Validating the Advantage of Using Ensembles Over a Single GAN Model for Calorimeter Simulations

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Introduction

- Monte Carlo simulations of calorimeter showers are very time demanding. Generative deep learning offers a faster alternative.
- Generative adversarial networks (GANs) can generate high-fidelity samples.
- However, GANs often suffer from mode collapse.
- Can we increase the diversity of generated samples using ensembling approach?

Training Data

- ECAL showers simulated for a prototype of an ILD detector.
- Events induced by a single electron (available on `Zenodo.org` [1]).
- Initial particle energies in range 2 − 500 GeV.
- Fixed incident angle of 60°.
- Energy depositions recorded in a cube grid with 25 × 25 × 25 cells where the layers in *z* axis correspond to the ECAL layers.
- High dynamic range of cell energies, high sparsity of images.

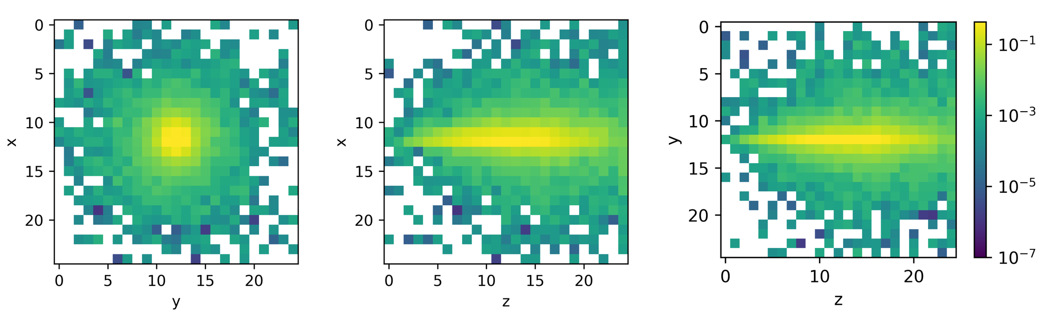


Fig. 1: 2D plots of simulated energy depositions in the ECAL.

Baseline GAN

- Custom conditional GAN based on 2D convolutional neural networks [2].
- 3-branch architecture in both generator and discriminator.
- Custom loss with 3 components:
  - true/fake loss (BCE),
  - loss on prediction of primary energy (MAPE),
  - loss on reconstruction of total deposited energy (MAPE).
- Training time: 4 hrs (GPU Tesla V100 32GB).
- Good quality of individual samples.
- Suffers from the mode collapse.

Conclusion

- An ensemble of 10 Conv2D GANs was successfully trained.
- Ensembling improved average features such as shower shapes and sampling fraction.
- By using the ensemble, we improved the variability of generated showers.
- However, the t-SNE algorithm distinguished samples generated by different GANs.

References

[1] Pierini M., Zhang M. *CLIC Calorimeter 3D images: Electron showers at Fixed Angle*, 2020. `zenodo.org/records/3603122`

[2] Rehm F., et al. *Validation of Deep Convolutional Generative Adversarial Networks for High Energy Physics Calorimeter Simulations*, 2021. `arxiv.org/abs/2103.13698`

[3] Tolstikhin I., et al. *AdaGAN: Boosting Generative Models*, 2017. `arxiv.org/abs/1701.02386`

Ensemble Structure and Training

Adapting the AdaGAN ensembling approach [3] to the Conv2D GAN for shower generation.

Steps:

1. Train the first GAN.
2. Retrieve the discriminator predictions for all training data.
3. Assign weights to training data based on the true/fake predicted probabilities:
   - ≈ 0.5 → low weight,
   - ≈ 1.0 → high weight.
4. Use weighted training data to train the next GAN for the ensemble.

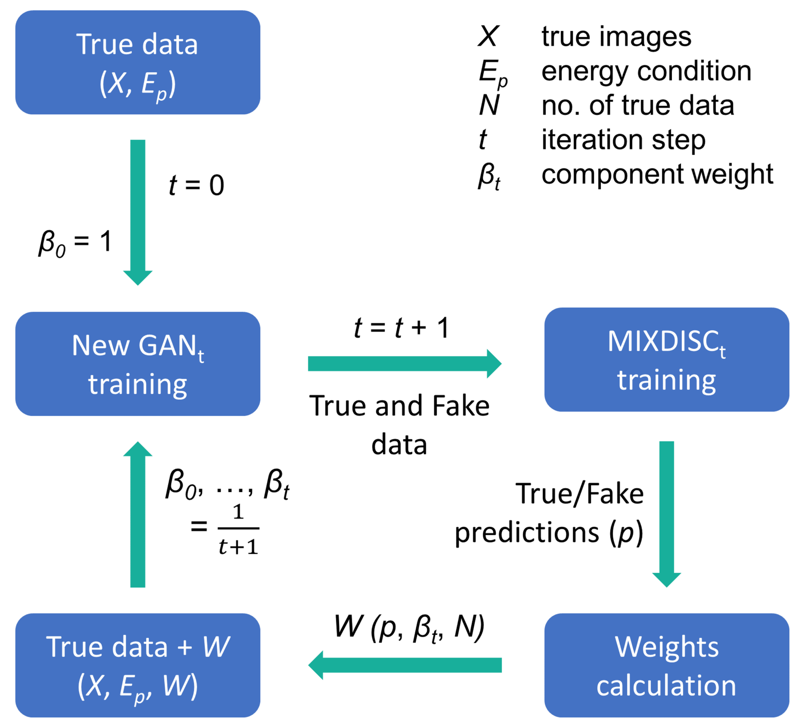
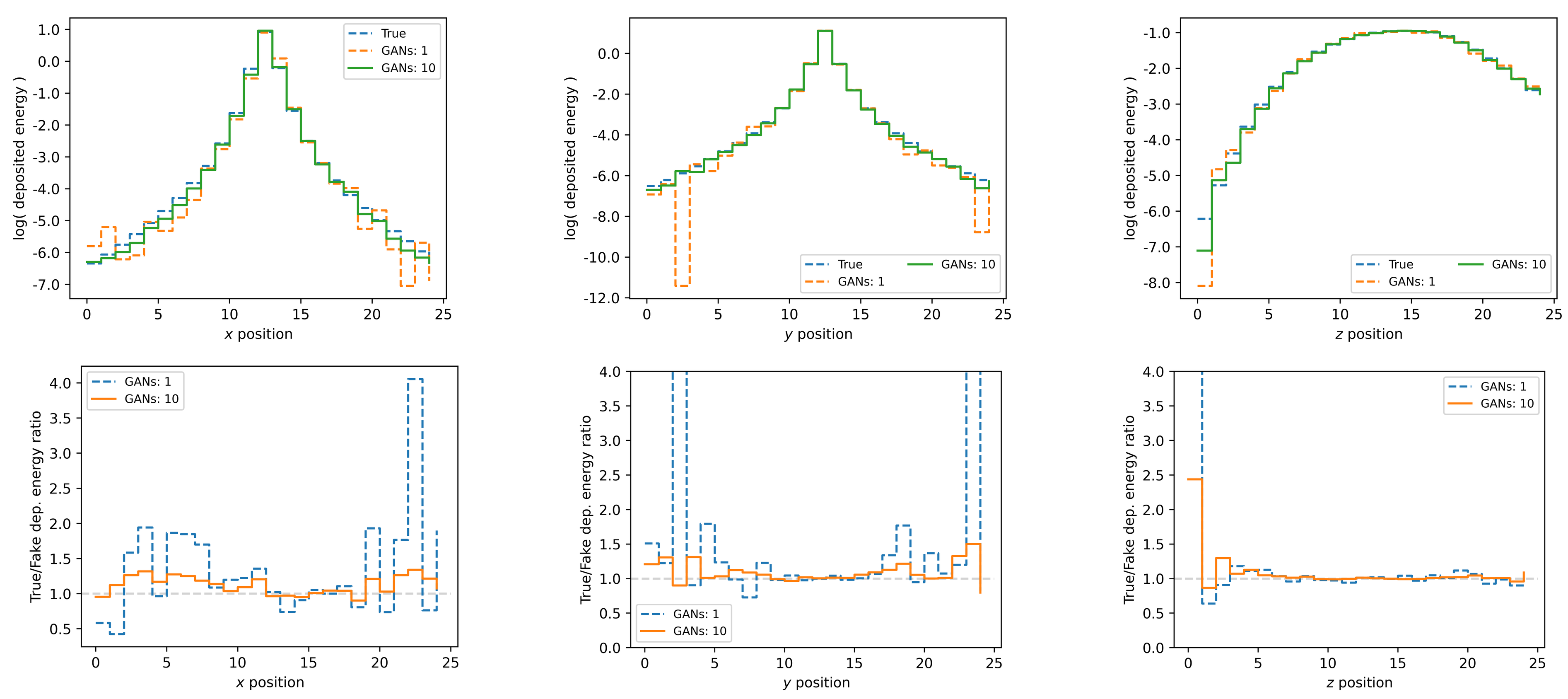


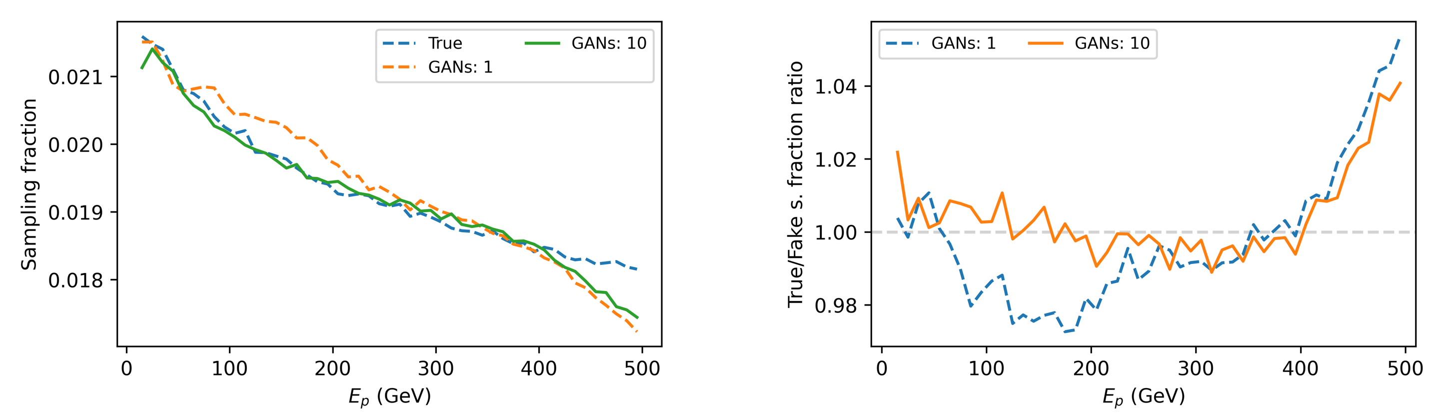
Fig. 2: Diagram of the ensemble training loop.

Sample Quality

Shower shapes The ensemble of GANs outperforms the single GAN model in matching the average shower shapes. A significant improvement is observed around the edges of the cube grid region.

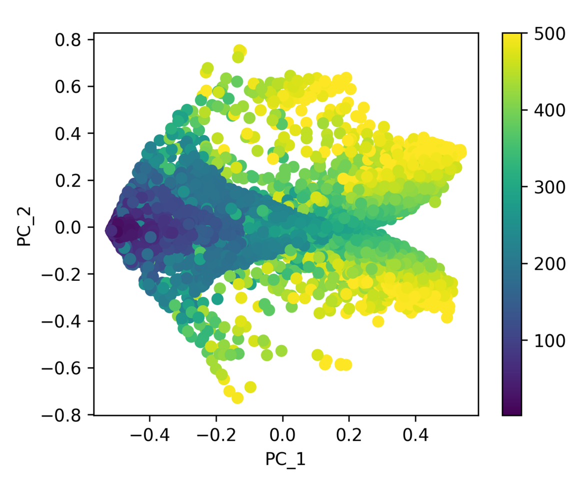


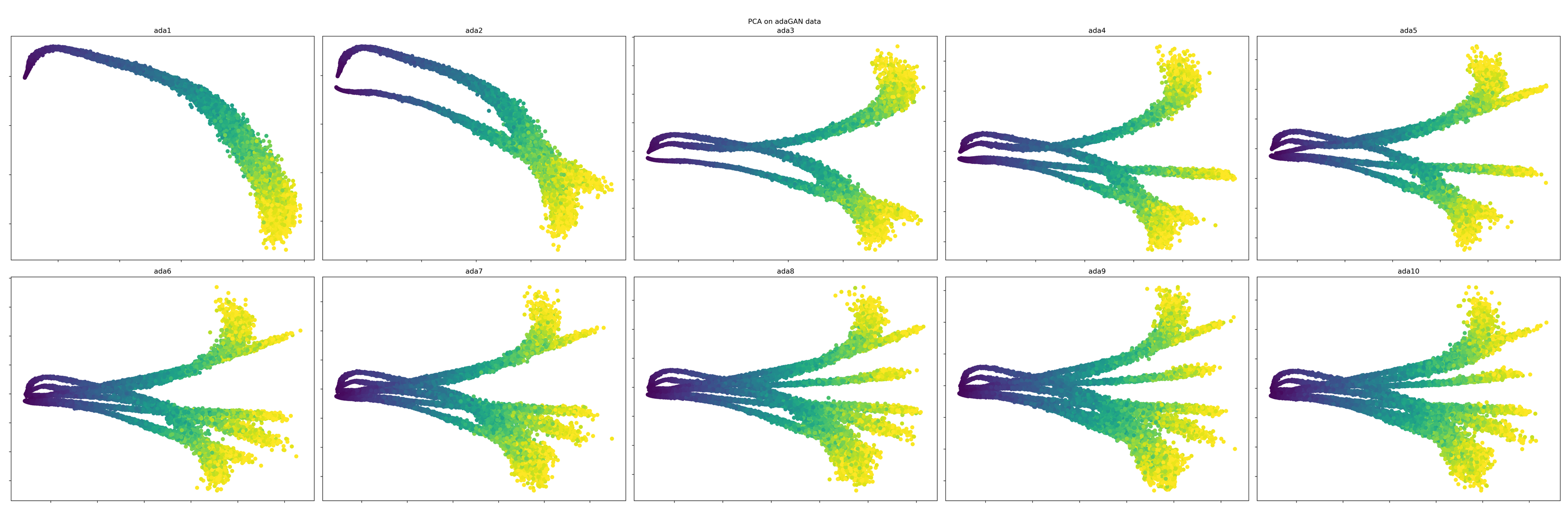
Sampling fraction is the ratio between the sum of deposited energies and the initial particle energy. The ensemble outperforms the single GAN model in matching this quantity.



Sample Variability

PCA on training data (left) Principal component analysis (PCA) fitted on the training data. The 1st and 2nd principle components (PCs) are visualized as a scatter plot.
PCA on generated data (right) Samples generated from ensembles of 1 − 10 GANs projected into the 1st and 2nd PCs fitted on the training data.
Colors of the points correspond to the initial particle energy in GeV.





t-SNE Visualization of the training samples (top) and ensemble-generated samples (bottom).