

Generative Networks for LHC

Tilman Plehn

Universität Heidelberg

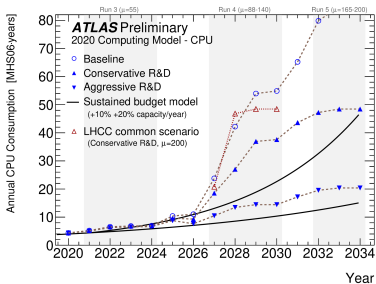
CMS 1/2021



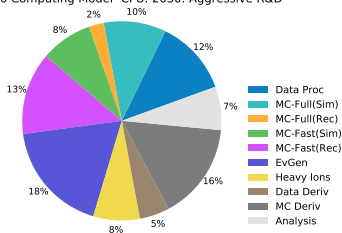
Simulations for future LHC runs

Unique: fundamental understanding of lots of data

- precision theory predictions
 - precision simulations
 - precision measurements
- ⇒ What's needed to keep the edge?



ATLAS Preliminary
2020 Computing Model -CPU: 2030: Aggressive R&D



Simulations for future LHC runs

Unique: fundamental understanding of lots of data

- precision theory predictions
 - precision simulations
 - precision measurements
- ⇒ What's needed to keep the edge?

Event generation towards HL-LHC

- simulated event numbers scaling with the expected events [factor 25]
- general move to NLO/NNLO as standard [5% error]
- higher relevant final-state multiplicities [jet recoil, extra jets, WBF, etc.]
- additional low-rate high-multiplicity backgrounds
- specific precision predictions not available in standard generators [N^3 LO in MC?]
- interpretation of measurements with general signal hypothesis [jets+MET]



Simulations for future LHC runs

Unique: fundamental understanding of lots of data

- precision theory predictions
 - precision simulations
 - precision measurements
- ⇒ What's needed to keep the edge?

Event generation towards HL-LHC

- simulated event numbers scaling with the expected events [factor 25]
- general move to NLO/NNLO as standard [5% error]
- higher relevant final-state multiplicities [jet recoil, extra jets, WBF, etc.]
- additional low-rate high-multiplicity backgrounds
- specific precision predictions not available in standard generators [N^3 LO in MC?]
- interpretation of measurements with general signal hypothesis [jets+MET]

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



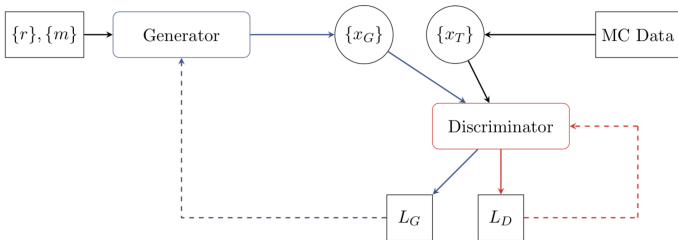
GAN algorithm

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**



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]
 - **generator** constructing $r \rightarrow x_G$ by minimizing [D needed]
- ⇒ **statistically independent copy of training events**

Generative network studies [review 2008.08558]

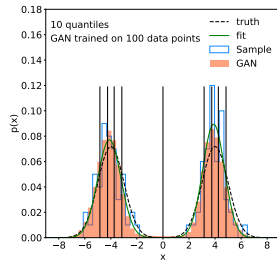
- **Jets** [de Oliveira (2017), Carrazza-Dreyer (2019)]
- **Detector simulations** [Paganini (2017), Musella (2018), Erdmann (2018), Ghosh (2018), Buhmann (2020)]
- **Events** [Ottens (2019), Hashemi, DiSipio, [Butter \(2019\)](#), Martinez (2019), Alanazi (2020), Chen (2020), Kansal (2020)]
- **Unfolding**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



GANplification

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

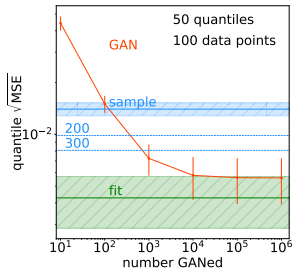
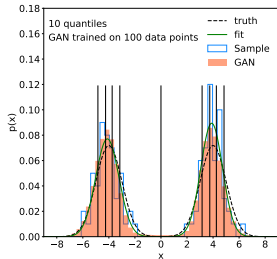
- true function known
compare GAN vs sampling vs fit
- quantiles with χ^2 -values



GANplification

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

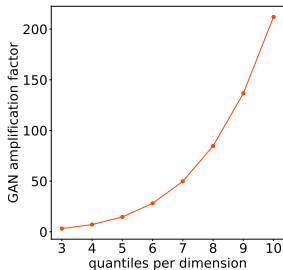
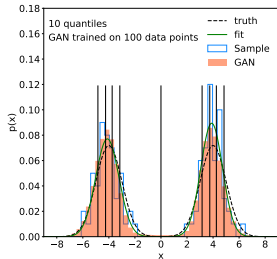
- true function known
compare GAN vs sampling vs fit
- quantiles with χ^2 -values
- fit like 500-1000 sampled points
GAN like 500 sampled points [amplification factor 5]



GANplification

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

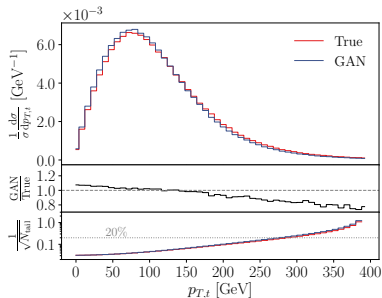
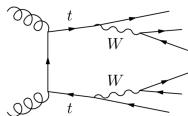
- true function known
compare GAN vs sampling vs fit
 - quantiles with χ^2 -values
 - fit like 500-1000 sampled points
GAN like 500 sampled points [amplification factor 5]
requiring 10,000 GANned events
 - 5-dimensional Gaussian shell
sparsely populated
amplification vs quantiles
 - fit-like additional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



How to GAN LHC events

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

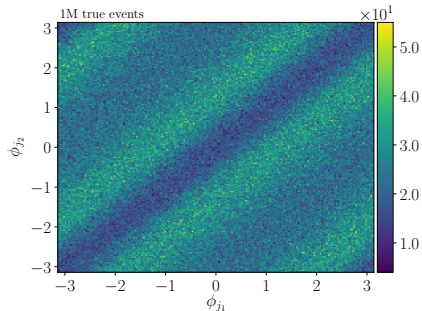
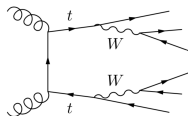
- medium-complex final state $t\bar{t} \rightarrow 6$ jets
- t/\bar{t} and W^\pm on-shell with BW $6 \times 4 = 18$ dof
- on-shell external states $\rightarrow 12$ dof [constants hard to learn]
- flat observables flat [phase space coverage okay]
- direct observables with tails [statistical error indicated]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



How to GAN LHC events

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

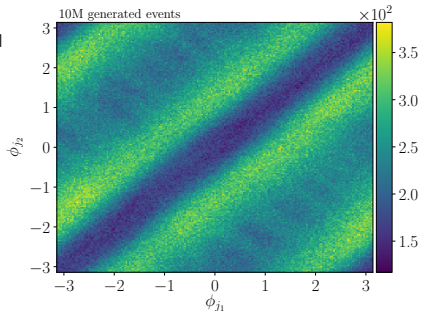
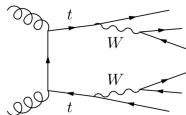
- medium-complex final state $t\bar{t} \rightarrow 6$ jets
- t/\bar{t} and W^\pm on-shell with BW $6 \times 4 = 18$ dof
- on-shell external states $\rightarrow 12$ dof [constants hard to learn]
- flat observables flat [phase space coverage okay]
- direct observables with tails [statistical error indicated]
- constructed observables similar
- improved resolution [1M training events]



How to GAN LHC events

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

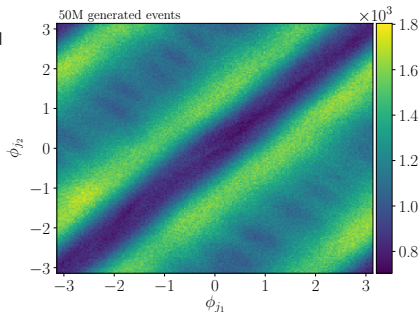
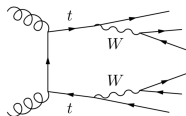
- medium-complex final state $t\bar{t} \rightarrow 6$ jets
- t/\bar{t} and W^\pm on-shell with BW $6 \times 4 = 18$ dof
- on-shell external states $\rightarrow 12$ dof [constants hard to learn]
- flat observables flat [phase space coverage okay]
- direct observables with tails [statistical error indicated]
- constructed observables similar
- improved resolution [10M generated events]



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
- improved resolution [50M generated events]
- **Proof of concept**



Chemistry of loss functions

GAN version of adaptive sampling

- generally 1D features

phase space boundaries

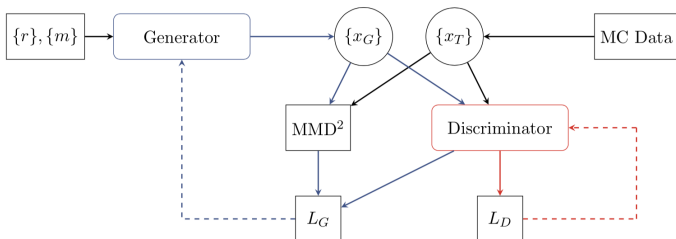
kinematic cuts

invariant masses [top, W]

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

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

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



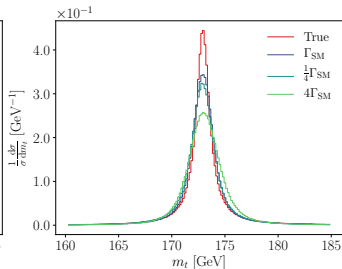
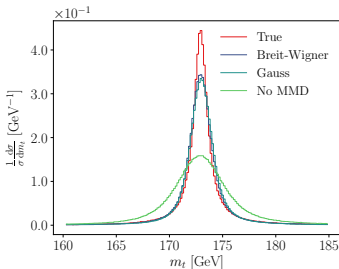
Chemistry of loss functions

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

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

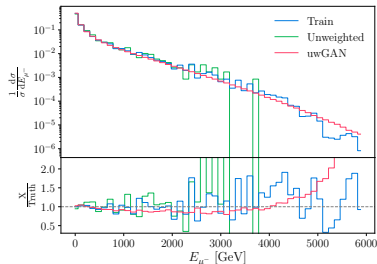
$$L_G \rightarrow L_G + \lambda_G \text{MMD}^2,$$



Unweighting

Gaining beyond GANplification [Butter, TP, Winterhalder; Clausius' talk]

- 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



How to GAN away detector effects

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

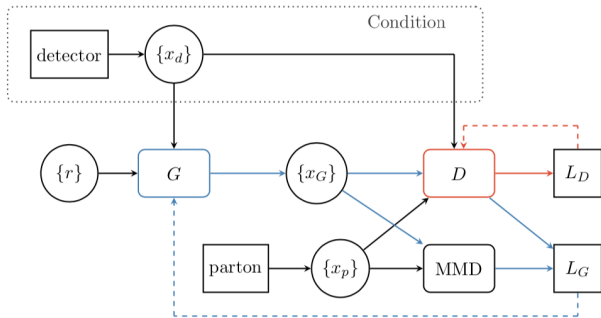
- detector simulation typical Markov process
- inversion possible, in principle [entangled convolutions]
- GAN task

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

\Rightarrow Full phase space unfolded

Conditional GAN

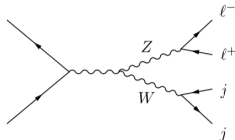
- map random numbers to parton level
hadron level as condition [matched event pairs]



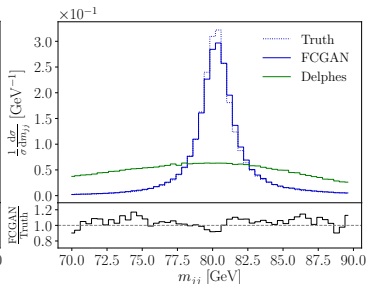
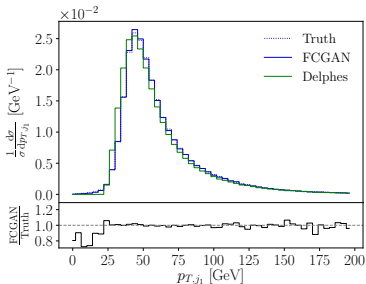
Detector unfolding

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]



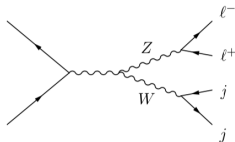
Simple application



Detector unfolding

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]

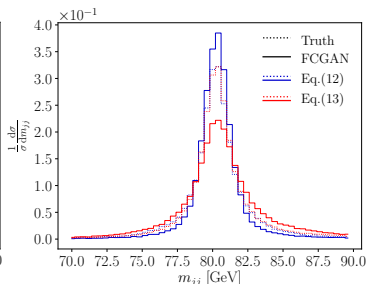
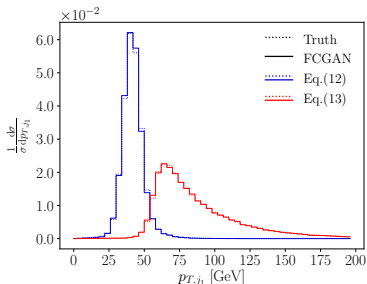


Simple application

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

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

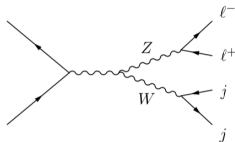
$$p_{T,j_1} > 60 \text{ GeV} \quad (13)$$



Detector unfolding

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]



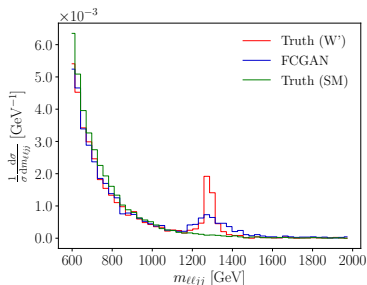
Simple application

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

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

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

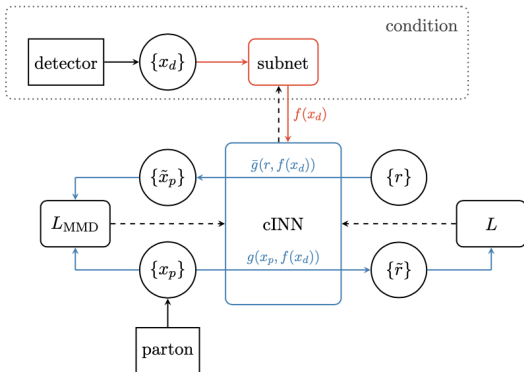
- model dependence of unfolding
 - train: SM events
test: 10% events with W' in s -channel
- ⇒ Working fine, but ill-defined



Unfolding as inverting

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

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



Unfolding as inverting

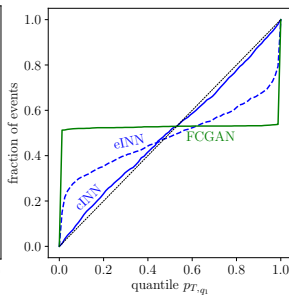
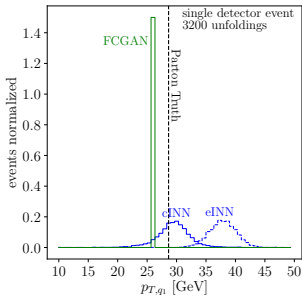
Invertible networks [Bellagente, Butter, Kasieczka, TP, Rousselot, Winterhalder, Arizzone, Köthe]

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

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

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

⇒ Proper statistical unfolding



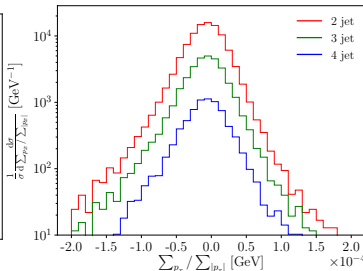
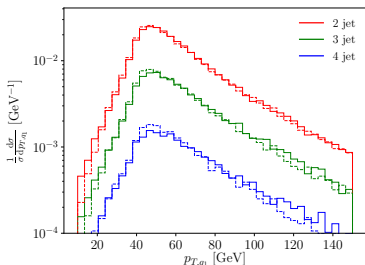
Unfolding as inverting

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 initial-state radiation

- 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]



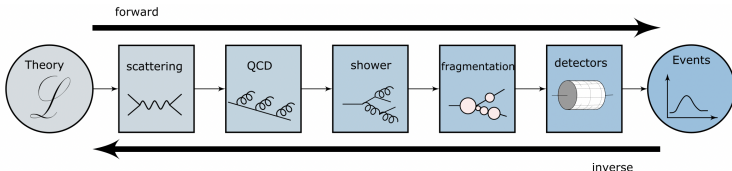
Unfolding as inverting

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 initial-state radiation

- 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]
- ⇒ **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?



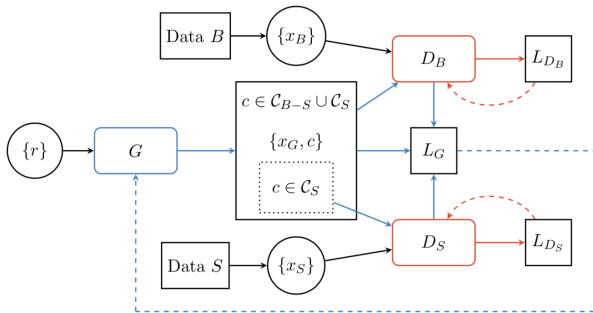
Backup: How to GAN event subtraction

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



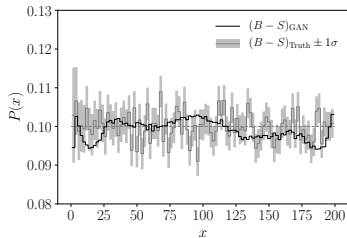
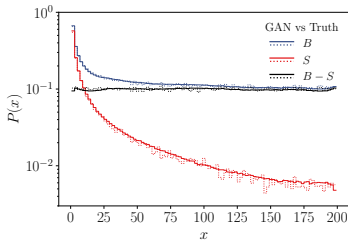
Subtracted events

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!)



Subtracted events

How to beat statistics by subtracting

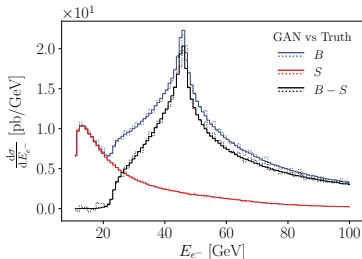
1- 1D toy example

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

– statistical fluctuations reduced (sic!)

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

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



Subtracted events

How to beat statistics by subtracting

1- 1D toy example

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

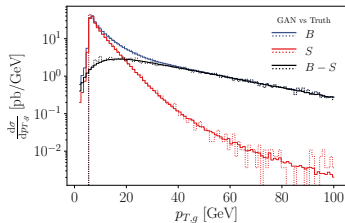
– statistical fluctuations reduced (sic!)

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

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

3- collinear subtraction [assumed non-local]

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



⇒ Applications in theory and analysis

