Fast Data-Driven simulation of Cherenkov Detectors Using Generative Adversarial Networks

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Outline

- Particle identification with Cherenkov detectors at LHCb
  - Fast simulation set-up
- Generative Adversarial Networks (GANs)
  - Basic architecture
  - JS and Wasserstein metrics and problems with them
  - Cramér and energy distances
- Results and discussion
Whilst the RICH detectors are primarily used for hadron identification, a distinct muon band can also be observed.

From The LHCb RICH Collaboration: Performance of the LHCb RICH detector at the LHC

The LHCb RICH Collaboration, Adinolfi, M., Aglieri Rinella, G. et al.
Information from RICH detectors

- PID with RICH is done with the maximum likelihood method
  - $\mathcal{L}(t_1, \ldots, t_N)$ – likelihood to observe a given picture, as a function of all track PIDs $t_i$ – hypothesized particle type for track $i$
  - A hypothesis $(t_1, \ldots, t_N)$ maximizing $\mathcal{L}$ is searched for

- For each track $i$, for each $x \in \{K, \mu, e, p, \text{below threshold}\}$, quantities $\text{DLL}_x$ are then calculated as:
  $$\log \mathcal{L}(t_k=t_k, k\neq i; t_i=x) - \log \mathcal{L}(t_k=t_k, k\neq i; t_i=\pi)$$
RICH simulation

• Accurate RICH simulation involves:
  - Tracing the particles through the radiators and delta-electron generation
    ‣ Delta-electrons contribute to Cherenkov light emissions
  - Cherenkov light generation
  - Photon propagation, reflection, refraction and scattering
  - Hybrid Photon Detector (photo-cathode + silicon pixel) simulation

• All this takes time & resources

• Given the growing demand on the number of simulated events, accurate simulation becomes unfeasible
RICH fast simulation

• A possible solution:
  - Bypass all those steps from Cherenkov light generation up to the high-level likelihood parameters (DLLs)
  - Learn the distribution of DLLs for given track parameters and sample from it, $P(\text{DLLs} | \text{<track params>})$

Derkach et al., NIMA 2019 (01) 031
Generative Adversarial Networks (GANs)

• Random variable $z$
• Two deterministic functions (neural nets)
  - generator $G(x, z)$
  - discriminator $D(x, y)$
• Generator maps $(x, z)$ to $y^{\text{gen}}$
• Discriminator distinguishes between $(x, y^{\text{gen}})$ and $(x, y^{\text{real}})$
• Training step («competition» between the two nets):
  - train discriminator to improve $(x, y^{\text{gen}})$ and $(x, y^{\text{real}})$ separation
  - train generator to increase the discriminator’s error rate
Discriminator metric

• Some of the options for the discriminator metric:
  - Binary cross-entropy between the real and generated samples
    ‣ Equilibrium when Jensen–Shannon divergence is minimized
    ‣ Problematic for distributions with different support; mode collapse problems
  - Wasserstein (aka Earth Mover’s) distance
    ‣ Discriminator => «Critic» (evaluates the metric)
    ‣ Naturally solves the non-equal support and mode collapse problems
    ‣ Suffers from biased gradients

arXiv:1406.2661
arXiv:1701.07875
GAN (Cramér / energy distance)

- Cramér distance between distributions $P$ and $Q$:
  \[
  l^2_2(P, Q) := \int_{-\infty}^{\infty} (F_P(x) - F_Q(x))^2 dx
  \]
- $F_P$ and $F_Q$ are CDFs
- This is (1/2 times) the 1-dimensional case of the Energy distance:
  \[
  \mathcal{E}(X, Y) := 2 \mathbb{E} \| X - Y \|_2 - \mathbb{E} \| X - X' \|_2 - \mathbb{E} \| Y - Y' \|_2
  \]
  \[
  X, X' \sim P \text{ and } Y, Y' \sim Q
  \]
- A GAN using this metric preserves all the nice properties of Wasserstein GAN, while solving the biased gradients problem
RICH fast simulation

- Dimensionality of $P(\text{DLLs} \mid \langle\text{track params}\rangle)$
  - 5 output DLLs
  - input: track momentum and pseudorapidity (+2)
  - input: omitting $\phi$ for simplicity (+0)
RICH fast simulation

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• DLLs depend not only on the given track’s parameters
  - overlapping circles at higher occupancies
  - input: total number of tracks in that event (+1)
RICH fast simulation

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- Training on real data (calibration channels)
  - using sPlot technique\(^1\) to extract signal distributions
  - loss function is weighted (with possibly negative weights)

Implementation details and input parameter distributions

- 10 hidden fully-connected layers for both generator and discriminator
  - 128 neurons each
  - ReLU activation
- 64-dimensional latent space (noise shape)
- 256-dimensional discriminator output
- 15 discriminator updates per 1 generator update
- RMSProp optimizer, exp decaying learning rate
RichDLLk
($\pi$ vs K)

3x3 bin plot over full P-ETA range
RichDLLk
($\pi$ vs K)

zoomed in to the most populated region
Differences between AUCs for real and generated samples (divided by error)

- Errors estimated using bootstrap technique
- Most differences are within just a few sigmas, larger deviations at low-stat regions

K vs π, using RichDLLk
μ vs π, using RichDLLmu
p vs π, using RichDLLp
Differences between AUCs for real and generated samples (absolute, generated – real)

- Absolute differences between AUCs are mostly in the 0.001-0.01 range

K vs π, using RichDLLk

μ vs π, using RichDLLmu

p vs π, using RichDLLp
Summary

• GANs are a promising tool for fast simulation models
• Can be trained in a background-contaminated environment, with the help of sPlot technique
  - negative weights don’t cause divergencies in our experiments
• Our model is doing well judging by the looks of generated vs real distributions
  - Some imperfections seen in the low-stat regions
  - AUC differences look reasonable
• Ongoing work to implement our model within the fast simulation framework of LHCb
  - Looking forward to evaluate our model in a real analysis environment
Backup
GAN (JS)

- Possible discriminator and generator losses – binary cross-entropy:

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

- This leads to equilibrium when Jensen-Shannon divergence between real and generated samples is minimized

- Problems:
  - vanishing gradients when discriminator too powerful
  - mode collapse (generating only a subset of the target distribution)
GAN (Wasserstein)

Another possible metric: Wasserstein distance (Earth Mover’s distance)

\[ W(\mathbb{P}_r, \mathbb{P}_g) = \inf_{\gamma \in \Pi(\mathbb{P}_r, \mathbb{P}_g)} \mathbb{E}(x,y) \sim \gamma \left[ \|x - y\| \right] \]

- \( \gamma \) – «optimal transport plan»
- This should solve the mode collapse and vanishing gradients problems
- Solution may not be optimal due to biased gradients (see arXiv: 1705.10743)