

# How to GAN for LHC

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# Machine Learning for LHC

## Fundamental understanding of LHC data

- LHC and dark matter data-driven, but never fundamental without theory
- just work with data and SM?
  1. simulation from first principles [Pythia, Sherpa]
  2. interpretation frameworks [SMEFT, SUSY]
  3. best use of the data [using 1, 2, our brains, and ML]
- 1991 visionaries: NN-based quark-gluon tagger

### USING NEURAL NETWORKS TO IDENTIFY JETS

Leif LÖNNBLAD\*, Carsten PETERSON\*\* and Thorsteinn RÖGNVALDSSON\*\*\*

*Department of Theoretical Physics, University of Lund, Sölvegatan 14A, S-22362 Lund, Sweden*

Received 29 June 1990



A neural network method for identifying the ancestor of a hadron jet is presented. The idea is to find an efficient mapping between certain observed hadronic kinematical variables and the quark-gluon identity. This is done with a neuron expansion in terms of a network of sigmoidal functions using a gradient descent procedure, where the errors are back-propagated through the network. With this method we are able to separate gluon from quark jets originating from Monte Carlo generated  $e^+e^-$  events with  $\sim 85\%$  approach. The result is independent of the MC model used. This approach for isolating the gluon jet is then used to study the so-called string effect.

In addition, heavy quarks (b and c) in  $e^+e^-$  reactions can be identified on the 50% level by just observing the hadrons. In particular we are able to separate b-quarks with an efficiency and purity, which is comparable with what is expected from vertex detectors. We also speculate on how the neural network method can be used to disentangle different hadronization schemes by compressing the dimensionality of the state space of hadrons.

⇒ Not that new...



## Simple classification done

SciPost Physics

Submission

## The Machine Learning Landscape of Top Taggers

G. Kasieczka (ed)<sup>1</sup>, T. Plehn (ed)<sup>2</sup>, A. Butter<sup>2</sup>, K. Cranmer<sup>3</sup>, D. Debnath<sup>4</sup>, B. M. Dillon<sup>5</sup>, M. Fairbairn<sup>6</sup>, D. A. Faroughy<sup>6</sup>, W. Federoz<sup>7</sup>, C. Gay<sup>7</sup>, L. Gonska<sup>8</sup>, J. F. Kammer<sup>9,10</sup>, P. T. Komiske<sup>10</sup>, S. Leis<sup>1</sup>, A. Lister<sup>7</sup>, S. Macaluso<sup>3,4</sup>, E. M. Metodiev<sup>10</sup>, L. Moore<sup>11</sup>, B. Nachman<sup>12,13</sup>, K. Nordström<sup>14,15</sup>, J. Pearson<sup>7</sup>, H. Qiu<sup>8</sup>, Y. Rath<sup>16</sup>, M. Rieger<sup>16</sup>, D. Shih<sup>4</sup>, J. M. Thompson<sup>7</sup>, and S. Varma<sup>6</sup>

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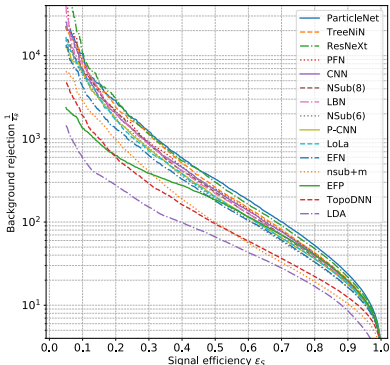
July 24, 2019

## Abstract

Based on the established task of identifying boosted, hadronically decaying top quarks, we compare a wide range of modern machine learning approaches. Unlike most established methods they rely on low-level input, for instance calorimeter output. While their network architectures are vastly different, their performance is comparatively similar. In general, we find that these new approaches are extremely powerful and great fun.

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# Beyond classification

## Phase space networks

- MC integration [Bendavit (2017)]
- NN Vegas [Klimek (2018), Carrazza (2020)]

## Event generation

- parton densities [NNPDF (since 2002)]
- amplitudes [Bishara (2019), Badger (2020)]
- neural importance sampling [Bothmann (2020)]
- i-flow in SHERPA [Gao (2020)]

## Generative networks

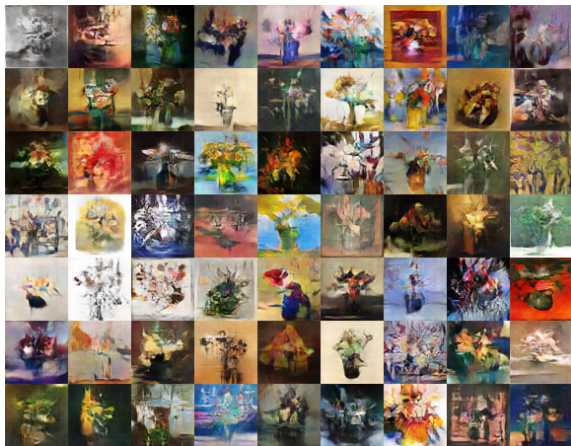
- Jet Images [de Oliveira (2017), Carazza (2019)]
- Detectors [Paganini (2017), Musella (2018), Erdmann (2018), Ghosh (2018), Buhmann (2020)]
- Event generation [Ottens (2019), Hashemi (2019), Di Sipio (2019), [Butter \(2019\)](#), Martinez (2019), Alanazi (2020)]
- Unfolding [Datta (2018), [Bellagente \(2019\)](#)]
- Templates for QCD factorization [Lin (2019)]
- Models [Erbin (2018), Otten (2018)]
- Event subtraction [[Butter \(2019\)](#)]



# Learning from art

## GANGogh [Bonafilia, Jones, Danyluk (2017)]

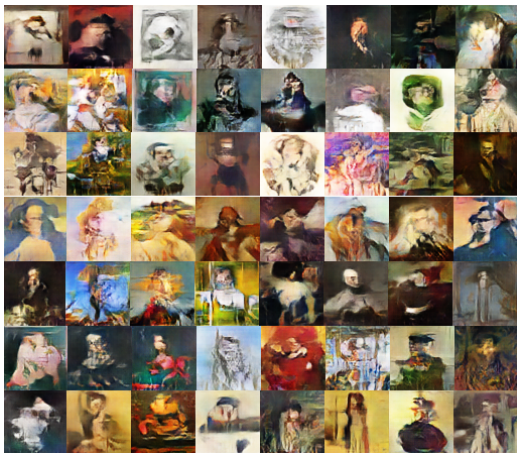
- old news: NNs turning pictures into art of a certain epoch but can they create **new pieces of art**?
- train on 80,000 pictures [organized by style and genre]
- map noise vector to images
- generate flowers



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# Learning from art

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## Edmond de Belamy [Caselles-Dupre, Fautrel, Vernier]

- trained on 15,000 portraits
  - sold for \$ 432.500
- ⇒ **all about marketing and sales**



# GAN basics

Basics

Events

Subtraction

Unfolding

Inverting

## MC crucial for LHC physics

- goal: **data-to-data** with fundamental physics input only
- MC challenges
  - higher-order precision in bulk
  - coverage of tails
  - inversion/unfolding to access fundamental QCD
- neural network benefits
  - best available interpolation**
  - structured latent space**
  - lightning speed, once trained
  - inversion solved
  - training on MC and/or data, anything goes
- GANs the cool kid
  - generator** trying to produce best events
  - discriminator** trying to catch generator
  - competing towards (Nash) equilibrium





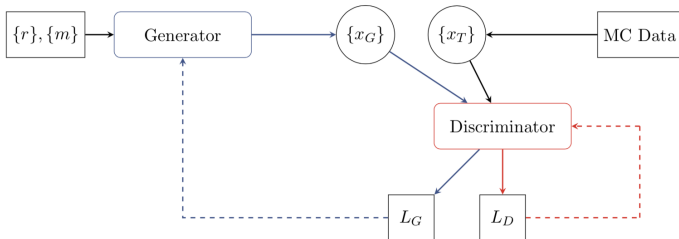
# GAN algorithm

## Example: LHC events

- training: true events  $\{x_T\}$  following  $p_T(x)$   
output: generated events  $\{r\} \rightarrow \{x_G\}$  following  $p_G(x)$
  - discriminator constructing  $D(x)$  [ $D(x) = 1, 0$  true/generator]  

$$L_D = \langle -\log D(x) \rangle_{x \sim P_T} + \langle -\log(1 - D(x)) \rangle_{x \sim P_G} \rightarrow -2 \log 0.5$$
  - generator giving events [ $D$  needed]  

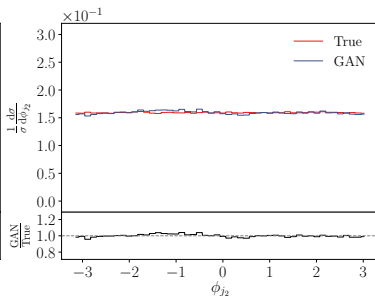
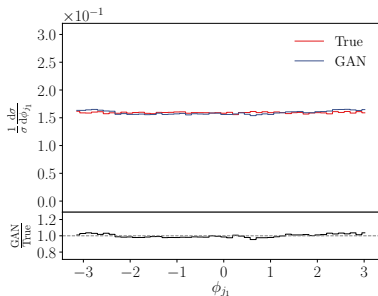
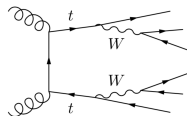
$$L_G = \langle -\log D(x) \rangle_{x \sim P_G}$$
  - loss function evaluated over batch
  - noise reduction/stabilization: gradient penalty [alternatively WGAN]
- $\Rightarrow$  statistically independent copy of training events



## 1– How to GAN LHC events

Idea: replace ME for hard process [Butter, TP, Winterhalder]

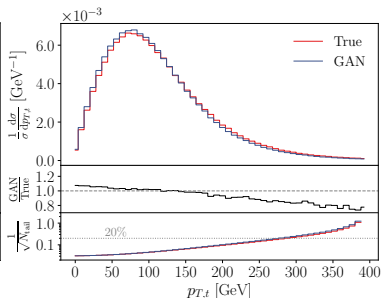
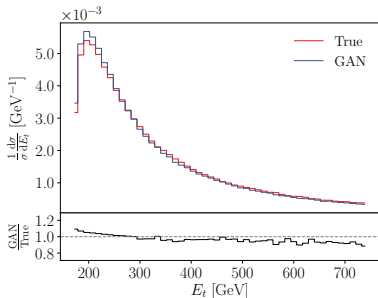
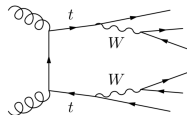
- medium-complex final state  $t\bar{t} \rightarrow 6$  jets
- $t/\bar{t}$  and  $W^\pm$  on-shell with BW  $6 \times 4 = 18$  dof
- on-shell external states  $\rightarrow 12$  dof [constants hard to learn]
- flat observables flat [phase space coverage okay]



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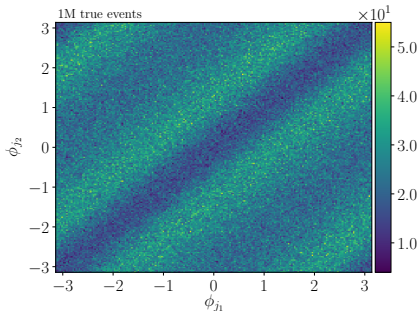
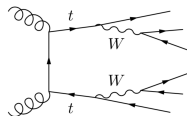
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- constructed observables similar



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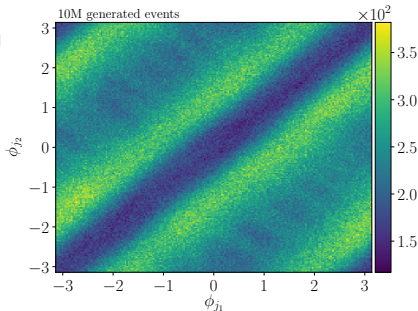
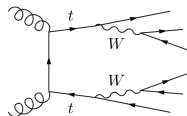
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- constructed observables similar
- improved resolution [1M training events]



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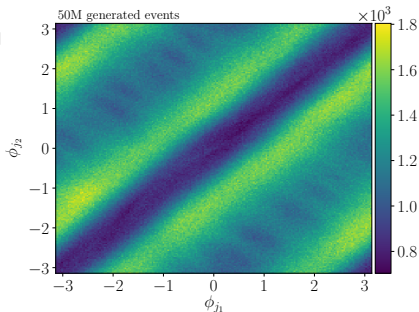
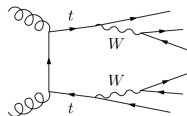
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- on-shell external states  $\rightarrow 12$  dof [constants hard to learn]
- flat observables flat [phase space coverage okay]
- direct observables with tails [statistical error indicated]
- constructed observables similar
- improved resolution [50M generated events]
- **concept promising**



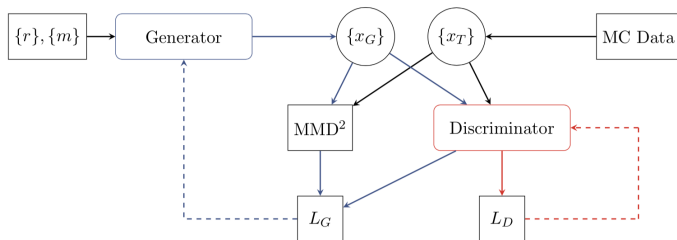
# Intermediate resonances

## GAN version of adaptive sampling

- generally 1D features  
phase space boundaries  
kinematic cuts  
invariant masses [top, W]
- batch-wise comparison of distributions, MMD loss with kernel  $k$

$$\text{MMD}^2 = \langle k(x, x') \rangle_{x, x' \sim P_T} + \langle k(y, y') \rangle_{y, y' \sim P_G} - 2 \langle k(x, y) \rangle_{x \sim P_T, y \sim P_G}$$

$$L_G \rightarrow L_G + \lambda_G \text{MMD}^2,$$



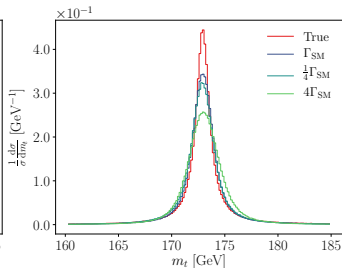
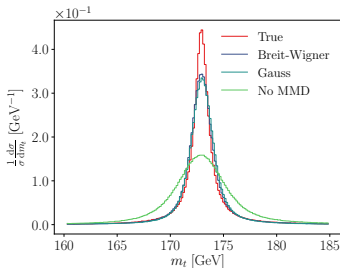
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$$L_G \rightarrow L_G + \lambda_G \text{MMD}^2,$$



⇒ minor impact of kernel function and width





## 2– How to GAN event subtraction

Idea: subtract event samples without bins [Butter, TP, Winterhalder]

- statistical uncertainty

$$\Delta_{B-S} = \Delta_{n_B N_B - n_S N_S} = \sqrt{\Delta_{n_B N_B}^2 + \Delta_{n_S N_S}^2} = \sqrt{n_B^2 N_B + n_S^2 N_S} > \max(B, S)$$

- applications in LHC physics

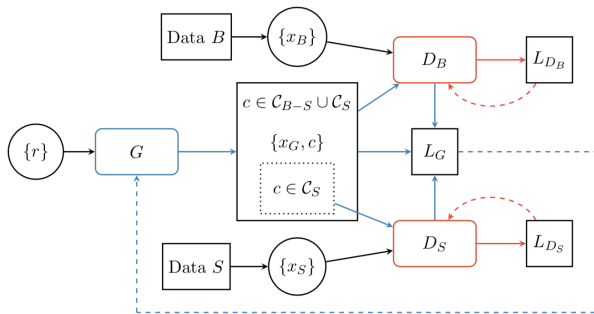
soft-collinear subtraction, multi-jet merging

on-shell subtraction

background/signal subtraction

- GAN setup

1. differential, steep class label
2. sample normalization



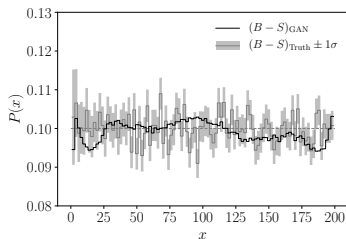
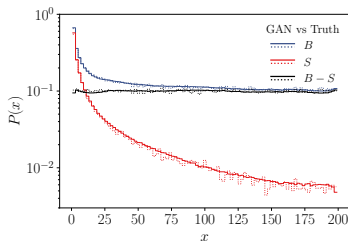
## Subtracted events

## How to beat statistics by subtracting

## 1- 1D toy example

$$P_B(x) = \frac{1}{x} + 0.1 \quad P_S(x) = \frac{1}{x} \Rightarrow P_{B-S} = 0.1$$

- statistical fluctuations reduced (sic!)



## Subtracted events

## How to beat statistics by subtracting

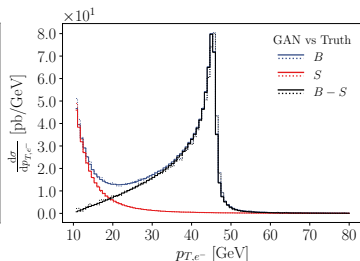
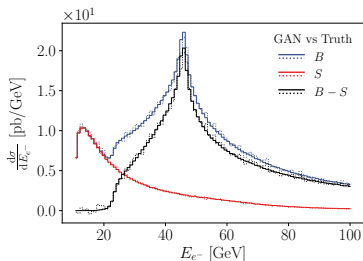
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## 2- event-based background subtraction [weird notation, sorry]

$$pp \rightarrow e^+e^- \text{ (B)} \quad pp \rightarrow \gamma \rightarrow e^+e^- \text{ (S)} \quad \Rightarrow \quad pp \rightarrow Z \rightarrow e^+e^- \text{ (B-S)}$$



## Subtracted events

## How to beat statistics by subtracting

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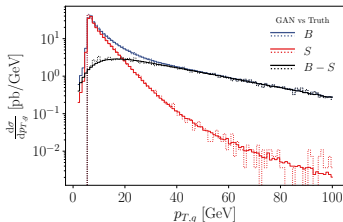
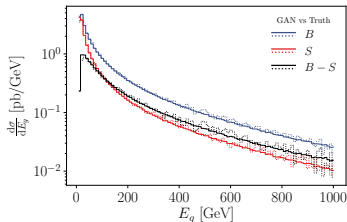
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## 3- collinear subtraction [assumed non-local]

$$pp \rightarrow Zg \quad (\text{B: matrix element, S: collinear approximation})$$



⇒ applications in theory and analysis



### 3– How to GAN away detector effects

Bottom line from SFitter etc [e.g. global SMEFT analyses]

- total rates without necessary information  
STXS model-dependent  
unfolded distributions extremely convenient [t $\bar{t}$  results]
- benefits  
access to hard matrix element/first-principles QCD  
matrix element method
- challenges  
non-invertible detector simulation  
model dependence

General: invert Markov processes [Bellagente, Butter, Kasiczka, TP, Winterhalder]

- detector simulation typical Markov process
- inversion possible, in principle [entangled convolutions]
- GAN task

partons  $\xrightarrow{\text{DELPHES}}$  detector  $\xrightarrow{\text{GAN}}$  partons

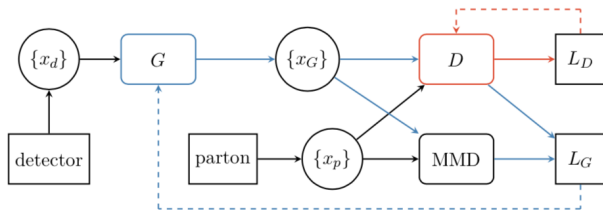
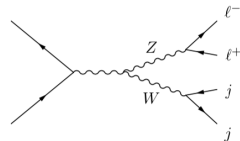
$\Rightarrow$  full phase space unfolded



## Standard GAN

## Reconstructing the parton level

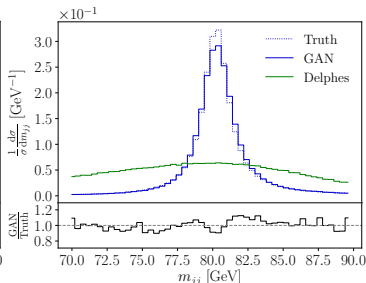
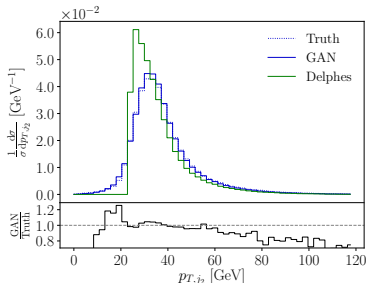
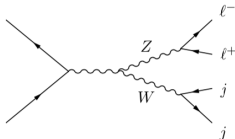
- $pp \rightarrow ZW \rightarrow (\ell\ell) (jj)$
- broad  $jj$  mass peak
- narrow  $\ell\ell$  mass peak
- modified  $2 \rightarrow 2$  kinematics
- fun phase space boundaries
- GAN same as event generation [with MMD]



# Standard GAN

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- fun phase space boundaries
- GAN same as event generation [with MMD]
- full inversion fine



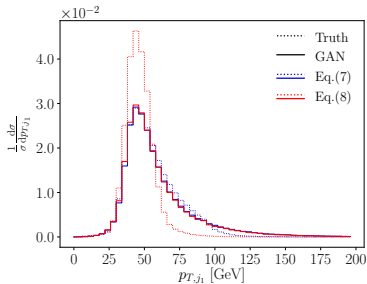
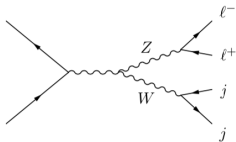
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## Reconstructing the parton level

- $pp \rightarrow ZW \rightarrow (\ell\ell) (jj)$
- broad  $jj$  mass peak
- narrow  $\ell\ell$  mass peak
- modified  $2 \rightarrow 2$  kinematics
- fun phase space boundaries
- GAN same as event generation [with MMD]
- full inversion fine
- **problem:** kinematics cuts in test data [88%, 38% events]

$$p_{T,j_1} = 30 \dots 100 \text{ GeV} \quad (7)$$

$$p_{T,j_1} = 30 \dots 60 \text{ GeV} \quad \text{and} \quad p_{T,j_2} = 30 \dots 50 \text{ GeV} \quad (8)$$

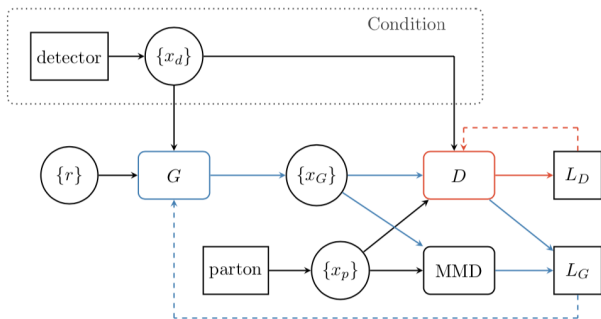




## Fully conditional GAN

## Proper sampling

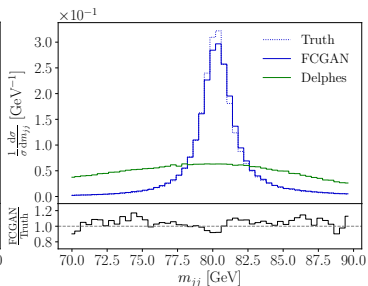
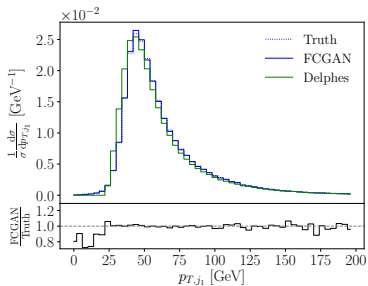
- map random numbers to parton level  
hadron level as condition [matched event pairs]



## Fully conditional GAN

## Proper sampling

- map random numbers to parton level  
hadron level as condition [matched event pairs]
- full inversion fine [again]



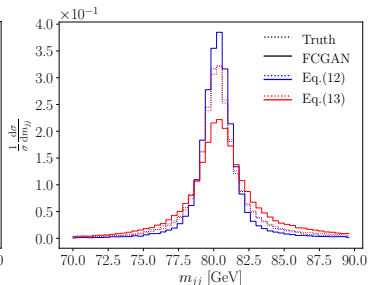
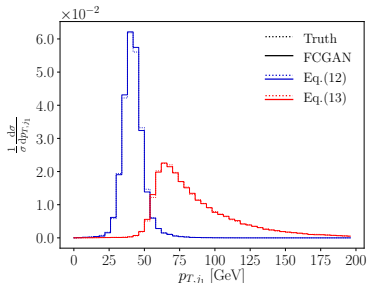
## Fully conditional GAN

## Proper sampling

- map random numbers to parton level  
hadron level as condition [matched event pairs]
- full inversion fine [again]
- tougher cuts challenging  $m_{jj}$  [14%, 39% events, no interpolation, MMD not conditional]

$$p_{T,j_1} = 30 \dots 50 \text{ GeV} \quad p_{T,j_2} = 30 \dots 40 \text{ GeV} \quad p_{T,e^-} = 20 \dots 50 \text{ GeV} \quad (12)$$

$$p_{T,j_1} > 60 \text{ GeV} \quad (13)$$



## Fully conditional GAN

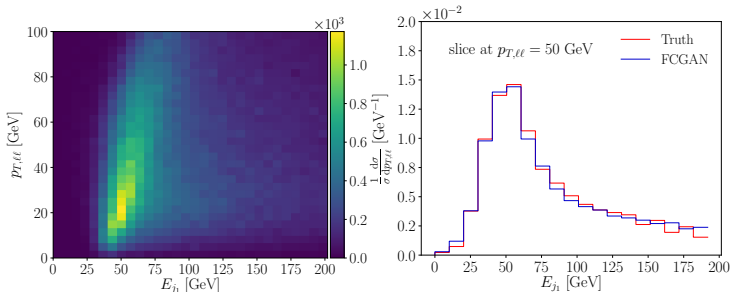
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$$p_{T,j_1} > 60 \text{ GeV} \quad (13)$$

- pretty pictures in 2D



⇒ 1.FCGAN unfolding works!



# BSM injection

Different training (MC) and actual data... [not in v1, thank you to Ben Nachman]

...or model dependence of unfolding

...or localization in latent space

– train: SM events

test: 10% events with  $W'$  in s-channel  $\Rightarrow$  any guesses?



## BSM injection

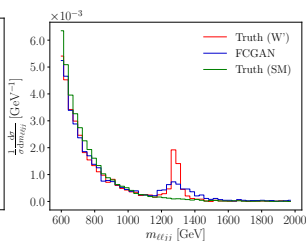
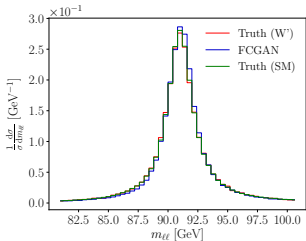
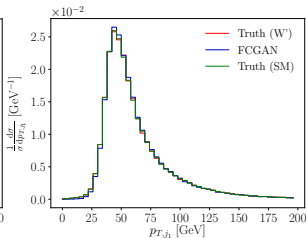
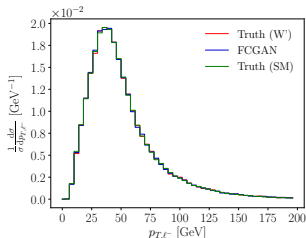
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## 4– Unfolding as inverting

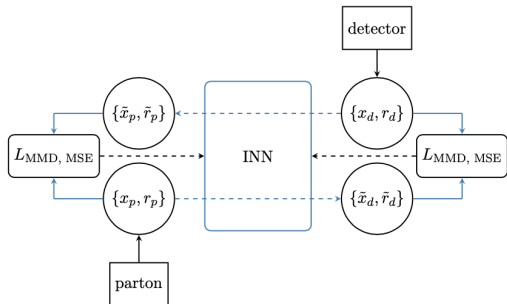
**Invertible networks?** [Bellagente, Butter, Kasieczka, TP, Rousselot, Winterhalder (soon)]

- network as bijective transformation — normalizing flow  
Jacobian tractable — normalizing flow  
evaluation in both directions — INN [Ardizzone, Kruse, Rother, Köthe]
- building block: coupling layer

$$x_d \sim g(x_p) \quad \text{with} \quad \frac{\partial g(x_p)}{\partial x_p} = \begin{pmatrix} \text{diag } e^{s_2(x_p, 2)} & \text{finite} \\ 0 & \text{diag } e^{s_1(x_d, 1)} \end{pmatrix}$$

- dimensions padded by random numbers

$$\begin{pmatrix} x_p \\ r_p \end{pmatrix} \xleftarrow{\text{PYTHIA, DELPHES: } g \rightarrow} \begin{pmatrix} x_d \\ r_d \end{pmatrix} \xrightarrow{\leftarrow \text{unfolding: } \bar{g}}$$



## 4– Unfolding as inverting

**Invertible networks?** [Bellagente, Butter, Kasieczka, TP, Rousselot, Winterhalder (soon)]

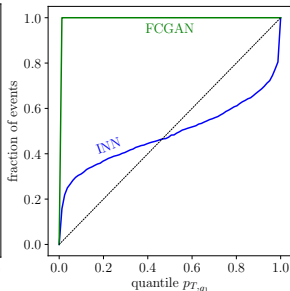
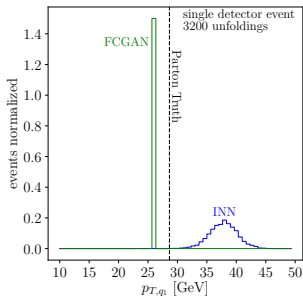
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$$x_d \sim g(x_p) \quad \text{with} \quad \frac{\partial g(x_p)}{\partial x_p} = \begin{pmatrix} \text{diag } e^{s_2(x_{p,2})} & & \\ & \dots & \\ & & 0 & \dots & \\ & & & \dots & \text{diag } e^{s_1(x_{d,1})} \end{pmatrix} \quad \begin{matrix} \text{finite} \\ \\ \\ \end{matrix}$$

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$$\begin{pmatrix} x_p \\ r_p \end{pmatrix} \xleftarrow{\text{PYTHIA, DELPHES: } g \rightarrow} \begin{pmatrix} x_d \\ r_d \end{pmatrix} \xrightarrow{\leftarrow \text{unfolding: } \bar{g}}$$

⇒ statistically promising

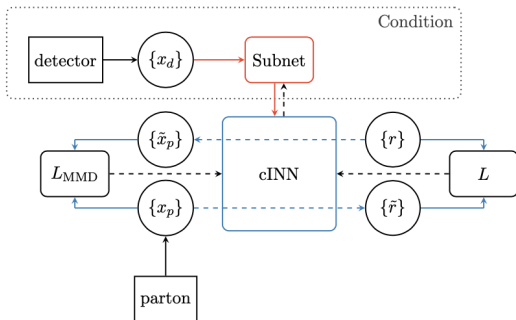




# Conditional INN

## Further improvement: conditional network

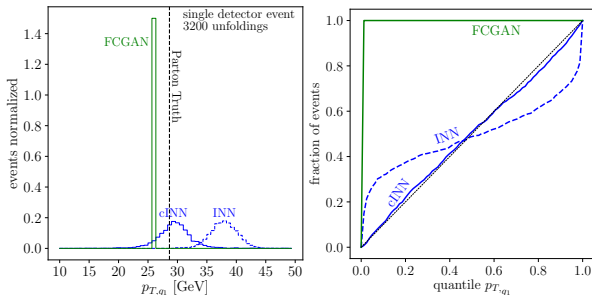
- same procedure as for GAN
- sampling parton level events from random numbers



# Conditional INN

## Further improvement: conditional network

- same procedure as for GAN
- sampling parton level events from random numbers
- calibration for statistical unfolding



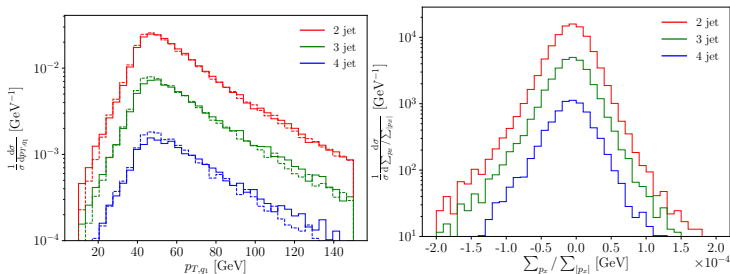
# Conditional INN

## Further improvement: conditional network

- same procedure as for GAN
- sampling parton level events from random numbers
- calibration for statistical unfolding

## Unfolding extra jets

- detector-level process  $pp \rightarrow ZW+\text{jets}$  [variable number of objects]
- parton-level hard process chosen  $2 \rightarrow 2$  [whatever you want]
- ME vs PS jets decided by network [including momentum conservation]



⇒ proper inversion, all working!



# Outlook

## Machine learning a great tool box

LHC physics really is big data

imagine classification was a starting point

jet classification largely established

generative networks exciting for theory

advantage 1: NN interpolation

advantage 2: latent space structures

advantage 3: training on MC and/or data

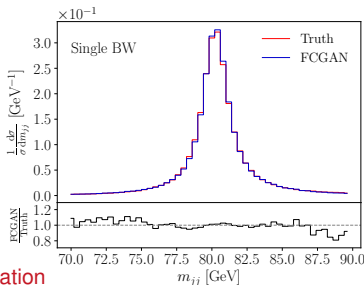
Any ideas?



## Dynamic MMD

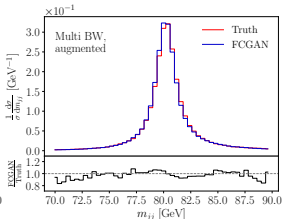
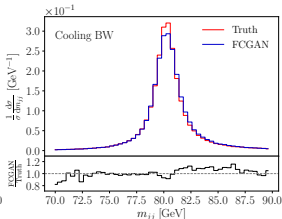
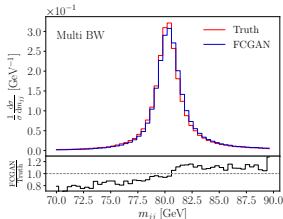
## Technical side-remark: dynamic MMD

- minimal input
- functional form of correlation  $m_{ij}$
- kernel shape (irrelevant) and resolution
- Adaptive resolution?



## Technical side-remark: dynamic MMD implementation

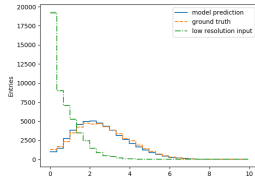
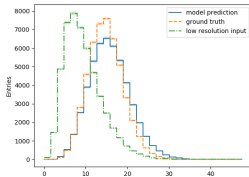
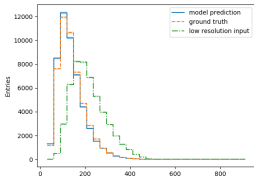
- multiple fixed-width kernels
  - multiple kernels for conditional input
  - cooling kernel [from SD of generator  $m_{ij}$ ]
- ⇒ Technical implementation still open...



# Superresolution GANs (preview)

## Getting inspired [Blecher, Butter, Keilbach, TP + Irvine]

- take high-resolution calorimeter images  
down-sample to 1/8th 1D resolution  
GAN inversion
- works because the GAN learn structure [showers are QCD]
- start from low-resolution calorimeter images  
GAN high-resolution images
- energy of constituents no.1,10,30



⇒ GANs are kind of magic

