Invertible Networks for LHC Theory

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Briefest introduction ever

Neural network just a function

– think $f_\theta(x)$ just as $f(x)$

– no parametrization, just very many values θ

– θ-space the cool space [latent space]

Construction through minimization

– define loss function L

– minimize through task

– evaluate $x \to f(x)$ in test/use case

LHC applications

– regression: parton momentum from jet constituents
matrix element over phase space

– classification: gluon/quark/bottom/top inside jet

– generation: sample $r \to f(r)$

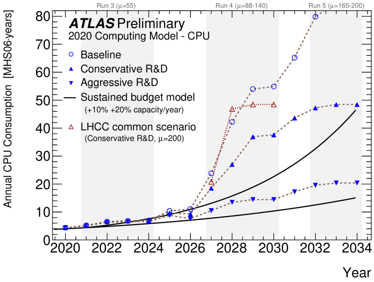
...

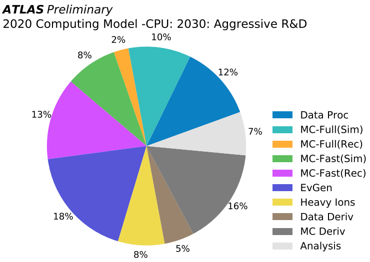
Challenges towards HL-LHC

Paradigm shift: model searches $\longrightarrow$ fundamental understanding of data

- precision QCD
- precision simulations
- precision measurements

$\Rightarrow$ Nothing fundamental without simulations [not even unsupervised...]





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10-year HL-LHC requirements

– 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^3LO in Pythia?]

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Three ways to use ML

- improve current tools: iSherpa, ML-MadGraph, etc
- new tools: 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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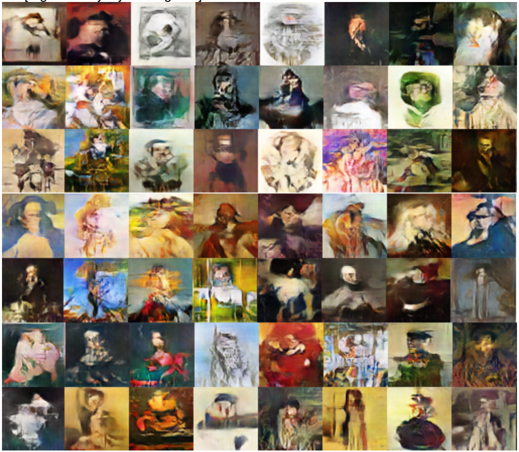

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– trained on 15,000 portraits

– sold for $432.500

$\Rightarrow$ ML all marketing and sales

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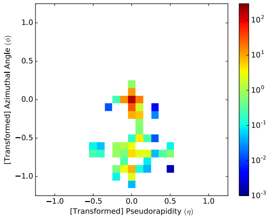
Jet portraits [de Oliveira, Paganini, Nachman (2017)]

– calorimeter or jet images
sparsity the technical challenge
1- reproduce valid jet images from training data
2- organize them by QCD vs W-decay jets
– high-level observables m, τ_{21} as check
⇒ GANs generating QCD jets



GAN algorithm

Generating events [phase space positions, possibly with weights]

- 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]

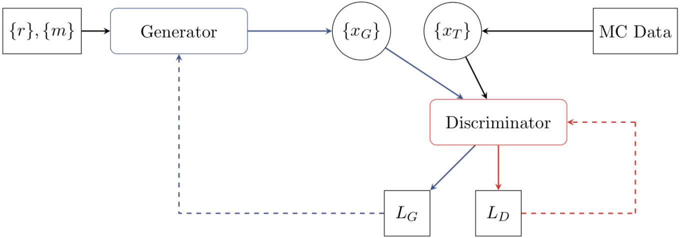
$$L_D = \big\langle -\log D(x) \big\rangle_{x_T} + \big\langle -\log(1 - D(x)) \big\rangle_{x_G}$$

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

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

- equilibrium $D = 0.5 \;\Rightarrow\; L_D/2 = L_G = -\log 0.5$

$\Rightarrow$ statistically independent copy of training events



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Generative network studies

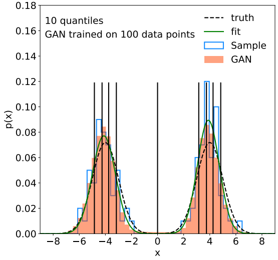
– Jets [de Oliveira (2017), Carrazza-Dreyer (2019)]
– Detector simulations [Paganini (2017), Musella (2018), Erdmann (2018), Ghosh (2018), Buhmann (2020,2021)]
– Events [Otten (2019), Hashemi, DiSipio, Butter (2019), Martinez (2019), Alanazi (2020), Chen (2020), Kansal (2020)]
– Unfolding [Datta (2018), Omnifold (2019), Bellagente (2019), Bellagente (2020), Vandegar (2020), Howard (2020)]
– Templates for QCD factorization [Lin (2019)]
– EFT models [Erbin (2018)]
– Event subtraction [Butter (2019)]
– Phase space [Bothmann (2020), Gao (2020), Klimek (2020)]
– Basics [GANplification (2020), DCTR (2020)]
– Unweighting [Verheyen (2020), Backes (2020)]
– Superresolution [DiBello (2020), Baldi (2020)]
– Parton densities [Carrazza (2021)]
– Uncertainties [Bellagente (2021)]

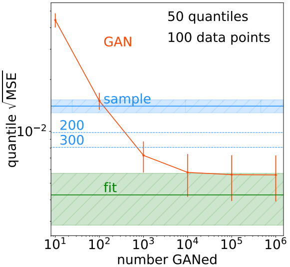
GANplification

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

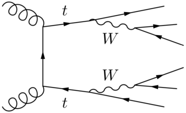
– true function known
  compare GAN vs sampling vs fit
– quantiles with χ^2-values
– fit like 500-1000 sampled points
  GAN like 500 sampled points [amplifictation factor 5]
  requiring 10,000 GANned events
– interpolation and resolution the key [NNPDF]

$\Rightarrow$ GANs beyond training data



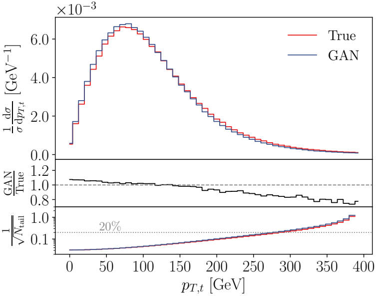


How to GAN LHC events



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]
  parton level, because it is harder
- flat observables flat [phase space coverage okay]
- standard observables with tails [statistical error indicated]



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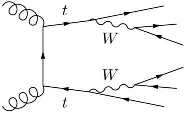

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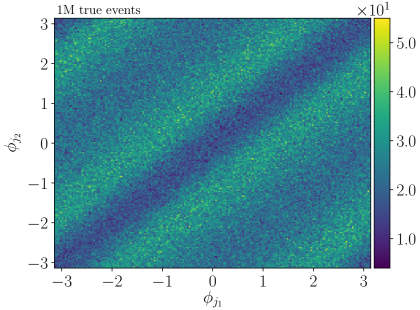
- improved resolution [1M training events]



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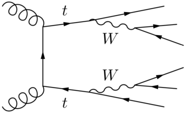

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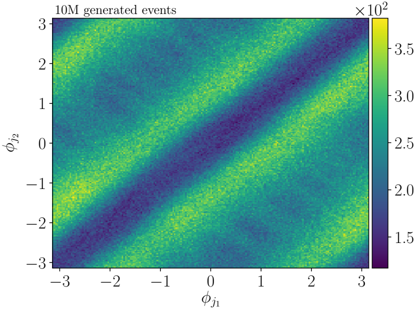

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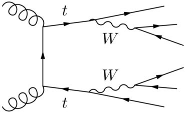

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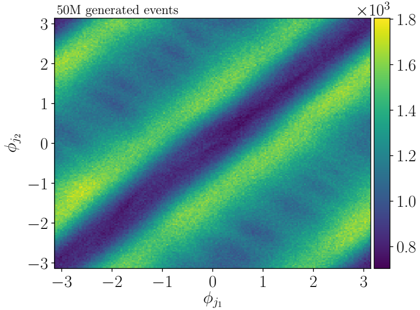
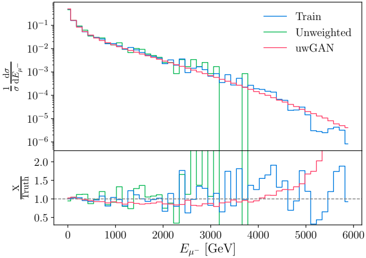
- improved resolution [50M generated events]
- Forward simulation working



Bonus: unweighting & errors without binning

Gaining from unweighting [Butter, TP, Winterhalder]

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



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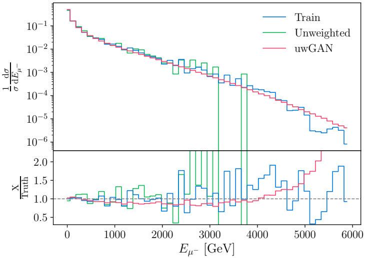
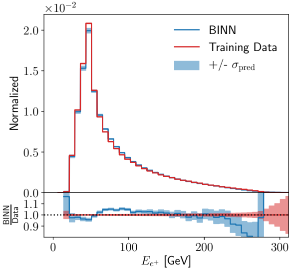


Events with error bars [Bellagente, Haußmann, Luchmann, TP]

(1) learn phase space density as usual

(2) learn error from weight distributions [Bayesian n

- generate events with error bars



How to GAN away detector effects

Goal: invert Monte Carlo [Bellagente, Butter, Kasiczka, TP, Winterhalder]

– parton shower, detector simulation typical examples [drawing random numbers]

– inversion possible, in principle [entangled convolutions, model assumed]

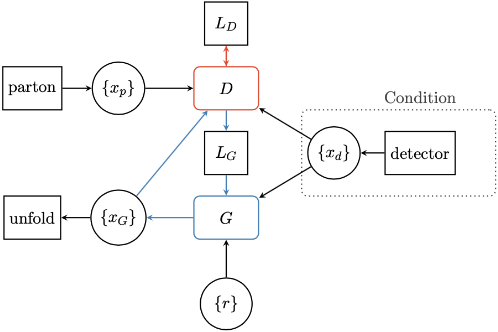
– GAN task

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

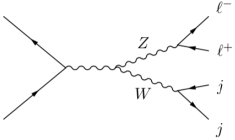
$\Rightarrow$ Full phase space unfolded

Conditional GAN

– random numbers $\longrightarrow$ parton level
hadron level as condition
matched event pairs



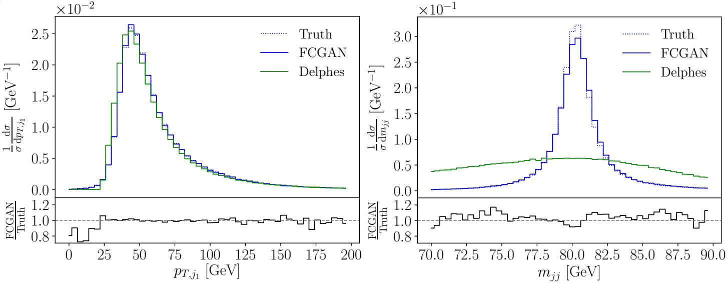
Detector unfolding



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]

Model (in)dependence



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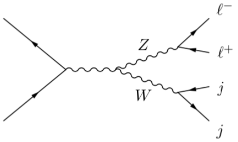

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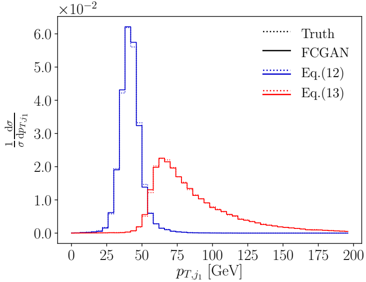
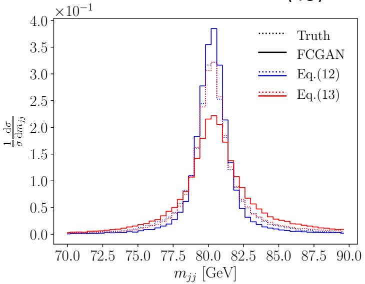
Model (in)dependence

– 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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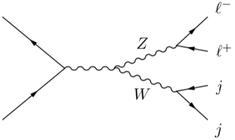

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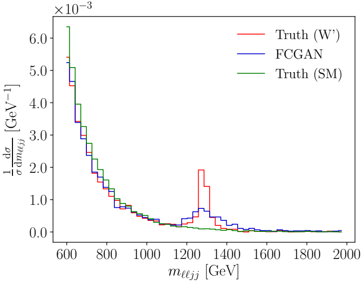
- model dependence [Thank you to BenN]
- train: SM events
  test: 10% events with W' in s-channel

$\Rightarrow$ Working fine, but ill-defined

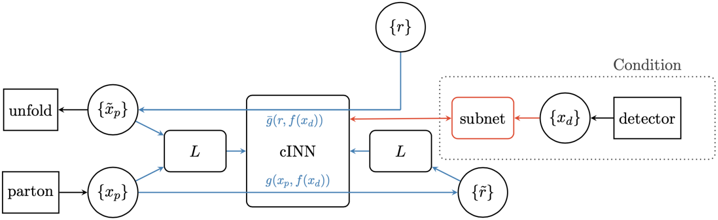


Proper inverting

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

- network as bijective transformation — normalizing flow
  Jacobian tractable [specifically: coupling layer]
  evaluation in both directions — INN [Ardizzone, Rother, Köthe]
- standard setup, random-number-padded working like FCGAN
- 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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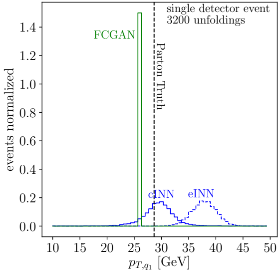
– performance on distributions like FCGAN
– parton-level probability distribution for single detector event

$\Rightarrow$ Well-defined statistical inversion



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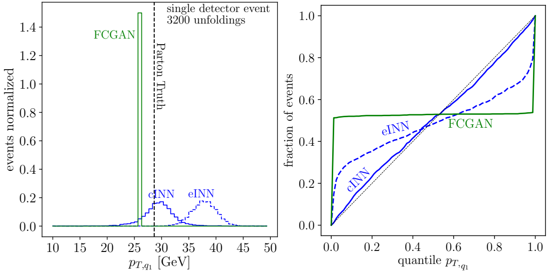

Invertible Networks

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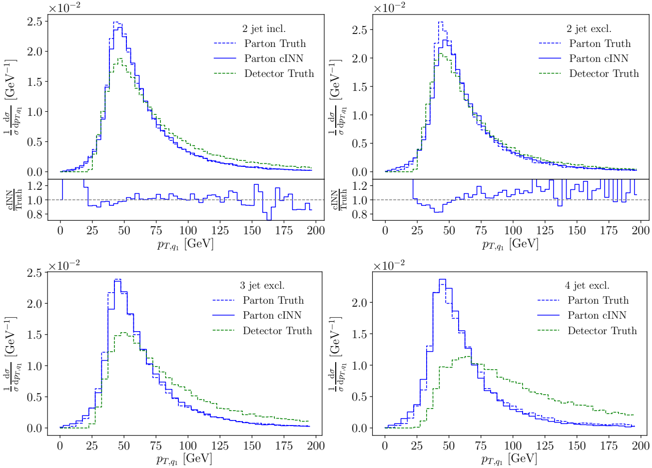
Inverting to hard process

What theorists want: undo ISR

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

– ME vs PS jets decided by network

– training jet-inclusively or jet-exclusively
parton-level hard process chosen $2 \to 2$



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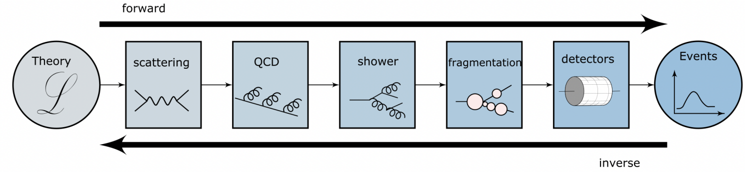
Towards systematic inversion

– detector unfolding known problem

– QCD parton from jet algorithm standard

– jet radiation possible

⇒ Invertible simulation in reach



Inverting to QCD

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

– condition jets with QCD parameters
  train model parameters $\longrightarrow$ Gaussian latent space
  test Gaussian sampling $\longrightarrow$ QCD parameter measurement

– going beyond C_A vs C_F [Kluth etal]

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

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

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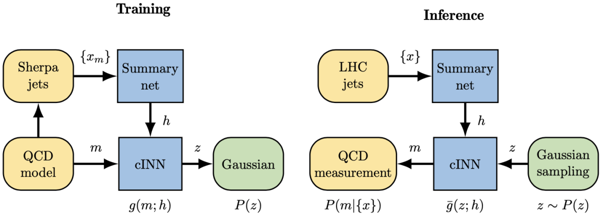

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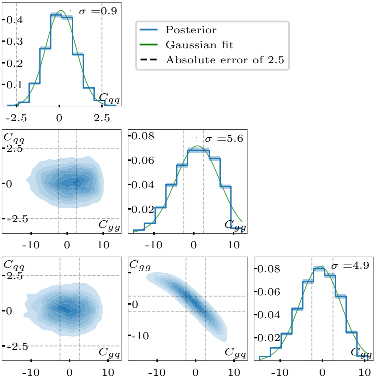
– idealized shower [Sherpa]



Inverting to QCD

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

– condition jets with QCD parameters
  train model parameters $\longrightarrow$ Gaussian latent space
  test Gaussian sampling $\longrightarrow$ QCD parameter measurement

– going beyond C_A vs C_F [Kluth etal]

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

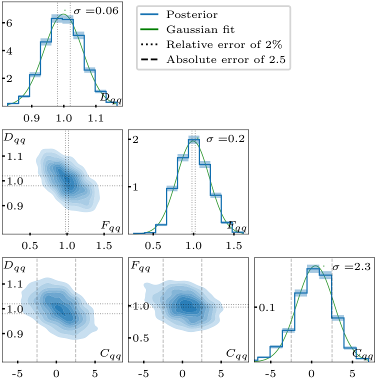
$$P_{gg} = 2C_A \left[D_{gg} \left(\frac{z(1-y)}{1-z(1-y)} + \frac{(1-z)(1-y)}{1-(1-z)(1-y)} \right) + F_{gg} z(1-z) + C_{gg} yz(1-z) \right]$$

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

– idealized shower [Sherpa]

– reality hitting...

– More ML-opportunities...



Machine learning for LHC theory

Machine learning for the LHC

– Classification/regression standard

  learning vs smart pre-processing
  uncertainties?
  experimental realities?

– GANs the cool kid

  generator trying to produce best events
  discriminator trying to catch generator

– INNs my theory hope

  flow networks for control
  condition for inversion
  Bayesian for errors

– Progress needs crazy ideas

Bonus: subtraction

Subtract samples without binning [Butter, TP, Winterhalder]

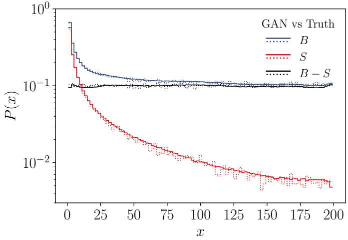
– statistical uncertainty

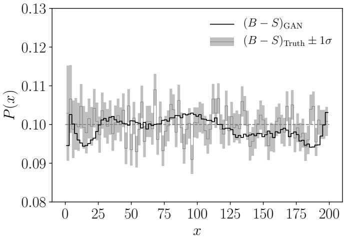
$$\Delta_{B-S} = \sqrt{\Delta_B^2 + \Delta_S^2} > \max(\Delta B, \Delta S)$$

– GAN setup: differential class label, sample normalization

– toy example

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





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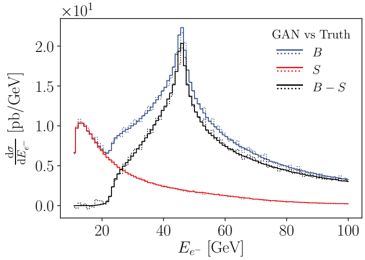
– event-based background subtraction [weird notation, sorry]

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



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– collinear subtraction [assumed non-local]

$pp \to Zg$ (B: matrix element, S: collinear approximation)