Generative models: their evaluation and their limitations

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based on A. Coccaro, M. Letizia, H. Reyes, RT, 2302.12024, and S. Grossi, M. Letizia, RT, 2409.16336

Why do we need generators in HEP

The need for the generation of "synthetic" data is a direct consequence of the scientific method:

*Simulation of an experiment is the only known way to deduce and estimate the **observable consequences** of a given **theoretical hypothesis***

It is critical in science for various reasons

- Help define the **expectation** for a given observable, which is essential to design the experiment
- It is at the basis of statistical inference, both **Frequentist** and **Bayesian**
    - **Statistical hypothesis testing** in the **Frequentist** approach requires the knowledge of the outcome of theoretically infinite experiments under a given (null) hypothesis
    - **Bayesian posterior inference** needs marginal integrals of the posterior distribution, which can (almost always) only be obtained through numerical integration (sampling)

Generators and generative models

Generator

An algorithm that, given a probability density function (PDF), can draw samples from it. The PDF may be known or unknown and there may be additional random noise in the generation process.

$$p(x|\theta) \xrightarrow{\text{(noise)}} \text{samples}$$

- Generation may be performed by directly drawing from the pdf (e.g. when cdf is known)
- MCMC techniques when no direct sampling is possible (Metropolis-Hasting, Gibbs Sampling, Affine Invariant, etc.)
- Examples in HEP are
  - **MadGraph**
  - **Pythia**
  - …
- Noise may be represented by **Delphes**, Full Detector Sym, etc.

Generative model

A model that learns the underlying PDF from some (train) data. The parameters determining the PDF are not known a priori but are extracted (fit) through the training process.

$$\begin{cases} \text{data} \\ p(\theta|\text{data}) \end{cases} \xrightarrow{\text{fit model}} \begin{cases} \hat{\theta} \\ p(x|\hat{\theta}) \end{cases} \xrightarrow{\text{(noise)}} \text{samples}$$

- The PDF estimated from data is rarely known analytically so that sampling is usually performed with dedicated techniques
- Examples are
  - Normalizing flows (density estimation for free)
  - Generative Adversarial Networks (GANs)
  - Variational AutoEncoders (VAEs)
  - Autoregressive models/Transformers (GPTs)
  - Diffusion models
  - …

Why do we want generative models?

- No generator exists

  Almost all commercial applications fall in this category (content creation, chatbots, machine translation, etc)

- Generator exists but is too slow/inefficient

  Almost all HEP applications. One may aim at two different results

  - ❑ Increase speed at fixed statistics
  - ❑ Increase statistics at fixed sampling time

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  Almost all HEP applications. One may aim at two different results

  - ☑ ✓ Increase speed at fixed statistics
  - ☐ ✗ Increase statistics at fixed sampling time

  *

*with some caveats

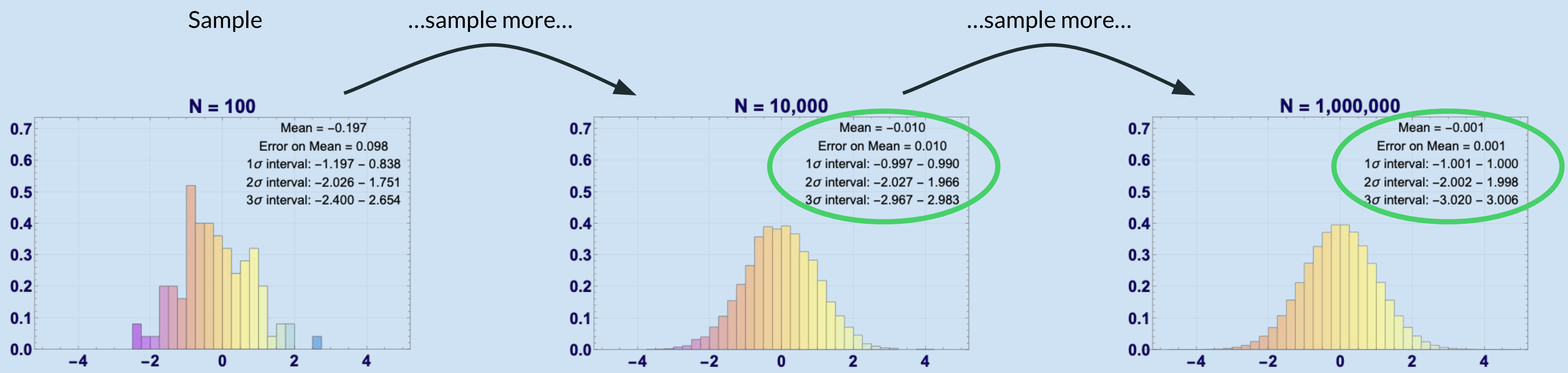
Statistical augmentation: generator

Generator $p(x|\theta) \xrightarrow{\text{(noise)}} \text{samples}$

- **Unbiased** sampling is possible (either through "exact" methods or MCMC)
- Statistics may be increased to reduce statistical uncertainty

$$\sigma_{\mu_{\text{gen}}} = \frac{\sigma_{\text{gen}}}{\sqrt{N_{\text{gen}}}}$$

- Example: Gaussian model with zero mean and unit variance (simplest possible generator)



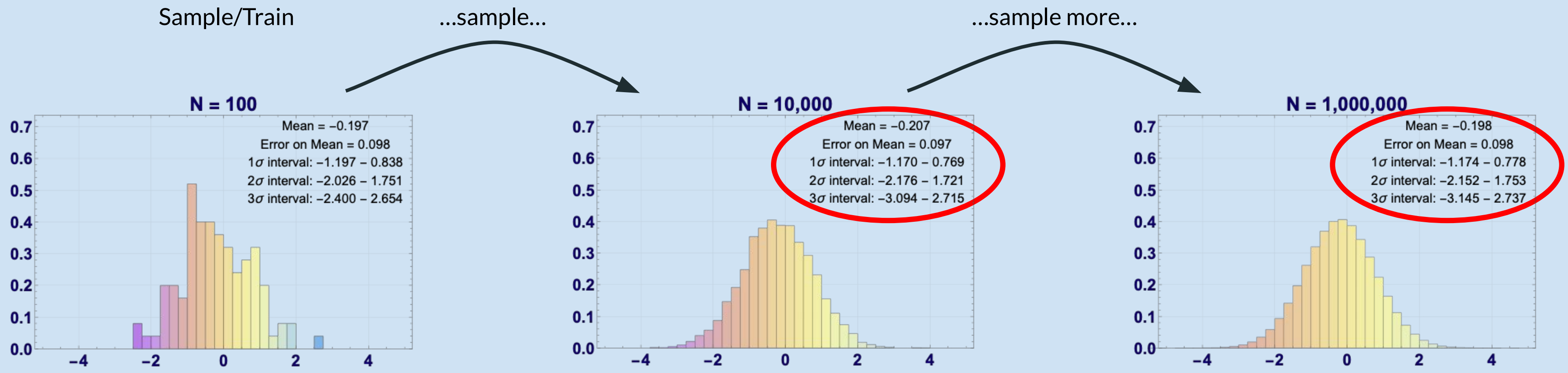
Statistical augmentation: GM

Generative model $\left\{ \begin{array}{l} \text{data} \\ p(\theta|\text{data}) \end{array} \right. \xrightarrow{\text{fit model}} \left\{ \begin{array}{l} \hat{\theta} \\ p(x|\hat{\theta}) \end{array} \right. \xrightarrow{\text{(noise)}} \text{samples}$

- Sampling is conditioned on the **train** data

$$\sigma_{\mu_{\text{gen}}} \approx \frac{\sigma_{\text{gen}}}{\sqrt{N_{\text{train}}}}$$

- Even though statistics increases, the uncertainty does not decrease for $N_{\text{gen}} \gg N_{\text{train}}$
- Example: Gaussian model fit to 100 points: **population mean/variance** are the **best unbiased estimators** of the mean/variance (simplest possible generative model, can even be sampled exactly!)



In practice it is even worse!

We now have an upper limit on the "fidelity" that a Generative Model can have:

*Samples generated by the **best** possible **Generative Model** are **indistinguishable** from samples generated by a generator built from the **true underlying model** within a **statistical uncertainty** determined by the size of the **training sample***

Reality is different and is affected by several effects:

- Data modeling: underlying model is generally not known
- Training efficiency: depending on the architecture, number of parameters, structure of the Generative Model, training, which usually is a numerical optimization task, may not yield the best result
- Hyperparameters: optimization of the GM may be difficult due to several hyperparameters on which it depends
- Noise in train data: data may contain further noise that "fool" the training procedure
- …

How do we evaluate fidelity of GMs?

This question obviously depends on some other questions:

- which level of precision do we need?
- on which observable do we need such precision?

The level of precision required in scientific applications is usually far above the one required in commercial ones!

A common strategy is to perform two-sample hypothesis testing

The approach depends on the information we have:

1. Both the generator and the GM PDFs are known (as for the Gaussians models)
2. PDFs are not known but we can generate both with some original generator and with the GM
3. We have a finite sample from the original distribution and can only draw samples with the GM

Two-sample hypothesis testing

Data: $x \sim p \mapsto X = \{x_i\},\ i = 1, \dots n,$
$y \sim q \mapsto Y = \{y_j\},\ j = 1, \dots m$

Hypothesis: $H_0 : p = q,$
$H_1 : p \neq q$

Test statistic: $t : (\mathcal{X})^n \times (\mathcal{X})^m \to \mathbb{R}$

Observation: $t_{\rm obs} = t(X, Y)$

Threshold: $\alpha = P(t \geq t_\alpha | H_0) = \int_{t_\alpha}^{\infty} f(t|H_0) dt$

p-value/Z-score: $\mathrm{p}_{\rm obs} = P(t \geq t_{\rm obs} | H_0),$ $\mathrm{Z}_{\rm obs} = \Phi^{-1}(1 - \mathrm{p}_{\rm obs})$

- Depending on the scenario the **null distribution** is computed with different techniques: Monte Carlo, re-sampling, etc.
- Two-sample tests are usually symmetric in *p* and *q*; adapting to a **goodness-of-fit testing** framework we turn *p* into a **reference** and *q* into an **alternative** (asymmetric test)

New hypothesis: $H_0 : X, Y \sim p$
$H_1 : X \sim p,\ Y \sim q$

Our approach

- **Non-parametric** two-sample testing beyond 1D is an open problem in statistics, due to the **curse of dimensionality** (volume grows exponentially, data become sparse, and tests loose power)
- Whenever available, **(log-)Likelihood-ratio** (LLR) is the **most powerful** test thanks to the **Neyman-Pearson** lemma (obviously LLR is a **parametric** test)
- Tests based on **classifiers** (Neural Networks, Kernel Methods, etc.) can approximate the LLR when it is not known (see A. Wulzer talk)
- Our goals are
  - Introduce a methodology to **test tests**
  - Test performance of efficient metrics based on **1D integral probability measures** (IPMs) such as Wasserstein Distance or KS test
  - Compare with **existing multivariate metrics**

The metrics

$$t_{\mathrm{SW}} = \frac{1}{K}\sum_{\theta\in\Omega_K}\left(\frac{1}{n}\sum_{i=1}^{n} |\, \underline{x}_i^{\theta} - \underline{x}_i^{\prime\theta} \,|\right)$$

Sliced Wasserstein distance (SW)

$$t_{\overline{\mathrm{KS}}} = \frac{1}{d}\sum_{I=1}^{d}\sqrt{\frac{nm}{n+m}}\,\sup_u |\, F_n^I(u) - G_m^I(u)|$$

Dimension averaged KS test ($\overline{\mathrm{KS}}$)

$$t_{\mathrm{SKS}} = \frac{1}{K}\sum_{\theta\in\Omega_K}\sqrt{\frac{nm}{n+m}}\,\sup_u |\, F_n^{\theta}(u) - G_m^{\theta}(u)\,|$$

Sliced KS test (SKS)

$$t_{\mathrm{MMD}} = \frac{1}{n(n-1)}\sum_{i=1}^{n}\sum_{j\neq i}^{n} k(x_i, x_j) + \frac{1}{m(m-1)}\sum_{i=1}^{m}\sum_{j\neq i}^{m} k(y_i, y_j) - \frac{2}{nm}\sum_{i=1}^{n}\sum_{j=1}^{m} k(x_i, y_j)\ ,$$

$$\text{with: } k(x, x') = \left(\frac{1}{d}x^T x' + 1\right)^4$$

Maximum Mean Discrepancy (MMD)

$$t_{\mathrm{FGD}} = \lim_{n,m\to\infty}\sum_{I=1}^{d}(\mu_{1,n}^I - \mu_{2,m}^I)^2 + \mathrm{tr}\left(\Sigma_{1,n} + \Sigma_{2,m} - 2\sqrt{\Sigma_{1,n}\Sigma_{2,m}}\right)$$

Fréchet Gaussian Distance (FGD)

$$t_{\mathrm{LLR}} = -2\log\frac{\mathcal{L}_{H_0}}{\mathcal{L}_{H_1}}$$

Log Likelihood Ratio (LLR)

Our methodology

- Start from **reference** p, and use it to compute the **null distribution**
- Define an **alternative** q by deforming p with well defined **deformations** depending on a **single parameter** $\boldsymbol{\varepsilon}$
- Since tests have very different performance for different sample size and deformation do not compare them at fixed ε, but at "**fixed precision**"
- In other words, build a meaningful comparison close to a **decision boundary** (in the same region of the null distribution)
- For **each deformation and sample size**, compute the **value of $\boldsymbol{\varepsilon}$ excluded** at some **Confidence Level** by each metric

Optimization problem

Given a value of the CL 1-α, there are two different optimization problems depending on whether the test is parametric or not

1. For non-parametric tests the null hypothesis **does not depend** on the alternative (deformed) distribution, and therefore on ε

$$\epsilon_\alpha = \arg\min_{\epsilon} \left| t(\epsilon) - t_0^\alpha \right|$$

2. For parametric (LLR) test, also the null hypothesis **depends** on the alternative distribution, and therefore on ε

$$\epsilon_\alpha = \arg\min_{\epsilon} \left| t(\epsilon) - t_0^\alpha(\epsilon) \right|$$

All tests have been performed for 95% and 99% CL and for varying sample size

Distributions/deformations

Toy distributions

- *d* dimensional multivariate Correlated Gaussians (CG) - *d* = 5, 20, 100
- mixture of *q* components *d* dimensional multivariate Gaussians (MoG) - (*d*,*q*) = (5,3), (20,5), (100,10)

N = 10K, 20K, 50K, 100K with Monte Carlo

Physics Datasets

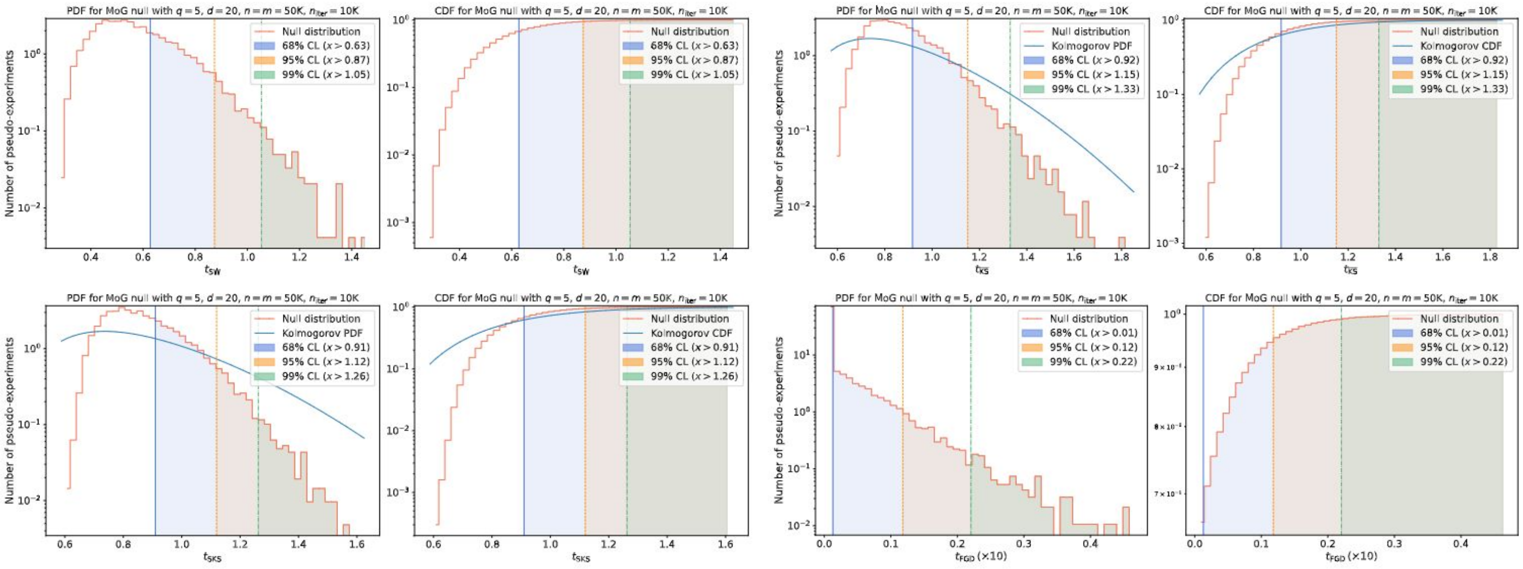
- JetNet gluon dataset with jet level features
- JetNet gluon dataset with (30) particle level features

N = 10K, 20K, 50K with re-sampling

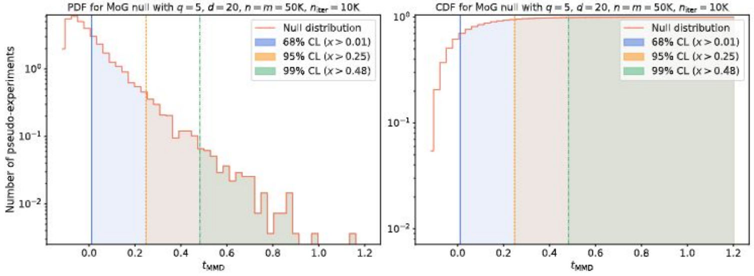
Deformations

$$
\begin{array}{llll}
(1) & \mu\text{-deformation}: & y_{iI} = x_{iI} + \delta_{\mu\, I}, & \delta_{\mu I} \sim \mathcal{U}_{[-\epsilon,\epsilon]} \\
(2) & \Sigma_{II}\text{-deformation}: & y_{iI} = \mu_I + c_{\Sigma I}(x_{iI} - \mu_I), & c_{\Sigma I} \sim \mathcal{U}_{[1,1+\epsilon]} \\
(3) & \Sigma_{I\neq I}\text{-deformation}: & y_{iI} = \sum_j P_{ij}^{(I)} x_{jI}, & P_{ij}^{(I)} = P_{ij}^{(I)}(\epsilon) \\
(4) & \text{pow}_{+}\text{-deformation}: & y_{iI} = \text{sign}(x_{iI})|x_{iI}|^{1+\epsilon}, & \epsilon \geq 0 \\
(5) & \text{pow}_{i}\text{-deformation}: & y_{iI} = \text{sign}(x_{iI})|x_{iI}|^{1-\epsilon}, & \epsilon \geq 0 \\
(6) & \mathcal{N}\text{-deformation}: & y_{iI} = x_{iI} + \delta_{iI}, & \delta_{iI} \sim \mathcal{N}_{0,\epsilon} \\
(7) & \mathcal{U}\text{-deformation}: & y_{iI} = x_{iI} + \delta_{iI}, & \delta_{iI} \sim \mathcal{U}_{-\epsilon,\epsilon}
\end{array}
$$

• MoG Toy models: null distributions



Mixture of Gaussians

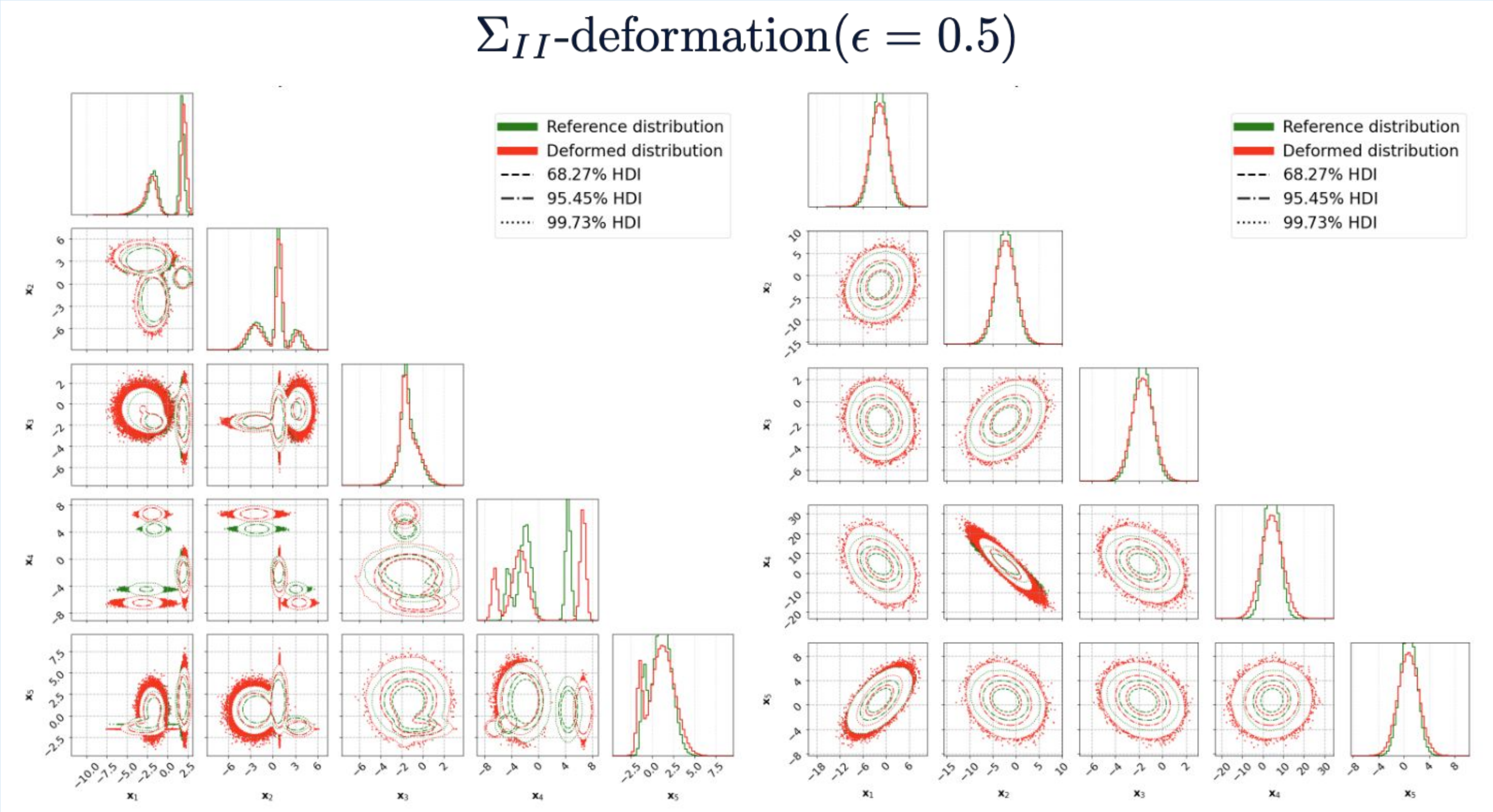


$q = 5,$

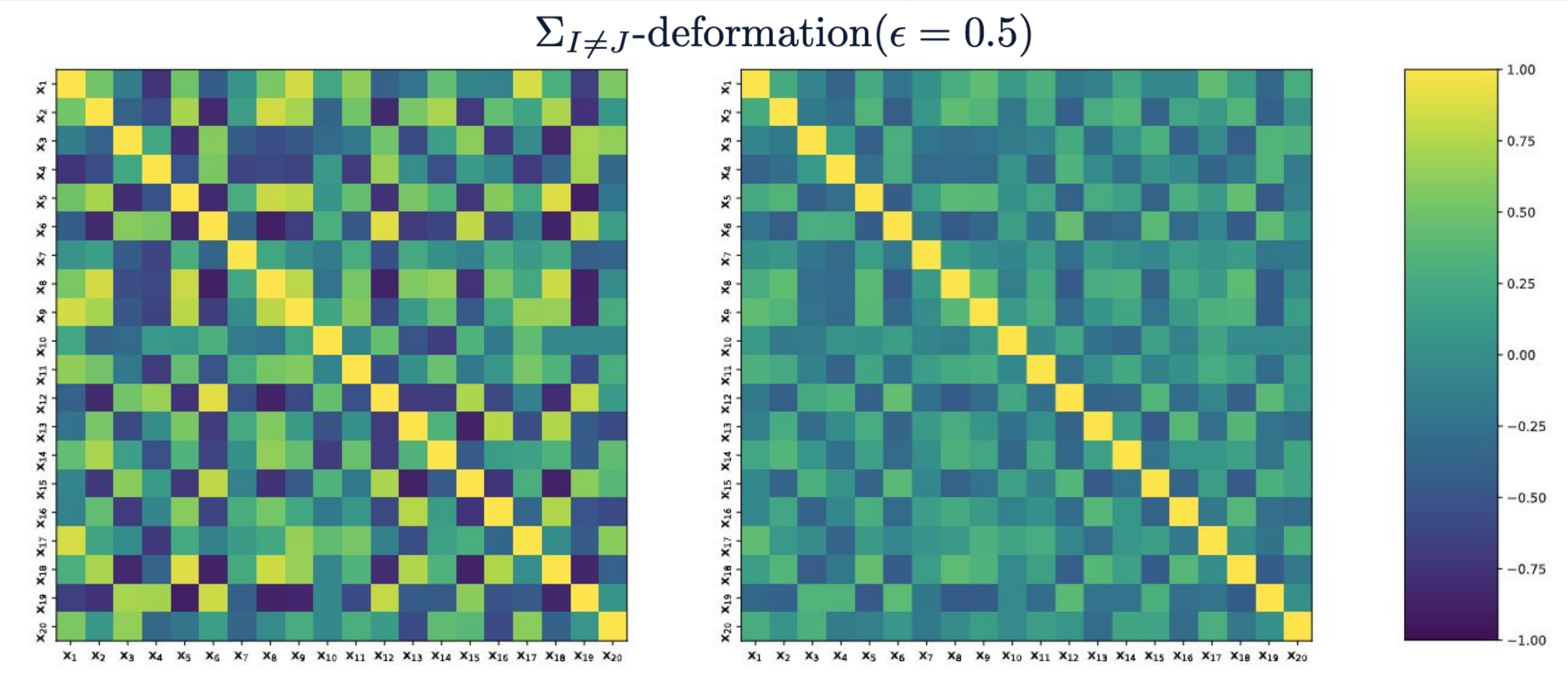
$d = 20,$

$m = n = 5 \cdot 10^4$

Toy models: deformations



Toy models: deformations



Toy models: results

MoG model with $d = 20$, $q = 5$, and $n = m = 5 \cdot 10^4$

	μ-deformation			Σ_{ii}-deformation		
Statistic	$\epsilon_{95\%CL}$	$\epsilon_{99\%CL}$	t (s)	$\epsilon_{95\%CL}$	$\epsilon_{99\%CL}$	t (s)
t_{SW}	$0.04957^{+0.018}_{-0.02}$	$0.06694^{+0.017}_{-0.017}$	3023	$0.01679^{+0.005}_{-0.0063}$	$0.02315^{+0.0045}_{-0.005}$	3197
$t_{\overline{\mathrm{KS}}}$	**$0.00482^{+0.0013}_{-0.0018}$**	**$0.00667^{+0.0011}_{-0.0013}$**	2966	**$0.00175^{+0.00052}_{-0.00068}$**	**$0.00248^{+0.00042}_{-0.00052}$**	3185
t_{SKS}	$0.03647^{+0.011}_{-0.014}$	$0.04821^{+0.011}_{-0.012}$	**2899**	$0.01329^{+0.003}_{-0.0043}$	$0.01759^{+0.0025}_{-0.003}$	**3022**
t_{FGD}	$0.05778^{+0.026}_{-0.027}$	$0.0787^{+0.023}_{-0.021}$	4047	$0.01945^{+0.0063}_{-0.0081}$	$0.02651^{+0.0053}_{-0.0056}$	4507
t_{MMD}	$0.04425^{+0.019}_{-0.018}$	$0.06215^{+0.017}_{-0.015}$	10204	$0.00923^{+0.0058}_{-0.0051}$	$0.01305^{+0.0053}_{-0.0044}$	11217
t_{LLR}	$0.00021^{+0.00013}_{-0.00014}$	$0.0003^{+0.00013}_{-0.00014}$	5911	$0.00007^{+0.00005}_{-0.00004}$	$0.0001^{+0.00005}_{-0.00004}$	6304

	$\Sigma_{i\neq j}$-deformation			pow_{+}-deformation		
Statistic	$\epsilon_{95\%CL}$	$\epsilon_{99\%CL}$	t (s)	$\epsilon_{95\%CL}$	$\epsilon_{99\%CL}$	t (s)
t_{SW}	$0.02162^{+0.0056}_{-0.008}$	$0.02935^{+0.0045}_{-0.0055}$	**3410**	$0.00581^{+0.0017}_{-0.0022}$	$0.00798^{+0.0015}_{-0.0017}$	**3157**
$t_{\overline{\mathrm{KS}}}$	$1.00146^{+0.00074}_{-0.00031}$	$1.00238^{+0.00055}_{-0.00031}$	3967	**$0.0004^{+0.00015}_{-0.00017}$**	**$0.00059^{+0.00013}_{-0.00014}$**	3363
t_{SKS}	$0.02306^{+0.0071}_{-0.0088}$	$0.03079^{+0.0062}_{-0.0072}$	3553	$0.0043^{+0.0009}_{-0.0013}$	$0.00565^{+0.00074}_{-0.0009}$	3193
t_{FGD}	**$0.00551^{+0.0015}_{-0.002}$**	**$0.00748^{+0.0013}_{-0.0013}$**	6327	$0.00702^{+0.0021}_{-0.0028}$	$0.00965^{+0.0016}_{-0.0019}$	4870
t_{MMD}	$0.01723^{+0.008}_{-0.0072}$	$0.02431^{+0.0069}_{-0.0064}$	11450	$0.00332^{+0.0018}_{-0.0017}$	$0.00467^{+0.0017}_{-0.0014}$	11801
t_{LLR}	-	-	-	$0.00002^{+0.00001}_{-0.00001}$	$0.00002^{+0.00001}_{-0.00001}$	6877

	pow_{-}-deformation			$\mathcal{N}$-deformation		
Statistic	$\epsilon_{95\%CL}$	$\epsilon_{99\%CL}$	t (s)	$\epsilon_{95\%CL}$	$\epsilon_{99\%CL}$	t (s)
t_{SW}	$0.00604^{+0.0017}_{-0.0023}$	$0.00825^{+0.0016}_{-0.0018}$	**3051**	$0.19318^{+0.025}_{-0.039}$	$0.22704^{+0.019}_{-0.026}$	**2403**
$t_{\overline{\mathrm{KS}}}$	**$0.00042^{+0.00015}_{-0.00018}$**	**$0.00061^{+0.00013}_{-0.00015}$**	3372	**$0.00751^{+0.002}_{-0.0024}$**	**$0.00993^{+0.0018}_{-0.002}$**	2934
t_{SKS}	$0.00441^{+0.00092}_{-0.0014}$	$0.00574^{+0.00077}_{-0.00094}$	3324	$0.15874^{+0.023}_{-0.034}$	$0.18473^{+0.019}_{-0.023}$	2726
t_{FGD}	$0.00722^{+0.0021}_{-0.0027}$	$0.00987^{+0.0016}_{-0.0019}$	4892	$0.18095^{+0.023}_{-0.038}$	$0.21269^{+0.016}_{-0.02}$	3756
t_{MMD}	$0.00353^{+0.0016}_{-0.0015}$	$0.00494^{+0.0014}_{-0.0012}$	11418	$0.43531^{+0.066}_{-0.11}$	$0.51609^{+0.045}_{-0.054}$	8642
t_{LLR}	$0.00002^{+0.00001}_{-0.00001}$	$0.00002^{+0.00001}_{-0.00001}$	6991	-	-	-

	$\mathcal{U}$-deformation			Timing
Statistic	$\epsilon_{95\%CL}$	$\epsilon_{99\%CL}$	t (s)	t^{null} (s)
t_{SW}	$0.33394^{+0.044}_{-0.068}$	$0.39248^{+0.033}_{-0.044}$	**2354**	338
$t_{\overline{\mathrm{KS}}}$	**$0.01211^{+0.003}_{-0.0035}$**	**$0.01575^{+0.0027}_{-0.003}$**	2835	**155**
t_{SKS}	$0.27395^{+0.041}_{-0.059}$	$0.3188^{+0.033}_{-0.04}$	2601	509
t_{FGD}	$0.31409^{+0.04}_{-0.07}$	$0.36919^{+0.027}_{-0.036}$	3643	2795
t_{MMD}	$0.75353^{+0.12}_{-0.18}$	$0.89336^{+0.078}_{-0.098}$	7700	13860
t_{LLR}	-	-	-	-

CG model with $d = 20$ and $n = m = 5 \cdot 10^4$

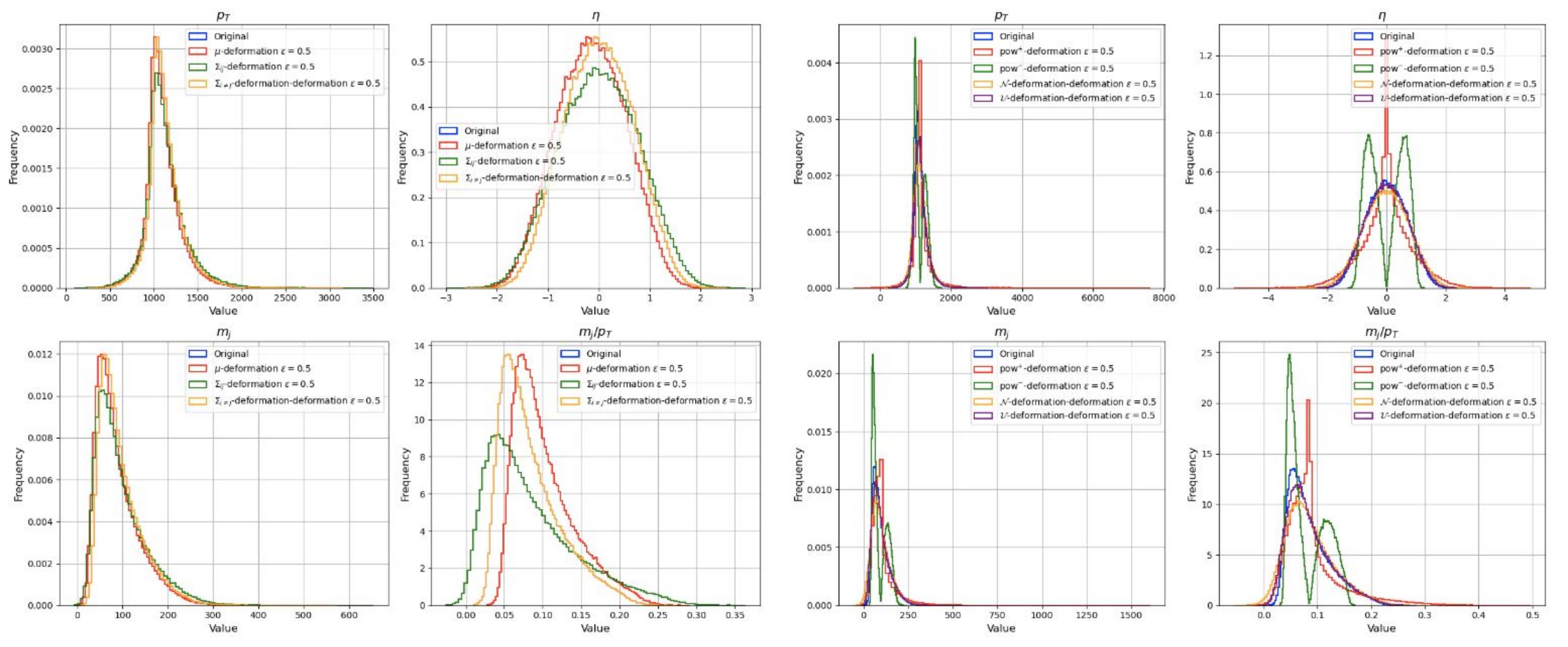
	μ-deformation			Σ_{ii}-deformation		
Statistic	$\epsilon_{95\%CL}$	$\epsilon_{99\%CL}$	t (s)	$\epsilon_{95\%CL}$	$\epsilon_{99\%CL}$	t (s)
t_{SW}	$0.04948^{+0.022}_{-0.021}$	$0.06621^{+0.021}_{-0.02}$	571	$0.02059^{+0.0066}_{-0.0078}$	$0.02732^{+0.0061}_{-0.0065}$	617
$t_{\overline{\mathrm{KS}}}$	**$0.04811^{+0.022}_{-0.021}$**	$0.06605^{+0.021}_{-0.02}$	**407**	$0.02898^{+0.011}_{-0.012}$	$0.04029^{+0.0097}_{-0.01}$	**434**
t_{SKS}	$0.04841^{+0.021}_{-0.021}$	**$0.06372^{+0.02}_{-0.02}$**	655	$0.02623^{+0.0087}_{-0.01}$	$0.03417^{+0.0082}_{-0.0086}$	694
t_{FGD}	$0.05029^{+0.026}_{-0.022}$	$0.06539^{+0.024}_{-0.02}$	1886	**$0.01695^{+0.007}_{-0.007}$**	**$0.02215^{+0.0065}_{-0.0059}$**	1994
t_{MMD}	$0.0596^{+0.028}_{-0.02}$	$0.08041^{+0.026}_{-0.02}$	7733	$0.02325^{+0.011}_{-0.0079}$	$0.03109^{+0.01}_{-0.0079}$	8173
t_{LLR}	$0.00556^{+0.0031}_{-0.003}$	$0.00795^{+0.003}_{-0.003}$	2441	$0.00153^{+0.001}_{-0.00098}$	$0.0022^{+0.00098}_{-0.00099}$	3081

	$\Sigma_{i\neq j}$-deformation			pow_{+}-deformation		
Statistic	$\epsilon_{95\%CL}$	$\epsilon_{99\%CL}$	t (s)	$\epsilon_{95\%CL}$	$\epsilon_{99\%CL}$	t (s)
t_{SW}	$0.02783^{+0.0077}_{-0.0099}$	$0.03884^{+0.0064}_{-0.0076}$	**1073**	$0.0046^{+0.0017}_{-0.0019}$	$0.00614^{+0.0016}_{-0.0017}$	642
$t_{\overline{\mathrm{KS}}}$	$1.02831^{+0.015}_{-0.015}$	$1.04211^{+0.0046}_{-0.012}$	1401	$0.00602^{+0.002}_{-0.0024}$	$0.00806^{+0.0019}_{-0.0019}$	**459**
t_{SKS}	$0.03839^{+0.011}_{-0.014}$	$0.05106^{+0.01}_{-0.012}$	1172	$0.00505^{+0.0017}_{-0.002}$	$0.00646^{+0.0016}_{-0.0017}$	747
t_{FGD}	**$0.00483^{+0.0012}_{-0.0014}$**	**$0.00631^{+0.0011}_{-0.0011}$**	3433	$0.00419^{+0.0019}_{-0.0018}$	$0.0054^{+0.0017}_{-0.0015}$	2765
t_{MMD}	$0.03094^{+0.017}_{-0.013}$	$0.04245^{+0.016}_{-0.013}$	8963	**$0.00358^{+0.0018}_{-0.0012}$**	**$0.00483^{+0.0016}_{-0.0013}$**	8839
t_{LLR}	-	-	-	$0.00042^{+0.00025}_{-0.00026}$	$0.00061^{+0.00025}_{-0.00025}$	2919

	pow_{-}-deformation			$\mathcal{N}$-deformation		
Statistic	$\epsilon_{95\%CL}$	$\epsilon_{99\%CL}$	t (s)	$\epsilon_{95\%CL}$	$\epsilon_{99\%CL}$	t (s)
t_{SW}	$0.00455^{+5}_{-0.0017}$	$0.00609^{+5}_{-0.0015}$	587	$0.28641^{+0.047}_{-0.065}$	$0.33654^{+0.037}_{-0.046}$	535
$t_{\overline{\mathrm{KS}}}$	$0.00575^{+0.002}_{-0.0022}$	$0.00773^{+0.0018}_{-0.0019}$	**461**	$0.32182^{+0.055}_{-0.08}$	$0.3832^{+0.045}_{-0.054}$	**393**
t_{SKS}	$0.00487^{+0.0017}_{-0.0019}$	$0.00632^{+0.0016}_{-0.0017}$	750	$0.28237^{+0.046}_{-0.066}$	$0.32811^{+0.038}_{-0.048}$	612
t_{FGD}	$0.00411^{+0.0017}_{-0.0015}$	$0.0054^{+0.0015}_{-0.0014}$	2758	**$0.16992^{+0.02}_{-0.03}$**	**$0.1944^{+0.014}_{-0.018}$**	2132
t_{MMD}	**$0.00346^{+0.0019}_{-0.0014}$**	**$0.00477^{+0.0018}_{-0.0014}$**	8990	$0.73852^{+0.086}_{-0.091}$	$0.85602^{+0.075}_{-0.062}$	5790
t_{LLR}	$0.00042^{+0.00025}_{-0.00026}$	$0.0006^{+0.00025}_{-0.00025}$	2930	-	-	-

	$\mathcal{U}$-deformation			Timing
Statistic	$\epsilon_{95\%CL}$	$\epsilon_{99\%CL}$	t (s)	t^{null} (s)
t_{SW}	$0.49513^{+0.079}_{-0.11}$	$0.5818^{+0.063}_{-0.078}$	512	313
$t_{\overline{\mathrm{KS}}}$	$0.55562^{+0.096}_{-0.14}$	$0.65585^{+0.083}_{-0.089}$	**378**	**127**
t_{SKS}	$0.48849^{+0.085}_{-0.11}$	$0.56476^{+0.072}_{-0.079}$	582	480
t_{FGD}	**$0.2926^{+0.036}_{-0.05}$**	**$0.33697^{+0.025}_{-0.034}$**	2042	3821
t_{MMD}	$1.28521^{+0.15}_{-0.17}$	$1.49004^{+0.11}_{-0.12}$	6502	13843
t_{LLR}	-	-	-	-

JetNet datasets: deformations



JetNet jet features: results

Jet features with $\mathbf{n = m = 5 \cdot 10^4}$

	μ-deformation			Σ_{ii}-deformation		
Statistic	$\epsilon_{95\%\text{CL}}$	$\epsilon_{99\%\text{CL}}$	t (s)	$\epsilon_{95\%\text{CL}}$	$\epsilon_{99\%\text{CL}}$	t (s)
t_{SW}	$0.03049^{+0.019}_{-0.013}$	$0.04713^{+0.015}_{-0.015}$	**1108**	$0.04623^{+0.017}_{-0.025}$	$0.06323^{+0.019}_{-0.015}$	**1141**
$t_{\overline{\text{KS}}}$	$\mathbf{0.01585^{+0.0043}_{-0.0063}}$	$\mathbf{0.01927^{+0.0043}_{-0.0056}}$	17004	$\mathbf{0.02085^{+0.0064}_{-0.008}}$	$\mathbf{0.02567^{+0.006}_{-0.0075}}$	21589
t_{SKS}	$0.02815^{+0.013}_{-0.014}$	$0.03444^{+0.012}_{-0.014}$	35328	$0.04838^{+0.018}_{-0.019}$	$0.06304^{+0.016}_{-0.02}$	27128
t_{FGD}	$0.03986^{+0.025}_{-0.013}$	$0.06157^{+0.019}_{-0.017}$	11779	$0.04333^{+0.028}_{-0.023}$	$0.05934^{+0.027}_{-0.022}$	18470
t_{MMD}	$0.04941^{+0.034}_{-0.021}$	$0.0712^{+0.03}_{-0.022}$	78077	$0.07669^{+0.072}_{-0.035}$	$0.11237^{+0.068}_{-0.035}$	71427
	$\Sigma_{i\neq j}$-deformation			pow_{+}-deformation		
Statistic	$\epsilon_{95\%\text{CL}}$	$\epsilon_{99\%\text{CL}}$	t (s)	$\epsilon_{95\%\text{CL}}$	$\epsilon^{\text{pow}_+}_{99\%\text{CL}}$	t (s)
t_{SW}	$0.30801^{+0.08}_{-0.11}$	$0.45956^{+0.071}_{-0.063}$	**1033**	$0.02535^{+0.0077}_{-0.011}$	$0.03745^{+0.0066}_{-0.0084}$	**1028**
$t_{\overline{\text{KS}}}$	$1.01892^{+0.0084}_{-0.01}$	$1.02245^{+0.011}_{-0.0035}$	19934	$\mathbf{0.0232^{+0.0074}_{-0.011}}$	$\mathbf{0.02698^{+0.01}_{-0.0092}}$	35049
t_{SKS}	$0.2959^{+0.12}_{-0.12}$	$0.40074^{+0.11}_{-0.054}$	32727	$0.02709^{+0.014}_{-0.012}$	$0.03452^{+0.017}_{-0.012}$	28409
t_{FGD}	$\mathbf{0.22063^{+0.053}_{-0.082}}$	$\mathbf{0.29862^{+0.045}_{-0.052}}$	13459	$0.02454^{+0.015}_{-0.014}$	$0.0321^{+0.017}_{-0.012}$	11640
t_{MMD}	$0.80374^{+0.26}_{-0.28}$	$1.05932^{+0.078}_{-0.1}$	31136	$0.02933^{+0.019}_{-0.015}$	$0.03749^{+0.021}_{-0.016}$	54684
	pow_{-}-deformation			$\mathcal{N}$-deformation		
Statistic	$\epsilon_{95\%\text{CL}}$	$\epsilon^{\text{pow}_-}_{99\%\text{CL}}$	t (s)	$\epsilon_{95\%\text{CL}}$	$\epsilon^{\mathcal{N}}_{99\%\text{CL}}$	t (s)
t_{SW}	$0.02553^{+0.0078}_{-0.0088}$	$0.03665^{+0.0074}_{-0.0068}$	**1080**	$0.12904^{+0.029}_{-0.034}$	$0.16235^{+0.02}_{-0.025}$	**981**
$t_{\overline{\text{KS}}}$	$\mathbf{0.02125^{+0.01}_{-0.0092}}$	$\mathbf{0.02649^{+0.0074}_{-0.009}}$	15925	$\mathbf{0.10579^{+0.014}_{-0.019}}$	$\mathbf{0.11672^{+0.012}_{-0.016}}$	28786
t_{SKS}	$0.02682^{+0.012}_{-0.012}$	$0.03607^{+0.01}_{-0.012}$	47622	$0.11163^{+0.022}_{-0.023}$	$0.12765^{+0.017}_{-0.023}$	38615
t_{FGD}	$0.02511^{+0.017}_{-0.012}$	$0.03353^{+0.016}_{-0.01}$	18451	$0.16887^{+0.046}_{-0.052}$	$0.19783^{+0.043}_{-0.036}$	13634
t_{MMD}	$0.03^{+0.02}_{-0.014}$	$0.04112^{+0.021}_{-0.012}$	39156	$0.25305^{+0.085}_{-0.11}$	$0.29551^{+0.081}_{-0.073}$	52861
	$\mathcal{U}$-deformation			Timing		
Statistic	$\epsilon_{95\%\text{CL}}$	$\epsilon^{\mathcal{U}}_{99\%\text{CL}}$	t (s)	t^{null} (s)		
t_{SW}	$0.22631^{+0.05}_{-0.064}$	$0.27734^{+0.044}_{-0.039}$	**916**	**129**		
$t_{\overline{\text{KS}}}$	$\mathbf{0.18246^{+0.022}_{-0.032}}$	$\mathbf{0.19931^{+0.018}_{-0.027}}$	32276	1907		
t_{SKS}	$0.18837^{+0.033}_{-0.048}$	$0.21334^{+0.027}_{-0.029}$	38491	4382		
t_{FGD}	$0.27796^{+0.1}_{-0.074}$	$0.34469^{+0.068}_{-0.062}$	19098	1794		
t_{MMD}	$0.49303^{+0.16}_{-0.18}$	$0.57279^{+0.12}_{-0.11}$	55838	3504		

Scaled Jet features with $\mathbf{n = m = 5 \cdot 10^4}$

	μ-deformation			Σ_{ii}-deformation		
Statistic	$\epsilon_{95\%\text{CL}}$	$\epsilon_{99\%\text{CL}}$	t (s)	$\epsilon_{95\%\text{CL}}$	$\epsilon_{99\%\text{CL}}$	t (s)
t_{SW}	$0.01623^{+0.0045}_{-0.0069}$	$0.02098^{+0.0049}_{-0.0059}$	12410	$0.02089^{+0.0073}_{-0.008}$	$0.02834^{+0.0077}_{-0.0079}$	**1054**
$t_{\overline{\text{KS}}}$	$0.01585^{+0.0043}_{-0.0063}$	$0.01927^{+0.0043}_{-0.0056}$	17174	$\mathbf{0.02085^{+0.0064}_{-0.008}}$	$\mathbf{0.02567^{+0.006}_{-0.0075}}$	38871
t_{SKS}	$\mathbf{0.0113^{+0.0044}_{-0.005}}$	$\mathbf{0.0141^{+0.0037}_{-0.0045}}$	32620	$0.02254^{+0.0074}_{-0.0099}$	$0.02773^{+0.0073}_{-0.0089}$	28803
t_{FGD}	$0.02106^{+0.0062}_{-0.0079}$	$0.02659^{+0.0058}_{-0.0069}$	**11583**	$0.02133^{+0.0078}_{-0.0097}$	$0.02741^{+0.0071}_{-0.008}$	14254
t_{MMD}	$0.06739^{+0.013}_{-0.021}$	$0.08802^{+0.013}_{-0.011}$	46972	$0.0318^{+0.015}_{-0.0083}$	$0.04328^{+0.014}_{-0.012}$	28709
	$\Sigma_{i\neq j}$-deformation			pow_{+}-deformation		
Statistic	$\epsilon_{95\%\text{CL}}$	$\epsilon_{99\%\text{CL}}$	t (s)	$\epsilon_{95\%\text{CL}}$	$\epsilon^{\text{pow}_+}_{99\%\text{CL}}$	t (s)
t_{SW}	$0.0503^{+0.016}_{-0.019}$	$0.07052^{+0.015}_{-0.014}$	**1008**	$0.02465^{+0.011}_{-0.0081}$	$0.03314^{+0.0099}_{-0.0095}$	**1025**
$t_{\overline{\text{KS}}}$	$1.02009^{+0.0072}_{-0.001}$	$1.02812^{+0.003}_{-0.008}$	16410	$0.0232^{+0.0074}_{-0.011}$	$0.02698^{+0.01}_{-0.0092}$	35198
t_{SKS}	$0.06201^{+0.02}_{-0.029}$	$0.07573^{+0.02}_{-0.024}$	35383	$0.0402^{+0.015}_{-0.015}$	$0.04921^{+0.015}_{-0.015}$	47807
t_{FGD}	$\mathbf{0.00627^{+0.0016}_{-0.0018}}$	$\mathbf{0.00809^{+0.0015}_{-0.0018}}$	14008	$0.02237^{+0.013}_{-0.011}$	$0.0281^{+0.011}_{-0.0084}$	24967
t_{MMD}	$0.0794^{+0.039}_{-0.031}$	$0.112^{+0.031}_{-0.026}$	29620	$\mathbf{0.01898^{+0.012}_{-0.0094}}$	$\mathbf{0.02472^{+0.012}_{-0.0076}}$	66075
	pow_{-}-deformation			$\mathcal{N}$-deformation		
Statistic	$\epsilon_{95\%\text{CL}}$	$\epsilon^{\text{pow}_-}_{99\%\text{CL}}$	t (s)	$\epsilon_{95\%\text{CL}}$	$\epsilon^{\mathcal{N}}_{99\%\text{CL}}$	t (s)
t_{SW}	$0.02527^{+0.011}_{-0.011}$	$0.03513^{+0.0084}_{-0.01}$	**993**	$0.11836^{+0.027}_{-0.028}$	$0.14062^{+0.018}_{-0.026}$	**910**
$t_{\overline{\text{KS}}}$	$\mathbf{0.02125^{+0.01}_{-0.0092}}$	$\mathbf{0.02649^{+0.0074}_{-0.009}}$	16472	$0.10579^{+0.014}_{-0.019}$	$0.11672^{+0.012}_{-0.016}$	31727
t_{SKS}	$0.03986^{+0.013}_{-0.017}$	$0.04873^{+0.013}_{-0.013}$	27407	$0.08577^{+0.024}_{-0.028}$	$0.10148^{+0.021}_{-0.026}$	25899
t_{FGD}	$0.02163^{+0.015}_{-0.0097}$	$0.02954^{+0.014}_{-0.0087}$	12892	$\mathbf{0.07833^{+0.0094}_{-0.019}}$	$\mathbf{0.08847^{+0.0084}_{-0.0069}}$	13246
t_{MMD}	$0.02133^{+0.013}_{-0.0086}$	$0.02924^{+0.011}_{-0.0081}$	68458	$0.26032^{+0.037}_{-0.057}$	$0.29897^{+0.028}_{-0.036}$	42149
	$\mathcal{U}$-deformation			Timing		
Statistic	$\epsilon_{95\%\text{CL}}$	$\epsilon^{\mathcal{U}}_{99\%\text{CL}}$	t (s)	t^{null} (s)		
t_{SW}	$0.20487^{+0.042}_{-0.048}$	$0.2434^{+0.032}_{-0.035}$	**877**	**123**		
$t_{\overline{\text{KS}}}$	$0.18018^{+0.024}_{-0.035}$	$0.19884^{+0.018}_{-0.027}$	25630	1913		
t_{SKS}	$0.14529^{+0.04}_{-0.056}$	$0.1719^{+0.035}_{-0.048}$	42277	4383		
t_{FGD}	$\mathbf{0.13545^{+0.014}_{-0.032}}$	$\mathbf{0.15299^{+0.015}_{-0.012}}$	12782	1787		
t_{MMD}	$0.45177^{+0.066}_{-0.091}$	$0.52083^{+0.05}_{-0.047}$	56078	3504		

JetNet particle features: results

Particle features with $\mathbf{n = m = 5 \cdot 10^4}$

Statistic	μ-deformation $\epsilon_{95\%CL}$	$\epsilon_{99\%CL}$	t (s)	Σ_{ii}-deformation $\epsilon_{95\%CL}$	$\epsilon_{99\%CL}$	t (s)
t_{SW}	$0.02633^{+0.0098}_{-0.013}$	$0.03714^{+0.0084}_{-0.0097}$	**849**	$0.02913^{+0.012}_{-0.0079}$	$0.04108^{+0.0093}_{-0.011}$	**824**
$t_{\overline{KS}}$	$\mathbf{0.0^{+0.0045}_{-0.0}}$	$\mathbf{0.00771^{+0.0022}_{-0.0068}}$	49525	$\mathbf{0.0^{+0.013}_{-0.0}}$	$\mathbf{0.01904^{+0.0086}_{-0.011}}$	55017
t_{SKS}	$0.01592^{+0.0046}_{-0.0061}$	$0.02334^{+0.0058}_{-0.0059}$	17572	$0.02735^{+0.0049}_{-0.01}$	$0.03362^{+0.0081}_{-0.0071}$	24987
t_{FGD}	$0.04749^{+0.012}_{-0.024}$	$0.06462^{+0.013}_{-0.013}$	30820	$0.04004^{+0.017}_{-0.012}$	$0.0556^{+0.018}_{-0.016}$	25551
t_{MMD}	$0.1396^{+0.1}_{-0.065}$	$0.21274^{+0.071}_{-0.065}$	18527	$0.06988^{+0.048}_{-0.031}$	$0.0986^{+0.037}_{-0.036}$	33217

Statistic	$\Sigma_{i\neq j}$-deformation $\epsilon_{95\%CL}$	$\epsilon_{99\%CL}$	t (s)	pow_+-deformation $\epsilon_{95\%CL}$	$\epsilon^{\text{pow}_+}_{99\%CL}$	t (s)
t_{SW}	$0.04883^{+0.012}_{-0.015}$	$0.06979^{+0.0097}_{-0.016}$	**1966**	$0.02745^{+0.011}_{-0.0075}$	$0.03872^{+0.0088}_{-0.011}$	**806**
$t_{\overline{KS}}$	$0.99933^{+0.0085}_{-0.014}$	$1.01732^{+0.006}_{-0.0079}$	11225	$\mathbf{0.0^{+0.0066}_{-0.0}}$	$\mathbf{0.01141^{+0.0073}_{-0.011}}$	46010
t_{SKS}	$0.04267^{+0.018}_{-0.012}$	$0.06018^{+0.014}_{-0.013}$	29568	$0.03594^{+0.021}_{-0.016}$	$0.05069^{+0.011}_{-0.014}$	24821
t_{FGD}	$\mathbf{0.02641^{+0.0058}_{-0.012}}$	$\mathbf{0.03966^{+0.006}_{-0.0079}}$	28408	$0.02459^{+0.013}_{-0.012}$	$0.03501^{+0.013}_{-0.012}$	25798
t_{MMD}	$0.25965^{+0.068}_{-0.086}$	$0.35327^{+0.073}_{-0.056}$	16061	$0.02054^{+0.014}_{-0.0071}$	$0.02657^{+0.013}_{-0.0091}$	26195

Statistic	pow_--deformation $\epsilon_{95\%CL}$	$\epsilon^{\text{pow}_-}_{99\%CL}$	t (s)	$\mathcal{N}$-deformation $\epsilon_{95\%CL}$	$\epsilon^{\mathcal{N}}_{99\%CL}$	t (s)
t_{SW}	$0.02745^{+0.011}_{-0.014}$	$0.03872^{+0.0088}_{-0.01}$	**809**	$0.10733^{+0.022}_{-0.026}$	$0.13357^{+0.016}_{-0.016}$	**691**
$t_{\overline{KS}}$	$\mathbf{0.0^{+0.0095}_{-0.0}}$	$\mathbf{0.01323^{+0.0069}_{-0.0085}}$	45685	$\mathbf{0.0656^{+0.016}_{-0.053}}$	$\mathbf{0.08707^{+0.013}_{-0.016}}$	7484
t_{SKS}	$0.03777^{+0.015}_{-0.017}$	$0.04837^{+0.014}_{-0.015}$	15966	$0.08456^{+0.013}_{-0.013}$	$0.09935^{+0.0089}_{-0.01}$	18276
t_{FGD}	$0.02241^{+0.019}_{-0.01}$	$0.0353^{+0.019}_{-0.011}$	26549	$0.14608^{+0.034}_{-0.038}$	$0.1758^{+0.023}_{-0.021}$	23330
t_{MMD}	$0.02077^{+0.017}_{-0.01}$	$0.02939^{+0.016}_{-0.0089}$	20263	$0.33827^{+0.088}_{-0.089}$	$0.37964^{+0.091}_{-0.073}$	19908

Statistic	$\mathcal{U}$-deformation $\epsilon_{95\%CL}$	$\epsilon^{\mathcal{U}}_{99\%CL}$	t (s)	Timing t^{null} (s)
t_{SW}	$0.1889^{+0.038}_{-0.046}$	$0.2351^{+0.028}_{-0.04}$	**625**	**150**
$t_{\overline{KS}}$	$\mathbf{0.10693^{+0.022}_{-0.086}}$	$\mathbf{0.14193^{+0.021}_{-0.019}}$	13565	2126
t_{SKS}	$0.14453^{+0.02}_{-0.028}$	$0.17795^{+0.0057}_{-0.023}$	17723	4818
t_{FGD}	$0.25168^{+0.053}_{-0.065}$	$0.30289^{+0.04}_{-0.036}$	23243	7351
t_{MMD}	$0.58039^{+0.17}_{-0.15}$	$0.6876^{+0.14}_{-0.14}$	25557	3880

Scaled Particle features with $\mathbf{n = m = 5 \cdot 10^4}$

Statistic	μ-deformation $\epsilon_{95\%CL}$	$\epsilon_{99\%CL}$	t (s)	Σ_{ii}-deformation $\epsilon_{95\%CL}$	$\epsilon_{99\%CL}$	t (s)
t_{SW}	$0.01334^{+0.0038}_{-0.0046}$	$0.01815^{+0.0037}_{-0.0029}$	**1116**	$0.0166^{+0.0059}_{-0.0063}$	$0.02125^{+0.006}_{-0.0034}$	**1079**
$t_{\overline{KS}}$	$\mathbf{0.0^{+0.0045}_{-0.0}}$	$\mathbf{0.00771^{+0.0022}_{-0.0049}}$	58835	$\mathbf{0.0^{+0.013}_{-0.0}}$	$0.01904^{+0.0086}_{-0.011}$	62555
t_{SKS}	$0.01275^{+0.0034}_{-0.0043}$	$0.01734^{+0.0036}_{-0.0028}$	18356	$0.02131^{+0.007}_{-0.0073}$	$0.02899^{+0.006}_{-0.0047}$	26542
t_{FGD}	$0.01627^{+0.003}_{-0.006}$	$0.02025^{+0.0024}_{-0.0047}$	39057	$0.01469^{+0.0034}_{-0.0057}$	$\mathbf{0.01805^{+0.0043}_{-0.0051}}$	27175
t_{MMD}	$0.01613^{+0.0049}_{-0.0058}$	$0.02141^{+0.0032}_{-0.0035}$	22841	$0.01606^{+0.0074}_{-0.0066}$	$0.02089^{+0.0055}_{-0.0061}$	33730

Statistic	$\Sigma_{i\neq j}$-deformation $\epsilon_{95\%CL}$	$\epsilon_{99\%CL}$	t (s)	pow_+-deformation $\epsilon_{95\%CL}$	$\epsilon^{\text{pow}_+}_{99\%CL}$	t (s)
t_{SW}	$0.03128^{+0.0068}_{-0.011}$	$0.04152^{+0.0061}_{-0.0067}$	**1424**	$0.01894^{+0.0055}_{-0.0072}$	$0.02425^{+0.0068}_{-0.0039}$	**1006**
$t_{\overline{KS}}$	$0.99134^{+0.016}_{-0.0078}$	$1.01532^{+0.008}_{-0.004}$	11987	$\mathbf{0.0^{+0.0066}_{-0.0}}$	$\mathbf{0.01141^{+0.0073}_{-0.011}}$	49091
t_{SKS}	$0.03809^{+0.011}_{-0.013}$	$0.0515^{+0.011}_{-0.0083}$	27313	$0.03552^{+0.0055}_{-0.013}$	$0.04366^{+0.01}_{-0.0066}$	15487
t_{FGD}	$\mathbf{0.0026^{+0.00076}_{-0.00089}}$	$\mathbf{0.00345^{+0.00052}_{-0.00076}}$	33338	$0.01534^{+0.0052}_{-0.0062}$	$0.01886^{+0.0045}_{-0.0055}$	24241
t_{MMD}	$0.01919^{+0.011}_{-0.0079}$	$0.02614^{+0.0089}_{-0.0065}$	20604	$0.01896^{+0.0074}_{-0.008}$	$0.02428^{+0.0068}_{-0.0071}$	27198

Statistic	pow_--deformation $\epsilon_{95\%CL}$	$\epsilon^{\text{pow}_-}_{99\%CL}$	t (s)	$\mathcal{N}$-deformation $\epsilon_{95\%CL}$	$\epsilon^{\mathcal{N}}_{99\%CL}$	t (s)
t_{SW}	$0.01909^{+0.0073}_{-0.0077}$	$0.02693^{+0.0061}_{-0.0068}$	**1006**	$0.10868^{+0.02}_{-0.017}$	$0.1277^{+0.011}_{-0.022}$	**886**
$t_{\overline{KS}}$	$\mathbf{0.0^{+0.0095}_{-0.0}}$	$\mathbf{0.01323^{+0.0069}_{-0.0085}}$	45323	$0.0656^{+0.016}_{-0.049}$	$0.08707^{+0.013}_{-0.019}$	22186
t_{SKS}	$0.0356^{+0.0093}_{-0.013}$	$0.04726^{+0.007}_{-0.011}$	22261	$0.10733^{+0.022}_{-0.017}$	$0.13357^{+0.016}_{-0.026}$	24344
t_{FGD}	$0.01543^{+0.007}_{-0.0065}$	$0.01852^{+0.0068}_{-0.0042}$	24968	$\mathbf{0.04853^{+0.0071}_{-0.0075}}$	$\mathbf{0.05702^{+0.0051}_{-0.006}}$	24273
t_{MMD}	$0.01859^{+0.0085}_{-0.0081}$	$0.02501^{+0.0083}_{-0.0064}$	27960	$0.26953^{+0.035}_{-0.052}$	$0.30333^{+0.029}_{-0.011}$	19782

Statistic	$\mathcal{U}$-deformation $\epsilon_{95\%CL}$	$\epsilon^{\mathcal{U}}_{99\%CL}$	t (s)	Timing t^{null} (s)
t_{SW}	$0.19116^{+0.035}_{-0.03}$	$0.22462^{+0.02}_{-0.039}$	**774**	**133**
$t_{\overline{KS}}$	$0.10693^{+0.022}_{-0.086}$	$0.14193^{+0.021}_{-0.019}$	10646	1972
t_{SKS}	$0.19116^{+0.035}_{-0.03}$	$0.22462^{+0.02}_{-0.039}$	16154	4379
t_{FGD}	$\mathbf{0.08969^{+0.006}_{-0.016}}$	$\mathbf{0.10215^{+0.0042}_{-0.016}}$	21825	6689
t_{MMD}	$0.48398^{+0.032}_{-0.088}$	$0.5512^{+0.022}_{-0.058}$	14676	3605

Full results

- TensorFlow2 code
  https://github.com/TwoSampleTests/GMetrics
- Code and results for toy models:
  https://github.com/TwoSampleTests/GenerativeModelsMetrics
- Code and results for JetNet datasets:
  https://github.com/TwoSampleTests/JetNetMetrics

Summary

- Generative models can replace generators only under specific assumptions
- Being able to evaluate the fidelity of generative models, especially in high dimensionality, is crucial
- We made a step forward defining novel simple and efficient metrics/tests
- We introduced a statistically robust methodology to compare metrics/tests
- We have validated our procedure on several datasets, both using Monte Carlo methods (when the PDFs are known) and resampling methods (when only numerical samples are available)
- We found that simple and efficient (highly parallelizable) extensions of 1D metrics show comparable performance to more complicated multivariate metrics

Thank you for your attention!