Domain Adaptation in Colliders: Reconcile Simulation and Data

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Introduction

There is always an uncertainty induced by simulation.

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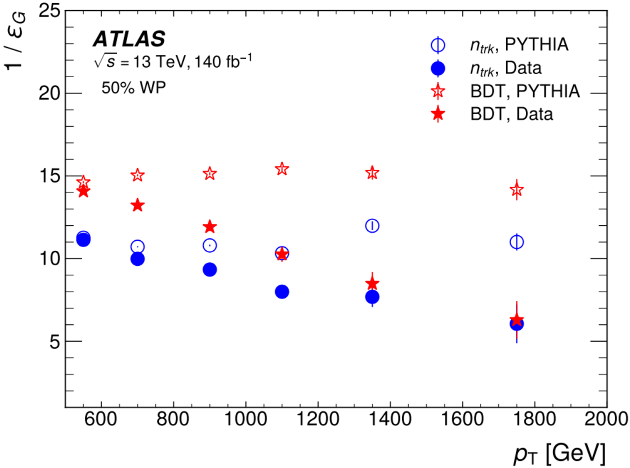
Typical working flow. Trained by simulation $\rightarrow$ Inference on data.

Domain difference between simulation and data:

- Parton shower
- Hadronization
- etc.

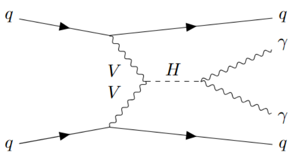
Introduction

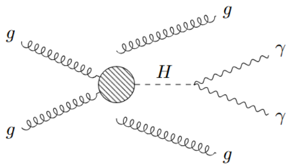


arXiv:2308.00716

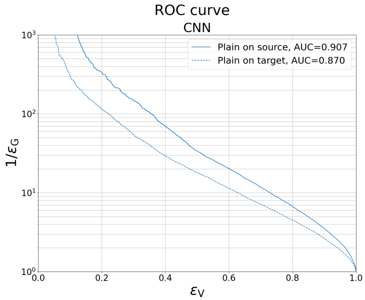
Introduction

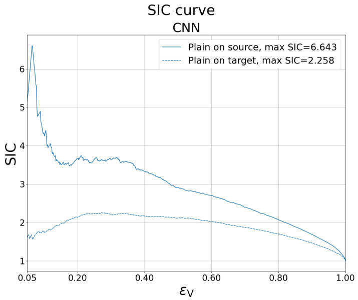
Assume a VBF Higss vs. ggF Higgs classification





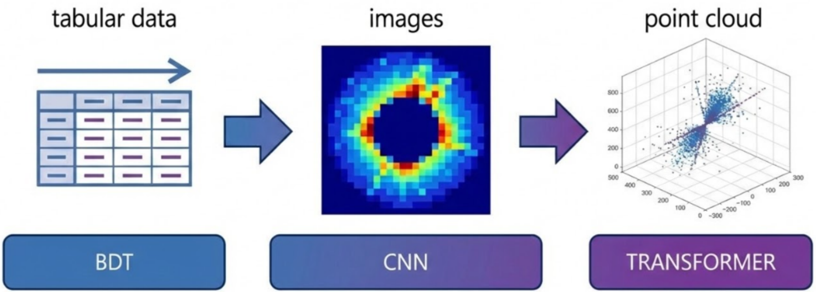
Train on Pythia, test on Pythia/Herwig





Introduction

Trend. We are accessing ever-increasingly granular information.



How to ensure the model does NOT learn the artifact in the simulation?

Introduction

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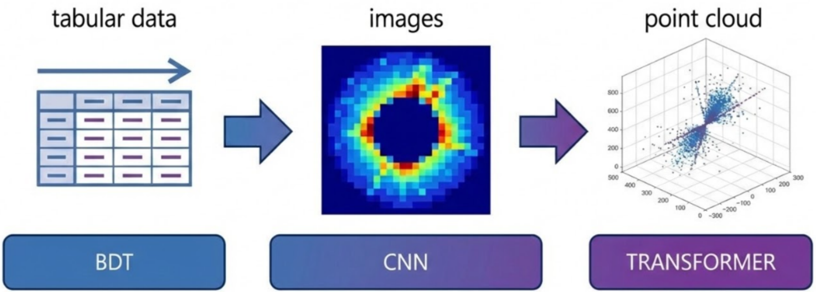


How to ensure the model does NOT learn the artifact in the simulation?

Unsupervised domain adaptation
Learn from simulation (with label) + data (without label)

Outline

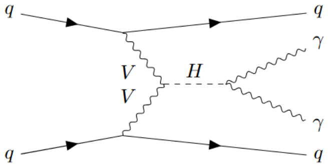
Table of Contents

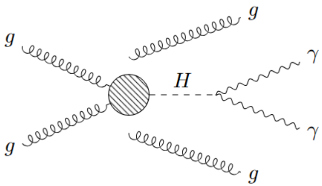
Dataset

Processes. Higgs production in pp collisions

- Signal: VBF Higgs with up to three jets
- Background: ggF Higgs with up to three jets

Assume the Higgs further decay to diphoton, $H \to \gamma\gamma$.





Dataset

Generation.

Domain	Generator		Shower & Hadronization		Detector
Pythia	NLO PWG	$\longrightarrow$	**Pythia**	$\longrightarrow$	ATLAS card
Herwig	NLO PWG	$\longrightarrow$	**Herwig**	$\longrightarrow$	ATLAS card

Two domains are needed to be adapted:

- **Source**/simulation/labeled: **Pythia VBF + Pythia ggF**
- **Target**/data/unlabeled: **Herwig VBF + Herwig ggF**

Dataset

Pre-selections.

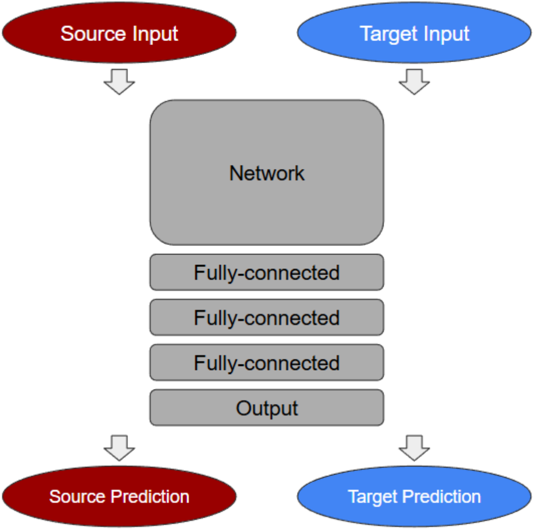
- $N_\gamma \geq 2$
- $N_j \geq 2$ with $p_{T,j} \geq 25$ GeV
- $\Delta\eta_{jj} \geq 2.5$
- $p_{T,H} < 200$ GeV

Pre-processing. Weight rescaling for each event to respect the xs

Pythia	N_{evt}	σ (pb)
VBF	242k	1.100(3)
ggF	97k	0.960(1)

Herwig	N_{evt}	σ (pb)
VBF	247k	1.123(1)
ggF	107k	1.072(3)

Unsupervised Domain Adaptation (UDA)



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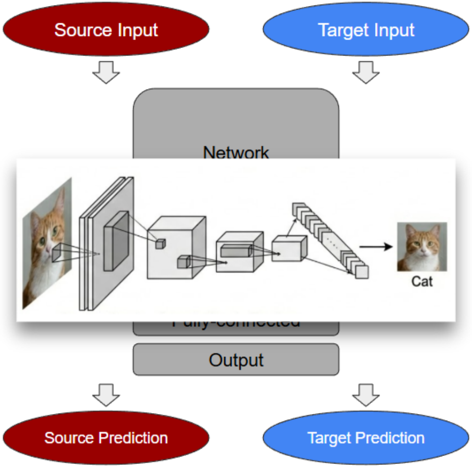

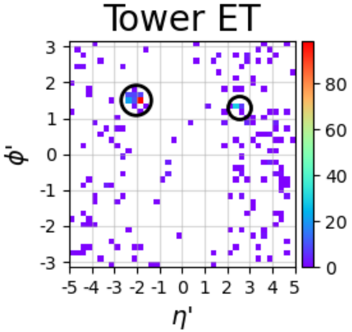

arXiv:2209.05518

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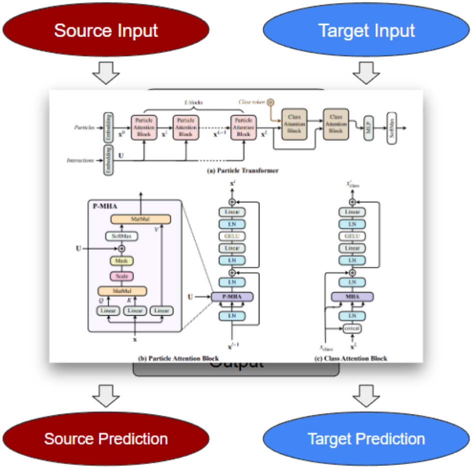
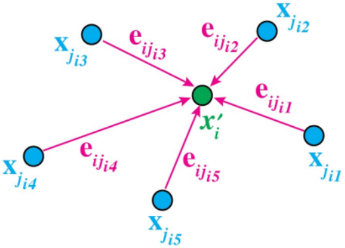


arXiv:2202.03772



arXiv:1801.07829

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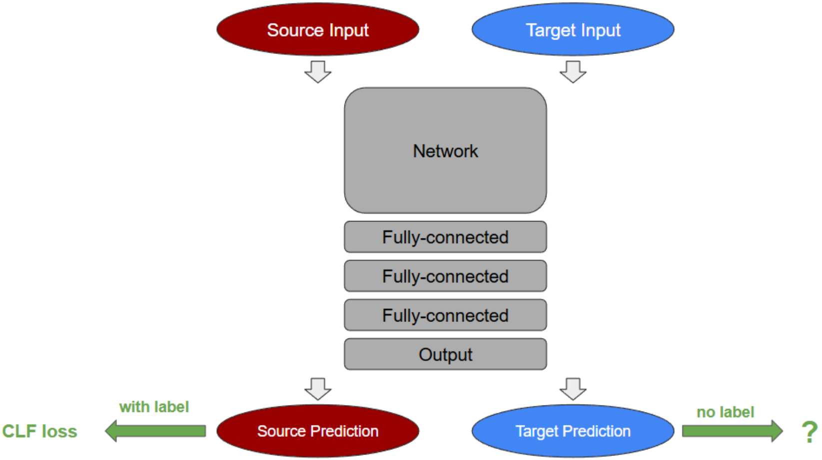

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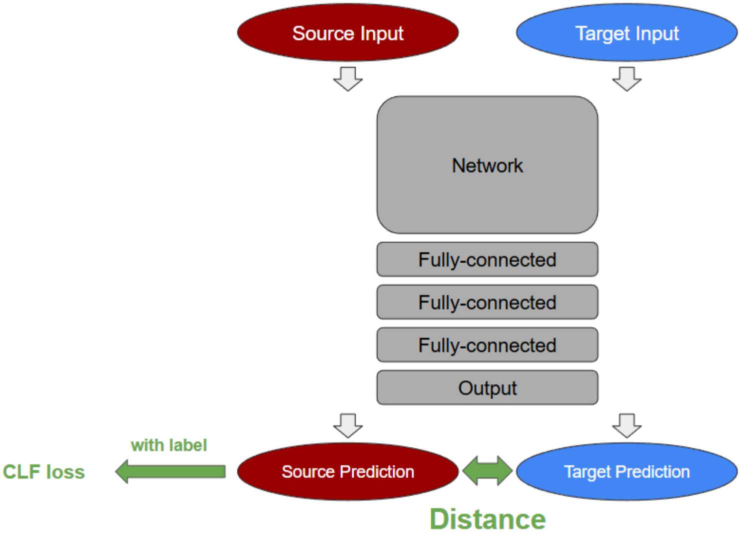


Unsupervised Domain Adaptation (UDA)

Idea. Align the representation of simulation and data.

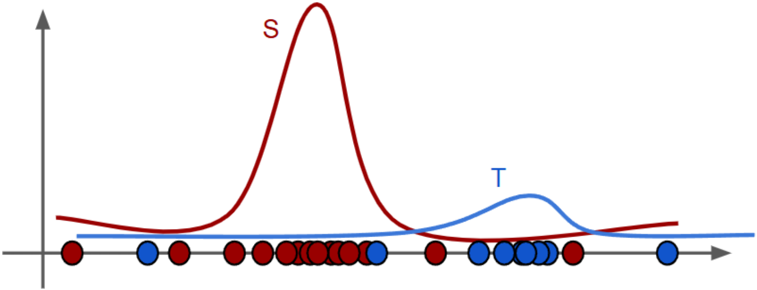
Introduce the **Maximum Mean Discrepancy (MMD)** as a distance of distributions. arXiv:1912.00320

$$\begin{aligned} \mathrm{MMD}^2(S,T) \equiv \mathbb{E}_{X\sim S}[k(X,X)] + \mathbb{E}_{Y\sim T}[k(Y,Y)] \\ - 2\mathbb{E}_{X\sim S, Y\sim T}[k(X,Y)], \end{aligned} \tag{1}$$

with the Gaussian kernel

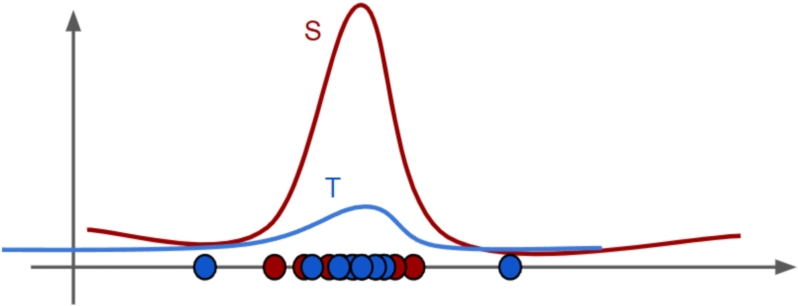
$$k(X,X') \equiv \exp\left(-\frac{\|X-X'\|^2}{\gamma}\right). \tag{2}$$

Unsupervised Domain Adaptation (UDA)



$$\text{distance} \sim ||\mathbb{E}_{X\sim S}\left[X\right] - \mathbb{E}_{Y\sim T}\left[Y\right]|| \quad (3)$$

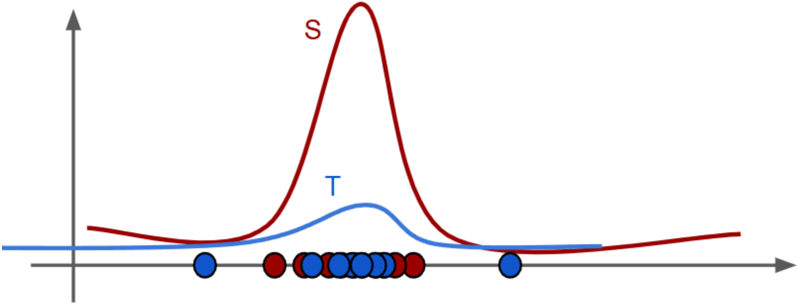
Unsupervised Domain Adaptation (UDA)



$$\text{distance} \sim \left|\left|\mathbb{E}_{X\sim S}\left[\left(X, X^2\right)\right] - \mathbb{E}_{Y\sim T}\left[\left(Y, Y^2\right)\right]\right|\right| \quad (4)$$

(5)

Unsupervised Domain Adaptation (UDA)

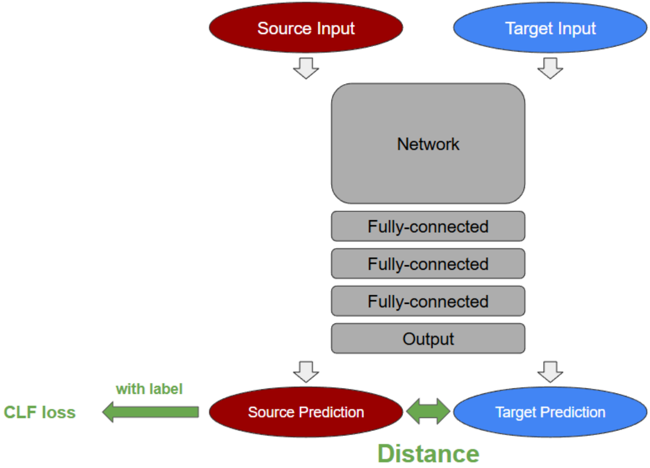


$$\text{distance} \sim \left|\left|\mathbb{E}_{X\sim S}\left[\left(X, X^2\right)\right] - \mathbb{E}_{Y\sim T}\left[\left(Y, Y^2\right)\right]\right|\right| \tag{4}$$

$\downarrow$ higher moment

$$\sim \left|\left|\mathbb{E}_{X\sim S}\left[e^X\right] - \mathbb{E}_{Y\sim T}\left[e^Y\right]\right|\right| \tag{5}$$

Unsupervised Domain Adaptation (UDA)



$$\mathcal{L} = \mathcal{L}_{\mathsf{CLF}}(\text{source}) + \lambda \cdot \mathrm{MMD}^2(\text{source}, \text{target}), \tag{6}$$

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Uncertainty

Toy measurement.

$$N_{\mathrm{V-like}} = \mathcal{L}(\sigma_{\mathrm{V}} \cdot \epsilon_{\mathrm{V}} + \sigma_{\mathrm{G}} \cdot \epsilon_{\mathrm{G}}) \tag{7}$$

$$N_{\mathrm{G-like}} = \mathcal{L}(\sigma_{\mathrm{V}} \cdot (1 - \epsilon_{\mathrm{V}}) + \sigma_{\mathrm{G}} \cdot (1 - \epsilon_{\mathrm{G}})). \tag{8}$$

$$\begin{pmatrix} \sigma_{\mathrm{V}} \\ \sigma_{\mathrm{G}} \end{pmatrix} = \frac{1}{\mathcal{L}} \frac{1}{\epsilon_{\mathrm{G}} - \epsilon_{\mathrm{V}}} \begin{pmatrix} \epsilon_{\mathrm{G}} - 1 & \epsilon_{\mathrm{G}} \\ 1 - \epsilon_{\mathrm{V}} & -\epsilon_{\mathrm{V}} \end{pmatrix} \begin{pmatrix} N_{\mathrm{V-like}} \\ N_{\mathrm{G-like}} \end{pmatrix}. \tag{9}$$

Uncertainty

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Sources of the uncertainty:

- Statistical: $N_{\text{V-like}}$, $N_{\text{G-like}} \sim$ Poisson
- Systematic: $\epsilon_{\mathrm{V}}(\mathrm{TPR})$, $\epsilon_{\mathrm{G}}(\mathrm{FPR})$

  $\rightsquigarrow$ Estimated by domain difference: $\Delta\epsilon_{\mathrm{V}}$, $\Delta\epsilon_{\mathrm{G}}$.

  ($\Delta\epsilon = \epsilon$ on source $- \epsilon$ on target)

Uncertainty

The variance of the cross section measurement:

$$(\Delta\sigma_{\rm V})^2 = \underbrace{\left(\frac{\partial\sigma_{\rm V}}{\partial N_{\rm V}}\right)^2 (\Delta N_{\rm V})^2 + \left(\frac{\partial\sigma_{\rm V}}{\partial N_{\rm G}}\right)^2 (\Delta N_{\rm G})^2}_{\text{statistical}}$$

$$+ \underbrace{\left(\frac{\partial\sigma_{\rm V}}{\partial \epsilon_{\rm V}}\right)^2 (\Delta \epsilon_{\rm V})^2 + \left(\frac{\partial\sigma_{\rm V}}{\partial \epsilon_{\rm G}}\right)^2 (\Delta \epsilon_{\rm G})^2}_{\text{systematic}} \quad (10)$$

$$= \frac{1}{(\epsilon_{\rm V} - \epsilon_{\rm G})^2} \left[\underbrace{\frac{(1-\epsilon_{\rm G})^2 N_{\rm V} + \epsilon_{\rm G}^2 N_{\rm G}}{\mathcal{L}^2}}_{\text{statistical}} + \underbrace{\sigma_{\rm V}^2 (\Delta\epsilon_{\rm V})^2 + \sigma_{\rm G}^2 (\Delta\epsilon_{\rm G})^2}_{\text{systematic}} \right], \quad (11)$$

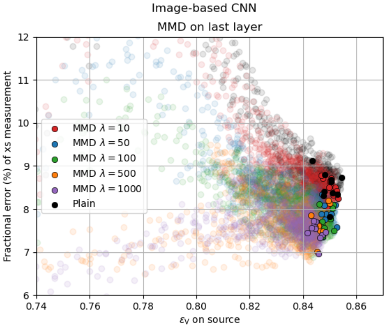
- $\mathcal{L} = 3\,\text{ab}^{-1}$,
- the working point with $\epsilon_{\rm G} = 0.2$.

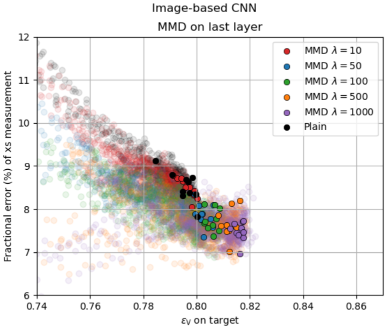
Uncertainty

Compare 10 runs for each of the following models:

- Plain
- MMD $\lambda = 10$
- MMD $\lambda = 50$
- MMD $\lambda = 100$
- MMD $\lambda = 500$
- MMD $\lambda = 1000$

Image-based CNN.



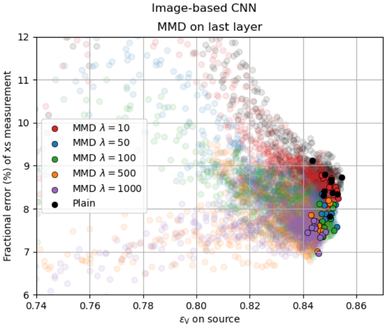


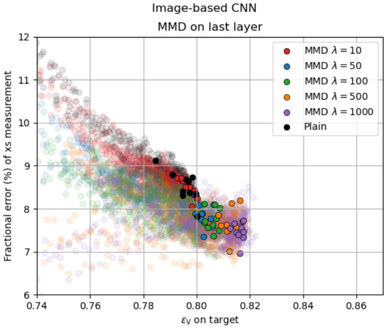
Each epoch in the training history is scattered.

The epoch with the largest source ϵ_V is marked to represent a run.

Uncertainty

Image-based CNN.

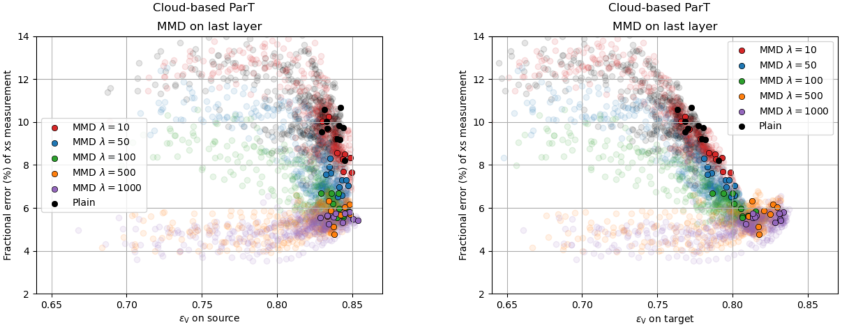




- Source ϵ_V is kept, and the uncertainty is reduced
- Target ϵ_V of MMD is even larger than the plain case.
- Uncertainty: $8\,\% - 9\,\%$ (plain) $\rightarrow$ $7\,\% - 8\,\%$ (MMD $\lambda = 1000$)

Uncertainty

Cloud-based ParT.



- Uncertainty: $9\,\% - 11\,\%$ (plain) $\rightarrow$ $5\,\% - 6\,\%$ (MMD $\lambda = 1000$)

Summary

- Systematic is an important ingredient in measurement.
- Introducing MMD helps to reduce the domain difference, and hence the systematic.
- The MMD can be readily applied to various types of networks and data representations.

Thank you for listening!

Backup - Epoch Selection

To perform epoch selection, the only viable information are

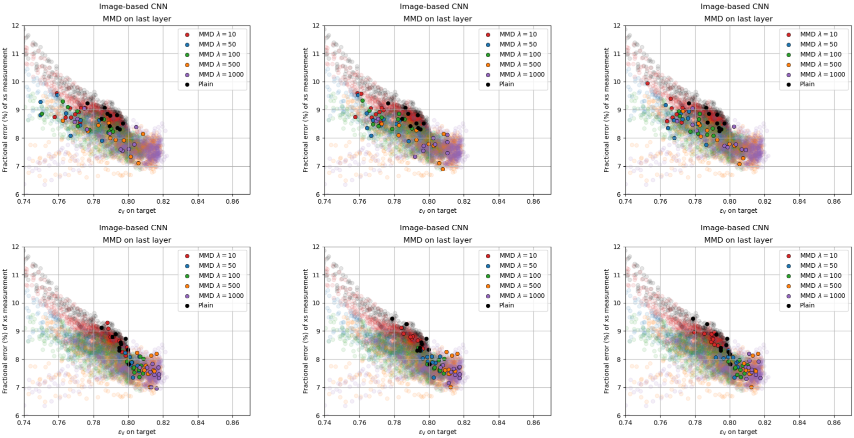
- ϵ_{V} on simulation;
- MMD between simulation and data.

Other possible selection strategies:

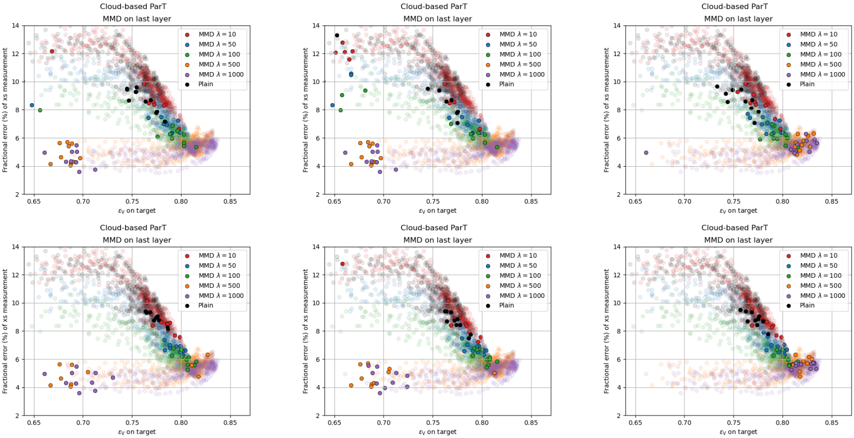
1. Selecting the epoch which has the least MMD on
   1. the third-to-last layer
   2. the second-to-last layer
   3. the last layer
2. First filter out the epochs with MMD less than 0.2 on
   1. the third-to-last layer
   2. the second-to-last layer
   3. the last layer,

   then among the remaining epochs, select the one with the highest ϵ_{V} on the source domain.

Backup - Epoch Selection



CNN: 1a (upper left), 1b (upper middle), 1c (upper right), 2a (lower left), 2b (lower middle), and 2c (lower right).

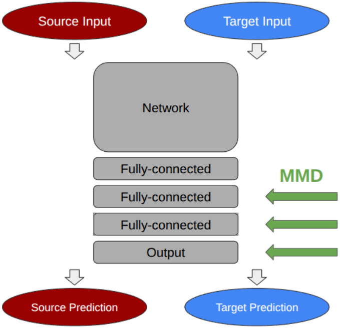


ParT: 1a (upper left), 1b (upper middle), 1c (upper right), 2a (lower left), 2b (lower middle), and 2c (lower right).

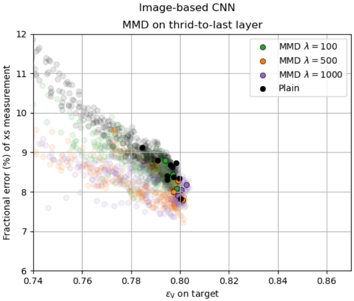
Backup - MMD Layers

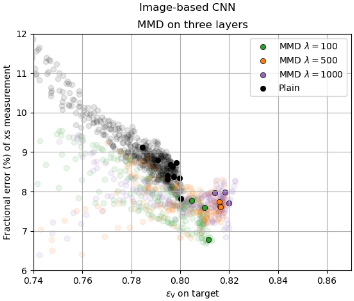
It is possible that the MMD can be applied on the hidden layers of the network.

$$\mathcal{L} = \mathcal{L}_{\text{clf}}(\text{source}) + \sum_{\ell \in \text{layers}} \lambda_\ell \cdot \mathrm{MMD}^2(\text{source}_\ell, \text{target}_\ell), \tag{12}$$



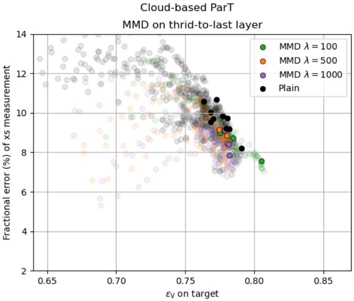
Backup - MMD Layers

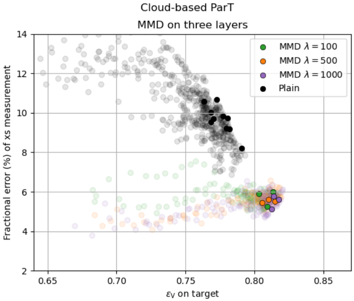




CNN: MMD is applied on the third-to-last (left), and all of the last three layers (right).

Backup - MMD Layers





ParT: MMD is applied on the third-to-last (left), and all of the last three layers (right).