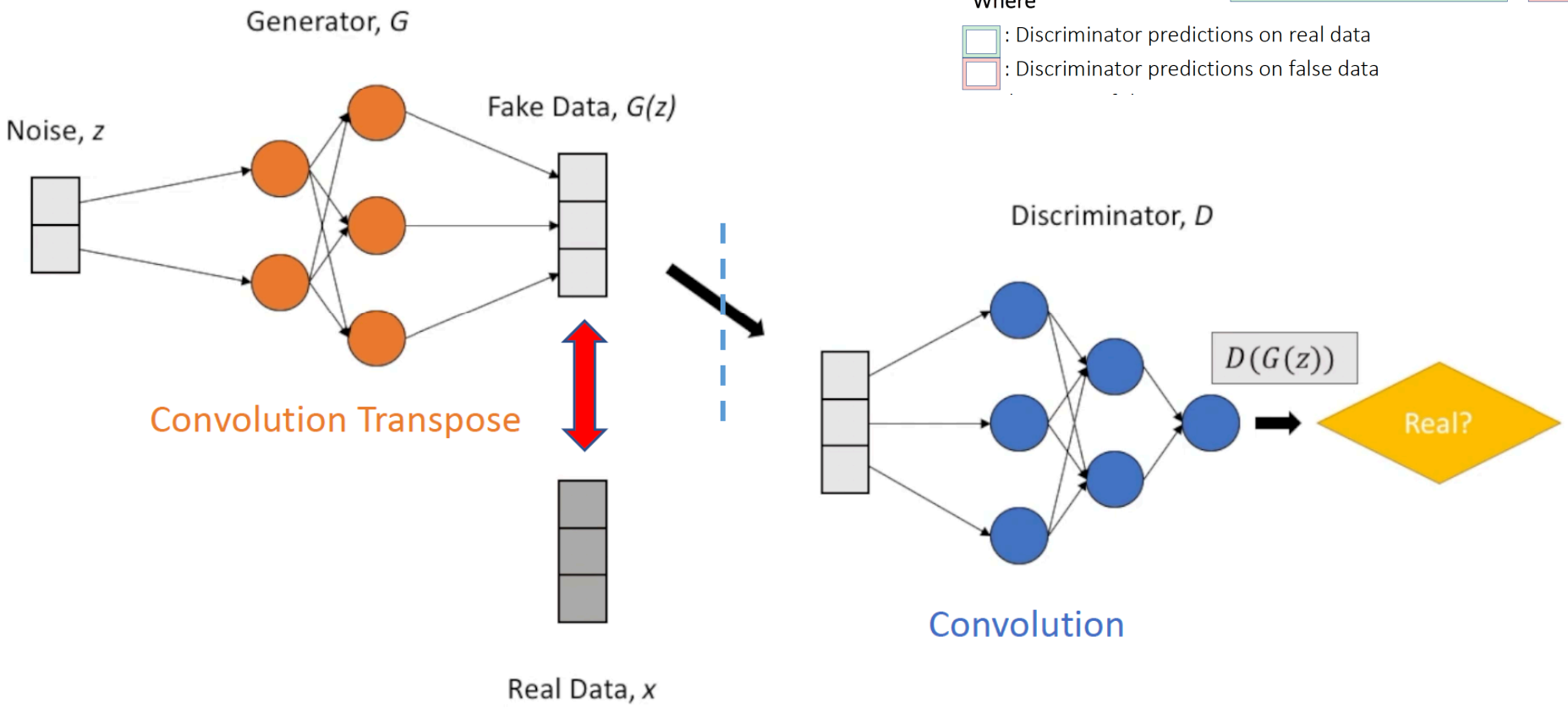
loss function

$$\min_{G}\max_{D} V(D,G) = \mathbb{E}_{x\sim p_{data}(x)}[logD(x)] + \mathbb{E}_{z\sim p_z(z)}\left[\log\left(1-D\left(G(z)\right)\right)\right]$$

Where

: Discriminator predictions on real data

: Discriminator predictions on false data



noise (z) is an input into the Generator network (G) that outputs Fake data G(z) as input into the Discriminator network (D), then D outputs D(G(z)) that can be classified as Real = 1 or Fake = 0. Fine tune G and D weights during non-supervised training

GANs in HEP

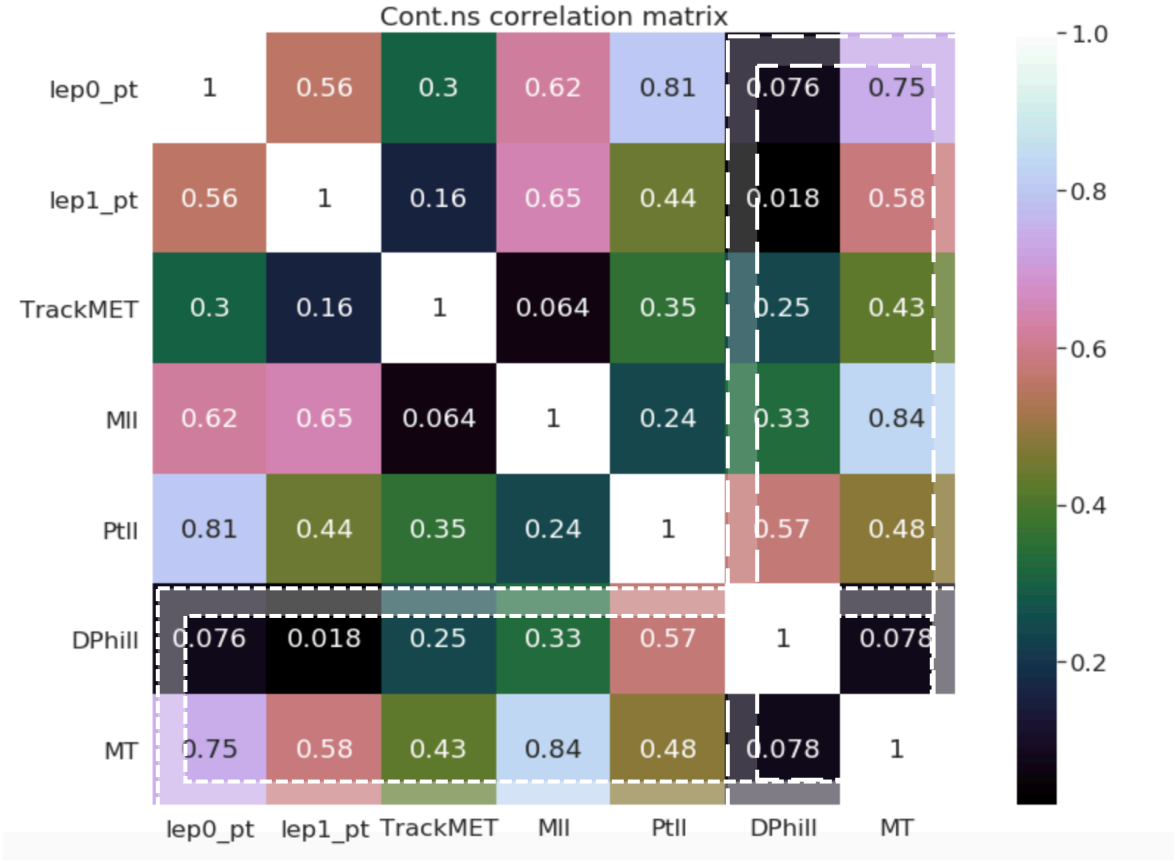
- Generative models can be viewed as:
  - a regression tasks that maps noise to structure, i.e. mimicking the Jacobian from a pre-defined distribution to target probability distribution
- shown great promise for accelerating simulations at the LHC
- useful for tasks such as sampling from the space of effective field theory models
- why GANs?
  - they can readily model asymmetric distributions and accommodate conditional features
  - they can be generic, accurate, fast and robust

Modeling

Features & preprocessing

Zero tail cut

```
lep0_pt : min: 27.000242 | max: 1736.1593
lep1_pt : min: 10.0000925 | max: 735.9781
TrackMET : min: 0.021143772 | max: 1328.2954
Mll : min: 10.001374 | max: 2178.0117
Ptll : min: 0.07439626 | max: 1728.6128
MT : min: 11.264636 | max: 2414.1794
```



5% tail cut

no of features: 6
applied cut: low = 0; high = 0.95
pretraining size: 424872K
training size: 800K
nb_epoch: 500K
CPU training duration: 7:15:53.97864

```
lep0_pt : min: 27.000242 | max: 159.03975
lep1_pt : min: 10.0000925 | max: 83.594124
TrackMET : min: 0.021143772 | max: 126.6691
Mll : min: 10.001374 | max: 257.86337
Ptll : min: 0.07439626 | max: 150.43474
MT : min: 11.264636 | max: 348.14563
```

Insights

- too much information loss
- evidence for possible convergence

Further modeling

no of features: 6
applied cuts: low = 0; high = 0.995
pretraining size: 424872K
training size: 800K
nb_epoch: 800K
CPU training duration: 09:26:54.29129

0.5% tail cut

```
lep0_pt : min: 27.000242 | max: 1736.1593
lep1_pt : min: 10.0000925 | max: 735.9781
TrackMET : min: 0.021143772 | max: 1328.2954
Mll : min: 10.001374 | max: 2178.0117
Ptll : min: 0.07439626 | max: 1728.6128
MT : min: 11.264636 | max: 2414.1794
```

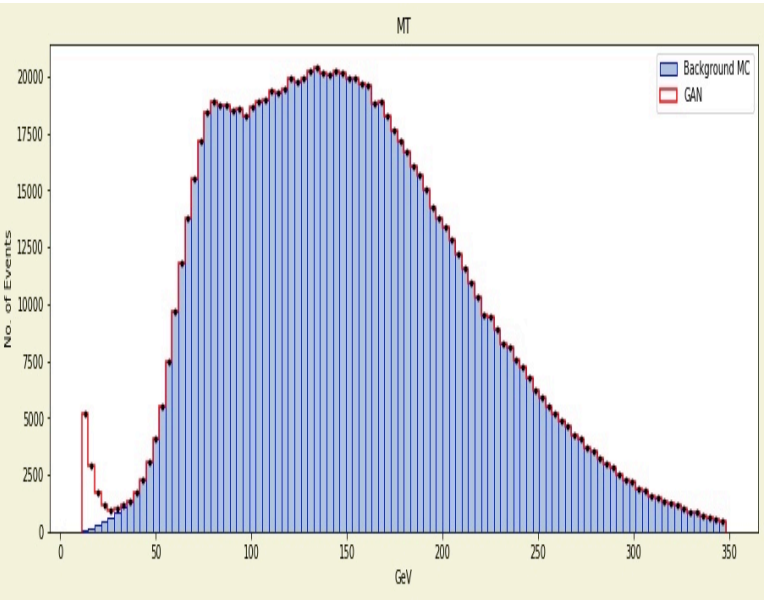
```
lep0_pt : min: 27.000242 | max: 283.32004
lep1_pt : min: 10.0000925 | max: 151.20517
TrackMET : min: 0.06590886 | max: 225.81873
Mll : min: 10.001374 | max: 477.63333
Ptll : min: 0.07439626 | max: 275.12195
MT : min: 11.264636 | max: 590.2197
```

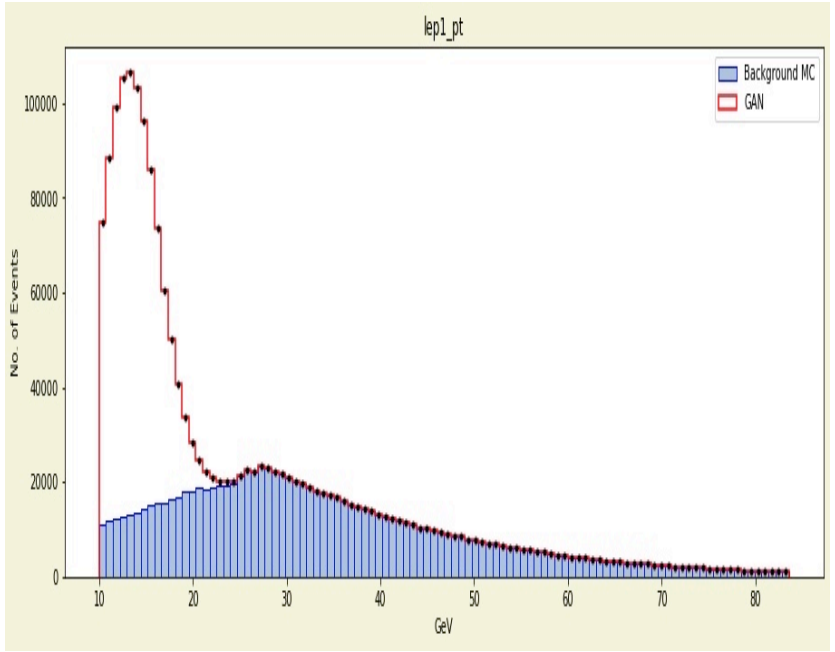
Models	No. Epochs	Time	Can Discriminate
Multilayer Perceptron (MLP)	1M	2:16:01.694724	False
Recurrent Neural Network (RNN)	150K	6:56:18.648813	False
Convolutional Neural Network (CNN)	500K	4:49:37.166094	True

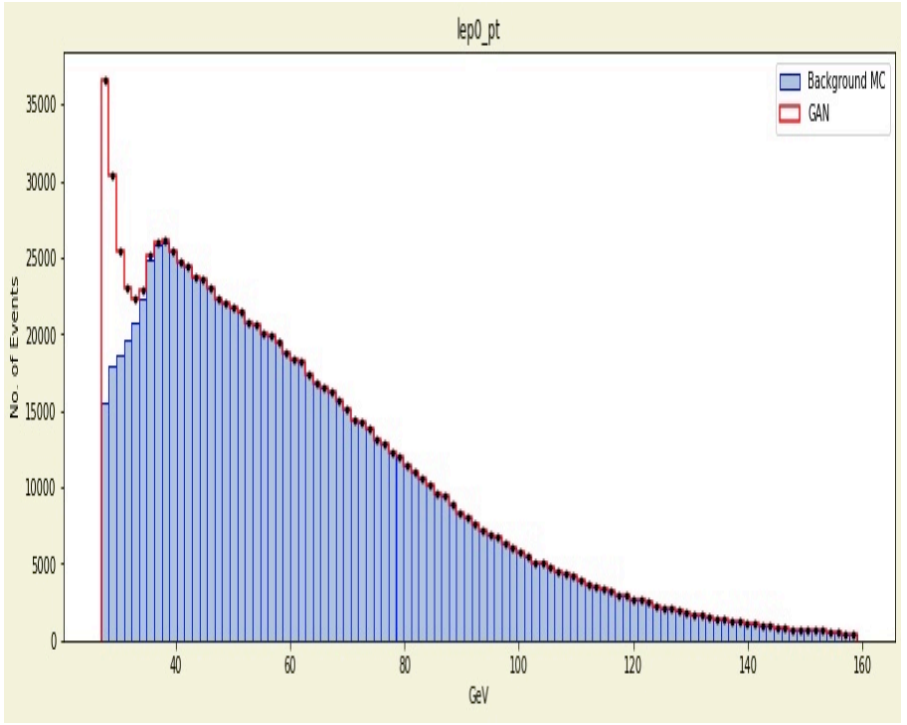
other architectures tried: fully connected, **RNNs**, **MLP** but **CNNs** yielded better performance and results, thanks to their superior ability to “learn" complex patterns.

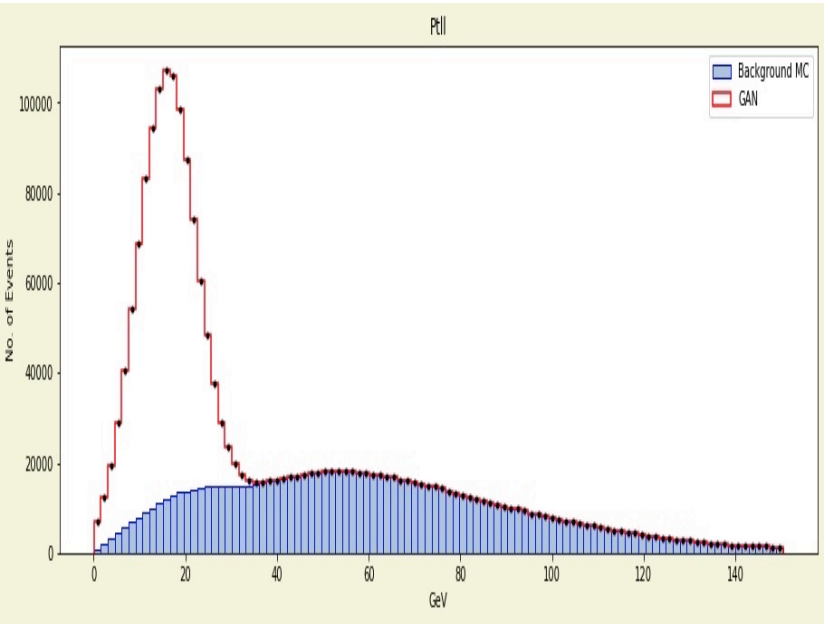
GAN Performance w/ 5% tail cuts

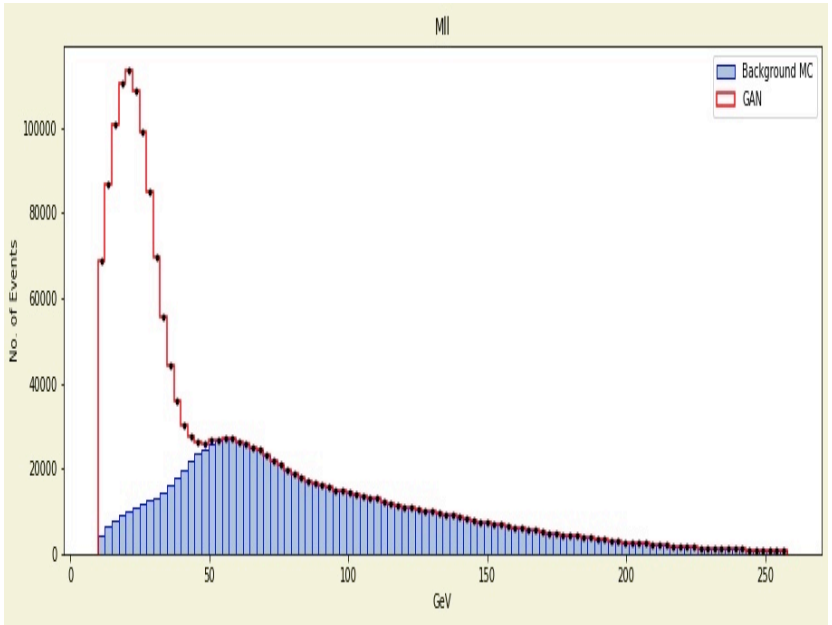
ATLAS Simulation Work in Progress

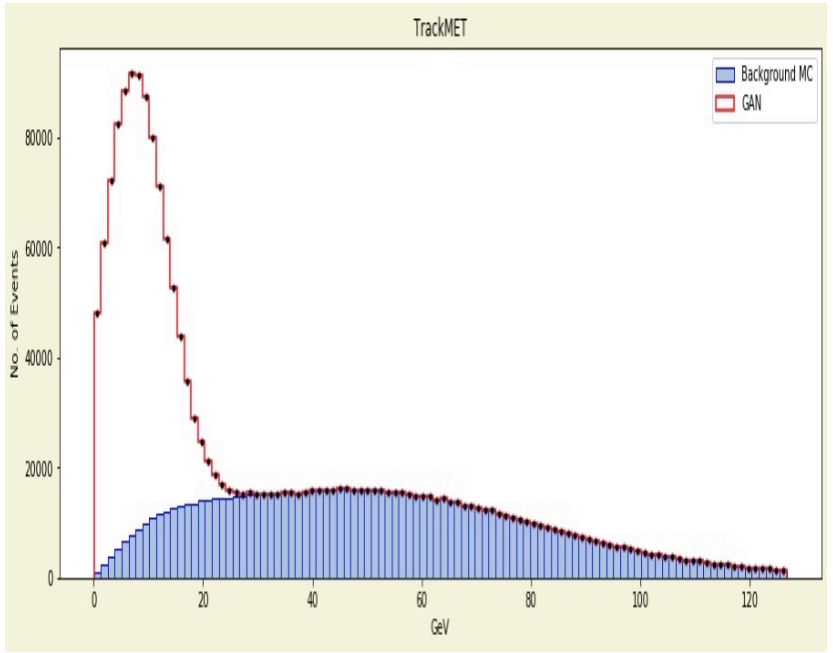






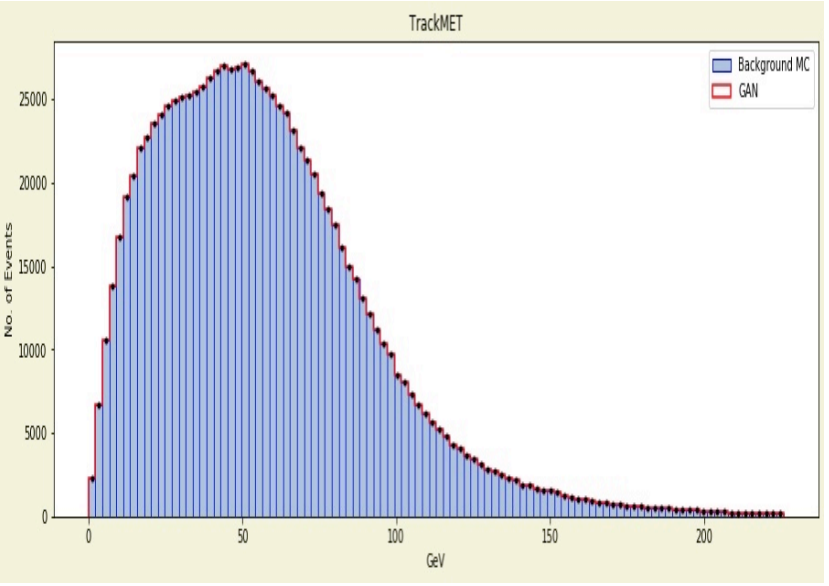


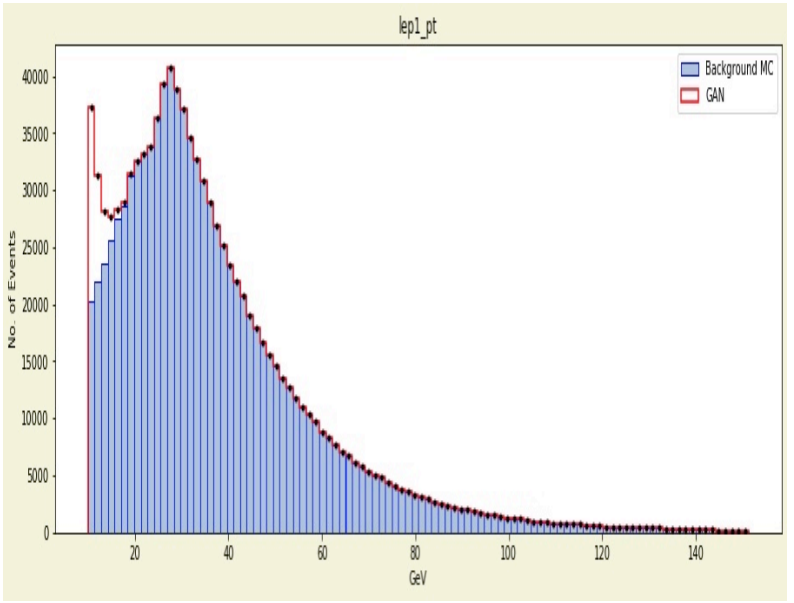


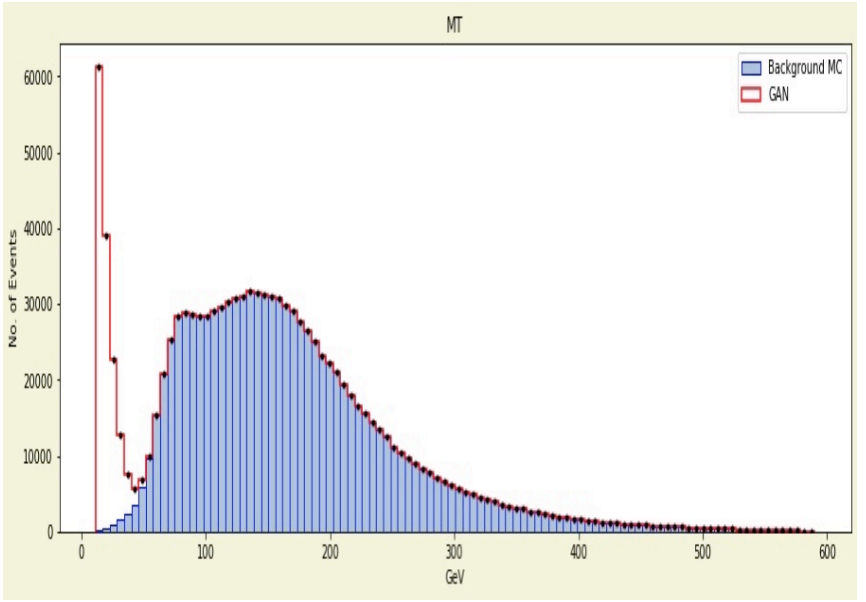


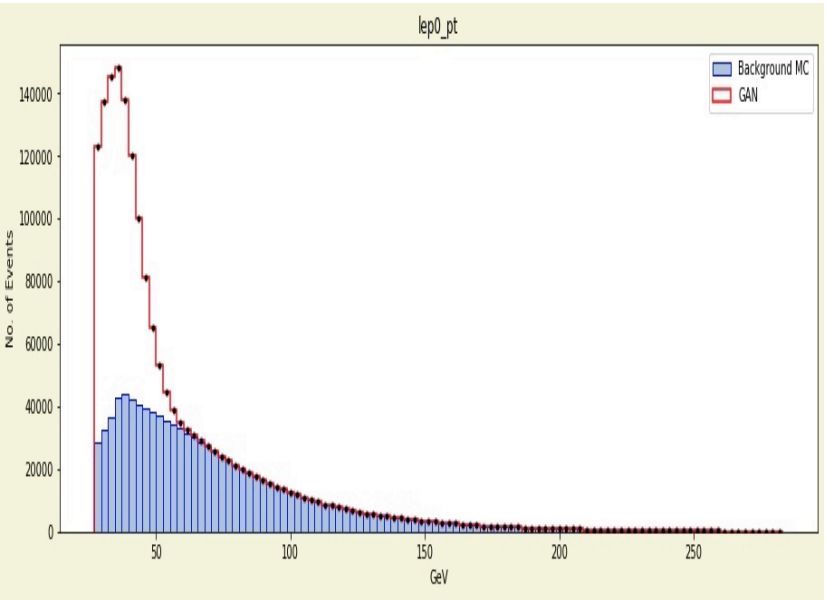
GAN Performance w/ 0.5% tail cuts

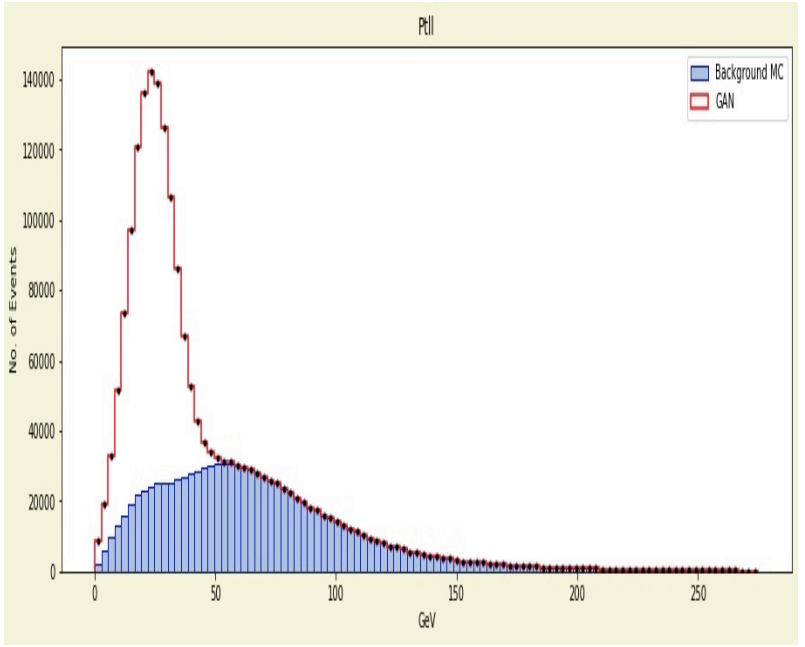
ATLAS Simulation Work in Progress

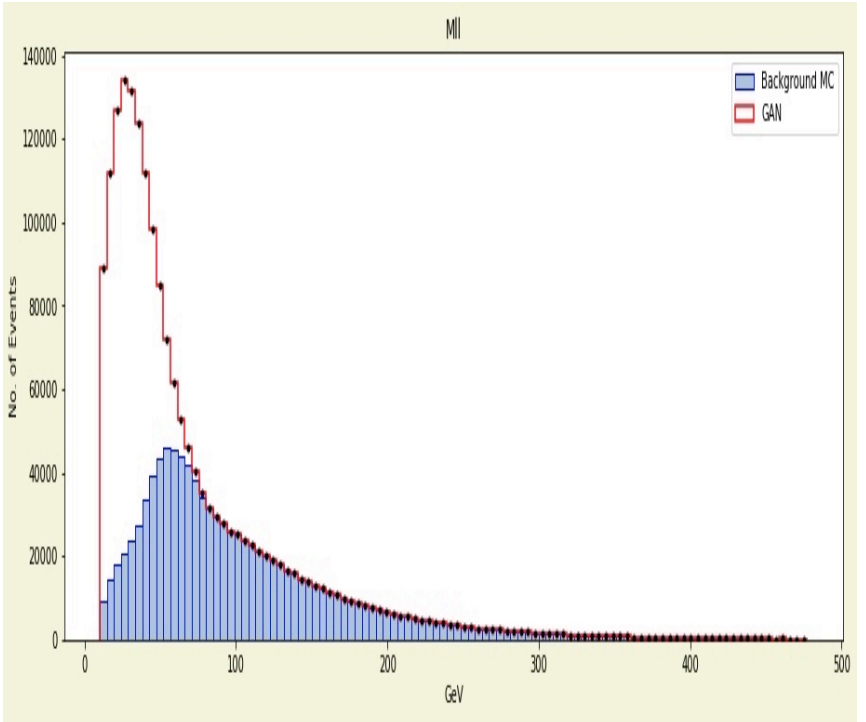






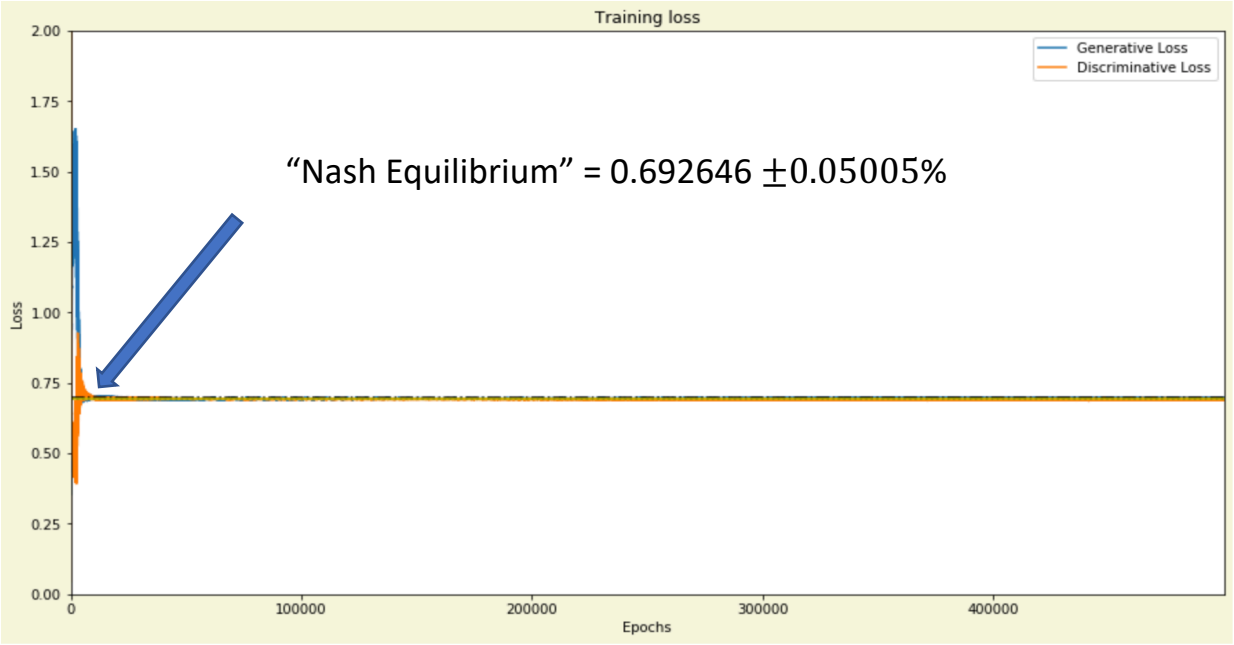


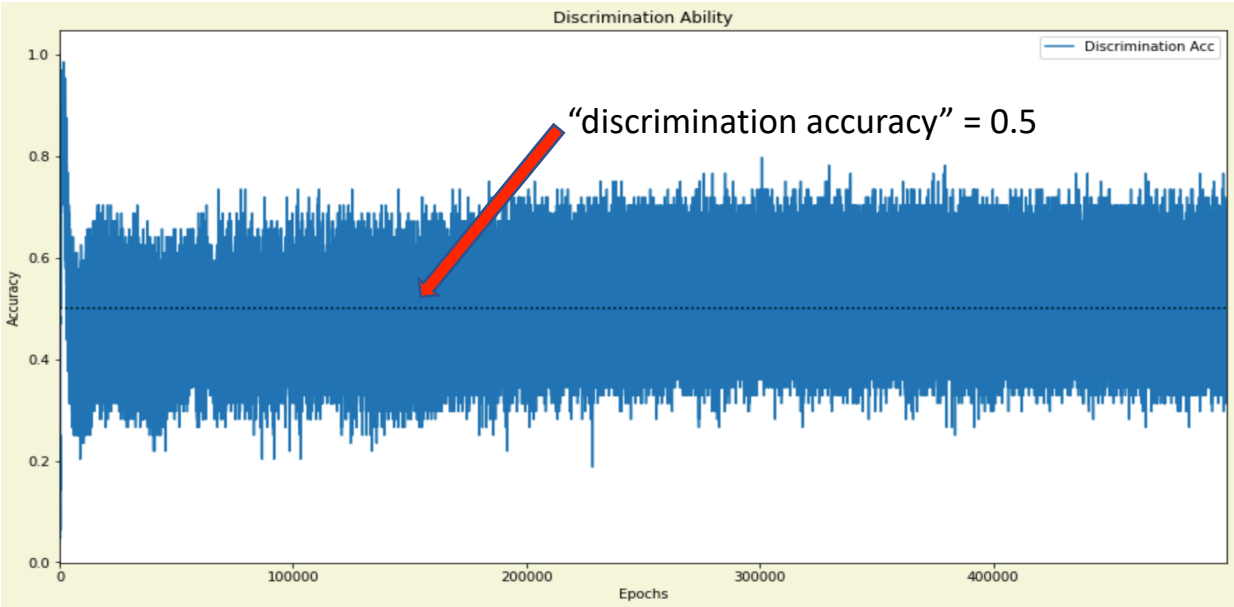




Current status

- training is a **minmax** game, not a Minimization
  - loss **stabilization & tuning**
  - no trivial way to measure the agreement for choosing the best training epoch
  - target goal is to end up with lowest χ^2
- cross-entropy loss converges to -ln(0.5)= 0.69314
- SWAN CPUs, takes ~100k epochs / 1hr





Conclusion & outlook

- more generative model techniques are applied to HEP
  - Variational Autoencoders (**VAE**), Mixture Density Networks (**MDN**), Adversarial AE, GANs, etc.
- Generative nets to speed up generation of large Monte Carlo samples
  - use small “key” MC generated data with high accuracy, use GAN to increase statistics
  - quality of the inputs should be much closer to the truth (MC data)
  - GANs are not a minimization, picking up the best epoch is not trivial (e.g. lowest χ^2)
- possible methods to consider:
  - direct training using TensorFlow on a GPU resourced environment
  - setup conditioning strategies for convergence speedup (TensorFlow)
  - use Auto-Encoder to handle arbitrary number of input variables
  - look into competing methods (β-VAE, Adversarial AE) …

Backup

Software packages

- Keras v2.2.4
- TensorFlow v2.0.0

- scikit-learn 0.22.1,
- Pandas, other libraries

- Input scaled in the [0,1] range

Parameters

- Generators: 64 random number ~U(0,1) → 6 physics quantities:
- Loss functions:
  - Generator: mean square error (MSE)
  - Discriminator: binary cross-entropy
- Optimizer(s):
  - Stochastic Gradient Descent (SGD)
  - Learning rate = 10-3 β1 = 0.5, β2 = 0.5 (slow gradient descent
  - with momentum)

References

- Generative Adversarial Networks: https://arxiv.org/pdf/1406.2661
- DijetGAN: A Generative-Adversarial Network Approach for the Simulation of QCD Dijet Events at the LHC: https://arxiv.org/pdf/1903.02433
- Event Generation and Statistical Sampling for Physics with Deep Generative VAE: https://arxiv.org/pdf/1901.00875
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- Deep Learning books