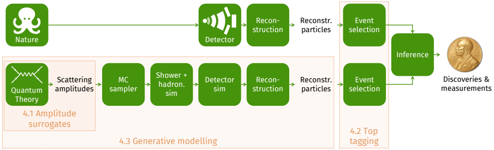
ML-Unfolding and More

Tilman Plehn

Universität Heidelberg

PHYSTAT, Stats meets ML, September 2024

LHC Theory



Turning data into knowledge

- QFT
  start with Lagrangian
  generate Feynman diagrams
- compute hard scattering
  compute decays
  compute jet radiation
- partons inside protons
  hadron-level QCD

$\rightarrow$ First-principle simulations, not modeling

HL-LHC: optimal inference with 10×more data

- statistical improvement $\sqrt{10} > 3$
- rate over phase space to $< 0.1\%$
- SBI starts with Simulation $\leftrightarrow$ theory [Giovanni De Crescenzo's poster]
- speed the key to precision

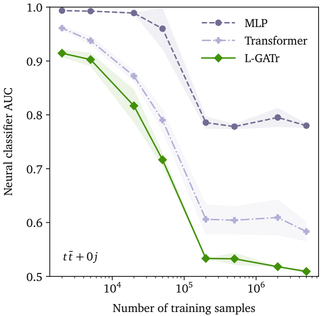
$\rightarrow$ MadNIS & Co [Ramon Winterhalder's talk,Nathan Hütsch's poster]

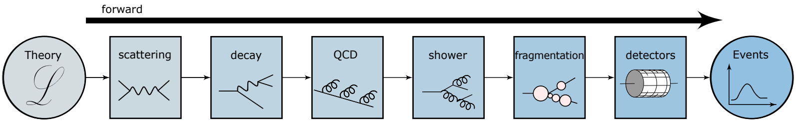
Generative AI

Forward simulations

- learn phase space density
  sample Gaussian $\to$ phase space
- Variational Autoencoder
  $\to$ low-dimensional physics
- Generative Adversarial Network
  $\to$ generator trained by classifier
- Normalizing Flow/Diffusion
  $\to$ (bijective) mapping [INN]
- JetGPT, ViT
  $\to$ non-local structures
- Equivariant L-GATr [Jonas Spinner's talk]
  $\to$ guarantee Lorentz symmetry

$\to$ Combinations: Transfermer, TraCFM,...





Generative AI

Forward simulations

- learn phase space density [with error bar]
  sample Gaussian $\to$ phase space
- Variational Autoencoder
- Generative Adversarial Network
- Normalizing Flow/INN/Diffusion
- JetGPT, ViT
- Equivariant L-GATr [Jonas Spinner's talk]

$\to$ Combinations: Transfermer, TraCFM,...

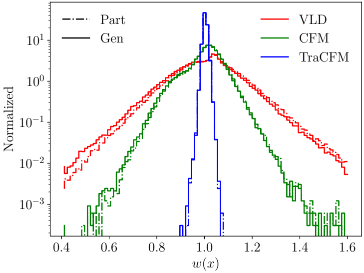
Quality control [Das, Favaro, Heimel, Krause, TP, Shih]

- classifier easier to train
  training vs generated [Neyman-Peason]

$$w(x_i) = \frac{D(x_i)}{1 - D(x_i)} = \frac{p_\text{train}(x_i)}{p_\text{gen}(x_i)}$$

- performance from width of distribution
- $w(x_i) \gg 1$ missing feature
  $w(x_i) \ll 1$ missing cut

$\to$ Systematic performance test



Transforming LHC physics

Number of searches [Aishik's talk]

- optimal inference: signal and background simulations
- CPU-limitation for many signals

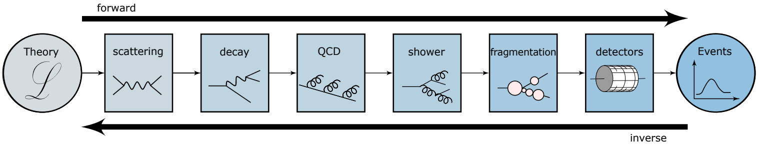
Optimal analyses

- theory limiting many analyses, but continuous progress
- analyses need to be updated

Public LHC data

- common lore:
  LHC data too complicated for amateurs [except Jesse]
- in truth:
  hard scattering and decay simulations public
  BSM physics not in hadronization and detector

$\rightarrow$ Unfold to suitable level [theoretically consistent?]



ML-Unfolding

Basic structure [reiterating Vini's talk]

- four phase space distributions

$$\begin{tikzcd}
p_\text{sim}(x_\text{part}) \arrow[rr, leftrightarrow, "\text{unfolding inference}"] \arrow[d, "p(x_\text{reco}|x_\text{part})"'] & & p_\text{unfold}(x_\text{part}) \\
p_\text{sim}(x_\text{reco}) \arrow[rr, leftrightarrow, "\text{forward inference}"] & & p_\text{data}(x_\text{reco}) \arrow[u, "p(x_\text{part}|x_\text{reco})"']
\end{tikzcd}$$

$\to$ ML for unbinned and high-dimensional unfolding?

ML-Unfolding

Basic structure [reiterating Vini's talk]

- four phase space distributions

$$
\begin{tikzcd}
p_\text{sim}(x_\text{part}) \arrow[r, leftrightarrow, "\text{unfolding inference}"] \arrow[d, "p(x_\text{reco} | x_\text{part})"'] & p_\text{unfold}(x_\text{part}) \\
p_\text{sim}(x_\text{reco}) \arrow[r, leftrightarrow, "\text{forward inference}"] & p_\text{data}(x_\text{reco}) \arrow[u, "p(x_\text{part} | x_\text{reco})"']
\end{tikzcd}
$$

$\rightarrow$ ML for unbinned and high-dimensional unfolding?

OmniFold [Andreassen, Komiske, Metodiev, Nachman, Thaler]

- learn $p_\text{sim}(x_\text{reco}) \leftrightarrow p_\text{data}(x_\text{reco})$ [Neyman-Pearson lemma, CWoLa]
- reweight $p_\text{sim}(x_\text{part}) \rightarrow p_\text{unfold}(x_\text{part})$

$$
\begin{tikzcd}
p_\text{sim}(x_\text{part}) \arrow[r, "\text{classifier weights}"] \arrow[d, leftrightarrow, "\text{pull/push weights}"'] & p_\text{unfold}(x_\text{part}) \\
p_\text{sim}(x_\text{reco}) \arrow[r, leftrightarrow, "\text{classifier weights}"] & p_\text{data}(x_\text{reco})
\end{tikzcd}
$$

$\rightarrow$ Driven by (now) established ML-classification

Unfolding by generation

Targeting conditional probability [Butter, TP, Winterhalder,...]

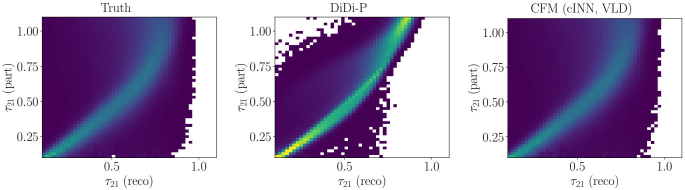
- just like forward ML-generation
- learn inverse conditional probability from $(x_\text{part}, x_\text{reco})$

$$\begin{tikzcd}
p_\text{sim}(x_\text{part}) \arrow[d, leftrightarrow, "\text{paired data}"'] & & p_\text{unfold}(x_\text{part}) \\
p_\text{sim}(x_\text{reco}) \arrow[rr, leftrightarrow, "\text{correspondence}"] & & p_\text{data}(x_\text{reco}) \arrow[u, "p_\text{model}(x_\text{part}|x_\text{reco})"']
\end{tikzcd}$$

Improvements crucial [Xavier Villadamigo's poster]

- make networks more precise $\to$ TraCFM
- remove training prior [Backes, Butter, Dunford, Malaescu]

$\to$ Success through generative progress



Unfolding top decays

Hadonic top decays [Sophia Palacios Schweitzer's poster]

- model dependence: simulation m_s vs data m_d

$$\begin{tikzcd}
p_\text{sim}(x_\text{part} | m_s) \arrow[d, "p(x_\text{reco} | x_\text{part})"'] & & p_\text{unfold}(x_\text{part} | m_s, m_d) \\
p_\text{sim}(x_\text{reco} | m_s) \arrow[rr, leftrightarrow, "\text{correspondence}"] & & p_\text{data}(x_\text{reco} | m_d) \arrow[u, "p_\text{model}(x_\text{part} | x_\text{reco}, m_s)"']
\end{tikzcd}$$

Unfolding top decays

Hadonic top decays [Sophia Palacios Schweitzer's poster]

- complete training bias $m_d \to m_s$ [too bad to reweight]

$$\begin{tikzcd}
p_\text{sim}(x_\text{part}|m_s) \arrow[d, "p(x_\text{reco}|x_\text{part})"'] & & p_\text{unfold}(x_\text{part}|m_s, \cancel{m_d}) \\
p_\text{sim}(x_\text{reco}|m_s) \arrow[rr, leftrightarrow, "\text{correspondence}"] & & p_\text{data}(x_\text{reco}|m_d) \arrow[u, "p_\text{model}(x_\text{part}|x_\text{reco}, m_s)"']
\end{tikzcd}$$

1. weaken bias by training on m_s-range
2. strengthen data by including batch-wise $m_d \sim M_{jjj} \in x_\text{reco}$

Unfolding top decays

Hadonic top decays [Sophia Palacios Schweitzer's poster]

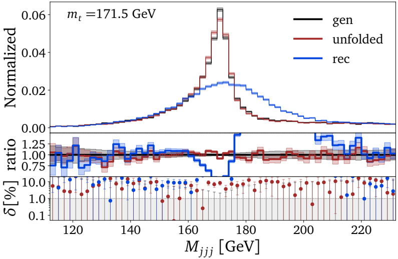
- complete training bias $m_d \to m_s$ [too bad to reweight]

$$
\begin{tikzcd}[column sep=huge]
p_\text{sim}(x_\text{part}|m_s) \arrow[d, "p(x_\text{reco}|x_\text{part})"'] & p_\text{unfold}(x_\text{part}|m_s, \cancel{m_d}) \\
p_\text{sim}(x_\text{reco}|m_s) \arrow[r, leftrightarrow, "\text{correspondence}"] & p_\text{data}(x_\text{reco}|m_d) \arrow[u, "p_\text{model}(x_\text{part}|x_\text{reco}, m_s)"']
\end{tikzcd}
$$

1. weaken bias by training on m_s-range
2. strengthen data by including batch-wise $m_d \sim M_{jjj} \in x_\text{reco}$

Preliminary unfolding results

- 4D for mass measurement



Unfolding top decays

Hadonic top decays [Sophia Palacios Schweitzer's poster]

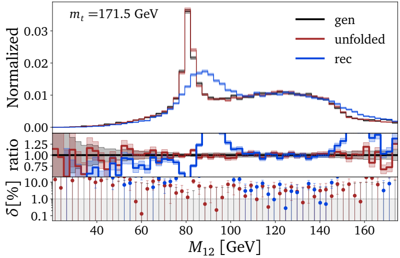
- complete training bias $m_d \to m_s$ [too bad to reweight]

$$\begin{tikzcd}
p_\text{sim}(x_\text{part}|m_s) \arrow[d, "p(x_\text{reco}|x_\text{part})"'] & & p_\text{unfold}(x_\text{part}|m_s, \cancel{m_d}) \\
p_\text{sim}(x_\text{reco}|m_s) \arrow[rr, leftrightarrow, "\text{correspondence}"] & & p_\text{data}(x_\text{reco}|m_d) \arrow[u, "p_\text{model}(x_\text{part}|x_\text{reco}, m_s)"']
\end{tikzcd}$$

1. weaken bias by training on m_s-range
2. strengthen data by including batch-wise $m_d \sim M_{jjj} \in x_\text{reco}$

Preliminary unfolding results

- 4D for calibrated mass measurement



Unfolding top decays

Hadonic top decays [Sophia Palacios Schweitzer's poster]

- complete training bias $m_d \to m_s$ [too bad to reweight]

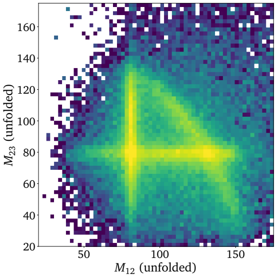
$$\begin{tikzcd}
p_\text{sim}(x_\text{part} | m_s) \arrow[d, "p(x_\text{reco} | x_\text{part})"'] & & p_\text{unfold}(x_\text{part} | m_s, \cancel{m_d}) \\
p_\text{sim}(x_\text{reco} | m_s) \arrow[rr, leftrightarrow, "\text{correspondence}"] & & p_\text{data}(x_\text{reco} | m_d) \arrow[u, "p_\text{model}(x_\text{part} | x_\text{reco}, m_s)"']
\end{tikzcd}$$

1. weaken bias by training on m_s-range
2. strengthen data by including batch-wise $m_d \sim M_{jjj} \in x_\text{reco}$

Preliminary unfolding results

- 4D for calibrated mass measurement
- 12D published data

$\to$ CMS data next

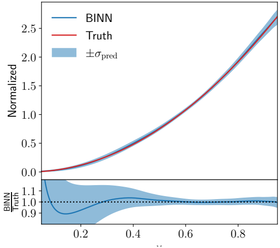


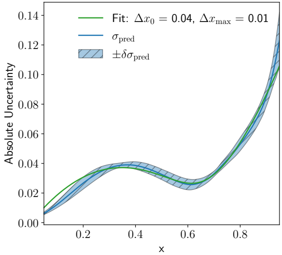
Learned uncertainties

Bayesian generative networks [Bellagente, Haussmann, Luchmann, TP; Bieringer, Diefenbacher, Kasieczka, Trabs]

- sampling phase space
  events with error bars on weights
- learned density & uncertainty
  reflecting network learning!

$\rightarrow$ INNs fitting functions





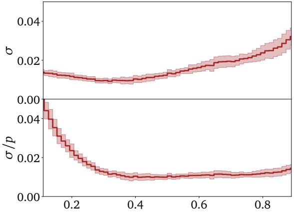
Learned uncertainties

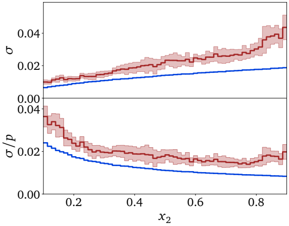
Bayesian generative networks [Bellagente, Haussmann, Luchmann, TP; Bieringer, Diefenbacher, Kasieczka, Trabs]

- sampling phase space
  events with error bars on weights
- learned density & uncertainty
  reflecting network learning!

→ INNs and DDPMs fitting functions

→ CFMs and transformers different





Learned uncertainties

Bayesian generative networks [Bellagente, Haussmann, Luchmann, TP; Bieringer, Diefenbacher, Kasieczka, Trabs]

- sampling phase space
  events with error bars on weights
- learned density & uncertainty
  reflecting network learning!

→ INNs and DDPMs fitting functions

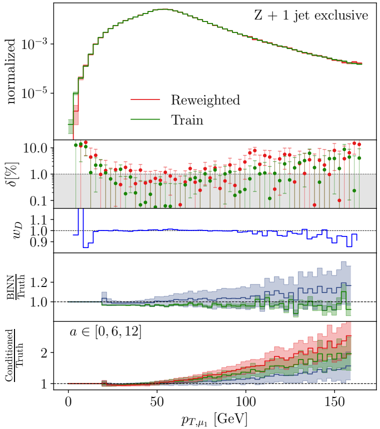
→ CFMs and transformers different

LHC events with uncertainties [Heimel, Vent...]

- statistical limitation from B-INN
- systematic limitation from condition

$$w = 1 + a \left(\frac{p_{T,j_1} - 15 \text{ GeV}}{100 \text{ GeV}} \right)^2$$

→ Comprehensive uncertainty control



Transforming LHC analyses

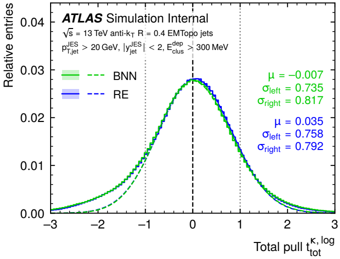
Calibration with uncertainties [Vogel, Loch, TP,...]

- interpretable topo-cluster phase space x
- learned calibration

$$\mathcal{R}^{\text{BNN}}(x) = \mathcal{R}(x) = \frac{E^{\text{EM}}(x)}{E^{\text{dep}}(x)}$$

- learned uncertainties $\Delta\mathcal{R}(x)$ [Nina Elmer's poster]
  Bayesian neural networks vs repulsive ensembles

$\to$ error vs data spread checked by pull



Transforming LHC analyses

Calibration with uncertainties [Vogel, Loch, TP,...]

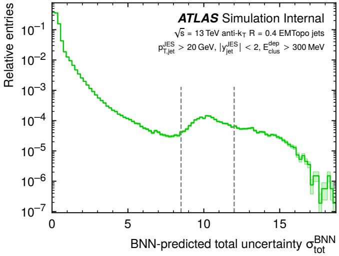
- interpretable topo-cluster phase space x
- learned calibration

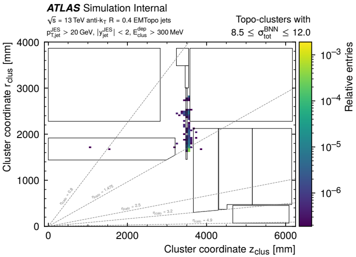
$$\mathcal{R}^{\text{BNN}}(x) = \mathcal{R}(x) = \frac{E^{\text{EM}}(x)}{E^{\text{dep}}(x)}$$

- learned uncertainties $\Delta\mathcal{R}(x)$ [Nina Elmer's poster]
  Bayesian neural networks vs repulsive ensembles

→ error vs data spread checked by pull

→ Understand data using uncertainties





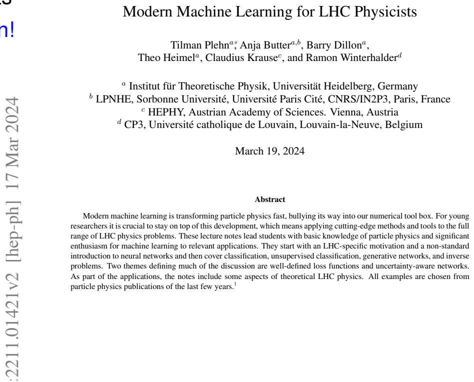
ML for LHC Theory

Developing ML for the best science

- just another numerical tool for a numerical field
- transformative new common language
- driven by external money
- 10000 Einsteins to...

  ...improve established tools
  ...develop new tools for exciting tasks
  ...transform through new ideas

$\rightarrow$ You are the golden generation!



arXiv:2211.01421v2 [hep-ph] 17 Mar 2024

Modern Machine Learning for LHC Physicists

Tilman Plehn[a*], Anja Butter[a,b], Barry Dillon[a],
Theo Heimel[a], Claudius Krause[c], and Ramon Winterhalder[d]

[a] Institut für Theoretische Physik, Universität Heidelberg, Germany
[b] LPNHE, Sorbonne Université, Université Paris Cité, CNRS/IN2P3, Paris, France
[c] HEPHY, Austrian Academy of Sciences. Vienna, Austria
[d] CP3, Université catholique de Louvain, Louvain-la-Neuve, Belgium

March 19, 2024

Abstract

Modern machine learning is transforming particle physics fast, bullying its way into our numerical tool box. For young researchers it is crucial to stay on top of this development, which means applying cutting-edge methods and tools to the full range of LHC physics problems. These lecture notes lead students with basic knowledge of particle physics and significant enthusiasm for machine learning to relevant applications. They start with an LHC-specific motivation and a non-standard introduction to neural networks and then cover classification, unsupervised classification, generative networks, and inverse problems. Two themes defining much of the discussion are well-defined loss functions and uncertainty-aware networks. As part of the applications, the notes include some aspects of theoretical LHC physics. All examples are chosen from particle physics publications of the last few years.[1]