Accelerating Simulation with GANs


Luke de Oliveira
Vai Technologies & Lawrence Berkeley National Lab

Joint work with:

Ben Nachman
Lawrence Berkeley National Lab

Michela Paganini
Yale University & Lawrence Berkeley National Lab

@lukede0
lukedeo@vaitech.io
https://ldo.io
Outline

• Introduction to Generative Adversarial Networks
• Learning to produce calorimeter showers
• Concluding remarks
• What is an adversary? Best to think about context of games

• As we design our “game,” we have a goal in mind for it’s outcome

• We can pit multiple players (usually neural networks) against each other with cost functions to minimize/maximize while playing, usually want to characterize emergent behavior / convergence of such a game
Generative Adversarial Networks (GAN)

Turn generative modeling into a two player, non-cooperative game.

- The **Generator** tries to produce real looking samples.
- The **Discriminator** tries to tell fake/real.
Setting up the Classical GAN system

\[ V(D, G) = \mathbb{E}_{x \sim p_{\text{data}}(x)}[\log D(x; \theta_D)] + \mathbb{E}_{z \sim p_z(z)}[\log(1 - D(G(x; \theta_G); \theta_D))] \]

- First term, probability that a real sample is classified as real
- Second term, probability that a fake sample is classified as fake
- Generator wants to minimize this, discriminator wants to maximize this
GANs in HEP

• Ultimate goal: quickly and accurately simulate particles interacting with individual detector components - speed up slow simulation

• Intermediary goal: can we speed up calorimeter simulation, which is the current bottleneck?

• First step: can we learn to generate jet images using a Generative Adversarial Network?
Jet Images: Particle Physics → Computer Vision

• Now quite ubiquitous: unroll a detector to treat depositions like an image

• For a more detailed explanation and related links, see Benjamin Nachman’s talk from ACAT 2017

• Jet image: 2D representation of the radiation pattern within a jet

A jet image

Average over thousands of jet images
Qualitative Assessment

GAN-generated signal - background

Real signal - background

5 random Jet Images

nearest LAGAN-generated neighbor
Checking Physical Properties

\[ p_T^2(I) = \left( \sum_{i=0}^{N} I_i \cos(\phi_i) \right)^2 + \left( \sum_{i=0}^{N} I_i \sin(\phi_i) \right)^2 \]

\[ m^2(I) = \left( \sum_{i=0}^{N} I_i \right)^2 - p_T^2(I) - \left( \sum_{i=0}^{N} I_i \sinh(\eta_i) \right)^2 \]

\text{n-subjettiness} \quad \text{jet mass}
CALOGAN

Calorimeter Images

- Closer and closer to raw detector output ($e^+, \pi^+, y$)
- Goal: obtain simulation speedups with GAN

**Challenges:**
- spatio-temporal dependence
- sparsity
- dynamic range
- location specificity

**Advantages:**
- compositionality
- quantifiable properties

arXiv:1705.02355
Open Dataset of Calo Images

- 3 layer, heterogeneous segmentation and resolution (designed to approximate ATLAS LAr calorimeter)

<table>
<thead>
<tr>
<th>Layer</th>
<th>z segmentation [mm]</th>
<th>η segmentation [mm]</th>
<th>φ segmentation [mm]</th>
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- 3 types of particle: $e^+$, $\pi^+$, $\gamma$

- Variable position and angle of incidence (5cm in x and y; 0°, 5° and 20° in theta and phi)

- Open, available, re-usable, citable
Model Requirements

- Obey (to an approximation) conservation of energy and other physical traits such as sparsity
- Allow conditioning on physical attributes (incident angle, energy, etc.)
- Model sequential relationship through layers
CaloGAN Architecture

Generator

Discriminator
CaloGAN Architecture

Generator

Attentional Component

Discriminator

arXiv:1705.02355
CaloGAN Architecture

Generator

Conditioning

Attentional Component

Discriminator

arXiv:1705.02355
Performance at Calo Level

**Figure 2.** Nearest GAN-generated neighbors (bottom) for seven random GEANT4-generated $e^+$ showers (bottom) for the first layer (left), second layer (middle), and last layer (right) of the calorimeter.

**Figure 3.** Interpolation across physical range of incident energy as a conditioning latent factor for $e^+$ showers, with energy increasing from 1 GeV to 100 GeV from left to right. Each point in the interpolation is an average of 10 showers, with each point along the traversal build from an identical latent prior $z$.

N.B., We also compare using shower shapes (see backup)
Computational Speed-up

- Since a GAN can be expressed using linear algebra primitives, can exploit modern computing platforms (such as GPU) and libraries (such as TensorFlow)
- With large batches, generation time per-particle decreases dramatically

<table>
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<th>Generation Method</th>
<th>Hardware</th>
<th>Batch Size</th>
<th>milliseconds/shower</th>
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Up to a $10^5$ speed-up compared to Geant4!

arXiv:1705.02355

N.B., See backup for benchmarking parameters
Concluding Remarks

• GANs have shown promise in learning complicated, high dimensional physical realizations

• GANs are extensible, and can easily incorporate domain constraints

• Speed-up from GANs compared to traditional modeling is promising

• Achievements so far using basic GAN formulation! Doesn’t include recent work on ProgressiveGANs or Spectral Normalization - can only get better!
Thanks!
Backup
Attribute Conditioning

**Figure 4.** Interpolation across physical range of $x_0$ as a conditioning latent factor for $e^+$ showers. Note in the ATLAS coordinate system, $x$ represents the vertical direction in this dataset. Each point in the interpolation is an average of 10 showers, with each point along the traversal build from an identical latent prior $z$.

**Figure 5.** Interpolation across physical range of $\theta$ as a conditioning latent factor for $e+$ showers, with $\theta$ increasing from left to right. Each point in the interpolation is an average of 10 showers subtracted from the middle point along the interpolation path, with each point along the traversal build from an identical latent prior $z$. 
Verification with 1D projections

Physical one-dimensional statistics of the shower probability distribution can help us verify how well our surrogate performs.
Attribute Regression

As a byproduct, the CaloGAN learns to regress out initial conditions.
Benchmarking Parameters

• Numerical results are obtained over an average of 100 runs.

• Geant4 and CaloGAN on CPU are benchmarked on nearly identical compute-nodes on the PDSF distributed cluster at the National Energy Research Scientific Computing Center (NERSC).

• CaloGAN on GPU hardware is benchmarked on an Amazon Web Service (AWS) p2.8xlarge instance, where a single NVIDIA® K80 is used for the purposes of benchmarking.