

# Precision Simulations Using Machine Learning

Tilman Plehn

Universität Heidelberg

Glasgow, April 2023



# LHC physics vs data scientist

## LHC questions

- How to trigger from 3 PB/s to 300 MB/s?



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Data compression [Netflix]



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- How to analyze events with 4-vectors?



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Simulation-based inference [Edinburgh Ultra-Mini 2007]
- **How to treat uncertainties??**



# Shortest ML-intro ever

## Fit-like approximation [ask NNPDF]

- approximate known  $f(x)$  using  $f_\theta(x)$
- no parametrization, just very many values  $\theta$
- new representation/latent space  $\theta$

## Construction and control

- define loss function
- minimize loss to find best  $\theta$
- compare  $x \rightarrow f_\theta(x)$  for training/test data

## LHC applications

- regression  $x \rightarrow f_\theta(x)$
- classification  $x \rightarrow f_\theta(x) \in [0, 1]$
- generation  $r \sim \mathcal{N} \rightarrow f_\theta(r)$
- conditional generation  $r \sim \mathcal{N} \rightarrow f_\theta(r|x)$
- ...

→ [Transforming numerical science](#)



# Networks with error bar

## Training-related uncertainties

- different trainings  
different initializations  
different data sets
  - histogram network output:  $f_{\theta}(x) \pm \Delta f(x)$
- Bayesian network:  $\Delta f_{\theta}(x)$  from  $\Delta \theta$  [Yarin Gal (2016)]

## Energy measurement with NN

- expectation value from probability distribution

$$\langle E \rangle = \int dE E p(E) \rightarrow \int dE E p_{\theta}(E)$$

- energy  $p(E|\theta)$  encoded in network parameters  
parameters  $p(\theta|T)$  trained on data  $T$

$$p_{\theta}(E) = \int d\theta p(E|\theta) p(\theta|T)$$

- Prediction by sampling weights

$$\langle E \rangle = \int dE d\theta E p(E|\theta) p(\theta|T) = \int dE d\theta E p(E|\theta) q(\theta)$$



# Constructing the loss function

## Training means encoding $p(\theta|T)$

- so-called variational approximation [think  $q(\theta)$  as Gaussian with mean and width]

$$p(E) = \int d\theta p(E|\theta) p(\theta|T) \stackrel{!}{=} \int d\theta p(E|\theta) q(\theta)$$

- similarity through minimized KL-divergence

$$D_{\text{KL}}[q(\theta), p(\theta|T)] = \int d\theta q(\theta) \log \frac{q(\theta)}{p(\theta|T)}$$



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- Bayes' theorem to replace  $p(\theta|T)$

$$\begin{aligned} D_{\text{KL}}[q(\theta), p(\theta|T)] &= \int d\theta q(\theta) \log \frac{q(\theta)p(T)}{p(T|\theta)p(\theta)} \\ &= D_{\text{KL}}[q(\theta), p(\theta)] - \int d\theta q(\theta) \log p(T|\theta) + \log p(T) \int d\theta q(\theta) \end{aligned}$$

- normalize distributions, ignore irrelevant terms, so minimize

$$D_{\text{KL}}[q(\theta), p(\theta|T)] \approx D_{\text{KL}}[q(\theta), p(\theta)] - \int d\theta q(\theta) \log p(T|\theta)$$



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$$D_{\text{KL}}[q(\theta), p(\theta|T)] \approx D_{\text{KL}}[q(\theta), p(\theta)] - \int d\theta q(\theta) \log p(T|\theta)$$

→ Loss combining likelihood and regularization

$$L = - \int d\theta q(\theta) \log p(T|\theta) + D_{\text{KL}}[q(\theta), p(\theta)]$$

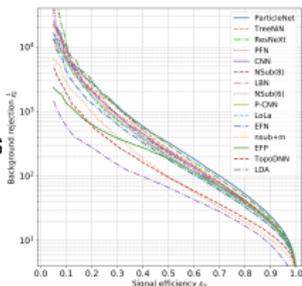


## ML-applications for analysis

## Top tagging [supervised classification]

- ‘hello world’ of LHC-ML
- end of QCD-taggers
- different NN-architectures

→ Non-NN left in the dust...



SciPost Physics

Submission

## The Machine Learning Landscape of Top Taggers

G. Kaselka<sup>1(a)</sup>, T. Plehn<sup>1(a)</sup>, A. Butter<sup>2</sup>, K. Craner<sup>3</sup>, D. Debanji<sup>4</sup>, B. M. Ertel<sup>5</sup>, M. Fairhead<sup>6</sup>, D. A. Ferguson<sup>7</sup>, W. Florko<sup>8</sup>, C. Gao<sup>9</sup>, L. Gornik<sup>7</sup>, J. F. Kerner<sup>10,11</sup>, P. T. Komke<sup>12</sup>, S. Linn<sup>13</sup>, A. Linte<sup>14</sup>, S. Maciocco<sup>15</sup>, E. M. Metodiev<sup>16</sup>, L. Moore<sup>17</sup>, B. Nefzaie<sup>18,19</sup>, K. Nishikida<sup>18,19</sup>, J. Pfaender<sup>18</sup>, H. Qiu<sup>20</sup>, Y. Ruan<sup>20</sup>, M. Sapper<sup>20</sup>, D. Saliu<sup>21</sup>, J. M. Thompson<sup>22</sup>, and S. Varrat<sup>23</sup>

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<sup>2</sup> Institut für Theoretische Physik, Universität Heidelberg, Germany  
<sup>3</sup> Center for Cosmology and Particle Physics and Center for Data Science, NYU, USA  
<sup>4</sup> NHCT, Dept. of Physics and Astronomy, Rutgers, The State University of NJ, USA  
<sup>5</sup> Joint Institute for Nuclear Research, Czechia  
<sup>6</sup> Theoretical Particle Physics and Cosmology, King's College London, United Kingdom  
<sup>7</sup> Department of Physics and Astronomy, The University of British Columbia, Canada  
<sup>8</sup> Department of Physics, University of California, Santa Barbara, USA  
<sup>9</sup> Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia  
<sup>10</sup> Center for Theoretical Physics, MIT, Cambridge, USA  
<sup>11</sup> CPJ, Universitat Catàlica de Leuven, Leuven-la-Neuve, Belgium  
<sup>12</sup> Physics Division, Lawrence Berkeley National Laboratory, Berkeley, USA  
<sup>13</sup> Sierra Inst. for the Theory of Computing, University of California, Berkeley, USA  
<sup>14</sup> National Institute for Subatomic Physics (NIKHEF), Amsterdam, Netherlands  
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<sup>16</sup> III. Physikalisches Institut A, RWTH Aachen University, Germany

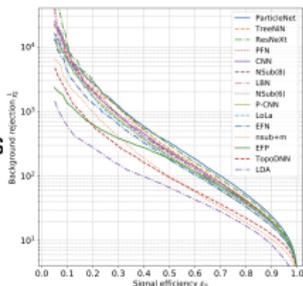


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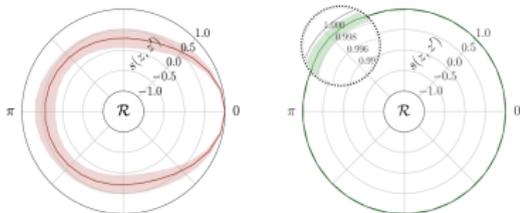
G. Kaselka (ed.), T. Plehn (ed.), A. Bhatti<sup>1</sup>, K. Craner<sup>2</sup>, D. Debnath<sup>3</sup>, R. M. Dikar<sup>4</sup>, M. Fairbrother<sup>5</sup>, D. A. Ferguson<sup>6</sup>, W. Florko<sup>7</sup>, C. Gay<sup>8</sup>, L. Gornik<sup>9</sup>, J. F. Kaniak<sup>10</sup>, P. T. Komar<sup>11</sup>, S. Litali<sup>12</sup>, A. Litali<sup>13</sup>, S. Maciocco<sup>14</sup>, E. M. Metodiev<sup>15</sup>, L. Moore<sup>16</sup>, B. Nandoriya<sup>17</sup>, K. Nandoriya<sup>18</sup>, J. Pfaender<sup>19</sup>, H. Qiu<sup>20</sup>, Y. Raha<sup>21</sup>, M. Sapper<sup>22</sup>, D. Saha<sup>23</sup>, J. M. Thompson<sup>24</sup>, and S. Varma<sup>25</sup>

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## Symmetric networks [contrastive learning, transformer network]

- rotations, translations, permutations, soft splittings, collinear splittings
- learn symmetries/augmentations

→ Symmetric latent representation



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Submissions

## Symmetries, Safety, and Self-Supervision

Barry M. Dikar<sup>1</sup>, Grigor Radicevic<sup>2</sup>, Hans Othlitzinger<sup>3</sup>, Tilman Plehn<sup>4</sup>, Peter Sorrensen<sup>5</sup>, and Lorenz Vogl<sup>6</sup>

- <sup>1</sup> Institut für Theoretische Physik, Universität Heidelberg, Germany
- <sup>2</sup> Institut für Experimentelle Physik, Universität Heidelberg, Germany
- <sup>3</sup> Heidelberg Collaboratory for Image Processing, Universität Heidelberg, Germany

August 11, 2021

## Abstract

Collider searches face the challenge of defining a representation of high-dimensional data such that physical symmetries are manifest, the discriminating features are retained, and the choice of representation is non-physicist agnostic. We introduce JetCLR to solve the mapping from low-level data to optimized observables through self-supervised contrastive learning. As an example, we construct a data representation for top and QCD jets using a permutation-invariant transformer-encoder network and visualize its symmetry properties. We compare the JetCLR representation with alternative representations using Boost classifier tests and find it to work quite well.



## Events and amplitudes

## Speeding up Sherpa and MadNIS [sampling]

- precision simulations limiting factor for Runs 3&4
  - unweighting critical
- Phase space sampling

	$gg \rightarrow Higgs$	$gg \rightarrow \tilde{t}\tilde{t}^*$	$gg \rightarrow \tilde{t}\tilde{t}^*$	$gg \rightarrow \tilde{t}\tilde{t}^*$	$gg \rightarrow Higgs$
$\epsilon_{cut}$	$1.1e-2$	$7.3e-3$	$6.8e-3$	$4.6e-4$	
$n_{full,MC}$	$8.7e-3$	$5.8e-3$	$4.7e-3$	$3.0e-4$	
$(n_{full}/n_{net})$	3032	2017	189	64	
$\mu_{full}^{MC}$	52.03	32.52	49.76	236.19	
$\mu_{full,MC}^{net}$	$2.4e-2$	$3.5e-2$	$2.1e-2$	$1.5e-2$	
$\mu_{net}^{MC}$	0.0669	0.9364	0.9364	0.9561	
$\mu_{net}^{MC}$	2.21	4.80	1.47	0.19	
$\sigma_{full}^{MC}$	30.40	19.14	27.76	35.34	
$\sigma_{full,MC}^{net}$	$4.3e-2$	$6.4e-2$	$3.1e-2$	$7.1e-2$	
$\sigma_{net}^{MC}$	0.0663	0.9360	0.9363	0.9321	
$\sigma_{net}^{MC}$	3.90	8.26	3.91	2.22	

Table 6: Performance measures for partonic channels contributing to  $gg \rightarrow 3$  jets production at the LHC.

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Substitutions

MCNET-21-13

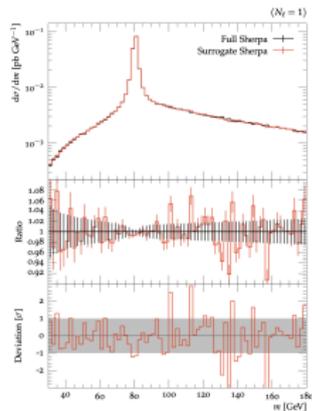
## Accelerating Monte Carlo event generation – rejection sampling using neural network event-weight estimates

K. Dönig<sup>1</sup>, T. Jocher<sup>2</sup>, S. Schwanze<sup>2</sup>, F. Siegel<sup>1</sup><sup>1</sup> Institut für Kern- und Teilchenphysik, TU Dresden, Dresden, Germany<sup>2</sup> Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany

September 27, 2021

## Abstract

The generation of unit-weight events for complex scattering processes presents a severe challenge to modern Monte Carlo event generators. Even when using sophisticated phase-space sampling techniques adapted to the underlying transition matrix elements, the efficiency for generating unit-weight events from weighted samples can become a limiting factor in practical applications. Here we present a novel two-staged unweighting procedure that makes use of a neural-network surrogate for the full event weight. The algorithm can significantly accelerate the unweighting process, while it still guarantees unbiased sampling from the correct target distribution. We apply, validate and benchmark the new approach in high-multiplicity LHC production processes, including  $2/W+4$  jets and  $0+3$  jets, where we find speed-up factors up to ten.



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	$gg \rightarrow Higgs$	$gg \rightarrow \gamma\gamma$	$gg \rightarrow Z\gamma$	$gg \rightarrow Higgs$	$gg \rightarrow Higgs$
$r_{full}$	$1.1e-2$	$7.3e-3$	$6.8e-3$	$6.6e-4$	$6.6e-4$
$r_{1+1,0+0}$	$8.7e-3$	$5.8e-3$	$4.7e-3$	$3.0e-4$	$3.0e-4$
$(r_{full}/r_{1+1,0+0})$	3013	3117	199	51	51
$r_{full}^{MC}$	52.03	32.12	49.75	236.19	236.19
$r_{full}^{MC,MC}$	$3.4e-2$	$3.8e-2$	$3.1e-2$	$3.0e-3$	$3.0e-3$
$r_{full}^{MC,MC}$	0.9889	0.9881	0.9904	0.9981	0.9981
$r_{full}^{MC,MC}$	2.21	1.89	1.47	0.19	0.19
$r_{full}^{MC,MC}$	30.40	19.14	27.78	35.31	35.31
$r_{full}^{MC,MC}$	$4.3e-2$	$4.4e-2$	$3.1e-2$	$2.1e-2$	$2.1e-2$
$r_{full}^{MC,MC}$	0.9563	0.9900	0.9943	0.9821	0.9821
$r_{full}^{MC,MC}$	3.90	8.26	3.91	2.22	2.22

Table 6: Performance measure for partonic channels contributing to  $gg \rightarrow 3$  jets production at the LHC.

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Submission

MCNET-21-33

### Accelerating Monte Carlo event generation – rejection sampling using neural network event-weight estimates

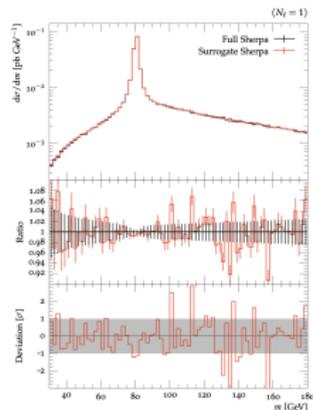
K. Dauterle<sup>1</sup>, T. Jausen<sup>1</sup>, S. Schwaner<sup>2</sup>, F. Singer<sup>1</sup>

<sup>1</sup> Institut für Kern- und Teilchenphysik, TU Dresden, Dresden, Germany  
<sup>2</sup> Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany

September 27, 2021

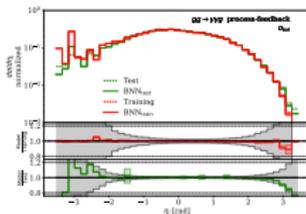
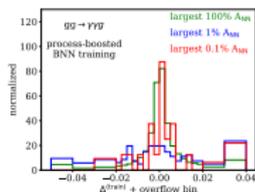
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## Speeding up amplitudes [precision regression]

- loop-amplitudes expensive
  - interpolation standard
- Precision NN-amplitudes



PREPARED FOR SUBMISSION TO JHEP

IFPP/20/138

### Optimising simulations for diphoton production at hadron colliders using amplitude neural networks

Joseph Aylott<sup>1</sup>, Simeon Badger<sup>2</sup>, Ryan Meehan<sup>3</sup>

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<sup>2</sup>Institute for Data Science, Durham University, Durham, DLU, UK, United Kingdom

<sup>3</sup>Department of Physics and Arnold Sommerfeld Center, Universität zu Tübingen, and DESY, Notke 85, 22607, Via F. D'Onofrio 1, 03020 Sesto San Giovanni, Italy

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**ABSTRACT:** Machine learning technology has the potential to dramatically optimise event generation and simulation. We continue to investigate the use of neural networks to approximate matrix elements for high-multiplicity scattering processes. We focus on the case of loop-induced diphoton production through gluon fusion, and develop a modular simulation method that can be applied to hadronic collider observables. Neural networks are trained using the one-loop amplitudes implemented in the *MadGraph5* library, and interfaced to the Sherpa Monte Carlo event generator, where we perform a detailed study for  $2+3$  and  $2+4$  scattering orders. We also consider how the trained networks perform when varying the kinematic cuts affecting the phase space and the reliability of the neural network simulations.



# Invertible event generation

## Precision NN-generators [Bayesian discriminator-flows]

- control through discriminator [GAN-like]
  - uncertainties through Bayesian networks
- Discussed later

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Submission

### Generative Networks for Precision Enthusiasts

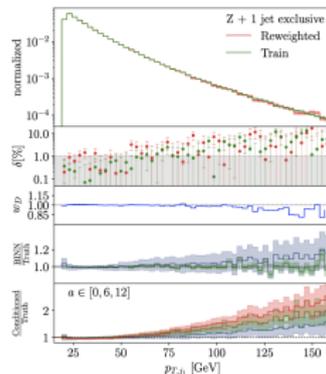
Anja Butter<sup>1</sup>, Theo Brandl<sup>1</sup>, Sander Hainzeck<sup>1</sup>, Tilman Kotze<sup>1</sup>,  
Tizian Plehn<sup>1</sup>, Armand Rouzeau<sup>2</sup>, and Sophia Viret<sup>1</sup>

<sup>1</sup> Institut für Theoretische Physik, Universität Heidelberg, Germany  
<sup>2</sup> Heidelberg Collaboratory for Image Processing, Universität Heidelberg, Germany

November 16, 2021

#### Abstract

Generative networks are opening new avenues in fast event generation for the LHC. We show how generative flow networks can reach percent-level precision for Monte Carlo distributions, how they can be trained jointly with a discriminator, and how this discriminator improves the generation. Our joint training relies on a novel coupling of the two networks which does not require a Nash equilibrium. We then estimate the generation uncertainties through a Bayesian network setup and through conditional data augmentation, while the discriminator ensures that there are no systematic inaccuracies compared to the training data.



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SIPhot Physics Submission

**Generative Networks for Precision Enthusiasts**

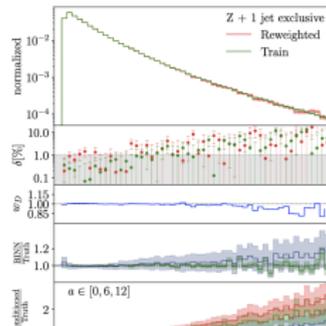
Andrius Buteris<sup>1</sup>, Tilman Plehn<sup>2</sup>, Sander Hirsiger<sup>1</sup>, Tobias Korte<sup>1</sup>,  
Tilman Plehn<sup>1</sup>, Armand Boudel<sup>1</sup>, and Sjoerd Vost<sup>1</sup>

<sup>1</sup> Institut für Theoretische Physik, Universität Heidelberg, Germany  
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November 16, 2021

### Abstract

Generative networks are opening new avenues in fast event generation for the LHC. We show how generative flow networks can reach percent-level precision for kinematic distributions, how they can be trained jointly with a discriminator, and how the discriminator improves the generation. Our joint training relies on a novel coupling of the two networks which does not require a Nash equilibrium. We then estimate the generator uncertainties through a Bayesian network using and through conditional data augmentation, while the discriminator ensures that there are no systematic inaccuracies compared to the training data.



## Unfolding and inversion [conditional normalizing flows]

- shower/hadronization unfolded by jet algorithm
- detector/decays unfolded e.g. in tops
- calibrated inverse sampling

→ Discussed later

SIPhot Physics Submission

**Invertible Networks or Partons to Detector and Back Again**

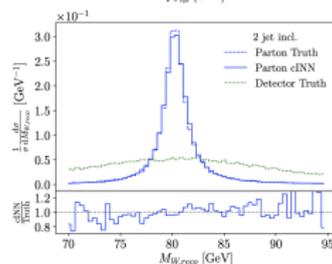
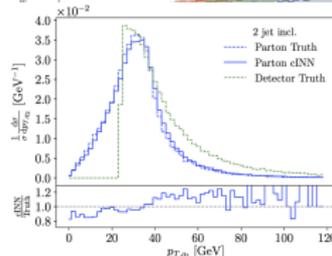
Marcio Bellagrosa<sup>1</sup>, Andrius Buteris<sup>1</sup>, Georgios Katsoulis<sup>1</sup>, Tilman Plehn<sup>1</sup>, Armand Boudel<sup>1</sup>,  
Ramon Winterhalder<sup>1</sup>, Lyndon Antonov<sup>1</sup>, and Ulrich Klöbe<sup>2</sup>

<sup>1</sup> Institut für Theoretische Physik, Universität Heidelberg, Germany  
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October 2, 2020

### Abstract

For simulations where the forward and the inverse directions have a physics meaning, invertible neural networks are especially useful. A conditional INN can learn a detector simulation in terms of high-level observables, specifically for ZW production at the LHC. It allows for a per-event statistical interpretation. Next, we show for a variable number of QCD jets. We model detector effects and QCD radiation to a pre-defined hard process, again with a per-event probabilistic interpretation over parton-level phase space.



# Modern generative networks

## Generative networks

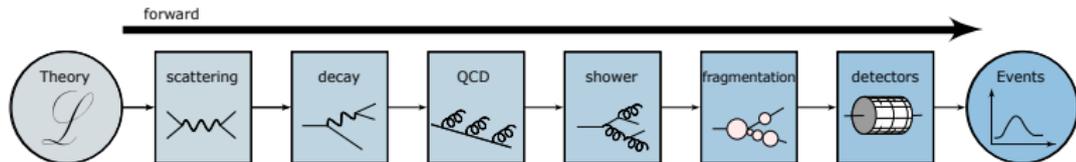
- generate **new** images, text blocks, etc
- encode density in target space  
sample from Gaussian into target space
- reproduce training data, statistically independently



# Modern generative networks

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  - reproduce training data, statistically independently
  - Variational Autoencoder  
→ low-dimensional physics, high-dimensional objects
  - Generative Adversarial Network  
→ generator trained by classifier
  - Normalizing Flow/Diffusion Model  
→ stable bijective mapping
  - Generative Pre-trained Transformer  
→ learning all structures
- **Pick best model for purpose**



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## Fundamental question: GANplification

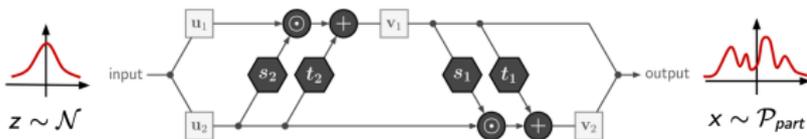
- first generated instances reproducing structures
- too many generated instances reproducing noise?



# Modern generative networks

## Normalizing flows — INN

- Gaussian latent space
  - bijective mapping
  - known Jacobian
  - likelihood loss
  - variety of coupling layers
- Perfect for speed and precision



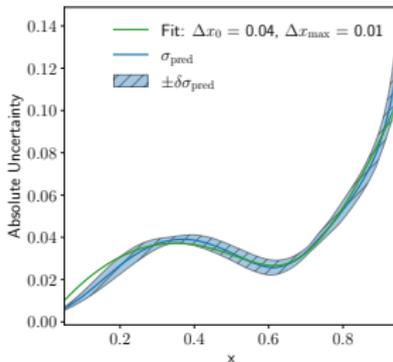
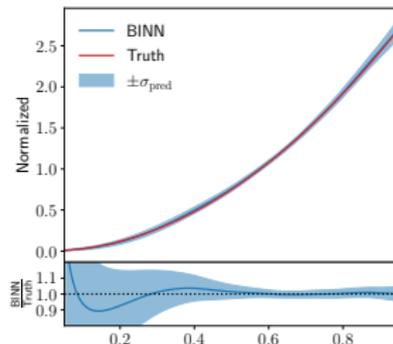
# Modern generative networks

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## INNs with uncertainties

- Bayesian NN for density estimation
  - events with error bars
  - density & uncertainty maps cross-talking
- Bayesian INNs just fits with error bars



# Precision generator

## ML-event generators

- useful ML-playground
- training from event samples  
no momentum conservation  
no detector effects [sharper structures]

1- top-quark pairs  $t\bar{t} \rightarrow 6$  jets [resonance peaks]

2-  $Z_{\mu\mu} + \{1, 2, 3\}$  jets [Z-peak, variable jet number, jet-jet topology]



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## INN-generator [Butter, Heimes, Hummerich, Krebs, TP, Rousselot, Vent]

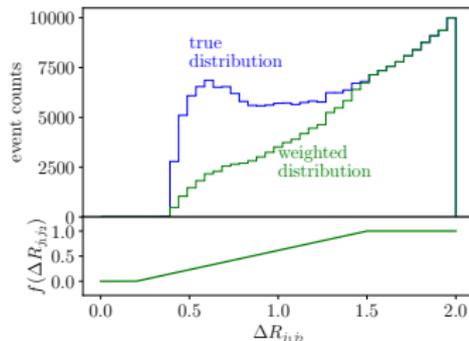
- challenging  $\Delta R_{jj}$  features
- opposite of importance sampling

$$w^{(1\text{-jet})} = 1$$

$$w^{(2\text{-jet})} = f(\Delta R_{j_1, j_2})$$

$$w^{(3\text{-jet})} = f(\Delta R_{j_1, j_2})f(\Delta R_{j_2, j_3})f(\Delta R_{j_1, j_3})$$

$$f(\Delta R) = \frac{\Delta R - R_-}{R_+ - R_-} \quad (\Delta R \in [R_-, R_+])$$



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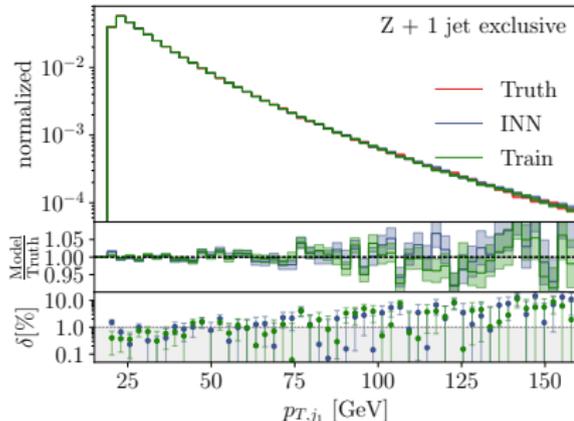
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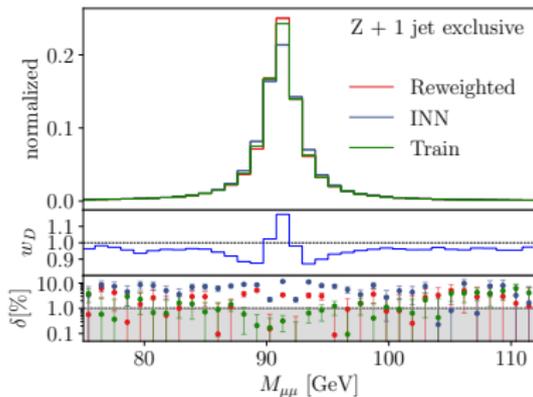
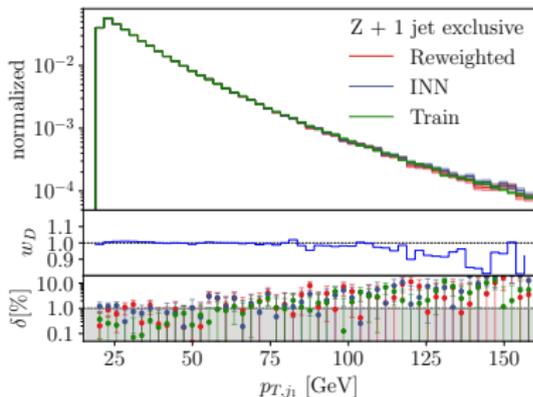
→ Per-cent precision in reach



## Controlled precision generator

## Discriminator: training vs generated

- probability output  $D = 0(\text{generator}), 1(\text{truth})$
  - decent generator  $D \approx 0.5$
  - additional event weight  $w_D = D/(1 - D)$
- Dual use — control & reweight



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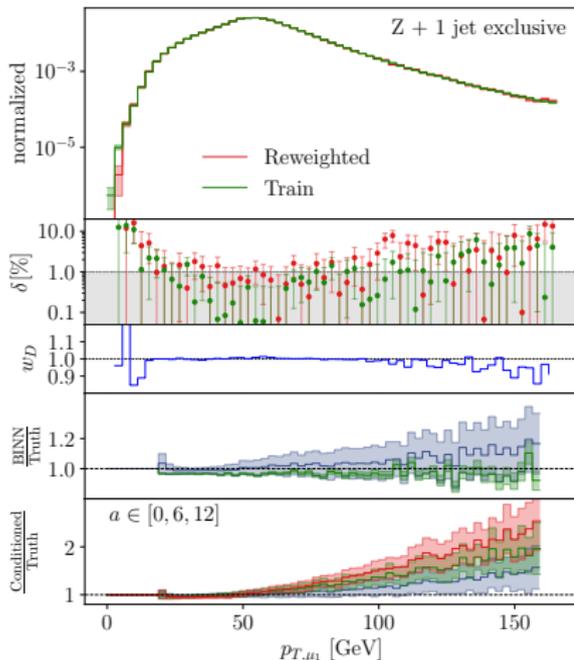
## Uncertainties

- training uncertainties from BINN
- low statistics challenging
- systematics from data augmentation
- adjust data in tails  $[a = 0 \dots 30]$

$$w = 1 + a \left( \frac{p_{T,j_1} - 15 \text{ GeV}}{100 \text{ GeV}} \right)^2$$

- train conditionally on smeared  $a$
- error bar from sampling  $a$

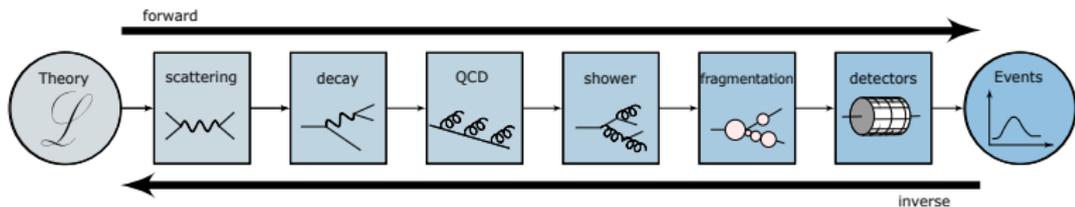
→ INNs for LHC standards



# Inverse simulation

## Invertible ML-simulation

- forward:  $r \rightarrow$  events trained on model
- inverse:  $r \rightarrow$  anything trained on model, conditioned on event



# Inverse simulation

## Invertible ML-simulation

- forward:  $r \rightarrow$  events trained on model
- inverse:  $r \rightarrow$  anything trained on model, conditioned on event
- individual steps known problems

detector unfolding

unfolding to QCD parton means jet algorithm

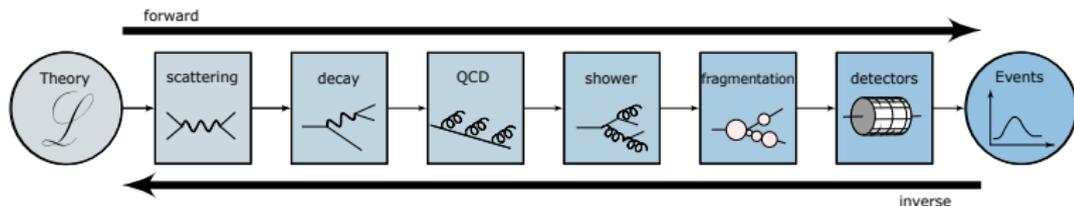
unfolding jet radiation known combinatorics problem

unfolding to hard process standard in top groups [needed for global analyses]

matrix element method an old dream

- improved through coherent ML-method

→ Free choice of data-theory inference point



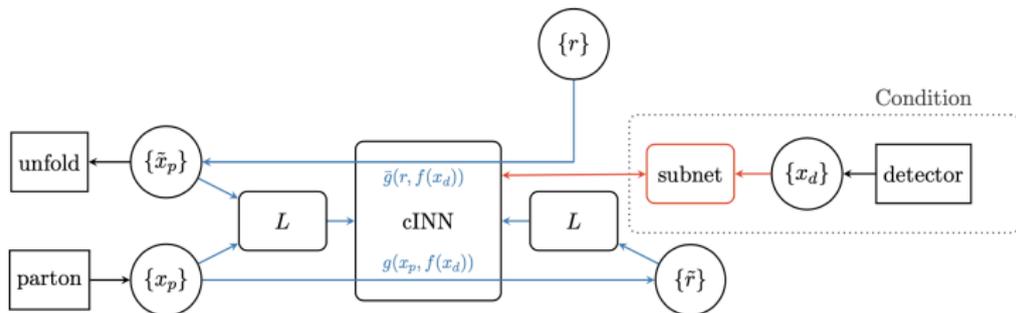
# Inverting to hard process

## Conditional INN

- partonic events  $x_p$  from  $\{r\}$ , given reco-event  $x_r$
- loss based on likelihood

$$\begin{aligned}
 L &= - \langle \log p(\theta | x_p, x_r) \rangle_{x_p, x_r} \\
 &= - \langle \log p(x_p | x_r, \theta) + \log p(\theta | x_r) - \log p(x_p | x_r) \rangle_{x_p, x_r} \\
 &= - \langle \log p(x_p | x_r, \theta) \rangle_{x_p, x_r} - \log p(\theta) + \text{const.} \\
 &= - \left\langle \log p(g(x_p | x_r)) + \log \left| \frac{\partial g(x_p | x_r)}{\partial x_p} \right| \right\rangle_{x_p, x_r} - \log p(\theta) + \text{const.}
 \end{aligned}$$

→ Stable and statistically calibrated



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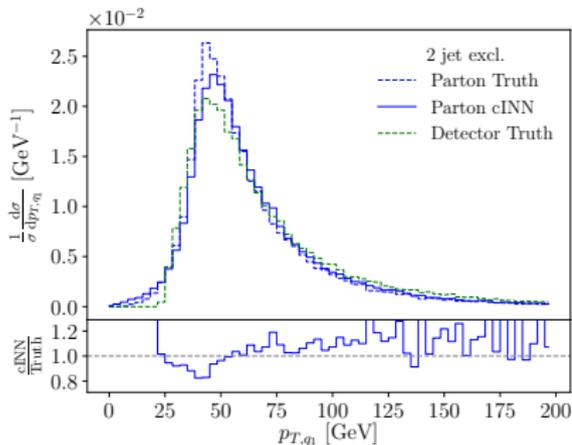
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## Undo detector and QCD jet radiation in $pp \rightarrow ZW + \text{jets}$

- hard process given
  - detector and reconstruction universal
  - jet radiation (approximately) universal
  - model-independence: Butter-Malaescu
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# Inverting to hard process

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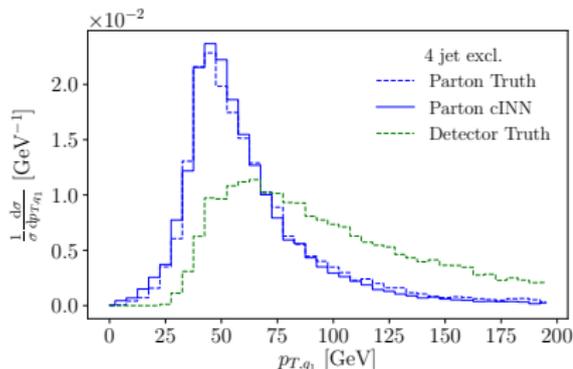
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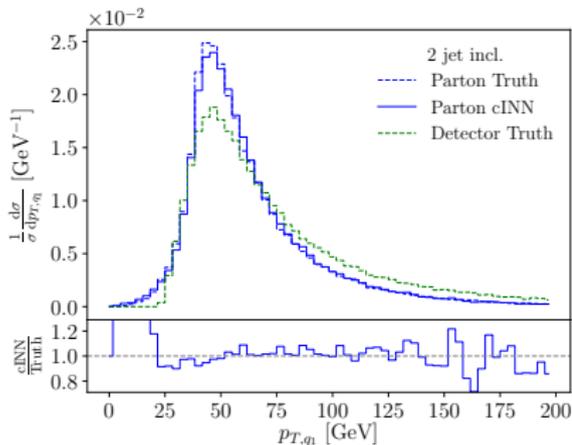
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# Optimal observables

## Measure model parameter $\theta$ optimally

- single-event likelihood

$$p(x|\theta) = \frac{1}{\sigma_{\text{tot}}(\theta)} \frac{d^m \sigma(x|\theta)}{dx^m}$$

- expanded in  $\theta$  around  $\theta_0$ , define score

$$\log \frac{p(x|\theta)}{p(x|\theta_0)} \approx (\theta - \theta_0) \left. \nabla_{\theta} \log p(x|\theta) \right|_{\theta_0} \equiv (\theta - \theta_0) t(x|\theta_0) \equiv (\theta - \theta_0) \mathcal{O}^{\text{opt}}(x)$$

- leading order parton level

$$p(x|\theta) \approx |\mathcal{M}|_0^2 + \theta |\mathcal{M}|_{\text{int}}^2 \quad \Rightarrow \quad t(x|\theta_0) \sim \frac{|\mathcal{M}|_{\text{int}}^2}{|\mathcal{M}|_0^2}$$



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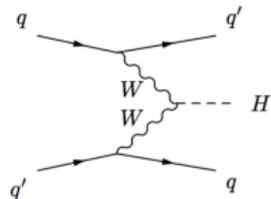
## CP-violating Higgs production

- unique CP-observable

$$t \propto \epsilon_{\mu\nu\rho\sigma} k_1^\mu k_2^\nu q_1^\rho q_2^\sigma \text{sign} [(k_1 - k_2) \cdot (q_1 - q_2)] \xrightarrow{\text{lab frame}} \sin \Delta\phi_{jj}$$

- CP-effect in  $\Delta\phi_{jj}$   
D6-effect in  $p_{T,j}$

⇒ Established LHC task



## Analytic formula for score

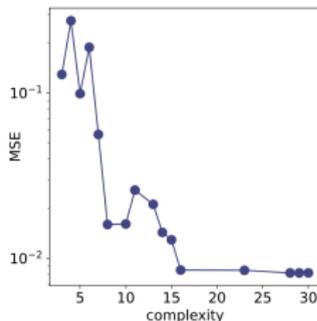
- function to approximate  $t(x|\theta)$
- phase space parameters  $x_p = p_T/m_H, \Delta\eta, \Delta\phi$  [node]
- operators  $\sin x, x^2, x^3, x + y, x - y, x * y, x/y$  [node]
- represent formula as tree [complexity = number of nodes]

⇒ Figures of merit

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n [g_i(x) - t(x, z|\theta)]^2 \rightarrow \text{MSE} + \text{parsimony} \cdot \text{complexity}$$

## Score around Standard Model

compl	dof	function	MSE
3	1	$a \Delta\phi$	$1.30 \cdot 10^{-1}$
4	1	$\sin(a\Delta\phi)$	$2.75 \cdot 10^{-1}$
5	1	$a\Delta\phi x_{p,1}$	$9.93 \cdot 10^{-2}$
6	1	$-x_{p,1} \sin(\Delta\phi + a)$	$1.90 \cdot 10^{-1}$
7	1	$(-x_{p,1} - a) \sin(\sin(\Delta\phi))$	$5.63 \cdot 10^{-2}$
8	1	$(a - x_{p,1}) x_{p,2} \sin(\Delta\phi)$	$1.61 \cdot 10^{-2}$
14	2	$x_{p,1} (a\Delta\phi - \sin(\sin(\Delta\phi))) (x_{p,2} + b)$	$1.44 \cdot 10^{-2}$
15	3	$-(x_{p,2} (a\Delta\eta^2 + x_{p,1}) + b) \sin(\Delta\phi + c)$	$1.30 \cdot 10^{-2}$
16	4	$-x_{p,1} (a - b\Delta\eta) (x_{p,2} + c) \sin(\Delta\phi + d)$	$8.50 \cdot 10^{-3}$
28	7	$(x_{p,2} + a) (bx_{p,1} (c - \Delta\phi) - x_{p,1} (d\Delta\eta + ex_{p,2} + f) \sin(\Delta\phi + g))$	$8.18 \cdot 10^{-3}$



## PySR

## Analytic formula for score

- function to approximate  $t(x|\theta)$
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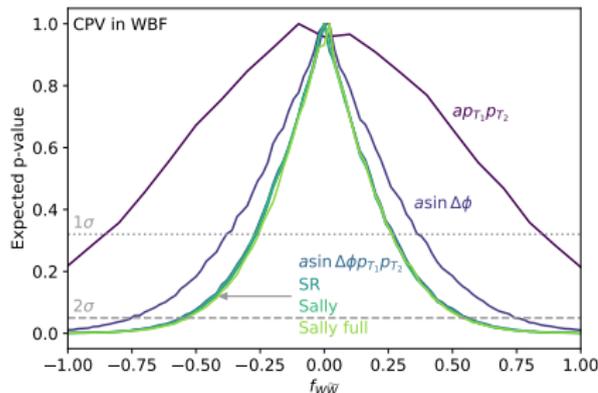
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## Score around Standard Model

- expected limits:  
very wrong formula  
wrong formula  
right formula  
MadMiner
- same within statistical limitation

⇒ New optimal observables next



# ML for LHC Theory

## ML-applications

- just another numerical tool for a numerical field
  - driven by money from data science and medical research
  - goals are...
    - ...improve established tasks
    - ...develop new tools for established tasks
    - ...transform through new ideas
  - xAI through...
    - ...precision control
    - ...uncertainties
    - ...symmetries
    - ...formulas
- Fun with good old LHC problems

## Modern Machine Learning for LHC Physicists

Tilman Plehn<sup>a</sup>, Anja Butter<sup>a,b</sup>, Barry Dillon<sup>a</sup>, and Claudius Krause<sup>a,c</sup>

<sup>a</sup> Institut für Theoretische Physik, Universität Heidelberg, Germany

<sup>b</sup> LPNHE, Sorbonne Université, Université Paris Cité, CNRS/IN2P3, Paris, France

<sup>c</sup> NHETC, Dept. of Physics and Astronomy, Rutgers University, Piscataway, USA

November 2, 2022

### Abstract

Modern machine learning is transforming particle physics, faster than we can follow, and bulging its way into our numerical tool box. For young researchers it is crucial to stay on top of this development, which means applying cutting-edge methods and tools to the full range of LHC physics problems. These lecture notes are meant to lead students with basic knowledge of particle physics and significant enthusiasm for machine learning to relevant applications as fast as possible. They start with an LHC-specific motivation and a non-standard introduction to neural networks and then cover classification, unsupervised classification, generative networks, and inverse problems. Two themes defining much of the discussion are well-defined loss functions reflecting the problem at hand and uncertainty-aware networks. As part of the applications, the notes include some aspects of theoretical LHC physics. All examples are chosen from particle physics publications of the last few years. Given that these notes will be outdated already at the time of submission, the week of ML4jets 2022, they will be updated frequently.



## Inverting to QCD

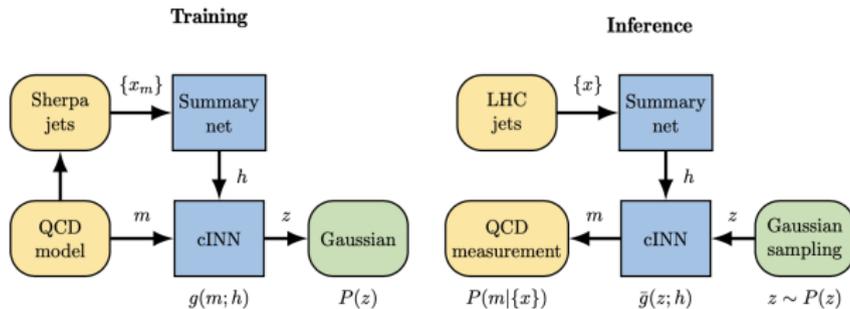
## cINN for inference [Bieringer, Butter, Heimes, Höche, Köthe, TP, Radev]

- condition jets with QCD parameters
- train model parameters  $\rightarrow$  Gaussian latent space
- test Gaussian sampling  $\rightarrow$  parameter measurement
- beyond  $C_A$  vs  $C_F$  [Kluth et al]

$$P_{qq} = C_F \left[ D_{qq} \frac{2z(1-y)}{1-z(1-y)} + F_{qq}(1-z) + C_{qq}yz(1-z) \right]$$

$$P_{gg} = 2C_A \left[ D_{gg} \left( \frac{z(1-y)}{1-z(1-y)} + \frac{(1-z)(1-y)}{1-(1-z)(1-y)} \right) + F_{gg}z(1-z) + C_{gg}yz(1-z) \right]$$

$$P_{gq} = T_R \left[ F_{gq} (z^2 + (1-z)^2) + C_{gq}yz(1-z) \right]$$



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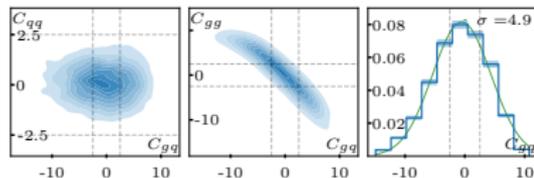
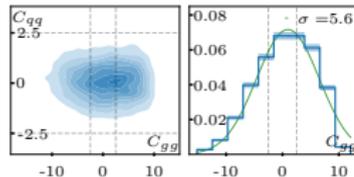
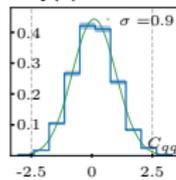
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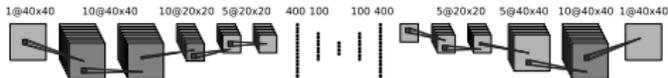
- idealized shower [Sherpa]
- More ML-opportunities...



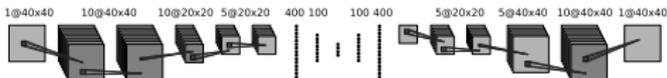
## Learning background only

## Unsupervised classification

- train on background only  
extract unknown signal from reconstruction error
  - reconstruct QCD jets → top jets hard to describe
  - reconstruct top jets → QCD jets just simple top-like jet
- Symmetric performance  $S \leftrightarrow B$ ?



## Learning background only

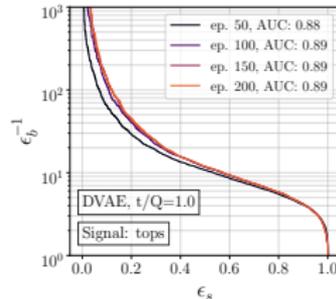
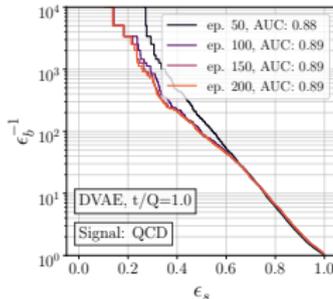
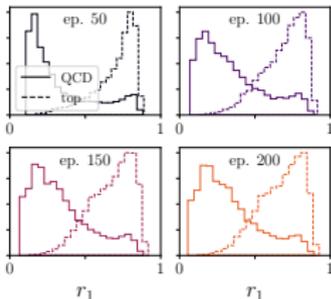


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## Moving to latent space

- anomaly score from latent space?
- VAE  $\rightarrow$  does not work
- GMVAE  $\rightarrow$  does not work
- Dirichlet VAE  $\rightarrow$  works okay
- density estimation  $\rightarrow$  does not work



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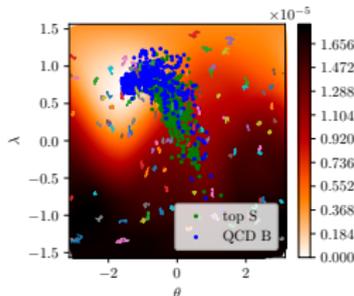
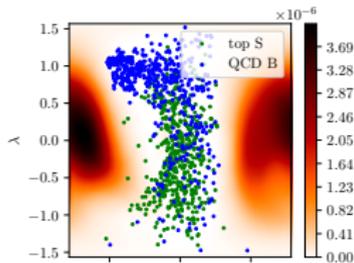
## Normalized autoencoder [penalize missing features]

- normalized probability loss
- Boltzmann mapping [ $E_\theta = \text{MSE}$ ]

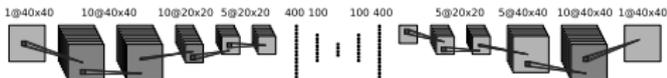
$$p_\theta(x) = \frac{e^{-E_\theta(x)}}{Z_\theta}$$

$$L = -\langle \log p_\theta(x) \rangle = \langle E_\theta(x) + \log Z_\theta \rangle$$

- inducing background metric
  - small MSE for data, large MSE for model
  - $Z_\theta$  from (Langevin) Markov Chain
- Symmetric autoencoder, at last



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