

Generative and Invertible Networks for LHC Theory

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Oxford 10/2020



Big data for LHC

LHC: fundamental understanding of lots of data

Basics

1- Jets

2- GANplification

3- Events

4- Subtraction

5- Unfolding

6- Inverting

– what do we really do?

1. theory framework [SMEFT, SUSY]
2. precision predictions [first-principles QFT]
3. compare simulated and measured events

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 neuronic 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.

⇒ What can we learn from Google and Facebook?



Generative networks

GANgogh [Bonafilia, Jones, Danyluk (2017)]

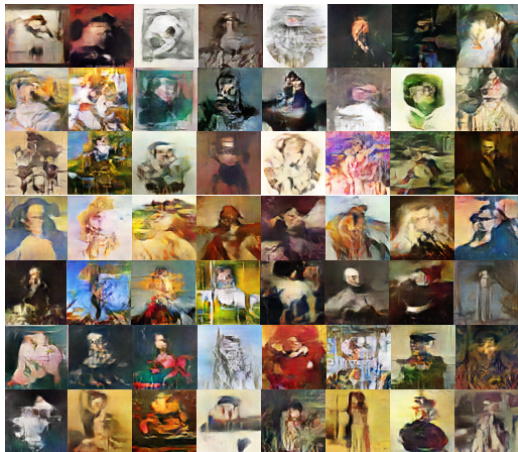
- neural network: learned function $f(x)$ [regression, classification]
- can networks create **new pieces of art**?
map random numbers to image pixels?
- train on 80,000 pictures [organized by style and genre]
- generate flowers



Generative networks

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

- trained on 15,000 portraits
 - sold for \$432,500
- ⇒ **ML all marketing and sales**



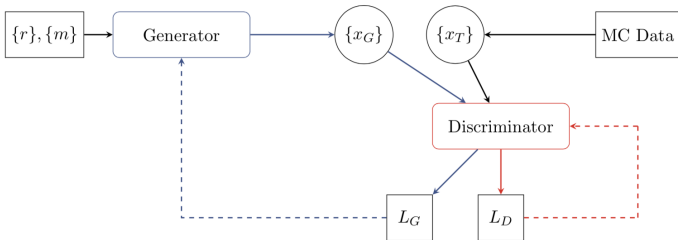
GAN algorithm

Generating events

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

$$L_D = \langle -\log D(x) \rangle_{x_T} + \langle -\log(1 - D(x)) \rangle_{x_G}$$
 - **generator** constructing $r \rightarrow x_G$ by minimizing [D needed]

$$L_G = \langle -\log D(x) \rangle_{x_G}$$
 - equilibrium $D = 0.5 \Rightarrow L_D = L_G = 1$
- \Rightarrow **statistically independent copy of training events**



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$$L_G = \langle -\log D(x) \rangle_{x_G}$$

⇒ **statistically independent copy of training events**

Generative network studies

- **Jet Images** [de Oliveira (2017), Carrazza-Dreyer (2019)]
- **Detector simulations** [Paganini (2017), Musella (2018), Erdmann (2018), Ghosh (2018), Buhmann (2020)]
- **Events** [Otten(2019), Hashemi (2019), Di Sipio (2019), **Butter (2019)**, Martinez (2019), Alanazi (2020), Chen (2020)]
- **Unfolding** [Datta (2018), Omnifold (1911), **Bellagente (2019)**, **Bellagente (2020)**]
- **Templates for QCD factorization** [Lin (2019)]
- **EFT models** [Erbin (2018)]
- **Event subtraction** [**Butter (2019)**]
- **Sherpa** [Bothmann (2020), Gao (2020)]
- **Basics** [GANplification (2020), DCTR (2020)]



1– Jet generation

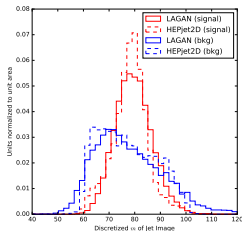
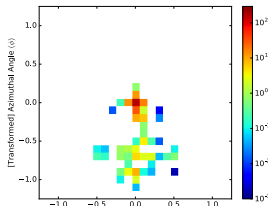
GANgogh for jet images [de Oliveira, Paganini, Nachman]

- start with calorimeter or jet images [η vs ϕ]
- sparsity the technical challenge [cf top tagging comparison]

- 1- reproduce valid jet images from training data
 - 2- organize them by QCD vs W -decay jets
 - high-level observables as check
- ⇒ **Generating jets** [Carrazza & Dreyer]

GAN questions

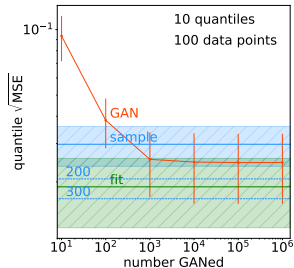
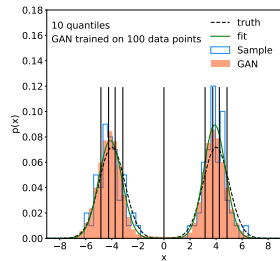
- use cases?
- control?
- uncertainty? [Bayesian networks?]
- gain?
- achievable precision?



2- GANplification

Gain beyond training data [Butter, Diefenbacher, Kasieczka, Nachman, TP]

- true function known
compare GAN vs sampling vs fit
- χ^2 -sum of quantiles



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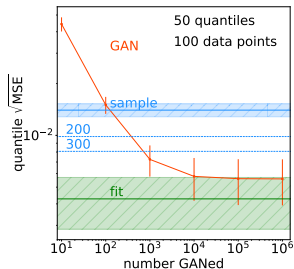
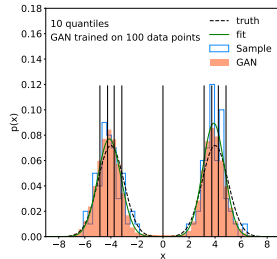
6- Inverting



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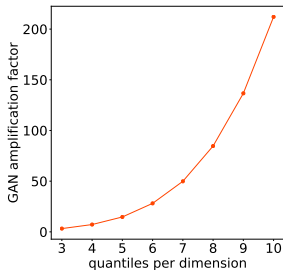
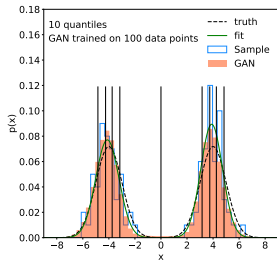
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compare GAN vs sampling vs fit
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- fit like 500-1000 sampled points
GAN like 500 sampled points [amplification factor 5]
requiring 10,000 GANned events



2- GANplification

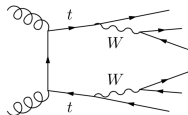
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- true function known
compare GAN vs sampling vs fit
 - χ^2 -sum of quantiles
 - fit like 500-1000 sampled points
GAN like 500 sampled points [amplification factor 5]
requiring 10,000 GANned events
 - 5-dimensional Gaussian shell
sparsely populated
amplification vs quantiles
 - fit-like additional information
 - interpolation and resolution the key [NNPDF]
- ⇒ GANs enhance training data



3– How to GAN LHC events

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

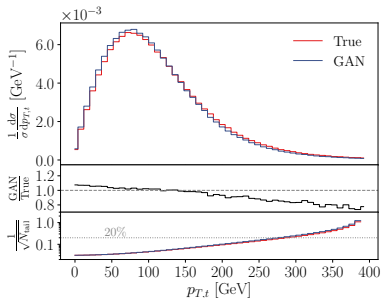


- medium-complex final state $t\bar{t} \rightarrow 6$ jets

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]

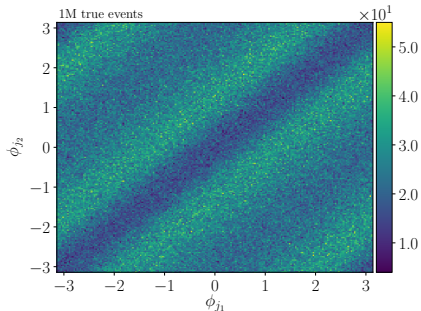
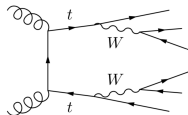
- flat observables flat [phase space coverage okay]
- direct observables with tails [statistical error indicated]
- constructed observables similar



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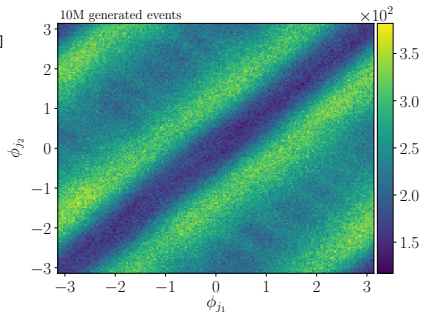
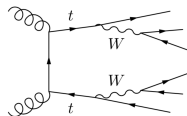
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- constructed observables similar
- improved resolution [1M training events]



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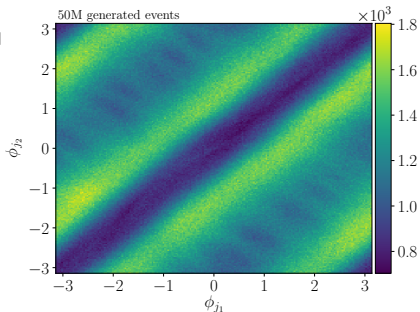
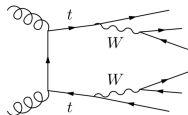
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- constructed observables similar
- improved resolution [10M generated events]



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- 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]
- direct observables with tails [statistical error indicated]
- constructed observables similar
- improved resolution [50M generated events]
- **Proof of concept**



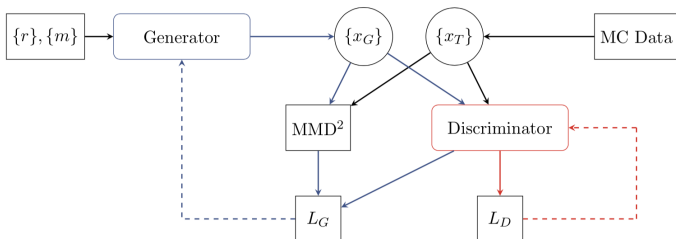
Chemistry of loss functions

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

$$\text{MMD}^2 = \langle k(x, x') \rangle_{x_T, x'_T} + \langle k(y, y') \rangle_{y_G, y'_G} - 2 \langle k(x, y) \rangle_{x_T, y_G}$$

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

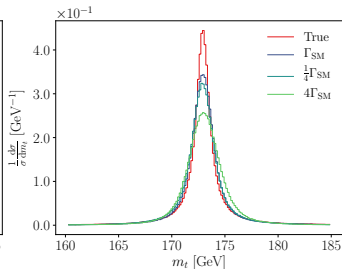
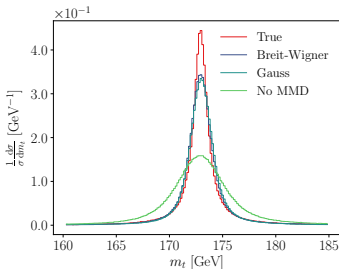


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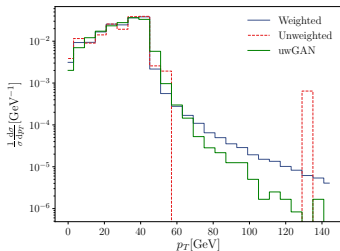
$$L_G \rightarrow L_G + \lambda_G \text{MMD}^2,$$



Unfolding

Gaining beyond GANplification [Butter, TP, Winterhalder]

- phase space sampling: weighted events [PS weight $\times |\mathcal{M}|^2$]
events: unweighted events [‘just events’]
- probabilistic unweighting weak spot of standard MC
- learn phase space from weighted events
generate unweighted events [(almost)]
- give us a few weeks...



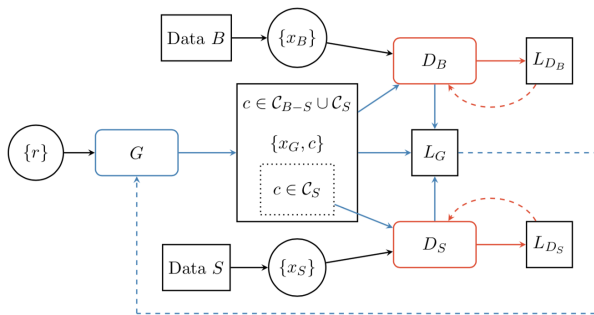
4– How to GAN event subtraction

Idea: subtract samples without binning [Butter, TP, Winterhalder]

- statistical uncertainty

$$\Delta_{B-S} = \sqrt{\Delta_B^2 + \Delta_S^2} > \max(\Delta_B, \Delta_S)$$

- 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



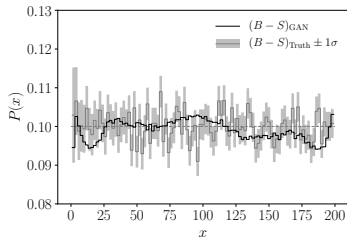
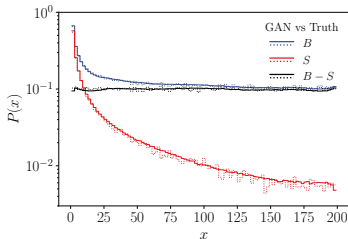
Subtracted events

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!)



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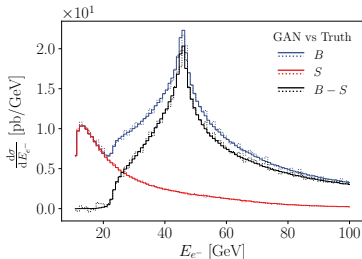
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2- event-based background subtraction [weird notation, sorry]

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



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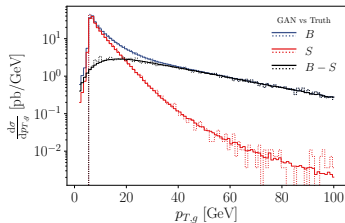
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3- collinear subtraction [assumed non-local]

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



⇒ Applications in theory and analysis



5– How to GAN away detector effects

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

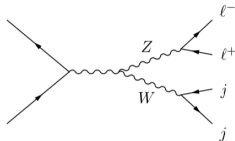
- detector simulation typical Markov process
- inversion possible, in principle [entangled convolutions]
- GAN task

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

\Rightarrow Full phase space unfolded

Reference process $pp \rightarrow ZW \rightarrow (\ell\ell)(jj)$

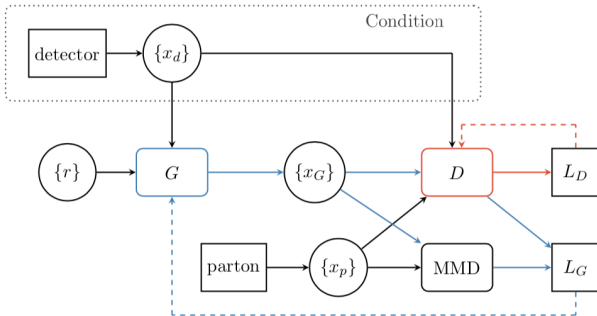
- broad jj mass peak
 - narrow $\ell\ell$ mass peak
 - modified $2 \rightarrow 2$ kinematics
 - fun phase space boundaries
 - GAN same as event generation [with MMD]
- \Rightarrow Perfect if training and test the same



Fully conditional GAN

Getting random sampling logic right

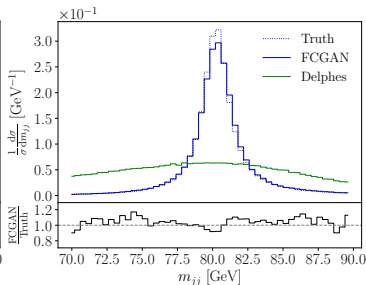
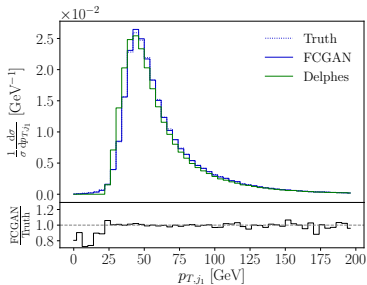
- map random numbers to parton level
hadron level as condition [matched event pairs]



Fully conditional GAN

Getting random sampling logic right

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



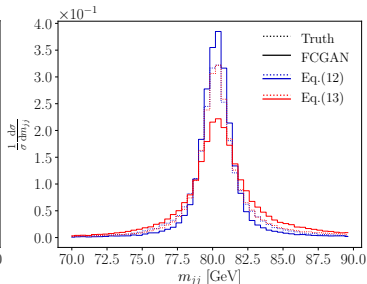
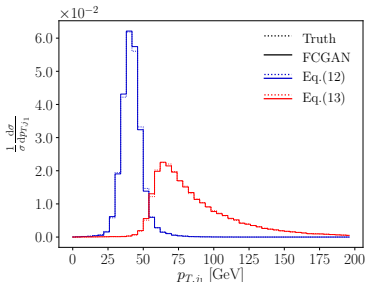
Fully conditional GAN

Getting random sampling logic right

- map random numbers to parton level
hadron level as condition [matched event pairs]
- full inversion fine
- detector-level cuts [14%, 39% events, no interpolation, MMD not conditional]

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

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



Fully conditional GAN

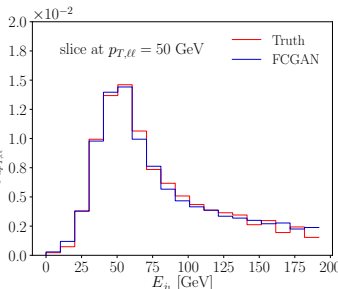
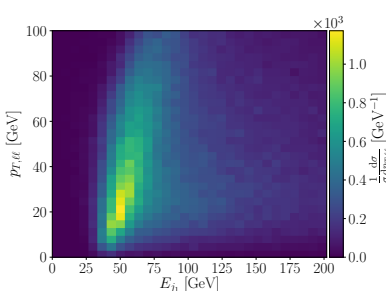
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- pretty pictures in 2D



⇒ 1.FCGAN unfolding at work



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?

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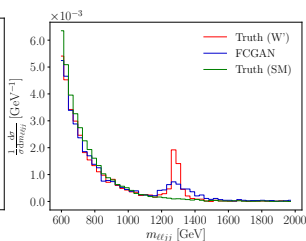
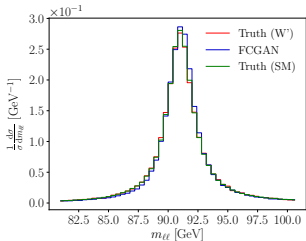
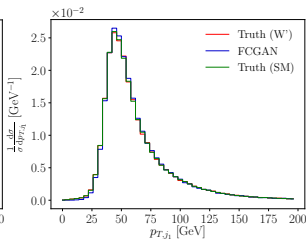
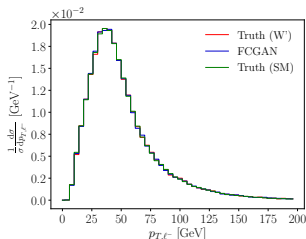
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...or model dependence of unfolding

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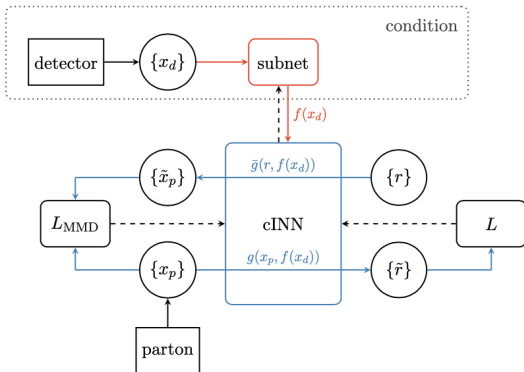
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6– Unfolding as inverting

Invertible networks [Bellagente, Butter, Kasieczka, TP, Rousselot, Winterhalder, Ardigzone, Köthe]

- network as bijective transformation — normalizing flow
Jacobian tractable — normalizing flow
evaluation in both directions — INN [Ardizzone, Rother, Köthe]
- building block: coupling layer
- conditional: parton-level events from $\{r\}$



6– Unfolding as inverting

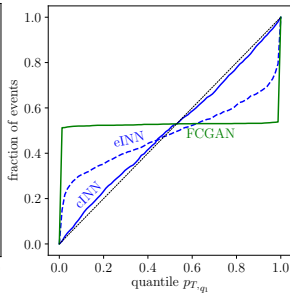
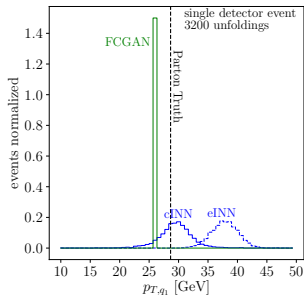
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Again $pp \rightarrow ZW \rightarrow (\ell\ell) (jj)$

- performance on distributions like FCGAN
- parton-level probability distribution for single detector event

⇒ **Proper statistical unfolding**



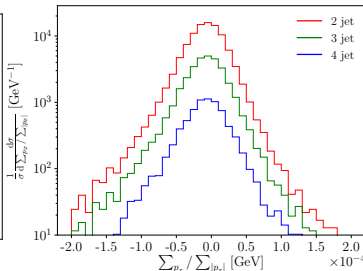
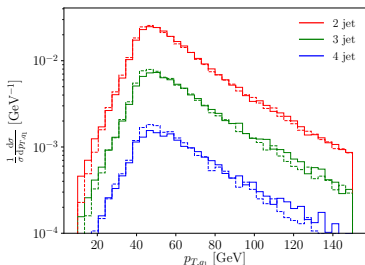
6– Unfolding as inverting

Invertible networks [Bellagente, Butter, Kasieczka, TP, Rousselot, Winterhalder, Ardizzone, Köthe]

- network as bijective transformation — normalizing flow
Jacobian tractable — normalizing flow
evaluation in both directions — INN [Ardizzone, Rother, Köthe]
- building block: coupling layer
- conditional: parton-level events from $\{r\}$

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]



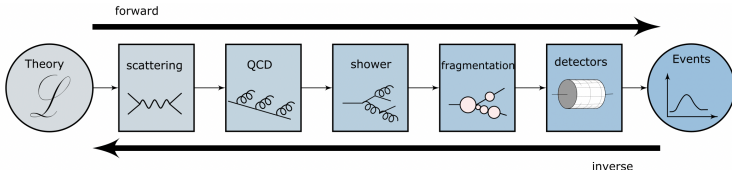
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- ⇒ How systematically can we invert?



Outlook

Machine learning for LHC theory

- goal: **data-to-data** with fundamental physics input
 - MC challenges
 - higher-order precision in bulk
 - coverage of tails
 - unfolding to access fundamental QCD
 - neural network benefits
 - best available interpolation**
training on MC and/or data, anything goes
lightning speed, once trained
 - GANs the cool kid
 - generator** trying to produce best events
 - discriminator** trying to catch generator,
 - INNs the theory hope
 - flow networks** to control spaces
 - invertible** network the new tool
- Any ideas?

