Generative Networks

Tilman Plehn

GAN basics

Generation

Inversion

Invertible LHC Simulations with Generative Networks

Tilman Plehn

Universität Heidelberg

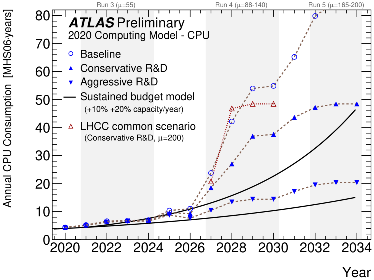
CAU BSM Workshop 2/2021

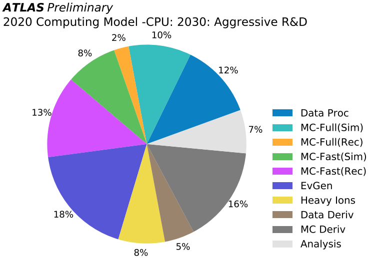
Orthogonal view on BSM searches

Searching for models $\longrightarrow$ fundamental understanding of data

- precision theory
- precision simulations
- precision measurements

$\Rightarrow$ What's needed to keep the edge?





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Precision event generation

- simulated event numbers $\sim$ expected events [factor 25 for HL-LHC]
- general move to NLO/NNLO [1%-2% error]
- higher relevant multiplicities [jet recoil, extra jets, WBF, etc.]
- new low-rate high-multiplicity backgrounds
- cutting-edge predictions not through generators [N^{3}LO in Pythia?]
- interpretation beyond specific models [jets+MET]

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Three ways to use ML

- improve current tools: iSherpa, ML-MadGraph, etc
- new ideas, like fast ML-generator-networks
- conceptual ideas in theory simulations and analyses

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

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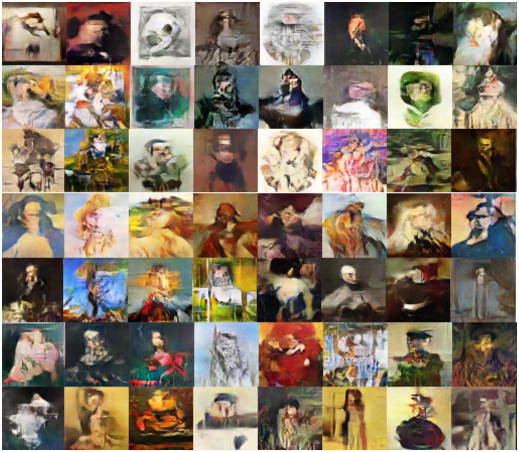

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Edmond de Belamy [Caselles-Dupre, Fautrel, Vernier]

– trained on 15,000 portraits

– sold for $432.500

$\Rightarrow$ ML all marketing and sales

GAN algorithm

Generating events

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

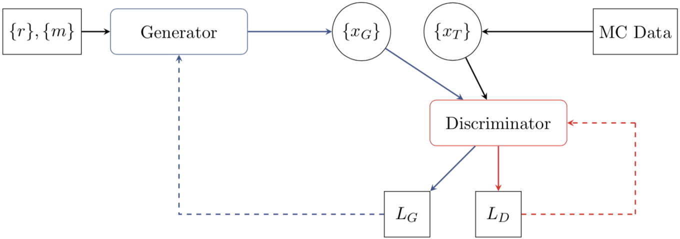
$$L_D = \Big\langle -\log D(x) \Big\rangle_{x_T} + \Big\langle -\log(1 - D(x)) \Big\rangle_{x_G}$$

– generator constructing $r \to x_G$ by minimizing [D needed]

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

– equilibrium $D = 0.5 \;\Rightarrow\; L_D = L_G = -\log 0.5$

$\Rightarrow$ statistically independent copy of training events



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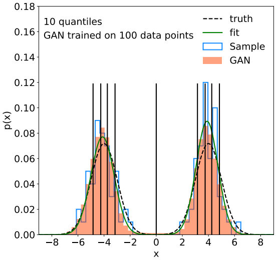
Generative network studies [review 2008.08558]

- Jets [de Oliveira (2017), Carrazza-Dreyer (2019)]
- Detector simulations [Paganini (2017), Musella (2018), Erdmann (2018), Ghosh (2018), Buhmann (2020)]
- Events [Otten (2019), Hashemi, DiSipio, Butter (2019), Martinez (2019), Alanazi (2020), Chen (2020), Kansal (2020)]
- Unfolding [Datta (2018), Omnifold (2019), Bellagente (2019), Bellagente (2020), Howard (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)]
- Unweighting [Verheyen (2020), Backes (2020)]
- Superresolution [DiBello (2020), Baldi (2020)]

GANplification

Warm-up: gain beyond training data [Butter, Diefenbacher, Kasieczka, Nachman, TP]

- true function known
  compare GAN vs sampling vs fit
- quantiles with χ^2-values



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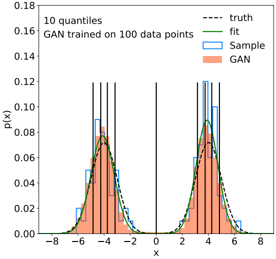
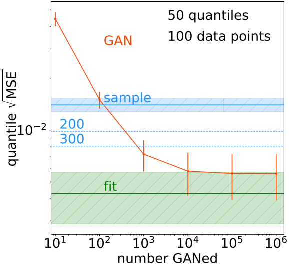
  GAN like 500 sampled points [amplifictation factor 5]
  requiring 10,000 GANned events





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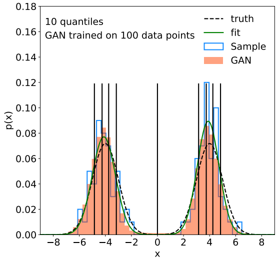
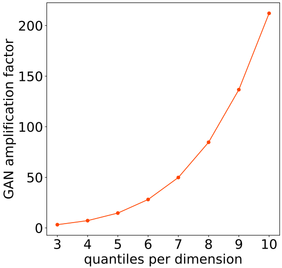
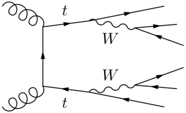
– 5-dimensional Gaussian shell
  sparsely populated
  amplification vs quantiles
– fit-like additional information
– interpolation and resolution the key [NNPDF]

$\Rightarrow$ GANs enhancing training data



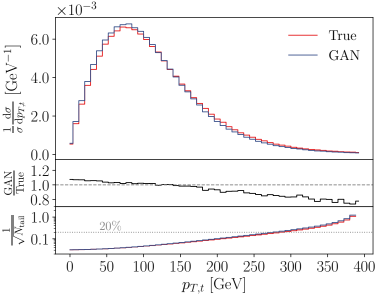


How to GAN LHC events



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

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



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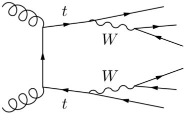

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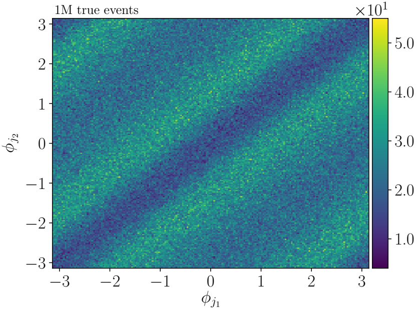

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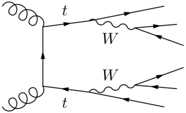

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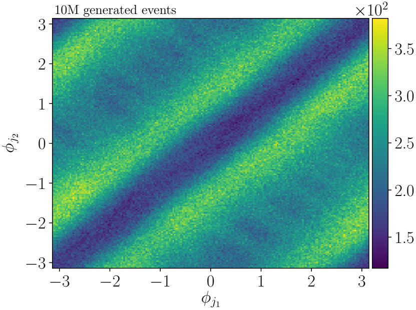

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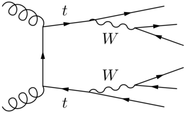

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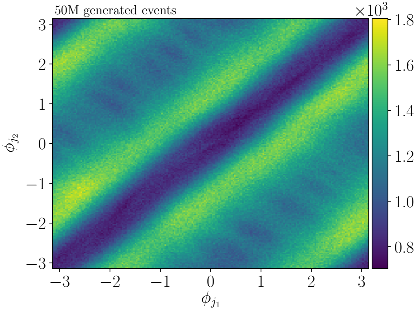
- reconstructed observables similar
- improved resolution [50M generated events]
- Forward simulation working



Chemistry of loss functions

GAN version of adaptive sampling

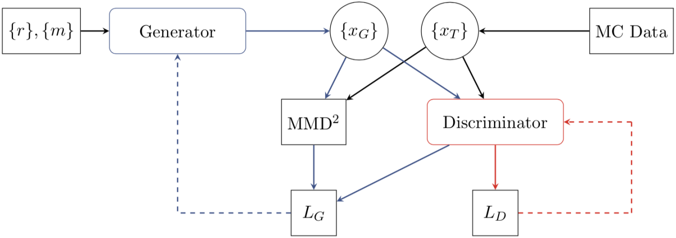
– generally 1D features

phase space boundaries
kinematic cuts
invariant masses [top, W]

– batch-wise comparison of distributions, MMD loss with kernel k

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

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



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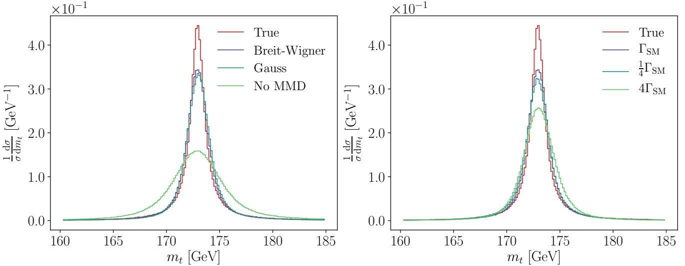
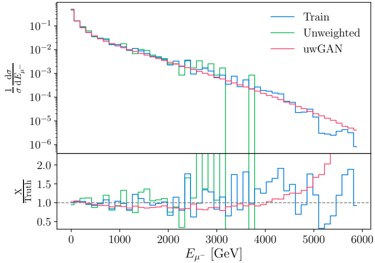


Unweighting

Gaining beyond GANpliflication [Butter, TP, Winterhalder]

- phase space sampling: weighted events [PS weight $\times |\mathcal{M}|^2$]
  events: constant weights
- probabilistic unweighting weak spot of standard MC
- learn phase space patterns [density estimation]
  generate unweighted events [through loss function]
- compare training, GAN, classic unweighting



Inverted simulation

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

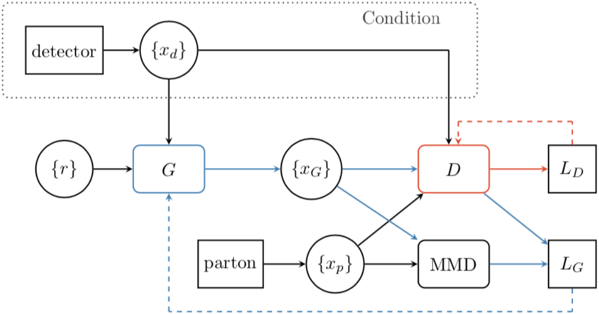
- detector simulation typical Markov process
- inversion possible, in principle [entangled convolutions]
- GAN task

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

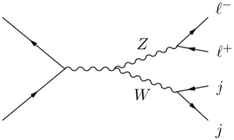
$\Rightarrow$ Full phase space unfolded

Conditional GAN

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



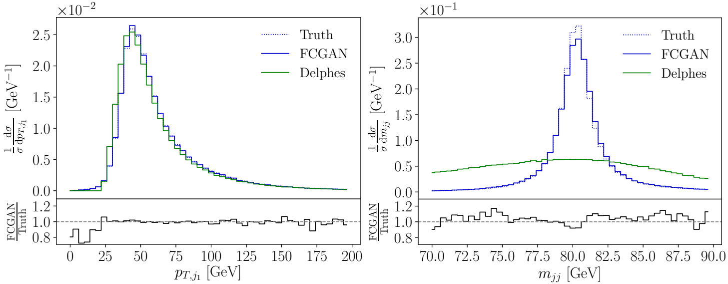
Detector unfolding



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

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

Simple application



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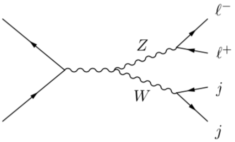

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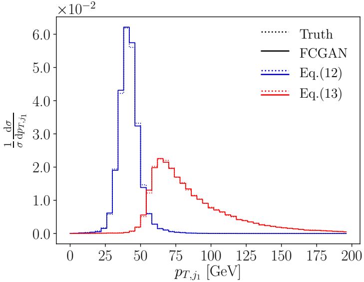
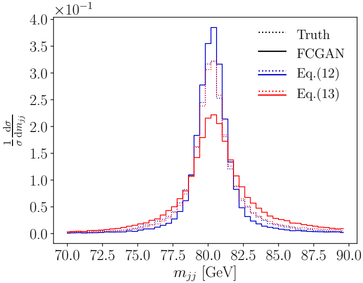
Simple application

– detector-level cuts [14%, 39% events, no interpolation, MMD not conditional]

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

$$p_{T,j_1} > 60\ \text{GeV} \tag{13}$$





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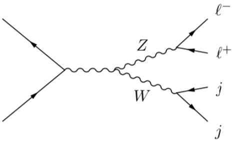

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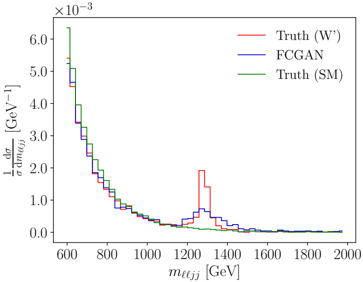
– model dependence of unfolding

– train: SM events
  test: 10% events with W' in s-channel

$\Rightarrow$ Working fine, but ill-defined

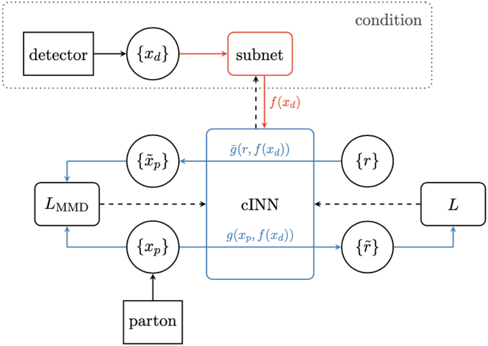


Unfolding as inverting

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

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

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



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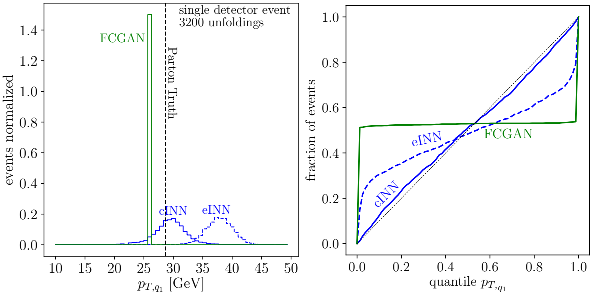
Properly defined unfolding [again $pp \to ZW \to (\ell\ell)\ (jj)$]

– performance on distributions like FCGAN

– parton-level probability distribution for single detector event

$\Rightarrow$ Proper statistical unfolding



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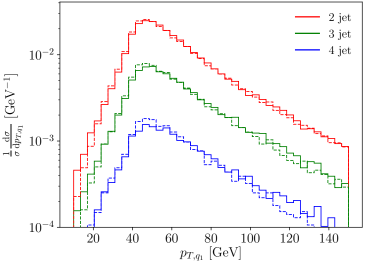
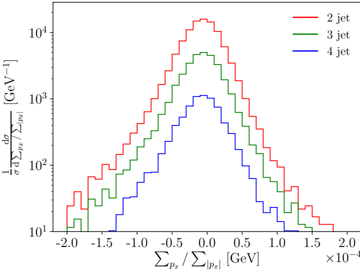
Unfolding initial-state radiation

– detector-level process $pp \to ZW$+jets [variable number of objects]

– parton-level hard process chosen $2 \to 2$ [whatever you want]

– ME vs PS jets decided by network [including momentum conservation]





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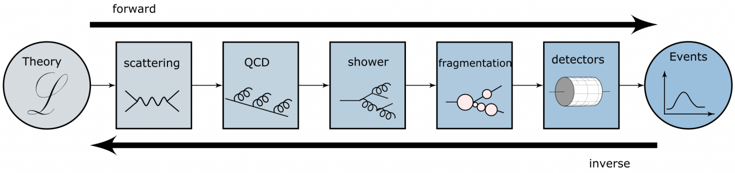
$\Rightarrow$ How systematically can we invert?



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?