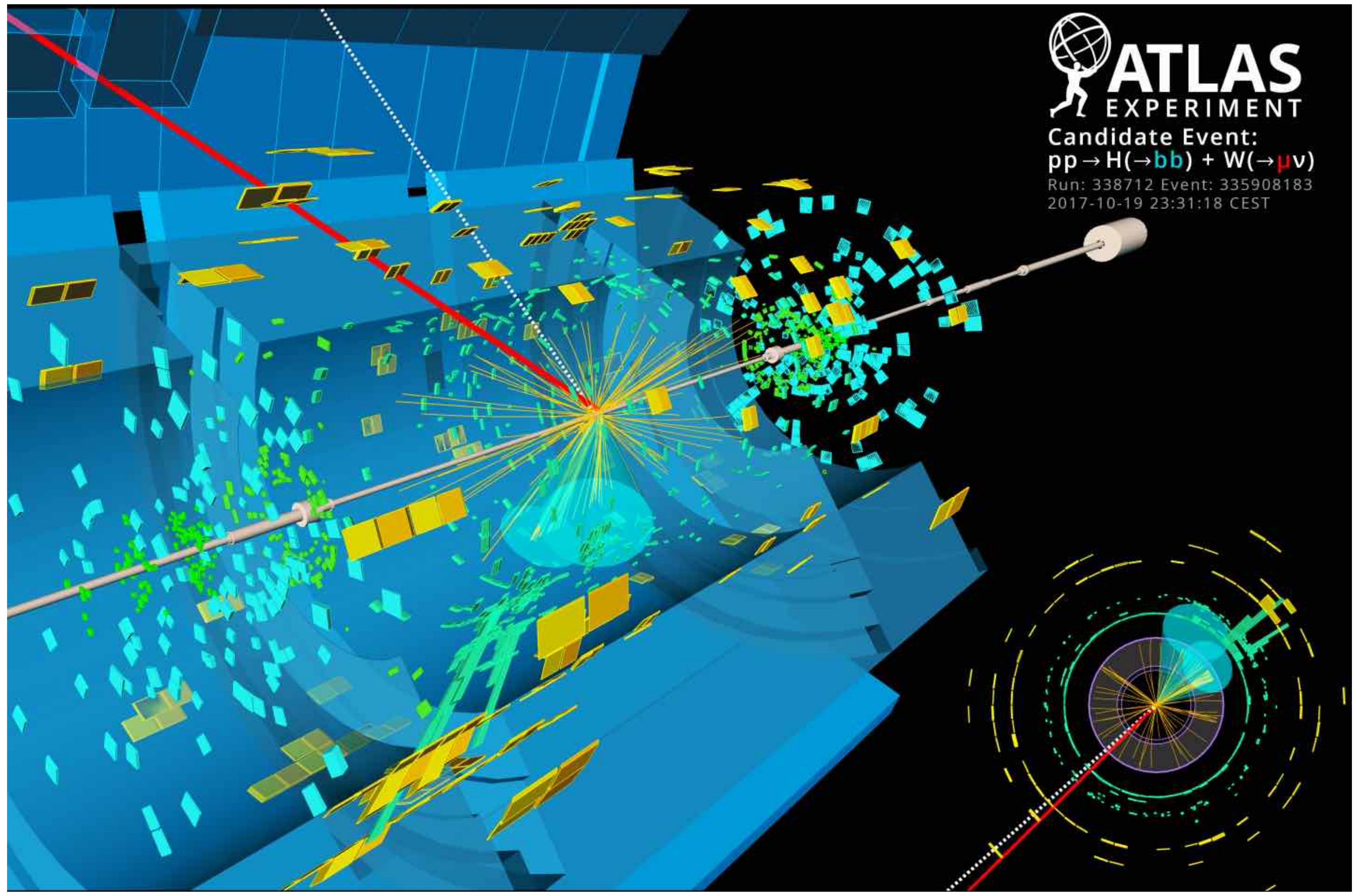
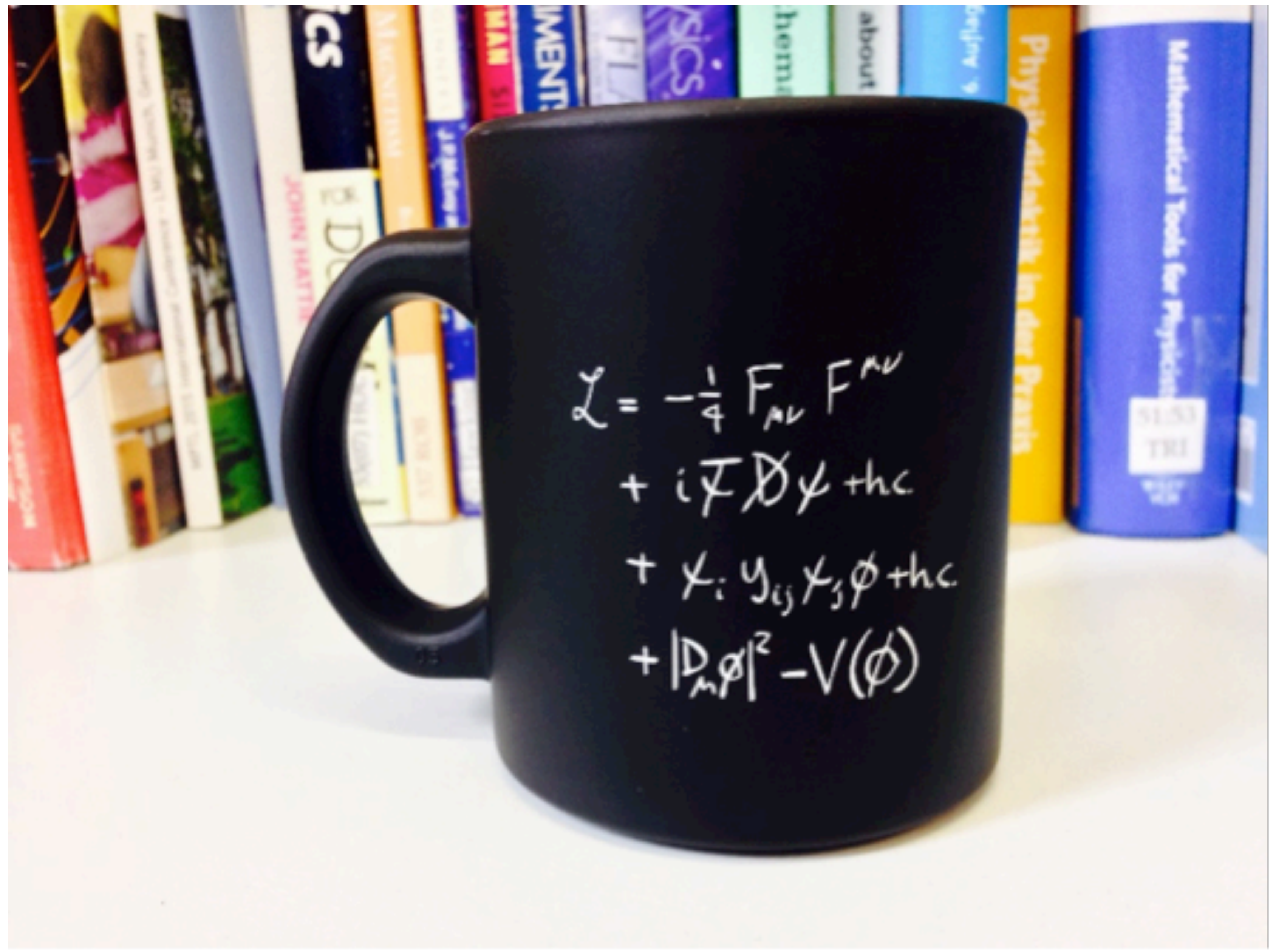
Boosting event generation & inference with new ML methods

IN2P3/IRFU Machine Learning Workshop

Anja Butter, ITP Heidelberg/LPNHE Paris

A biased view on LHC physics



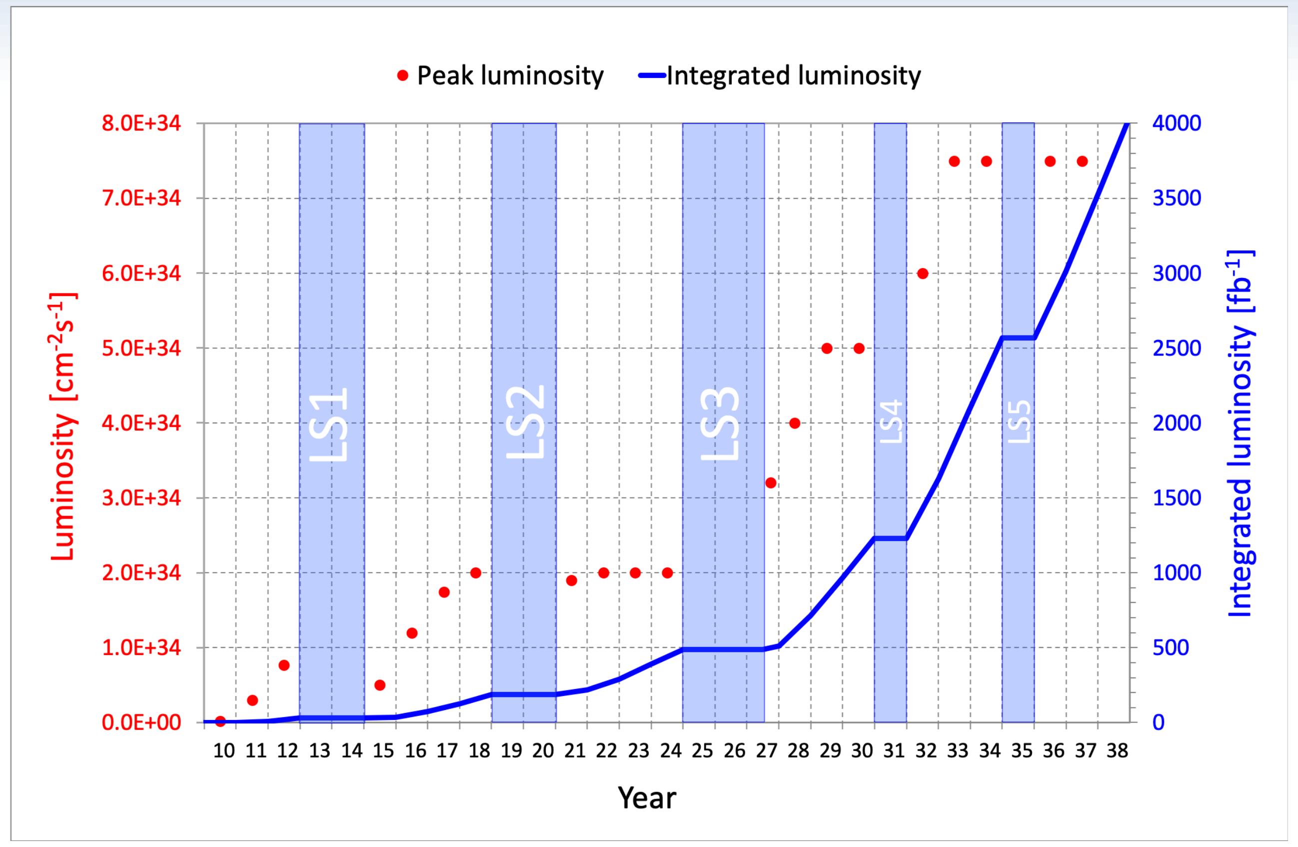


Setting
- Large Hadron Collider at CERN
- Proton collisions at 13 TeV
- **Huge** dataset ~1Pb/s before trigger selection

Goal
- Understand full dataset from **1st principles**
- Precision measurements of the SM
- Find signs of new physics (eg dark matter)

Open questions towards HL-LHC

A biased selection



- Facing **25 times** the amount of data
- What do we need to understand the data? (*read:* find new physics)

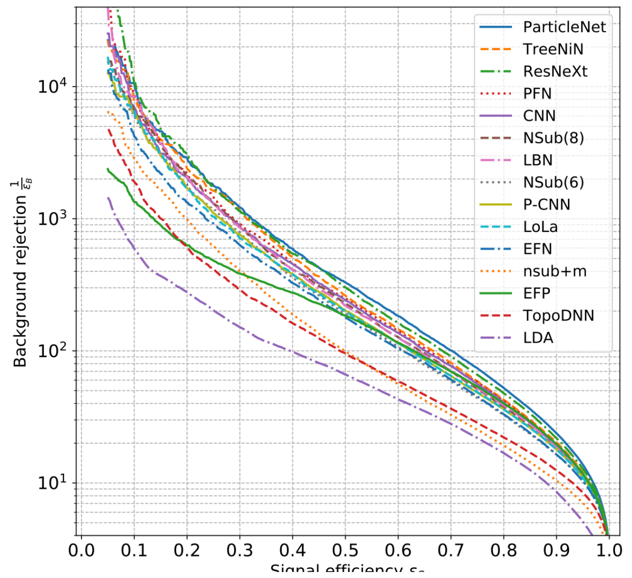
- **Precision predictions**
  - Higher order amplitudes
  - Event generation
  - Shower
  - Detector simulation

- **Optimized analysis for high-dimensional data**
  - Likelihood free inference
    - Optimal Observables, Unfolding
  - Anomaly detection
  - Uncertainty treatment

Problems beyond supervised classification/regression → How can machine learning help?

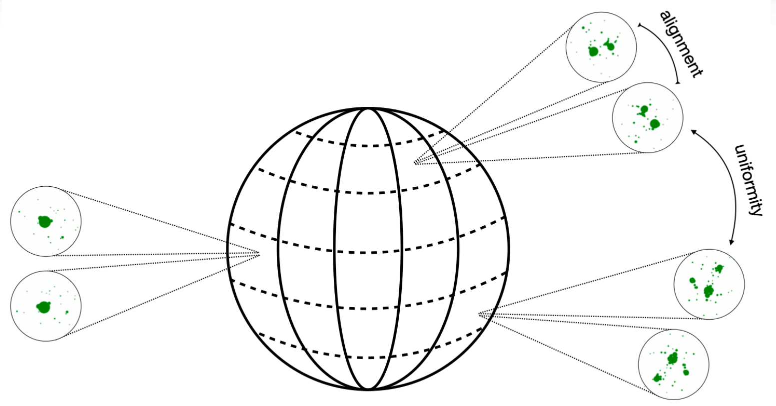
ML for big data in particle physics

Top tagging



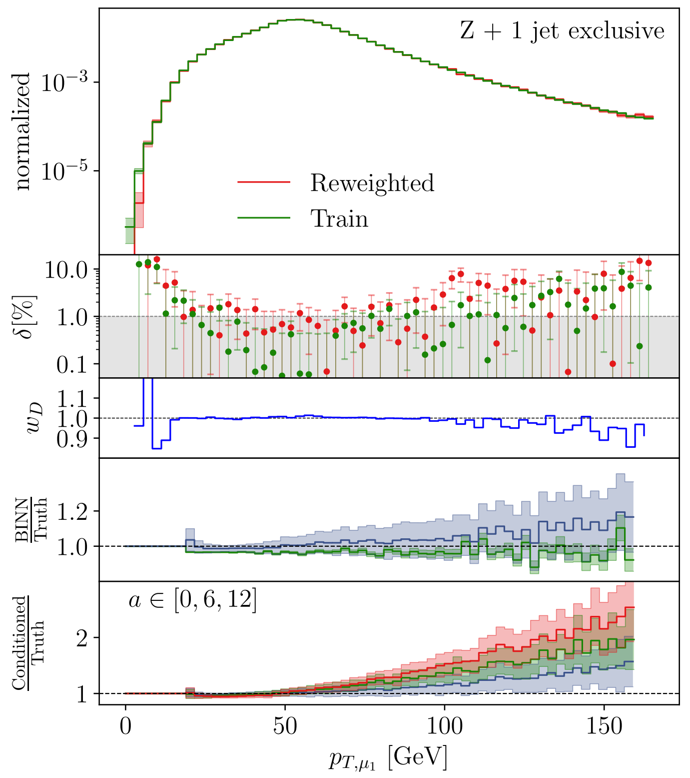
G. Kasieczka et al. [1902.09914]

Anomaly detection



B. Dillon et al. [2108.04253]

Event generation



A. Butter et al. [2110.13632]

Classification

Generative models

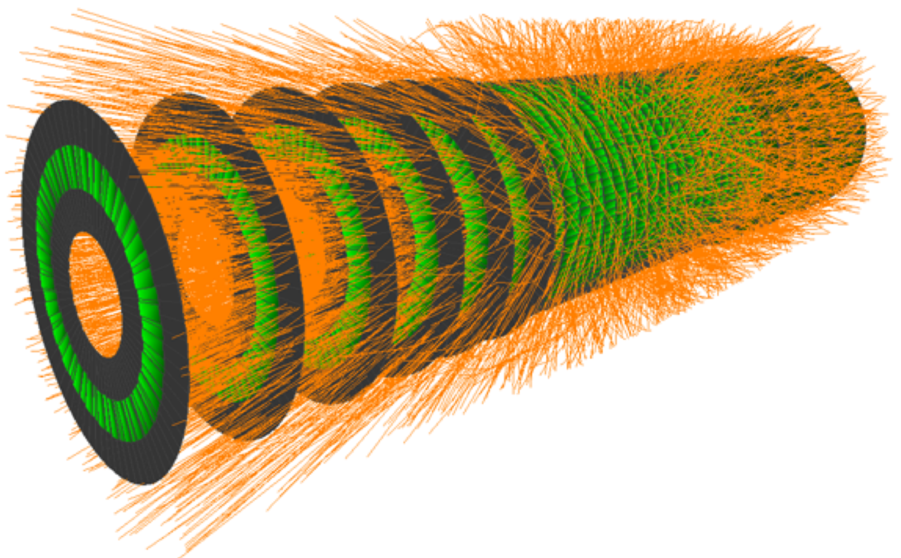
Graph networks

Bayesian networks

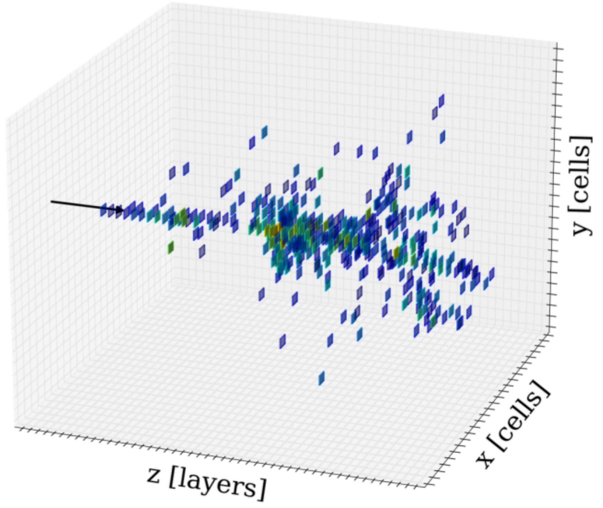
Regression

Track reconstruction

Kaggle challenge

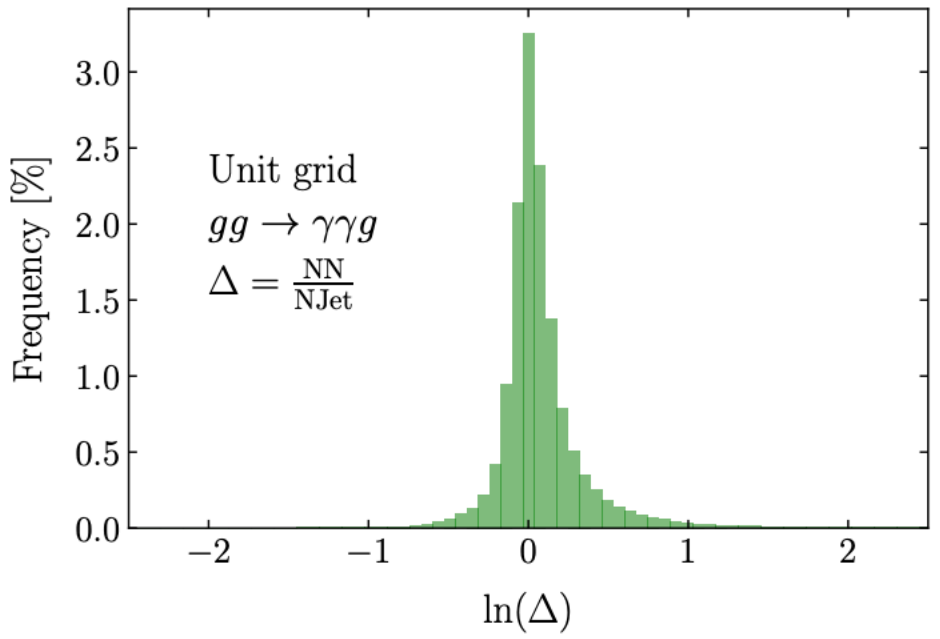


Detector simulation



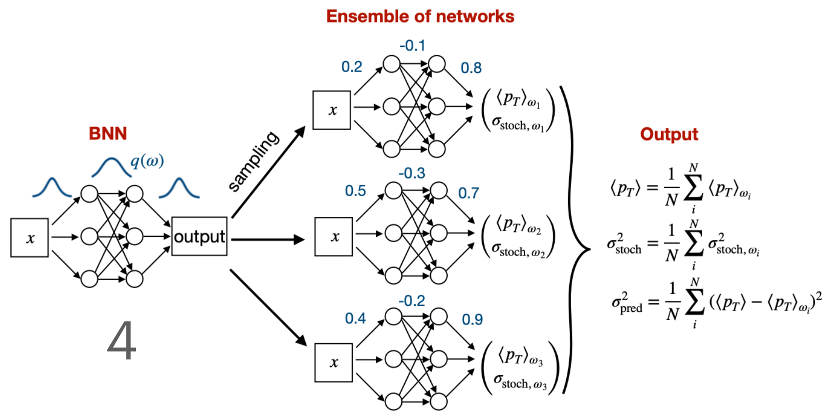
E. Buhmann et al. [2112.09709]

Amplitude estimation



J. Aylett-Bullock, et al. [2106.09474]

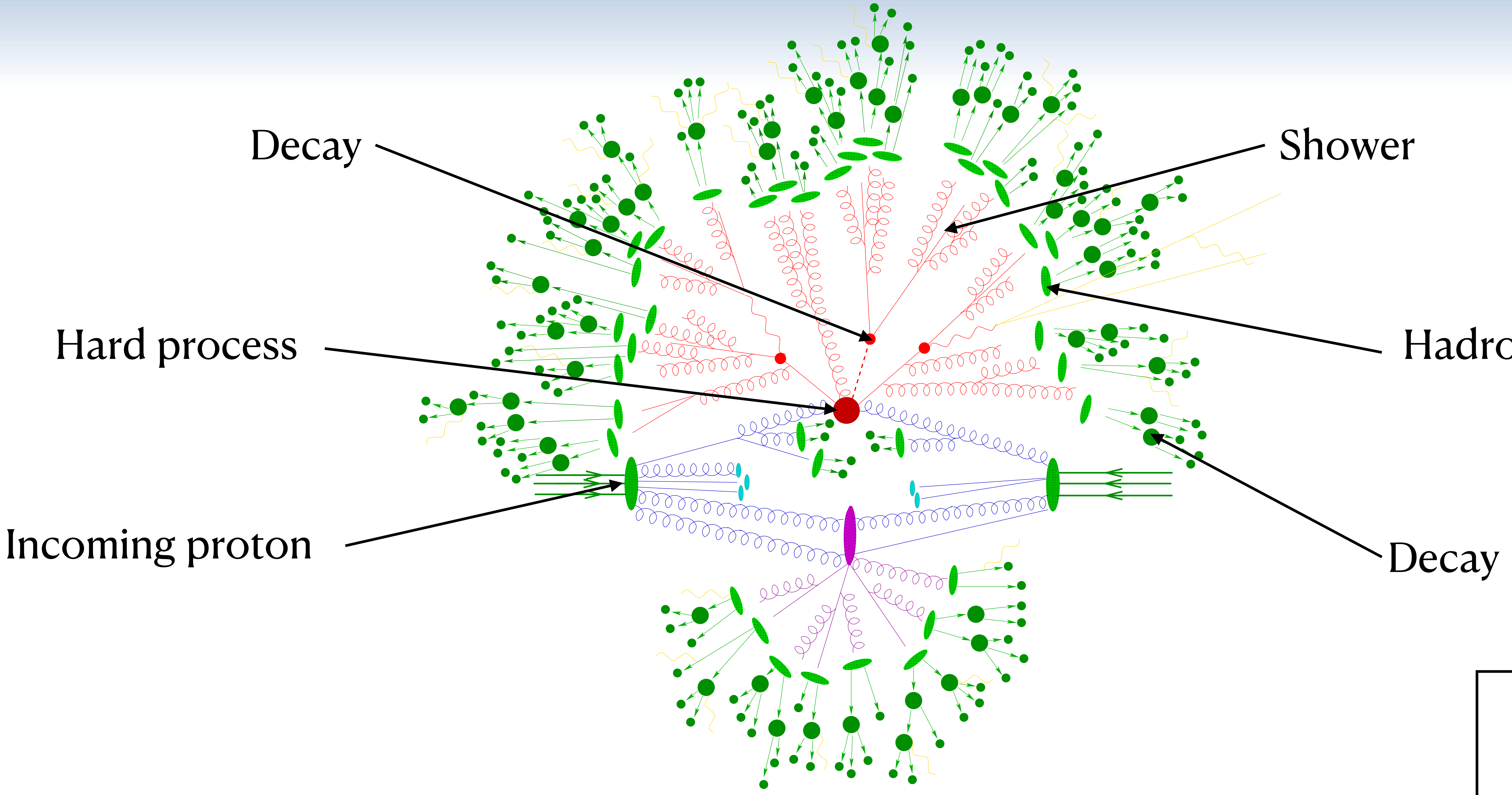
Jet calibration & uncertainties



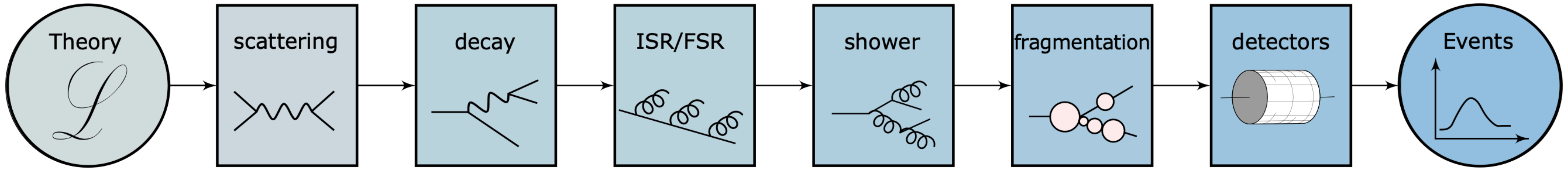
G. Kasieczka et al. [2003.11099]

Complete citations $\mathcal{O}(800)$
https://iml-wg.github.io/HEPML-LivingReview/

Event generation at the LHC



Simulation tool



ML at all stages
PDFs
Amplitudes
Phase space generation
Shower
Hadronization
Detector simulation

Complete references in 2203.07460

Monte carlo event generation

1. Generate phase space points

$\rightarrow$ set of four-momenta p_i

2. Calculate event weight

$$w_{\text{event}} = f(x_1, Q^2) f(x_1, Q^2) \times \mathscr{M}(x_1, x_2, p_1, \ldots, p_n) \times J(p_i(r))$$

PDF

Matrix element †

Phase space mapping

3. Unweighting †

keep events with $\frac{w_i}{w_{\max}} > r \in [0,1]$

† Bottlenecks

1. Slow **matrix element** calculation
   - Complexity grows exponentially with
     - # final state particles
     - Precision (LO, NLO, NNLO, ...)
2. Low **unweighting** efficiency
   - Discard most events if $w_i \ll w_{\max}$
   - Optimize phase space mapping
     ➡ $J(p_i(r)) = (f \times \mathscr{M})^{-1}$

Amplitudes

Calculation and Approximation

Approximating Amplitudes

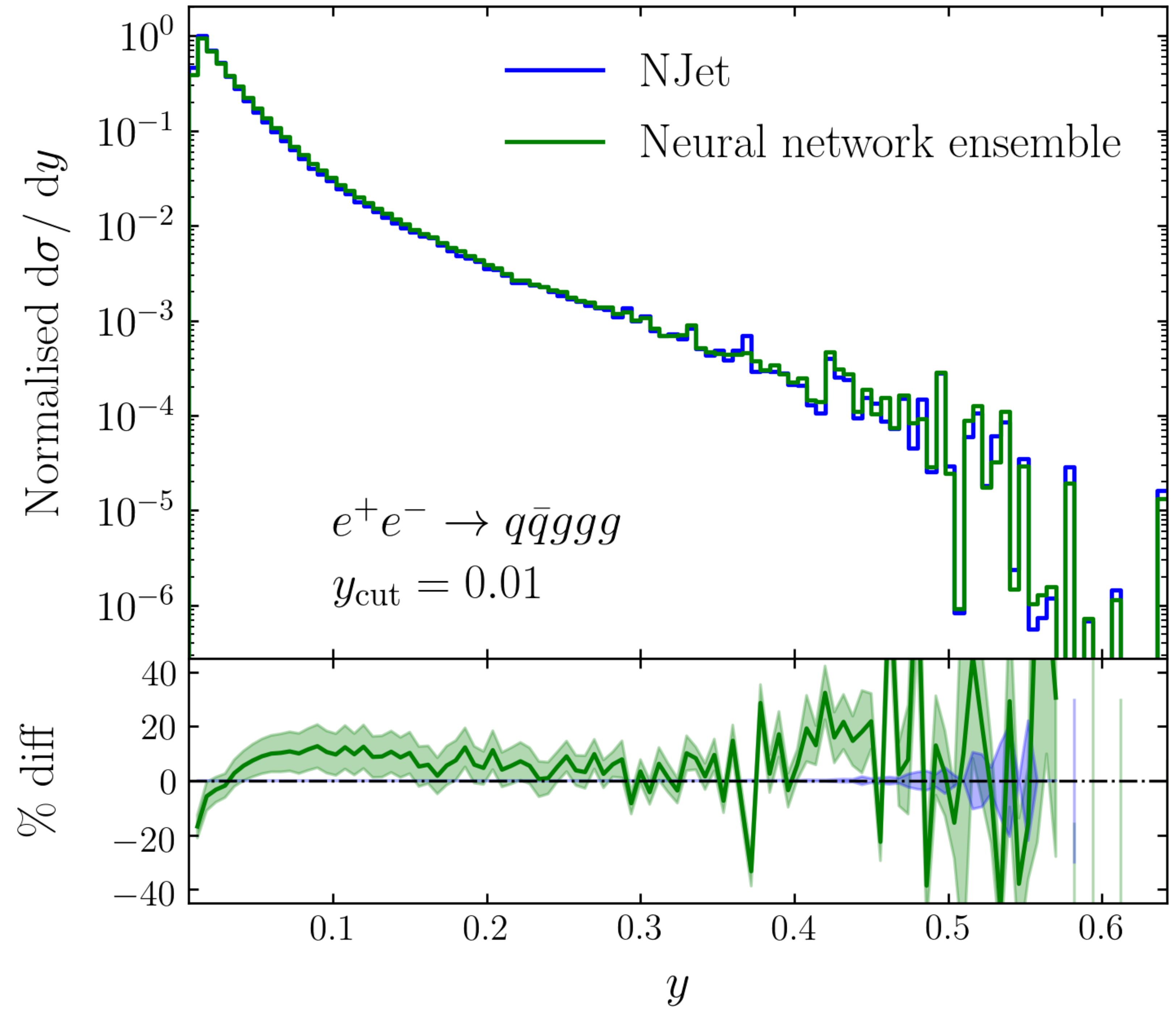
- Approximate matrix element with NN

- Regression problem
- Minimize distance between prediction and truth

$\Rightarrow \mathscr{L} = \left(NN(p_i) - \mathscr{M}(p_i)\right)^2$

+ Generalization of interpolation
+ Better scaling than grids for large dimensions

- Open questions
    - Limited precision
    - Overtraining vs interpolation



Badger, Bullock [2002.07516]

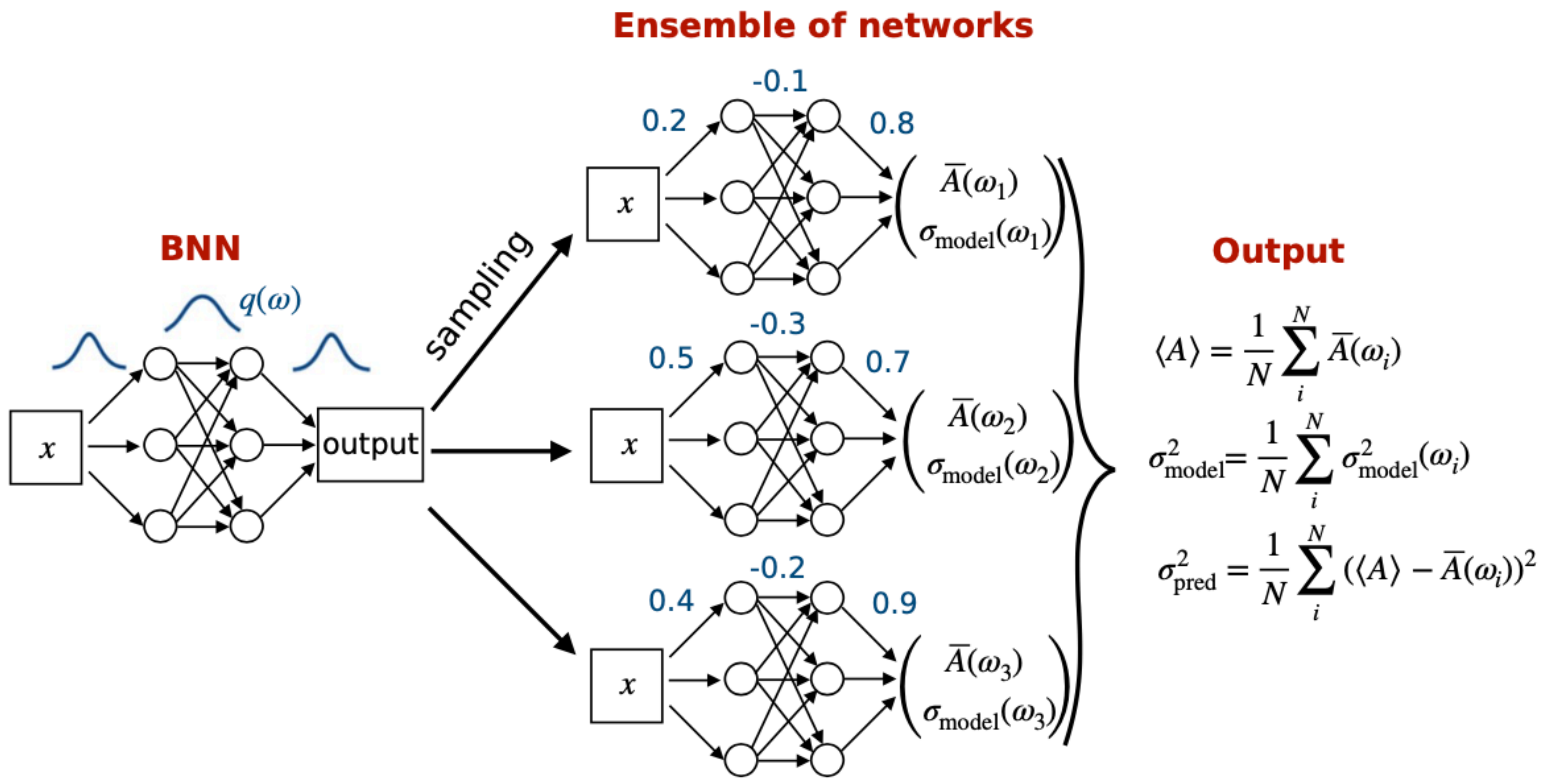
Uncertainties from Bayesian Neural Networks

Example $gg \to \gamma\gamma g(g)$, 90k training, 870k test amplitudes

Training data $T =$ (phase space points x', Amplitudes $A'(x')$)

For limited data there is **no unique solution**

$\to$ Find $p(A\,|\,T) = \int \mathrm{d}w\; p(A\,|\,w)p(w\,|\,T) \approx \int \mathrm{d}w\; p(A\,|\,w)q(w)$



Approximate $q(w)$ by minimizing KL divergence

$$\mathscr{L}_{BNN} = \mathrm{KL}[q(w), p(w)] - \int dw\; q(w)\;\log p(T\,|\,w)$$

Gaussian prior

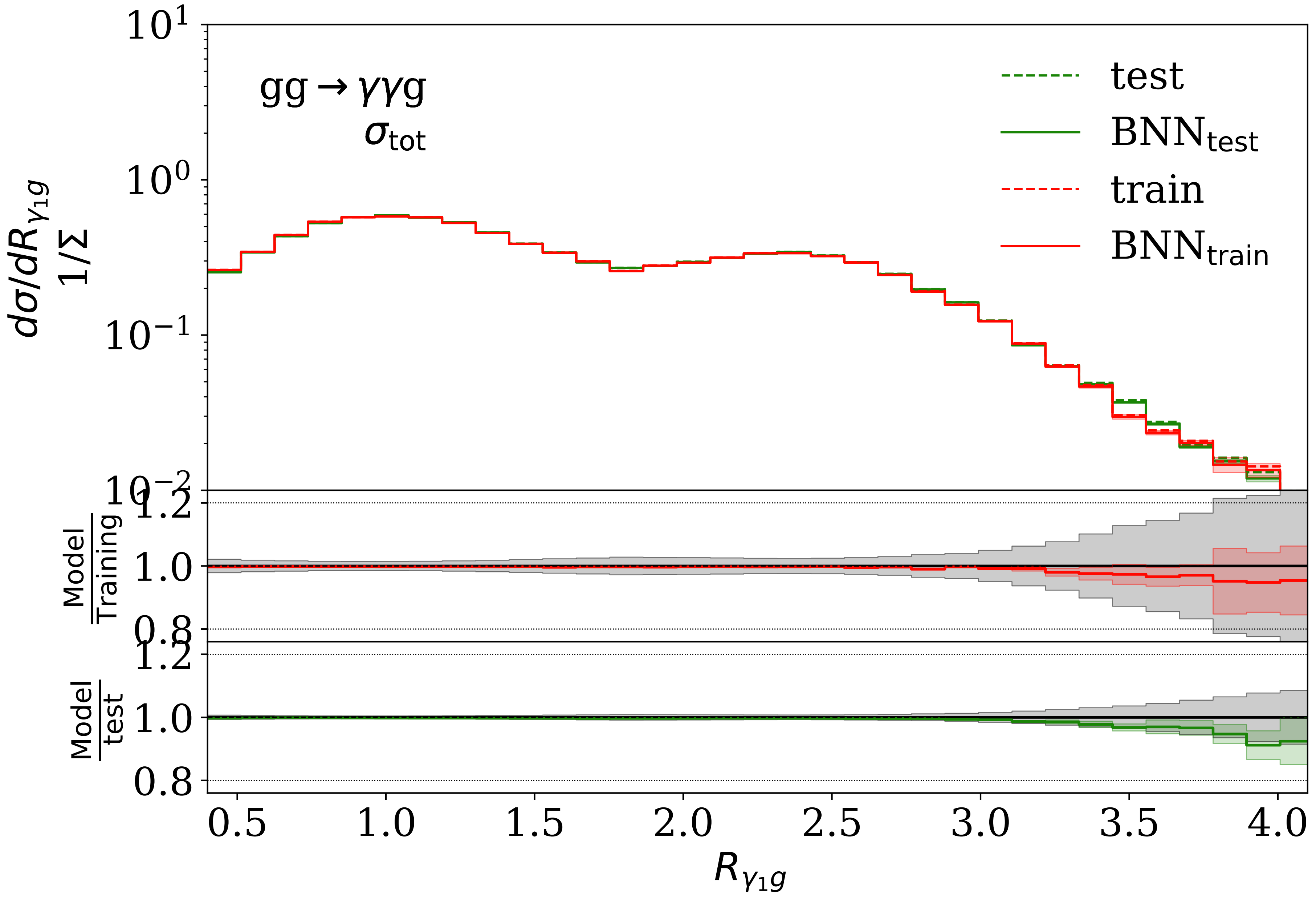
$$\frac{\sigma_q^2 - \sigma_p^2 + (\mu_q - \mu_p)^2}{2\sigma_p^2} + \log\frac{\sigma_p}{\sigma_q}$$

Gaussian uncertainty

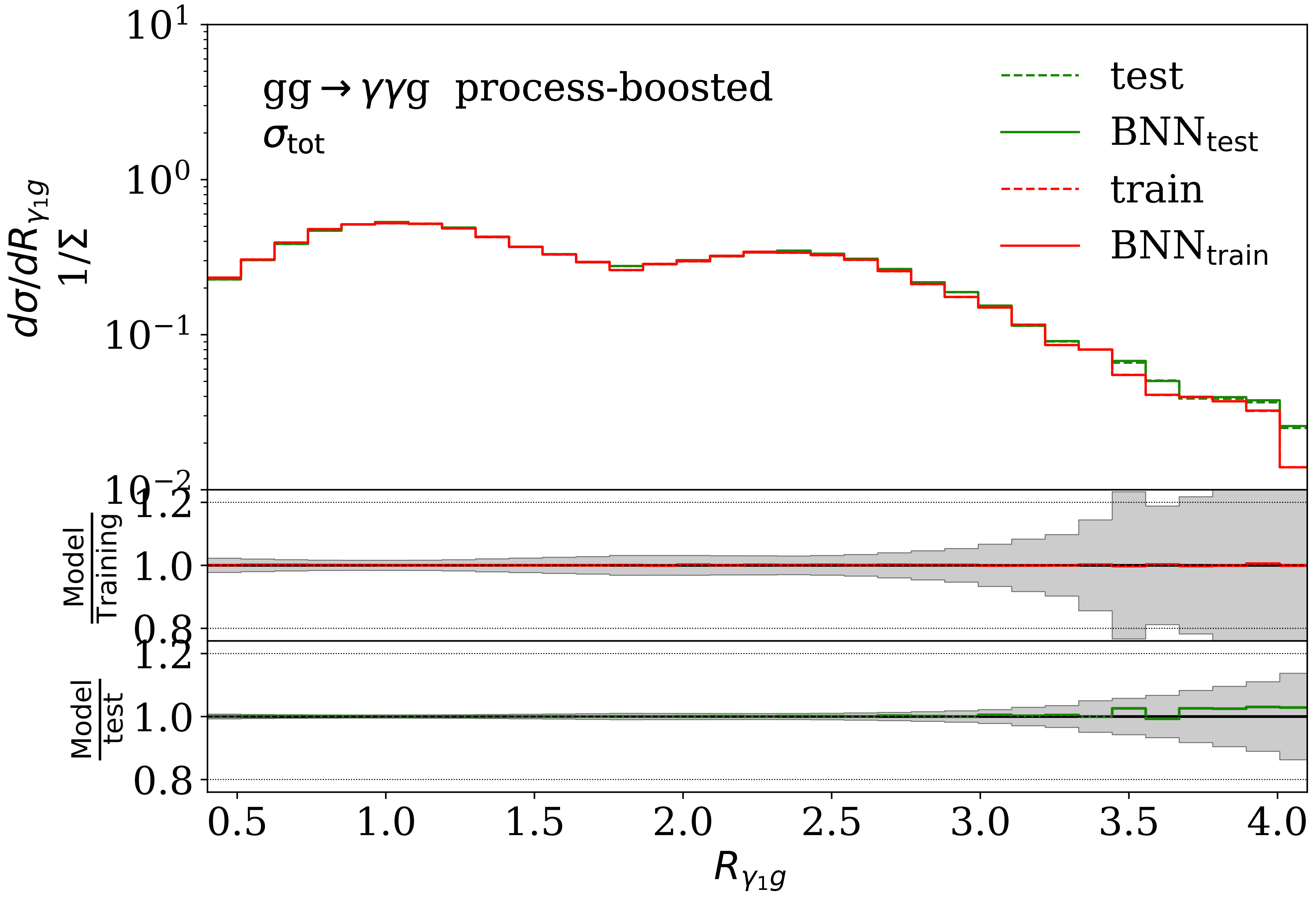
$$\frac{\left|\bar{A}_j(\omega) - A_j^{(\text{truth})}\right|^2}{2\sigma_{\text{model},j}(\omega)^2} + \log\sigma_{\text{model},j}(\omega)$$

Kinematic distributions

Standard BNN



Precision boosted BNN

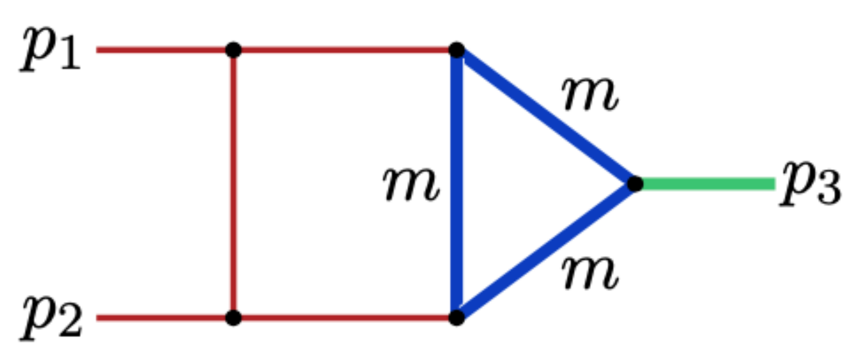


Gray shades indicate statistical limitation of training data...

Multi-loop calculations with INNs

Profiting from the Jacobian

Precision predictions based on loop diagrams



Analytic expression for loop amplitude

$$G = \int_{-\infty}^{\infty} \left(\prod_{l=1}^{L} \frac{\mathrm{d}^D k_l}{i\pi^{\frac{D}{2}}} \right) \prod_{j=1}^{N} \frac{1}{(q_j^2 - m_j^2 + i\delta)^{\nu_j}}$$

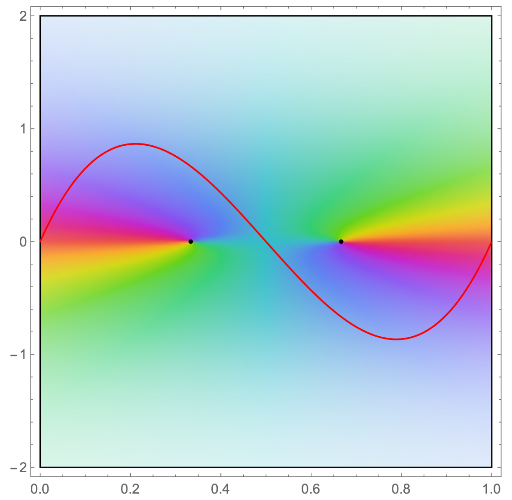
$$= \int_0^1 \prod_{j=1}^{N-1} \mathrm{d}x_j \, x_j^{\nu_j - 1} \frac{U^{\nu-(L+1)D/2}}{F^{\nu-LD/2}} = \int_0^1 \prod_{j=1}^{N-1} \mathrm{d}x_j \, I(\vec{x})$$

Rewrite with Feynman parameters

Still contains singularities

Solved by contour deformation due to Cauchy's theorem

$$\int_0^1 \prod_{j=1}^{N} \mathrm{d}x_j \, I(\vec{x}) = \int_0^1 \prod_{j=1}^{N} \mathrm{d}x_j \, \det\left(\frac{\partial \vec{z}(\vec{x})}{\partial \vec{x}} \right) I(\vec{z}(\vec{x}))$$

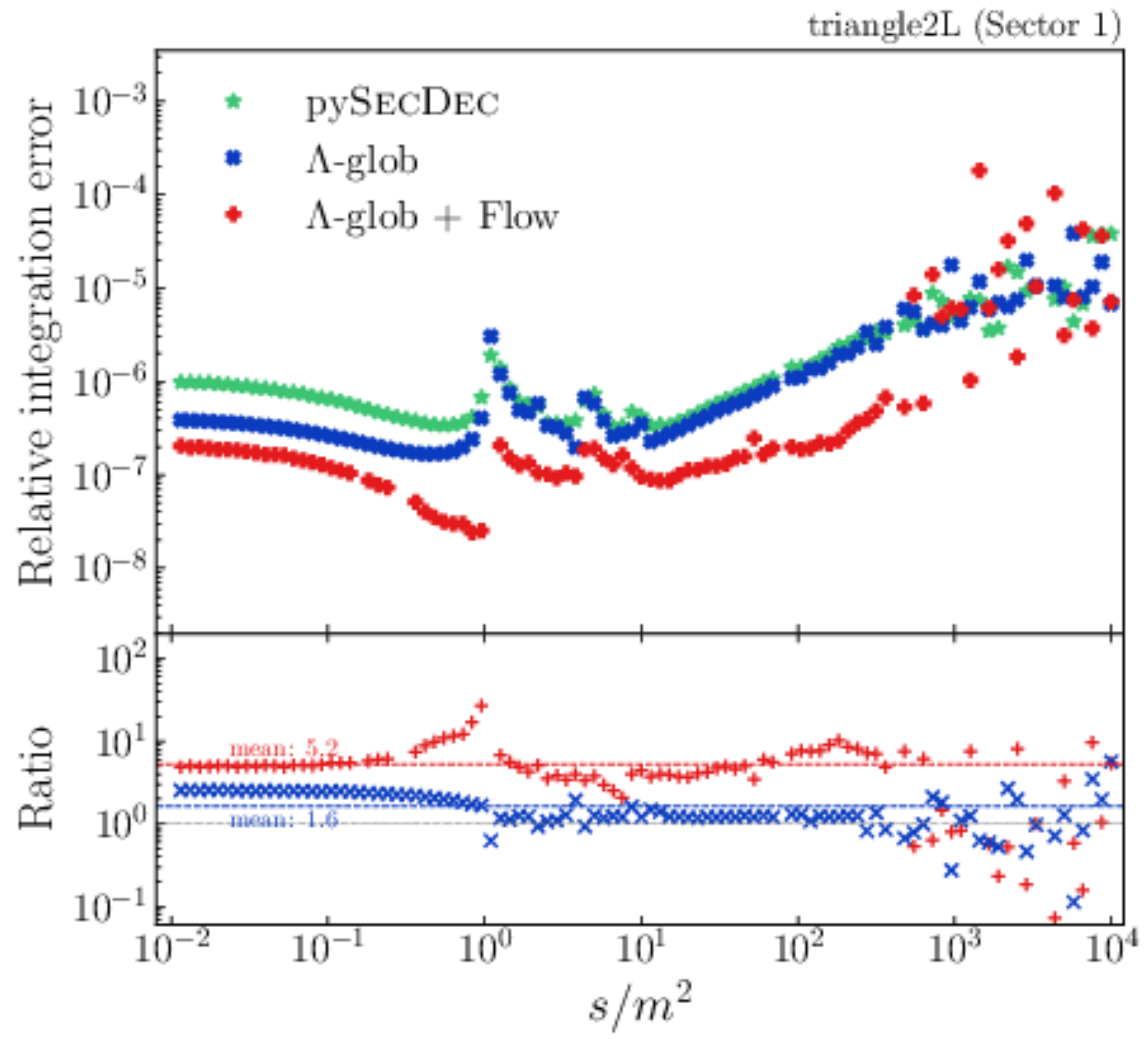


Optimal parametrization = minimal variance

Turn it into an ML Problem

Parametrization $\rightarrow z = \mathrm{INN}(x)$

Variance $\rightarrow \mathscr{L}$



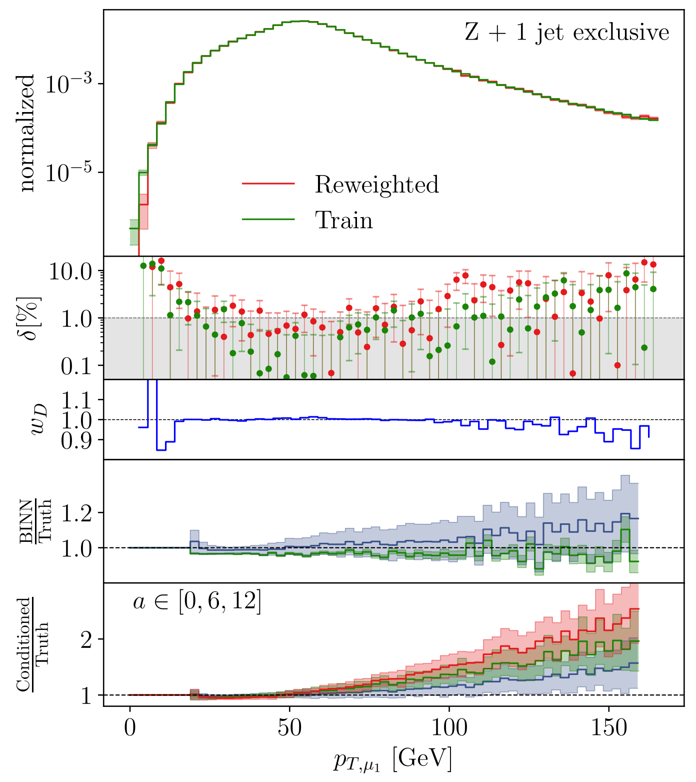
R. Winterhalder, et al. [2112.09145]

Event generation

Phase space sampling & End-To-End generation

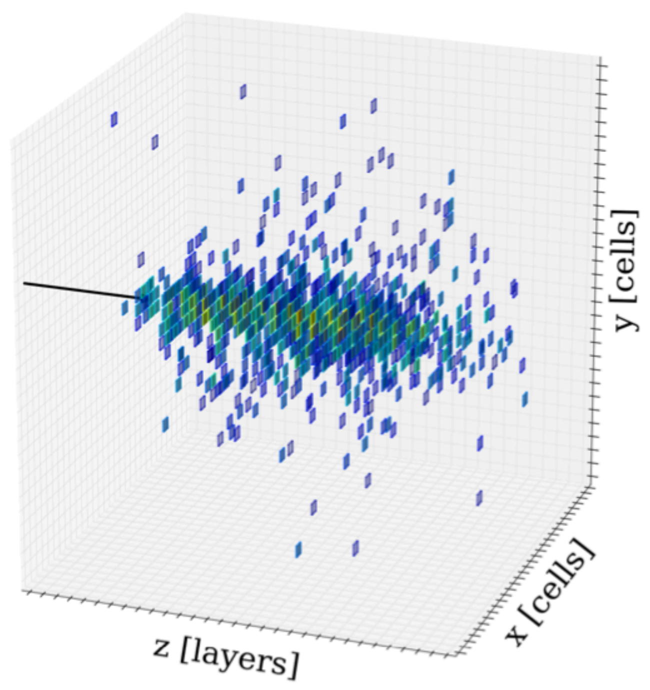
Forward simulations with generative networks

Event generation

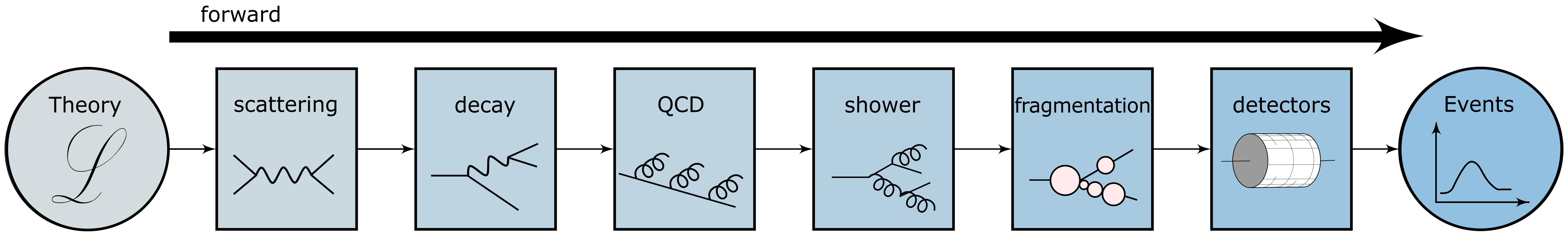


→ Otten et al.
→ Gao et al.
→ Bothmann et al.
→ Stienen et al.
→ AB, et al.
→ and many more

Detector simulation



→ CaloGAN by M. Paganini et al.
→ BIBAE by E. Buhman, S. Diefenbacher et a
→ CaloFlow by C. Krause , D. Shih
→ and many more



Further applications

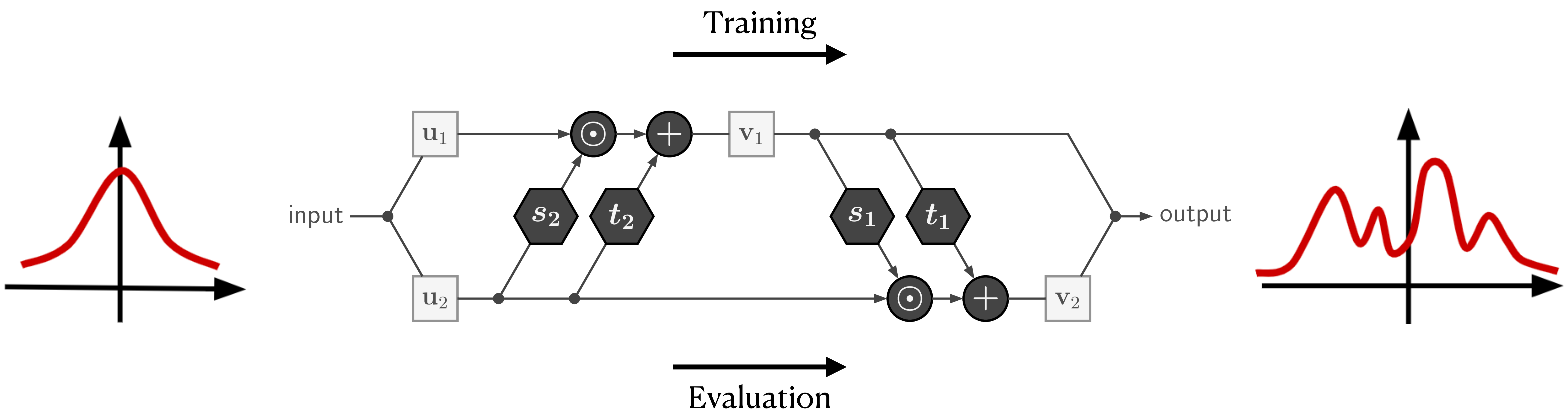
- End to end learning
- Data compression
- Amplification

Multiple possibilities for generative networks
GAN → first applications
VAE → compressed latent space
NF → highest control

Normalizing flows

Invertible networks for complex transformations

+ Bijective mapping
+ Tractable Jacobian → $p_x(x) = p_z(z) \cdot J_{NN}$
+ Fast evaluation in both direction



Training on density $t(x)$
→ Minimize difference

$$\begin{aligned}\mathscr{L} &= \log p_x(x)/t(x) \\ &= \log p_z(z(x))\ J_{NN} \,/\, t(x)\end{aligned}$$

Training on samples x
→ Maximize the log-likelihood

$$\begin{aligned}\mathscr{L} &= \log p(\theta\,|\,x) \\ &= \log p(z\,|\,\theta) + \log J_{NN} + p(\theta)\end{aligned}$$

Normalizing flows

Invertible networks for complex transformations

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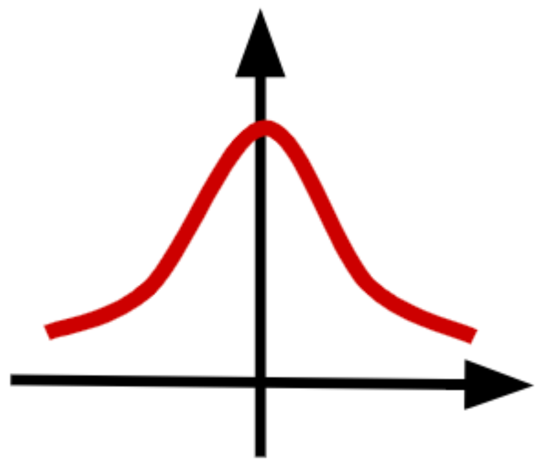

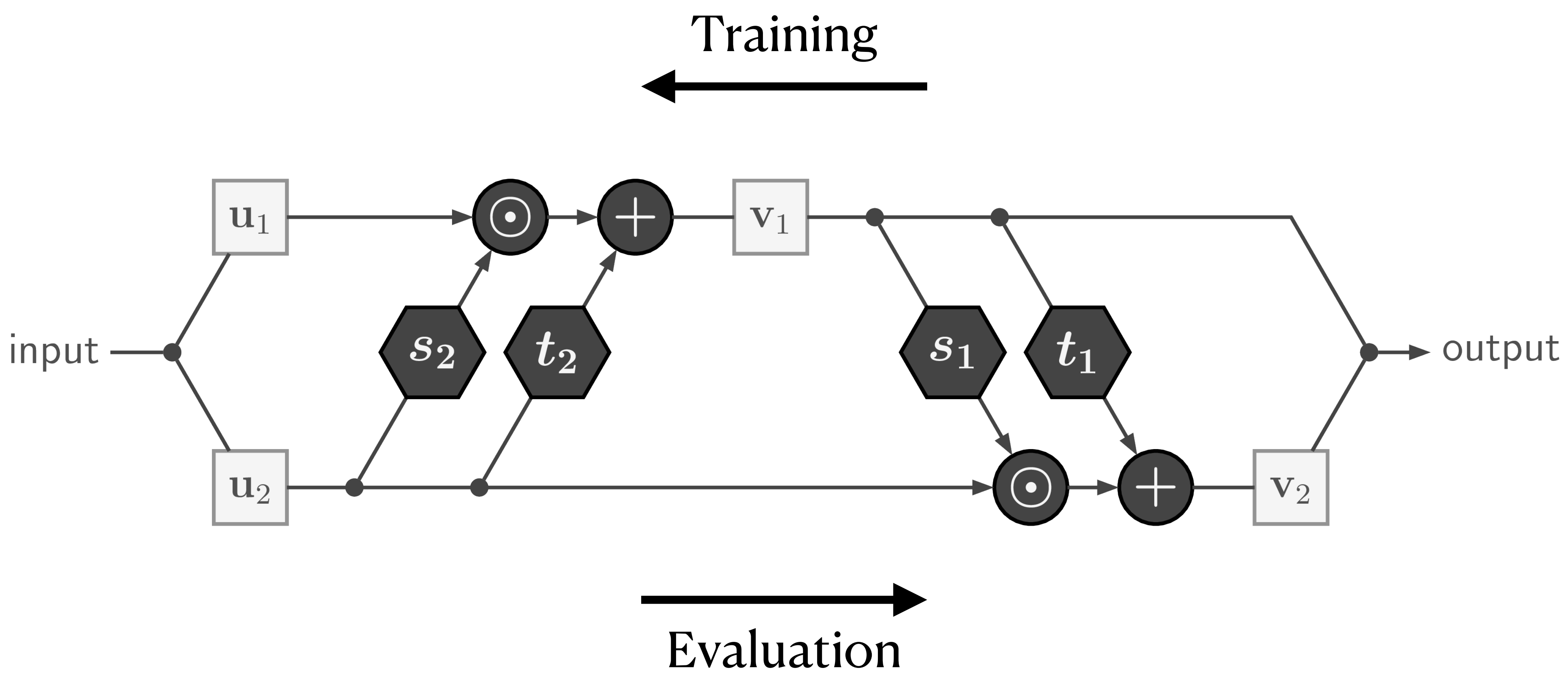

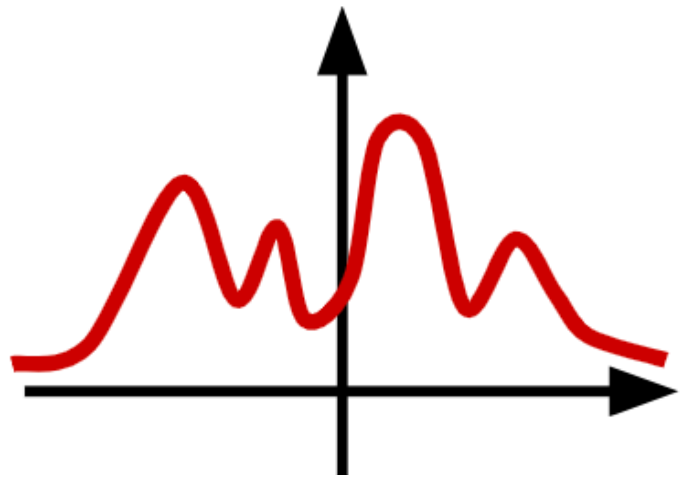

Training on density $t(x)$

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$$= \log p_z(z(x))\, J_{NN} \,/\, t(x)$$

Training on samples x

→ Maximize the log-likelihood

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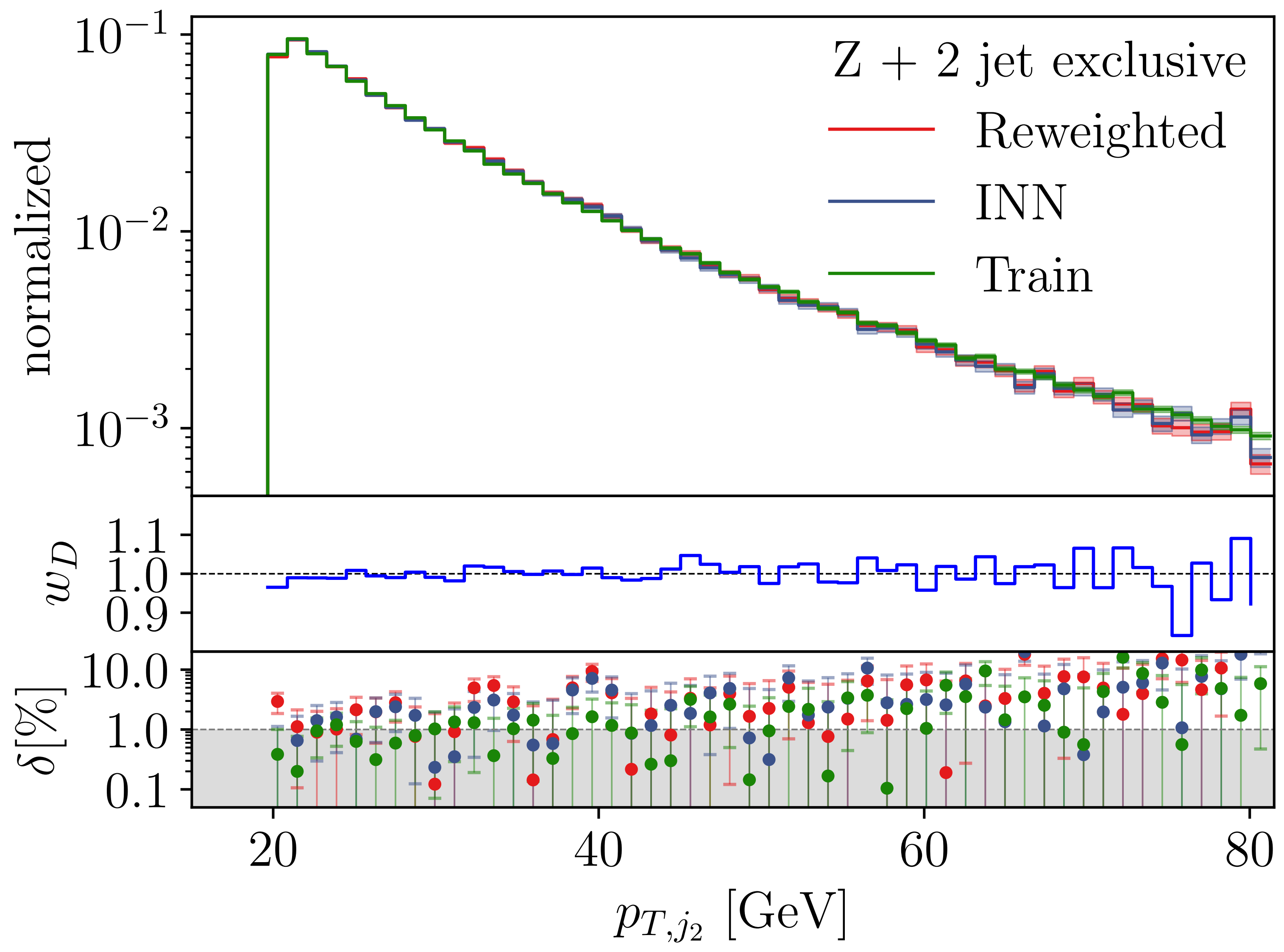
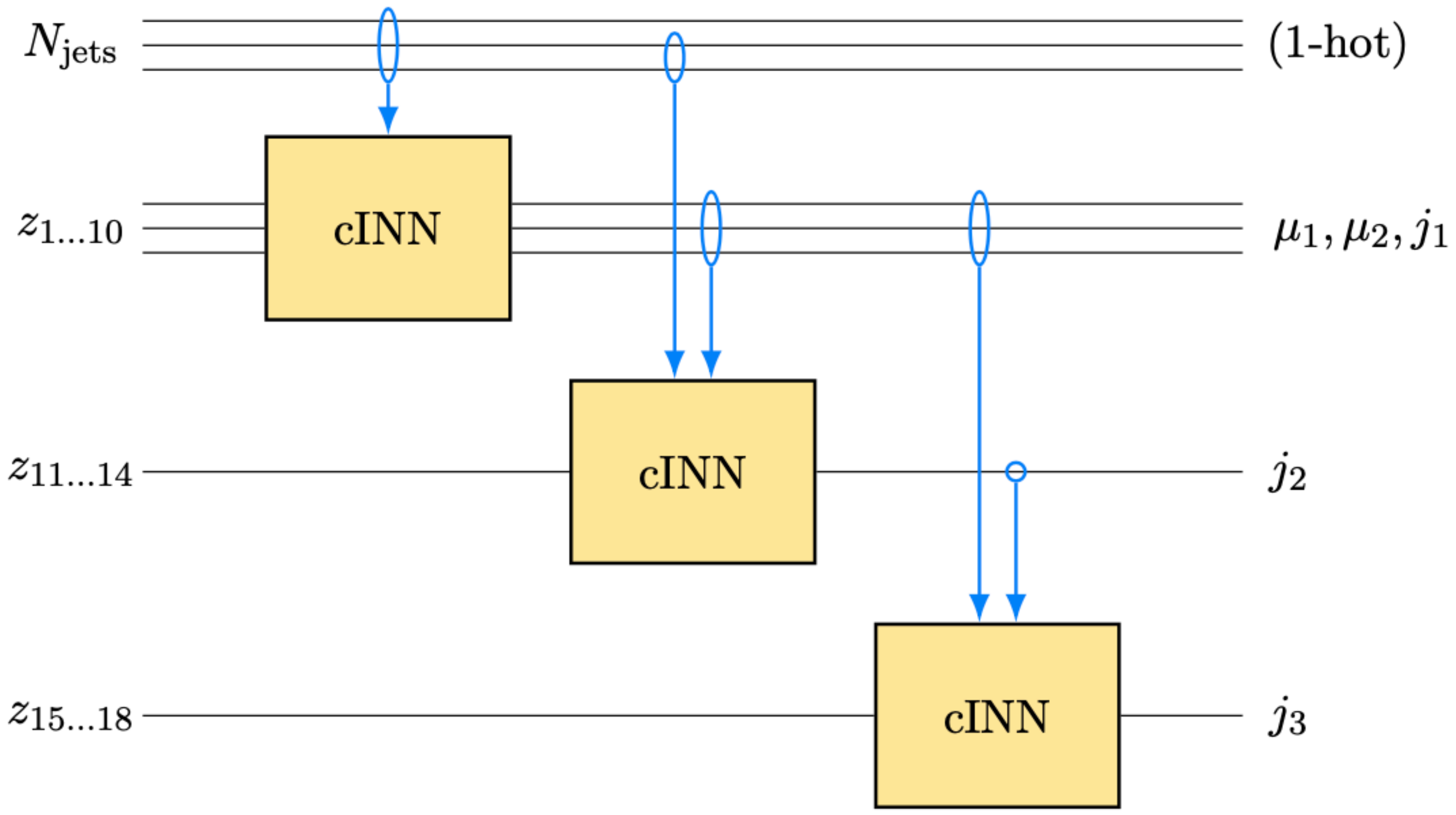
Putting flows to work

Event generation



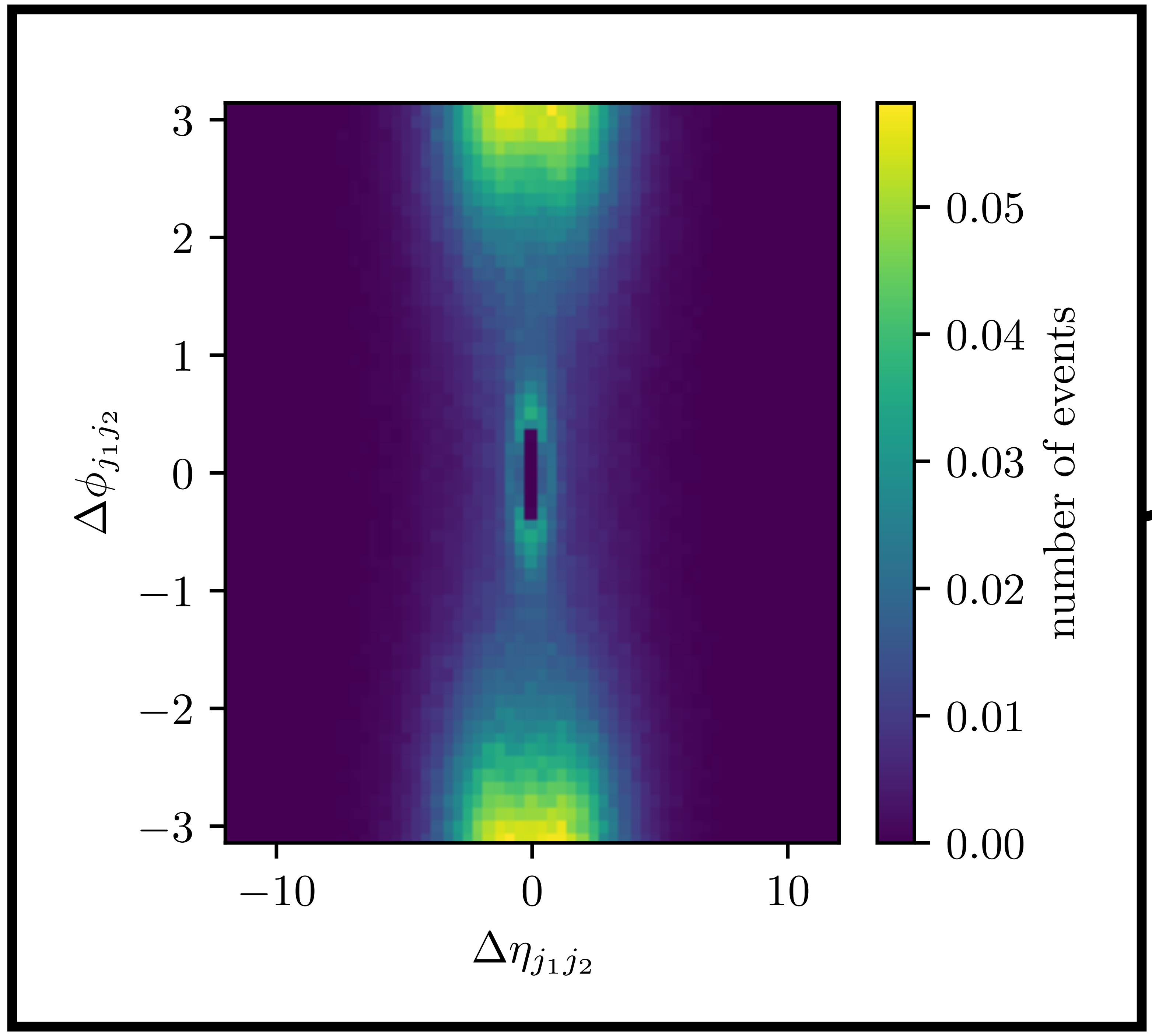


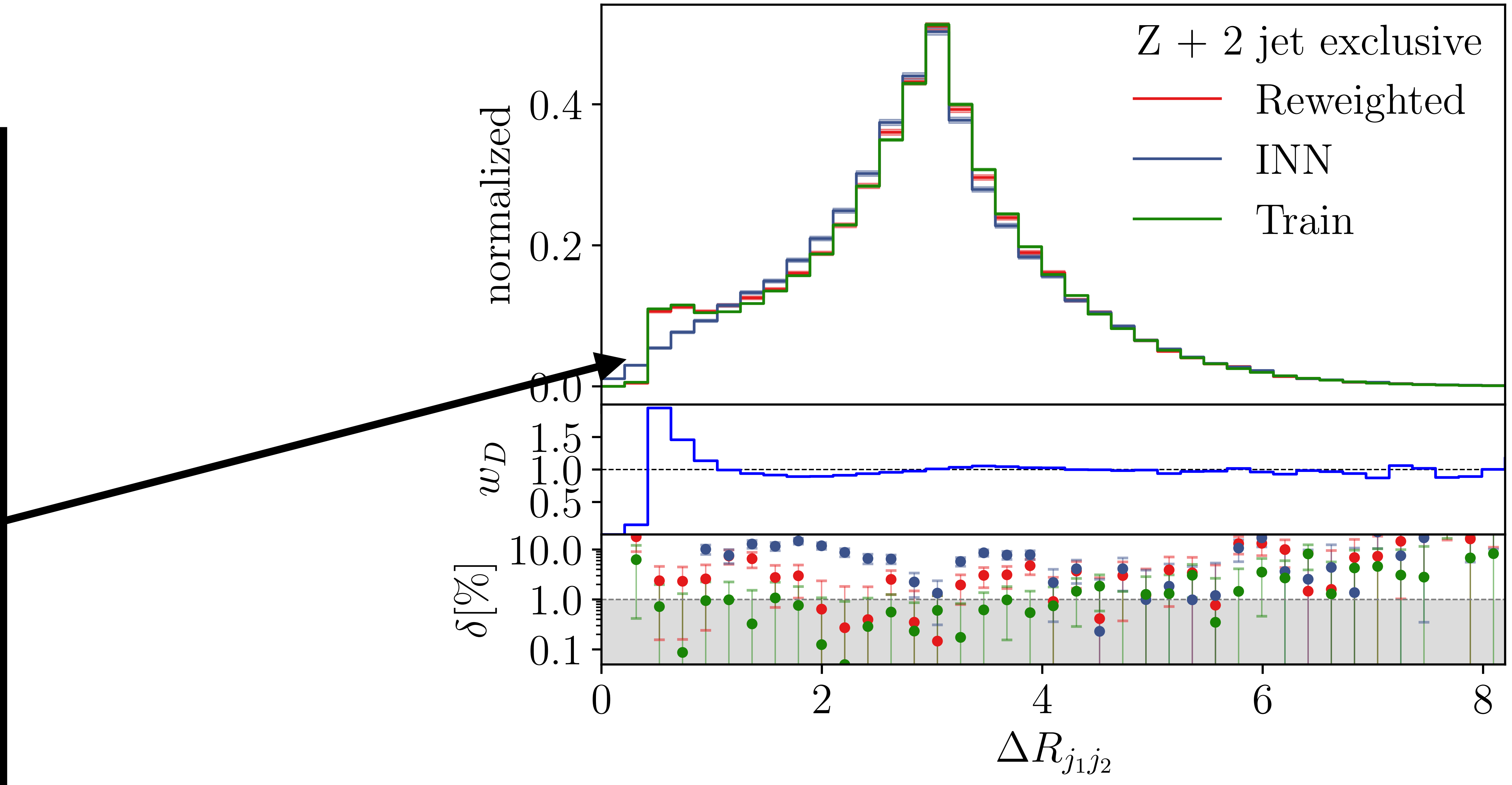
- Train normalizing flow on 4-momenta
- Include symmetries in feature representation
- Excellent performance for direct output

- Extend setup vor variable jet multiplicity

Challenges for normalizing flows

- Narrow features
- Topological holes (eg ΔR cuts)
  - no bijecive mapping possible
  - can only be approximated





Reweighting for Precision

- Classifier loss

$$\mathscr{L} = -\sum_{x\sim p_{data}} \log(D(x)) - \sum_{x\sim p_{INN}} \log(1 - D(x))$$

$$= -\int \mathrm{d}x \, p_{data}(x) \, \log(D(x)) + p_{INN}(x) \, \log(1 - D(x))$$

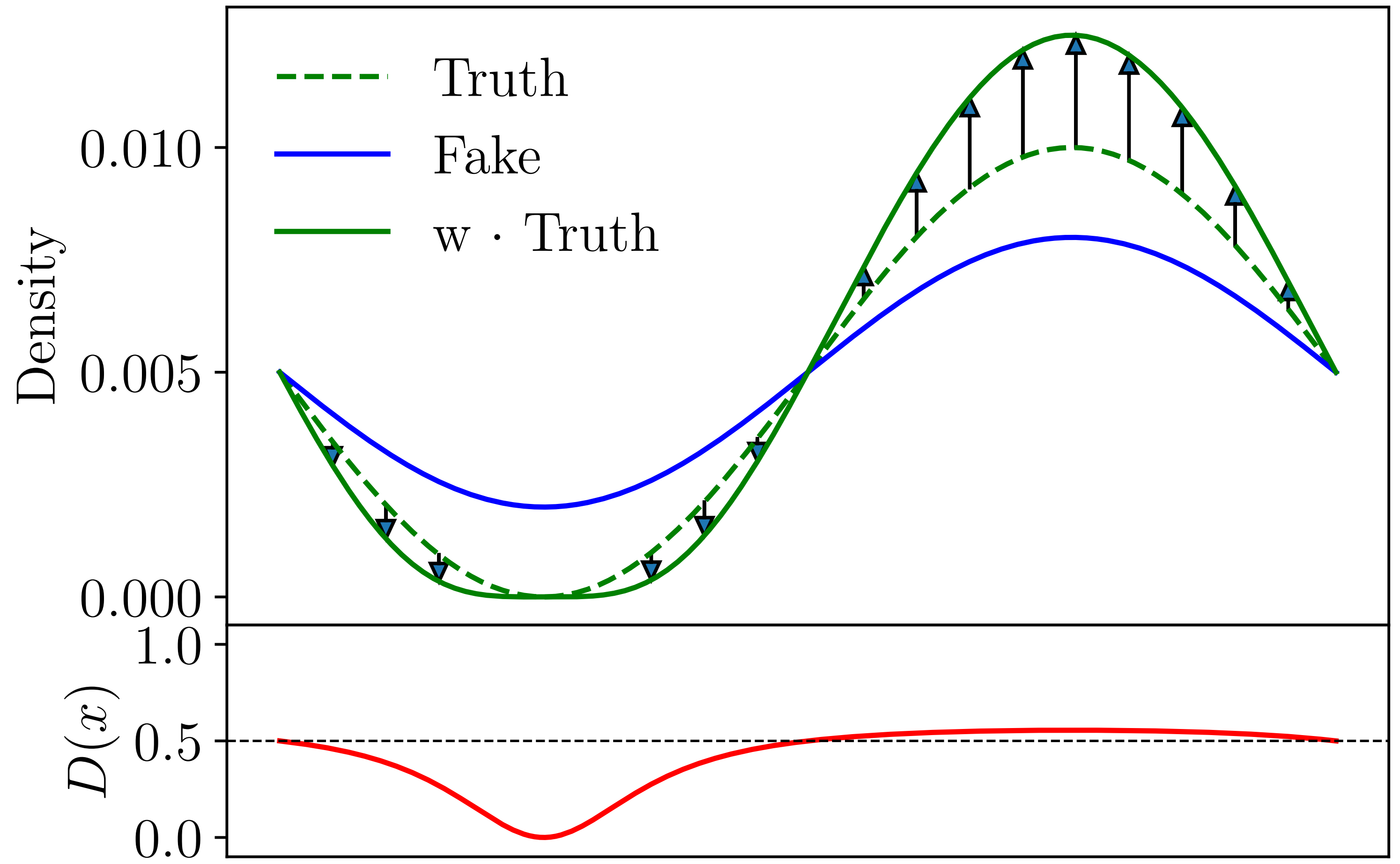
- Upon convergence obtain **reweighting factor**

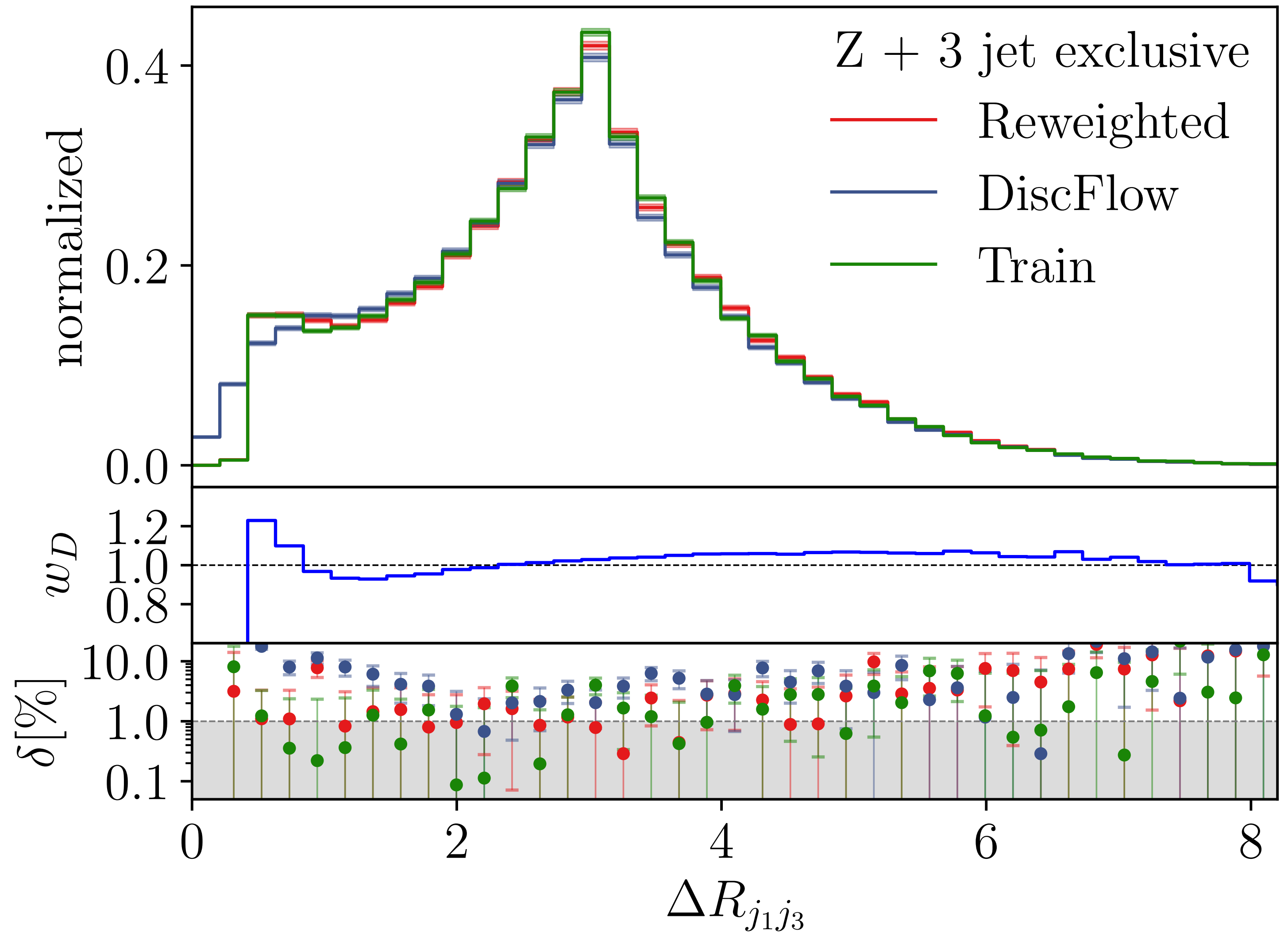
$$\Rightarrow \frac{p_{data}(x)}{p_{INN}(x)} = \frac{D(x)}{1 - D(x)} = w_D$$

- Use classifier feedback to enhance gradients

$$\mathscr{L}_{\text{DiscFlow}} \approx \int \mathrm{d}x \quad \underbrace{w_D(x)^\alpha P(x)}_{\text{reweighted truth}} \left(\frac{\psi(x;c)^2}{2} - \log J(x) \right)$$

$\Rightarrow$ Reduces range of reweighting factors





ML Uncertainties

When do we (not) need them?

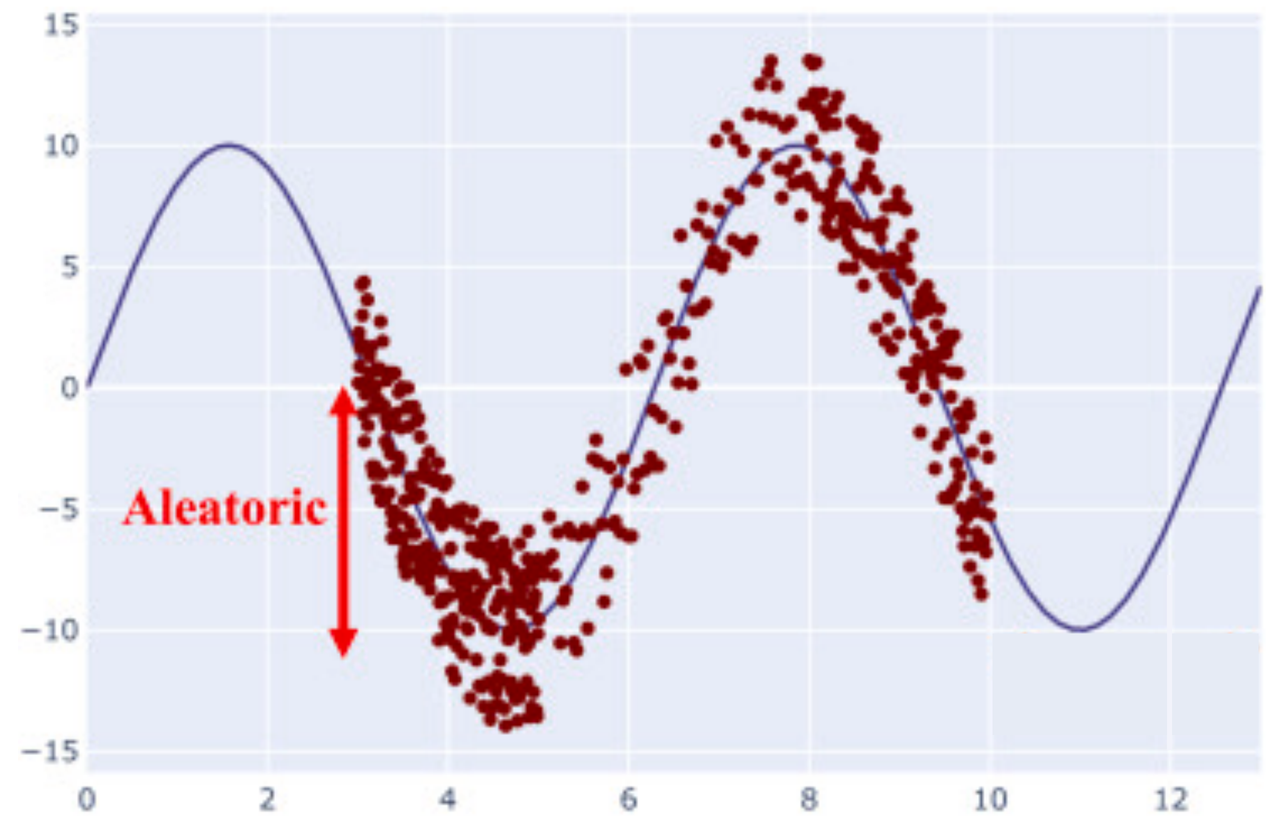
- Predictions with poorly trained NNs are sub-***optimal*** but not ***wrong***

- Example 1: **Phase space sampling**
  - Mapping induces Jacobian
  - Events obtain weight from ME × J
  - Bad mapping → small unweighting efficiency

- Example 2: INN for **integration**
  - Sub-optimal contour deformation
  - **High variance** of integral
  - Not efficient but not wrong

➡ **Control** comes from **simulation** !

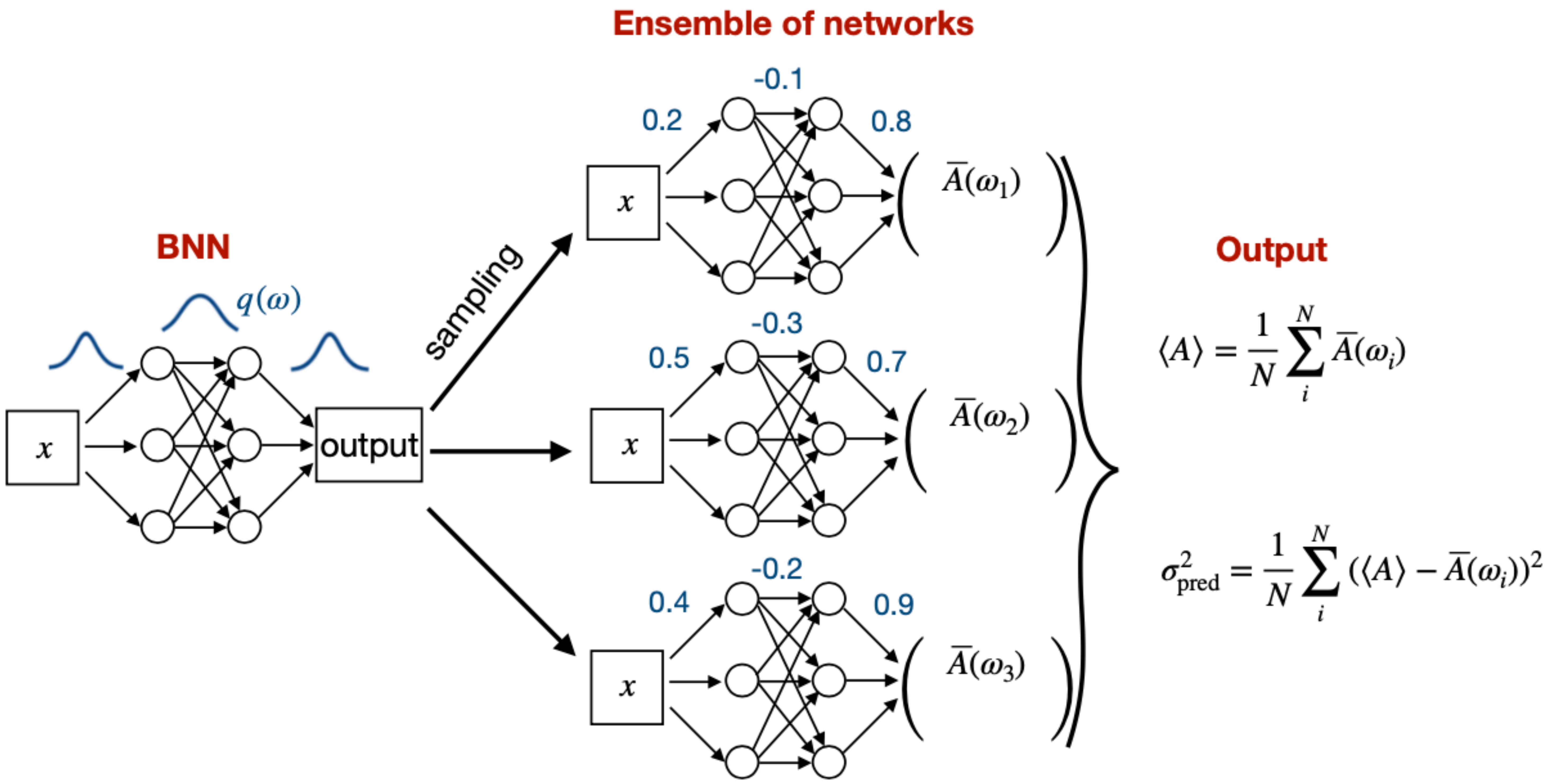
- Example 3: Data compression
  - Direct use of generator output



modified from M. Abdar [doi.org/10.1016/j.inffus.2021.05.008]

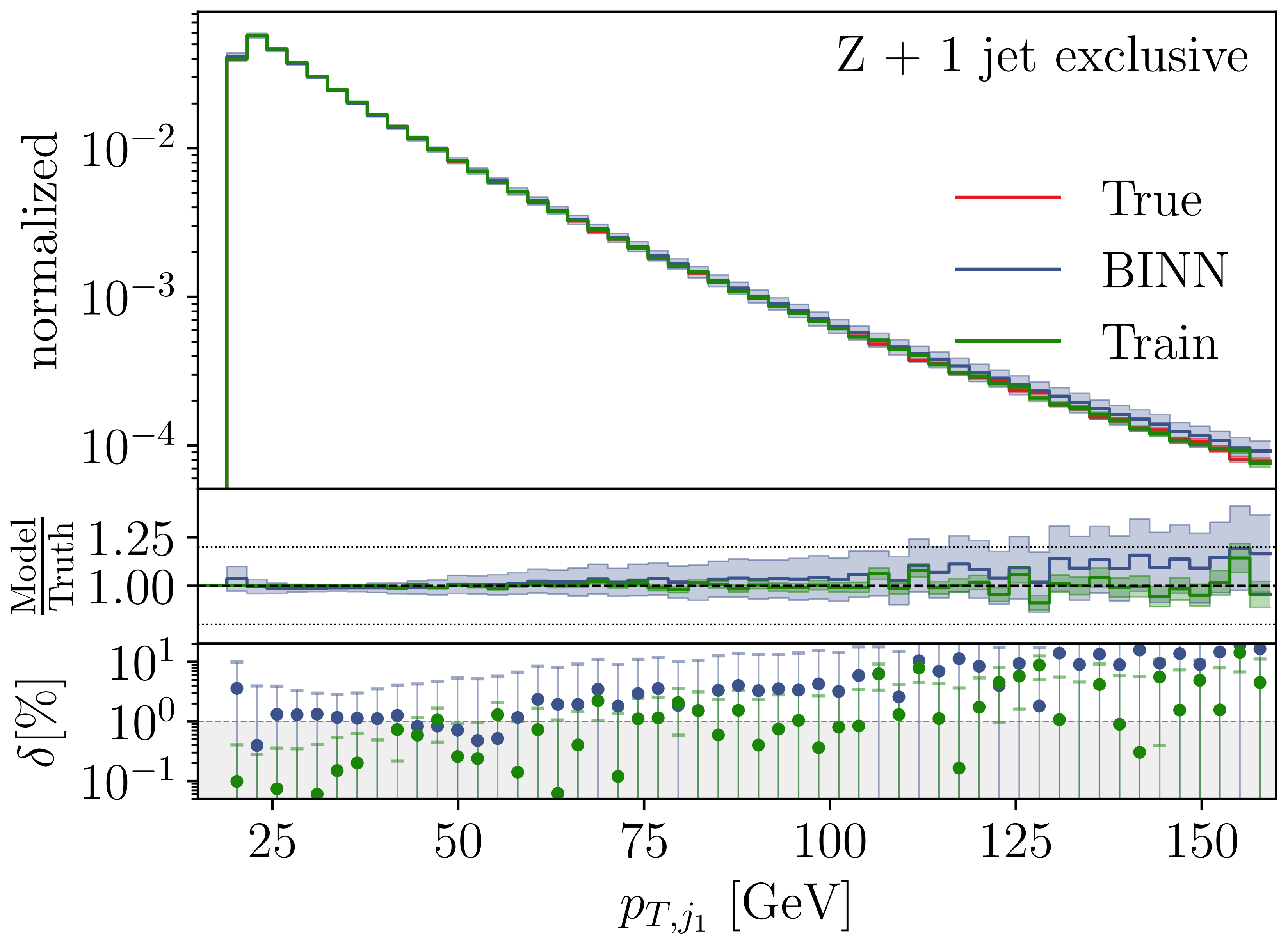
➡ How can we estimate this uncertainty?

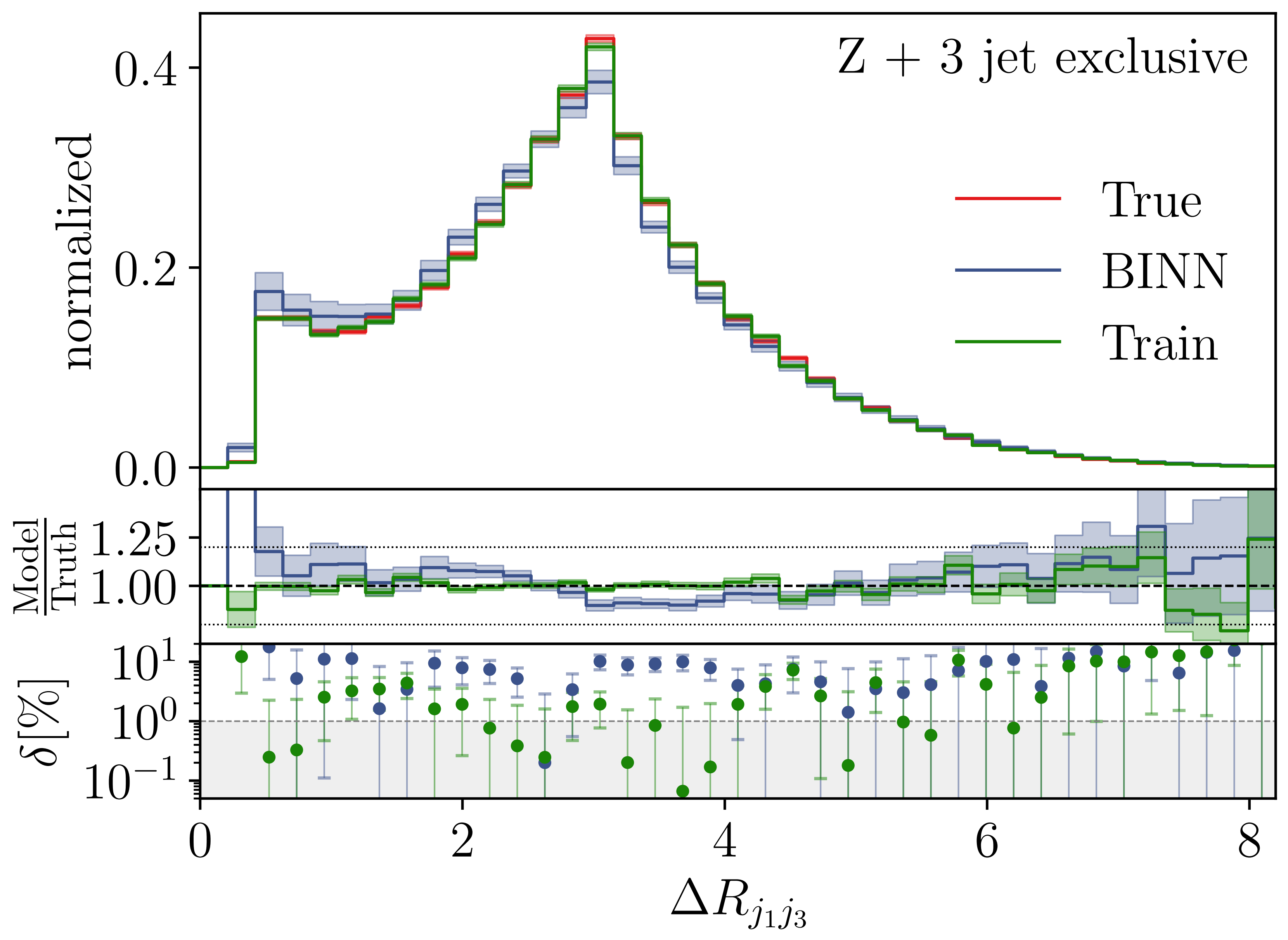
Bayesian Neural Network

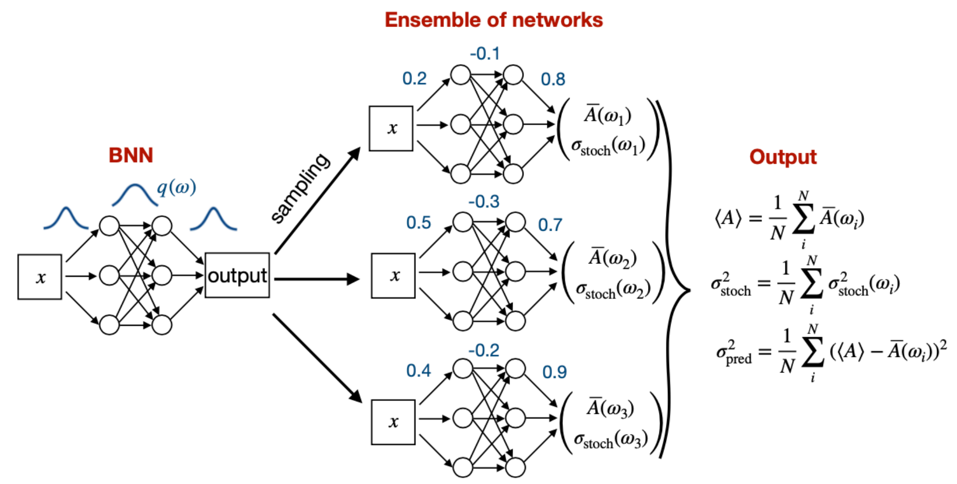


$$
\begin{aligned}
\mathscr{L} &= \mathscr{L}_{INN} + KL_{prior} \\
&= \sum_{n=1}^{N} \langle \log p_X(x_n \,|\, \theta) \rangle_{\theta \sim q_\Phi(\theta)} - KL(q_\Phi(\theta), p(\theta))
\end{aligned}
$$

Bayesian generative networks





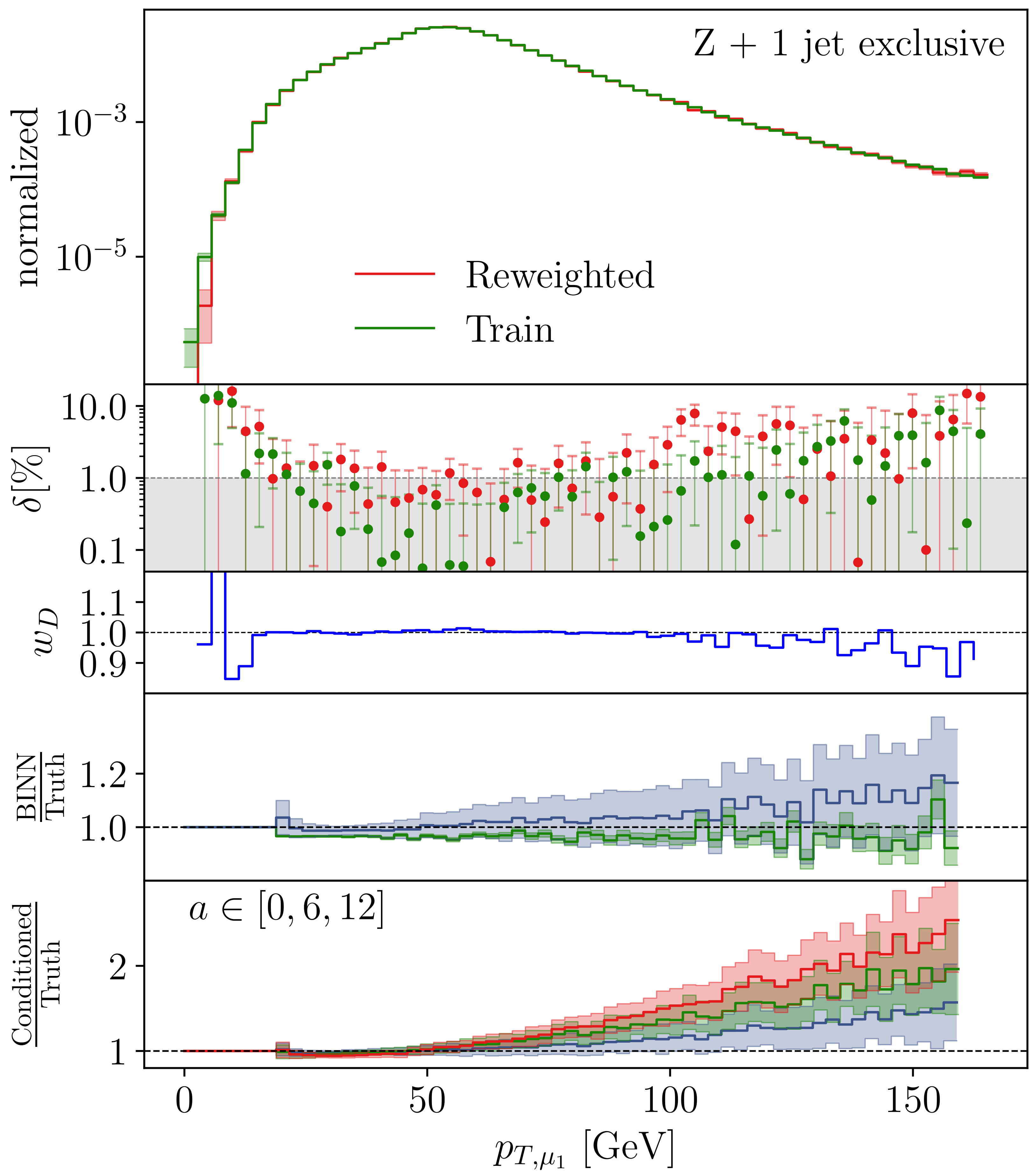


⇒ BINN captures uncertainty related to convergence and statistical uncertainties

⇒ BINN does not capture lack of expressiveness

Putting flows to work

Event generation



- Basis: INN
  - Phase space symmetries in architecture
- Control via classifier D
  - $$\frac{p_{\text{truth}}(x)}{p_{\text{INN}}(x)} = \frac{D(x)}{1 - D(x)}$$
- Precision via reweighting
  - Correct deviations of p_{INN}

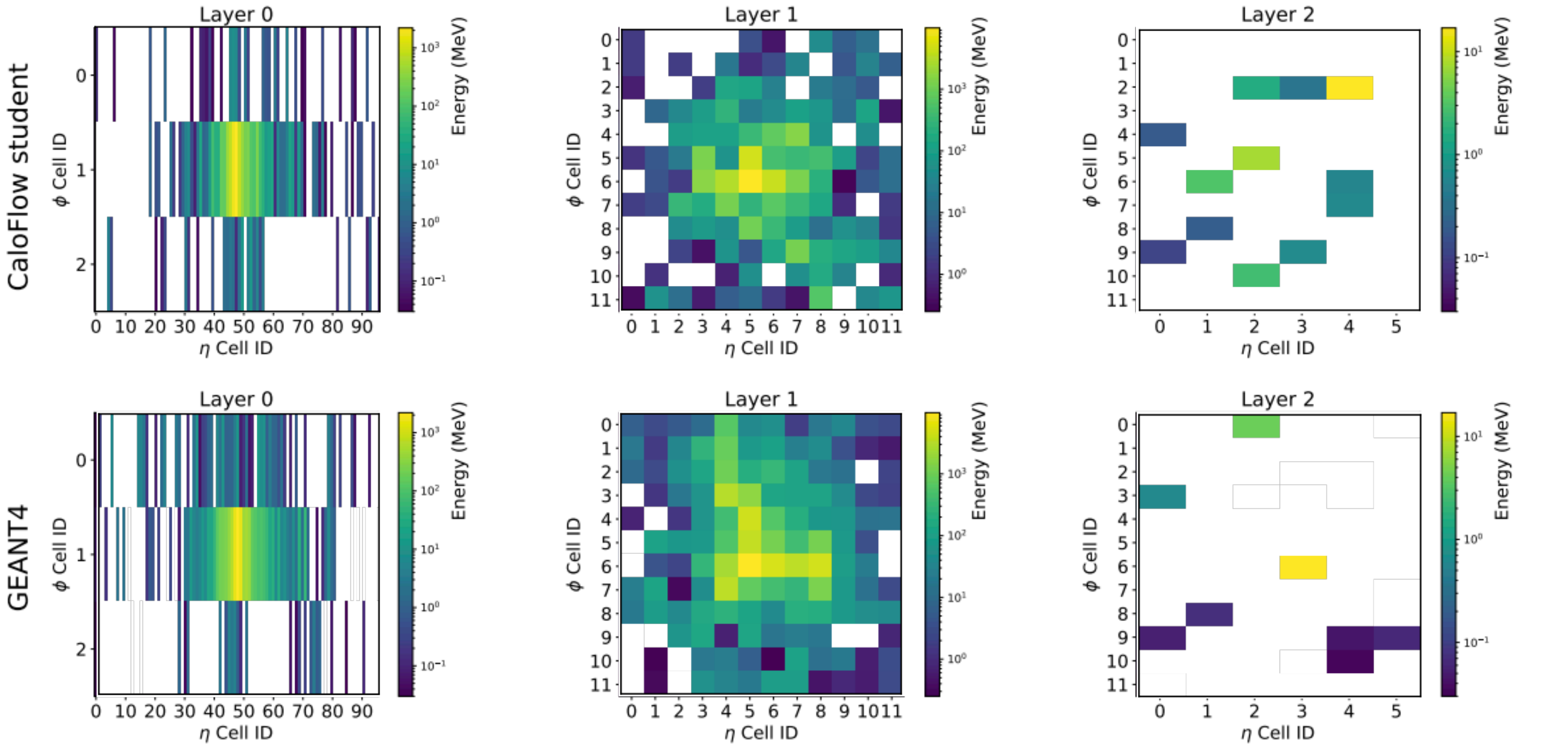
➡ Uncertainty estimation via Bayesian NN

➡ Uncertainty propagation via conditioning

Putting flows to work

Detector simulation

Challenge: large dimensionality $(3 \times 96, 12 \times 12, 12 \times 6)$



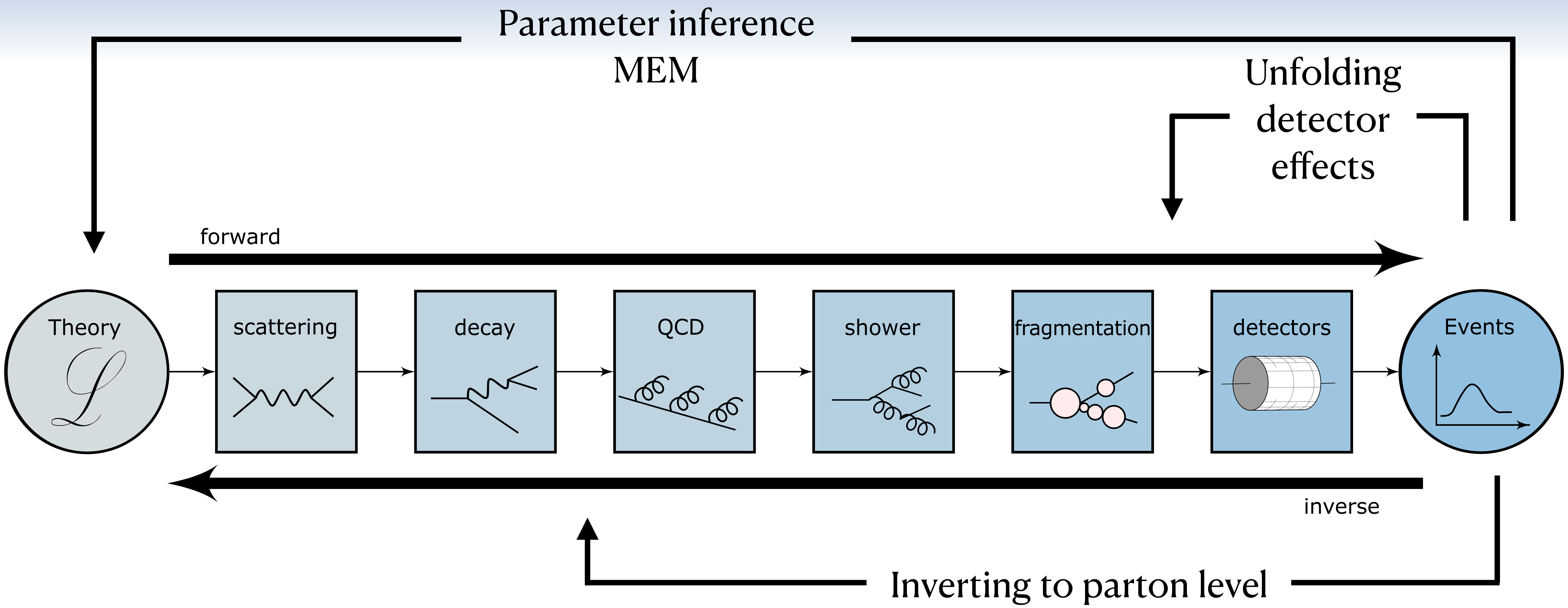
C. Krause & D. Shih [2110.11377]

π^+ shower individual & average

Inverting the simulation chain

Unfolding

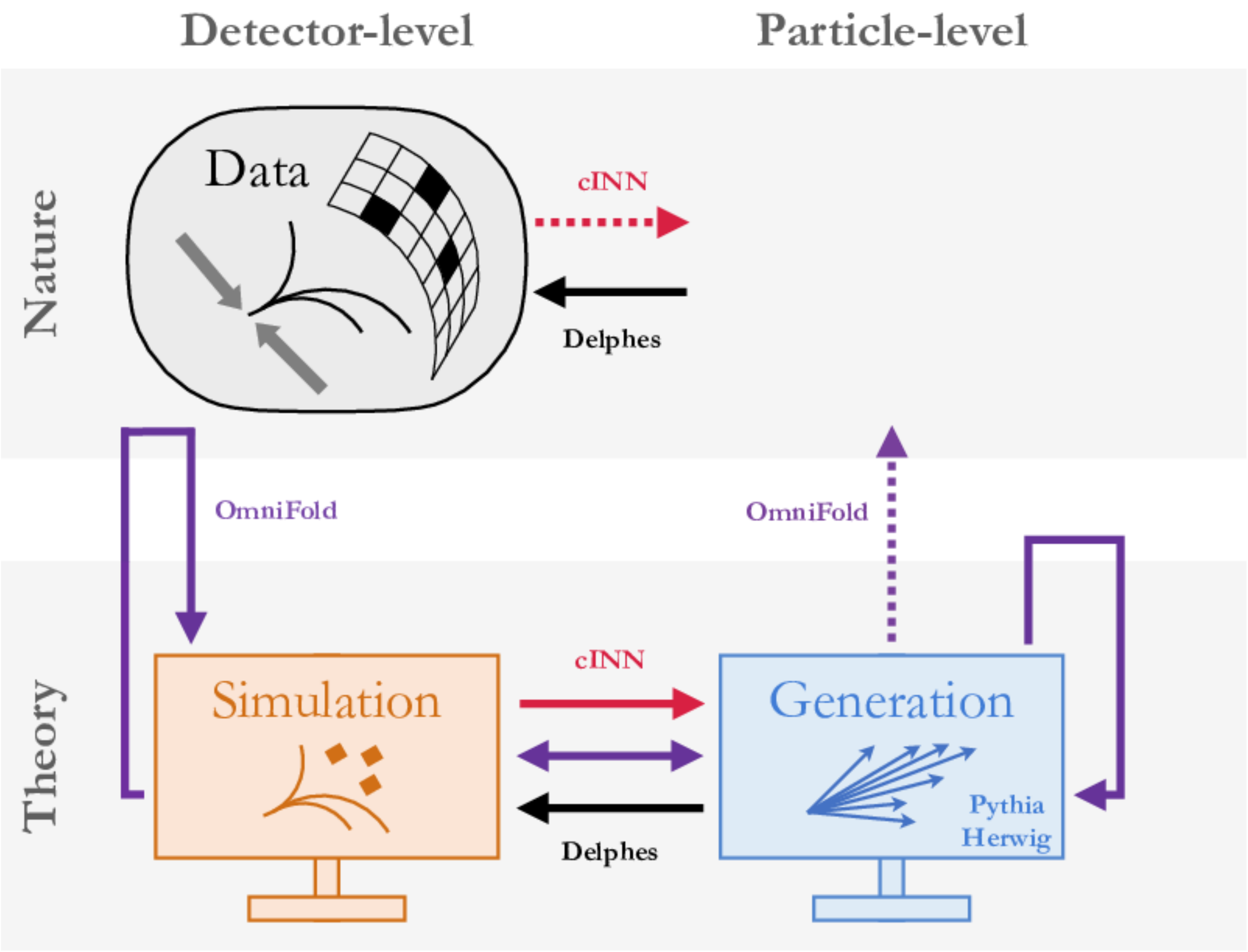
Inverting the simulation chain



Requirements
- ❑ Highdimensional
- ❑ Bin independent
- ❑ Statistically well defined

ML unfolding methods

High-dimensional. Bin independent. Robust.



M. Arratia et al. [2109.13243]

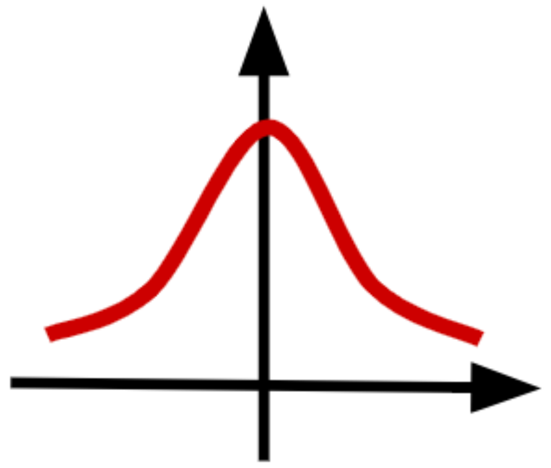
Classifier based aproach
Output: reweighted distribution of MC events

Density based approach
Output: probability density per unfolded event

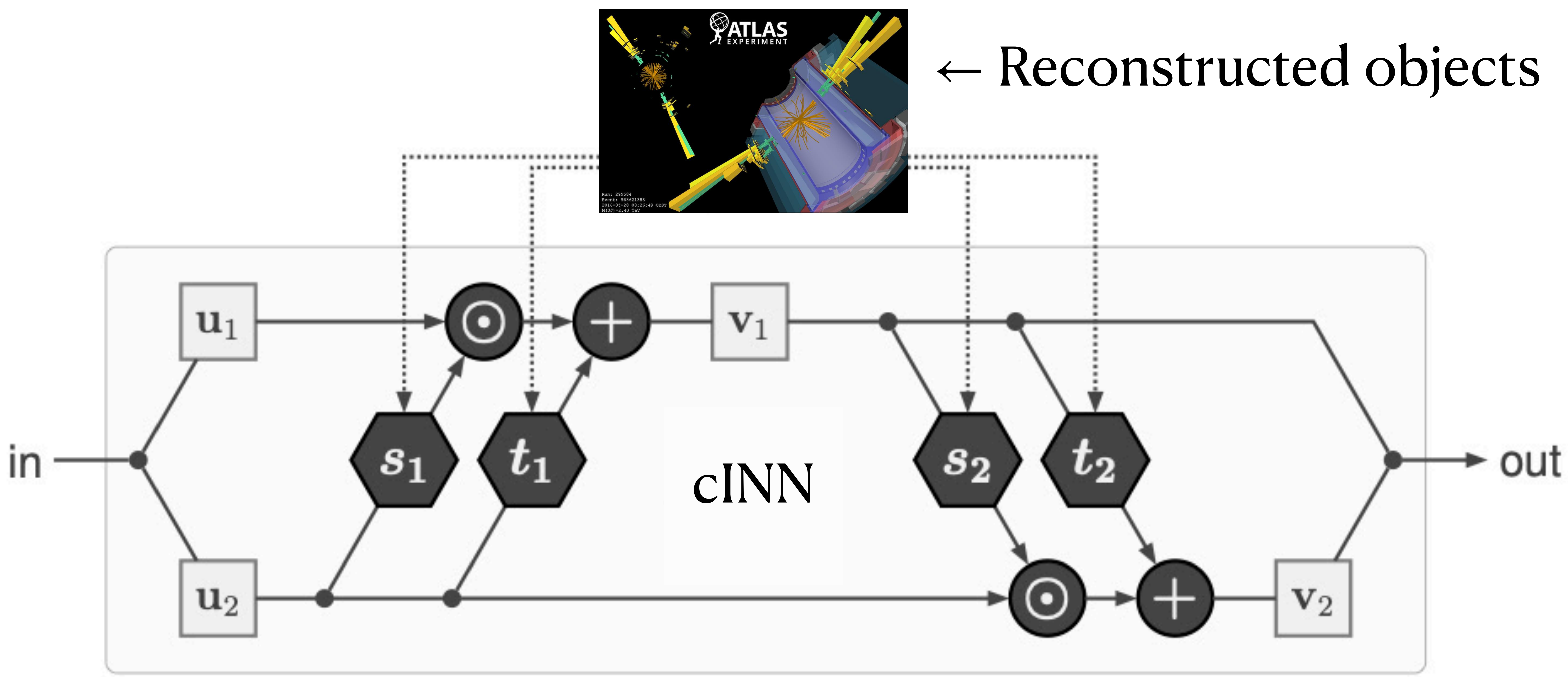
VAE alternative: OTUS by J. N. Howard et al.

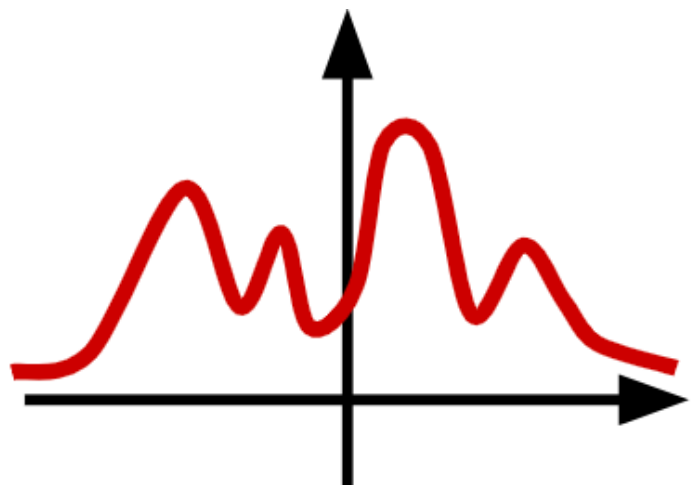
cINN unfolding

Given a reconstructed event:
What is the probability distribution at particle level?



Normal distribution
$z \sim \mathcal{N}$





Probability distribution
$x \sim P_{\text{parton}}$

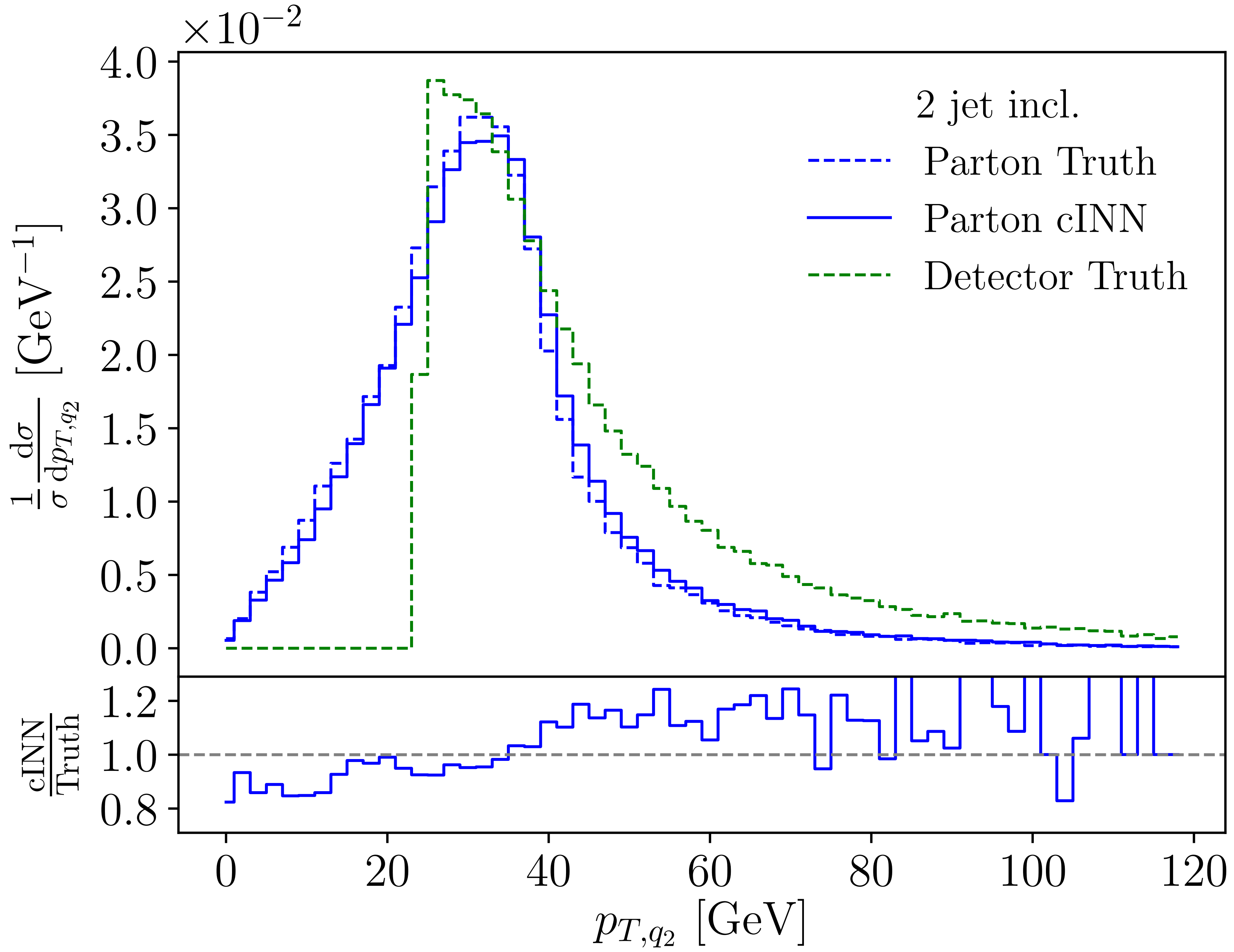
Training

Unfolding

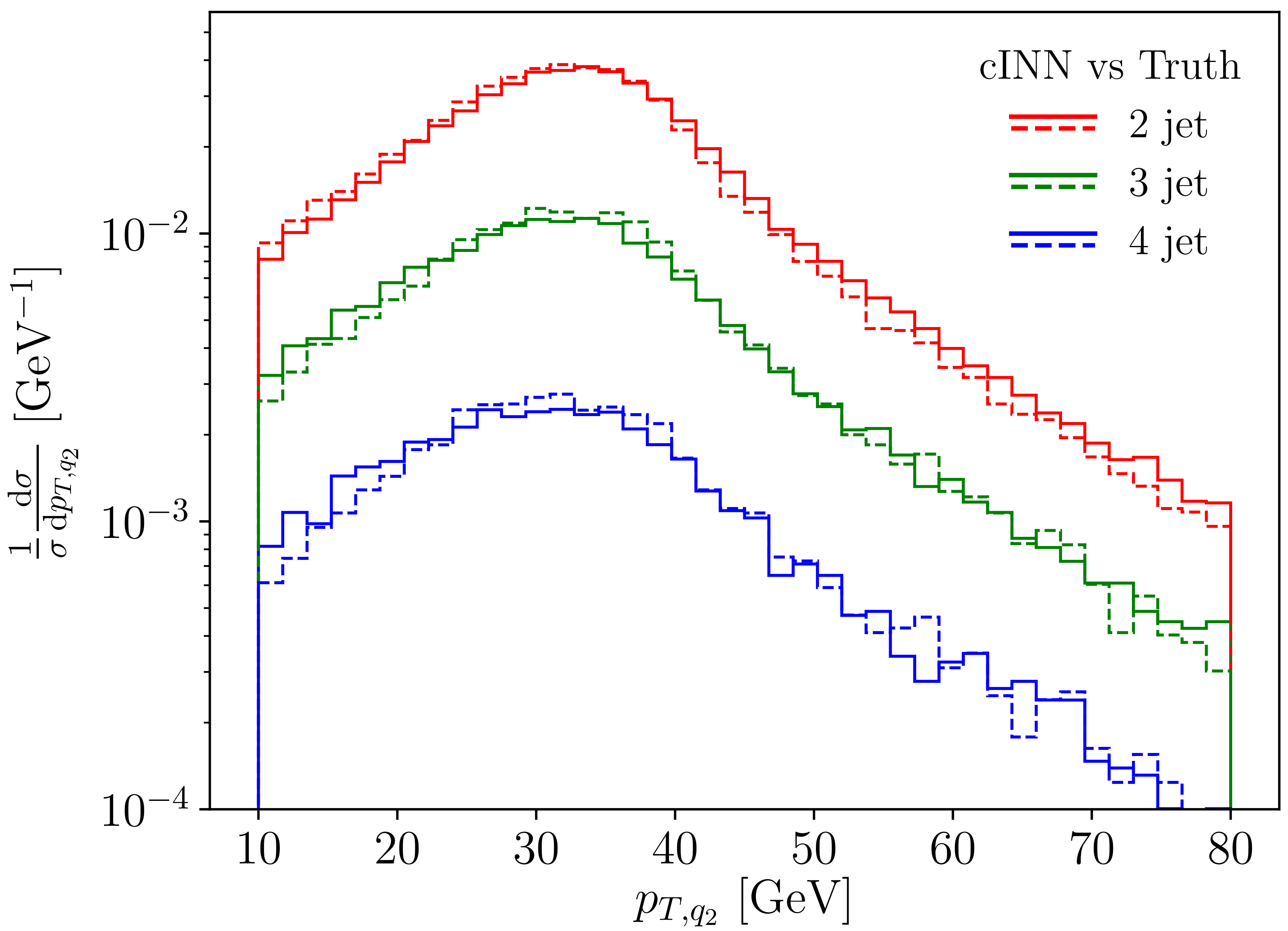
Inverting inclusive distributions

$pp > WZ > q\bar{q}l^+l^- +$ ISR $\rightarrow$ 2/3/4 jet events

Training on inclusive dataset



Evaluate exclusive 2/3/4 jet events

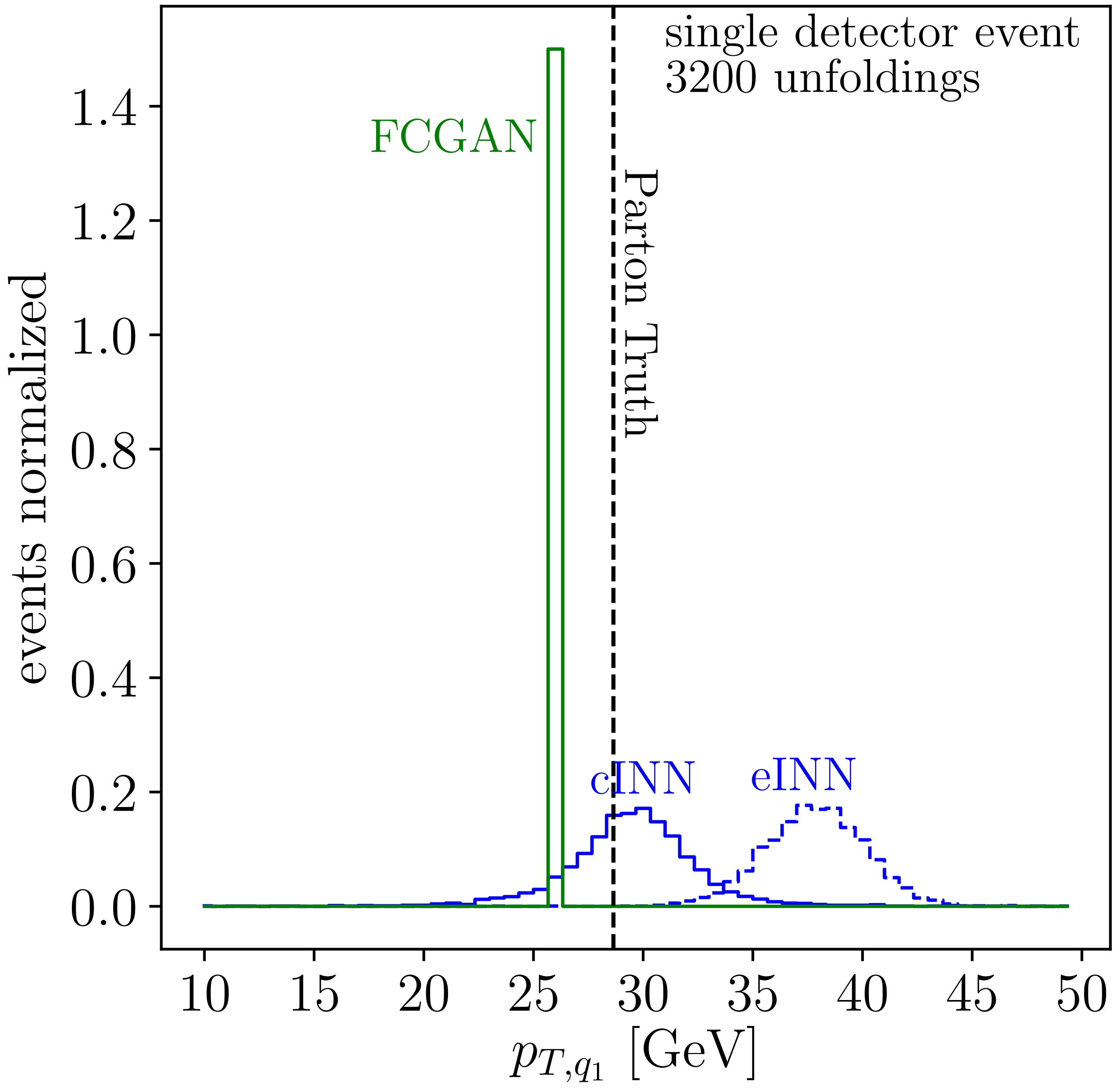


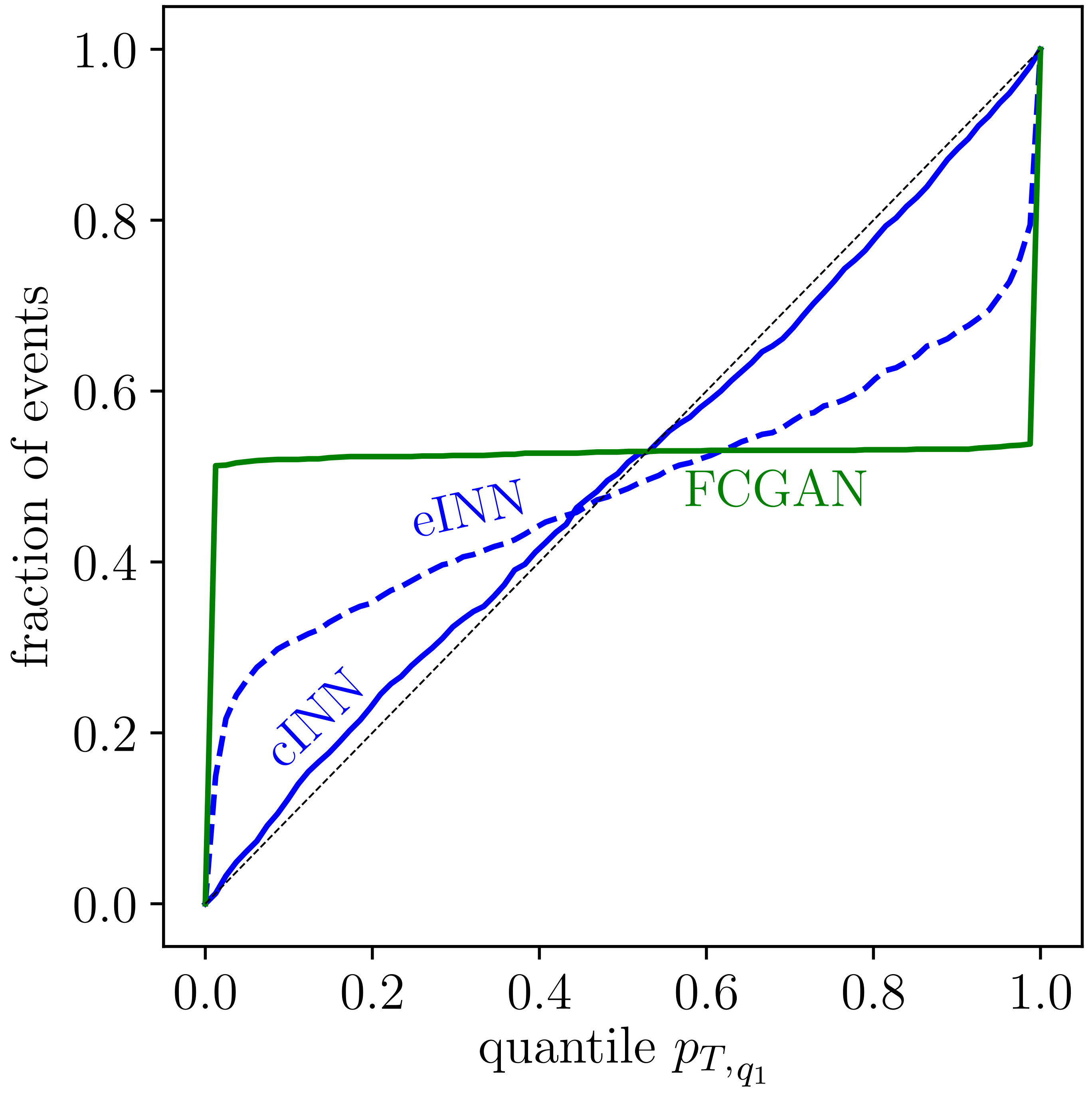
- [x] High-dimensional
- [x] Bin-independent
- [ ] Statistically well defined ?

M. Bellagente et al. [2006.06685]

Event-wise unfolding

No deterministic mapping!
Check calibration of probability density for individual event unfolding



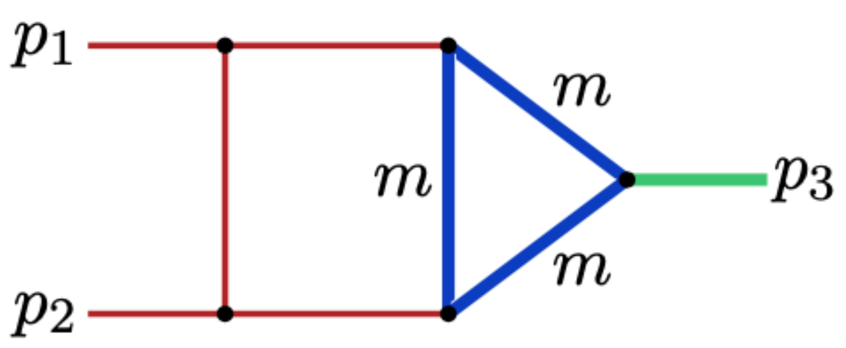


- ☑ High-dimensional
- ☑ Bin-independent
- ☑ Statistically well defined

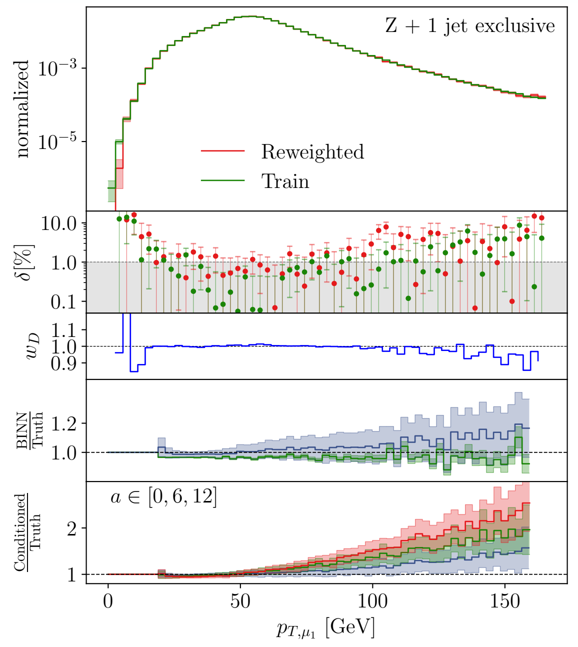
M. Bellagente et al. [2006.06685]

ML 4 LHC Event generation

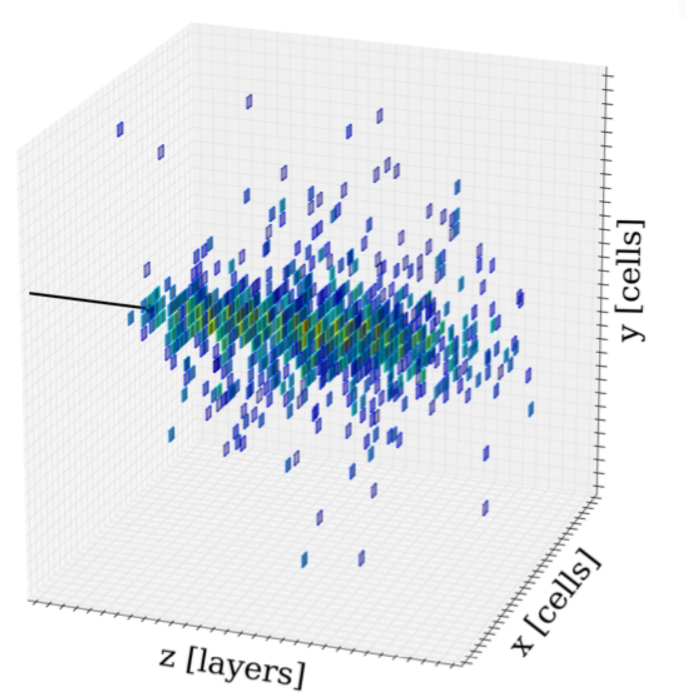
Amplitude estimation

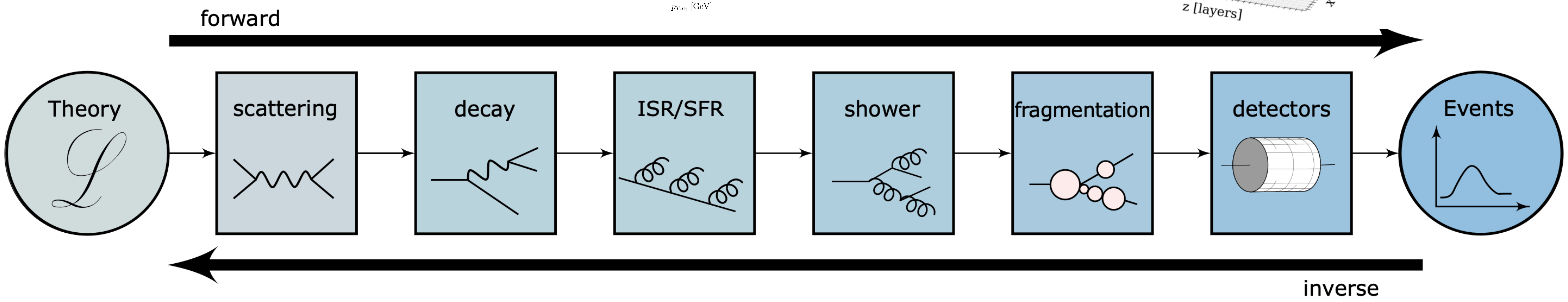


Phase space sampling

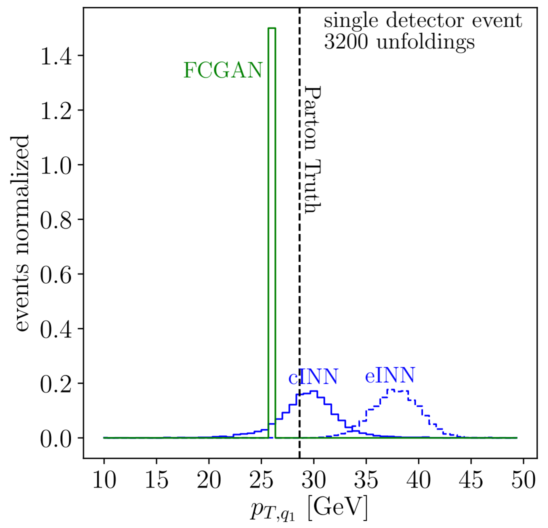


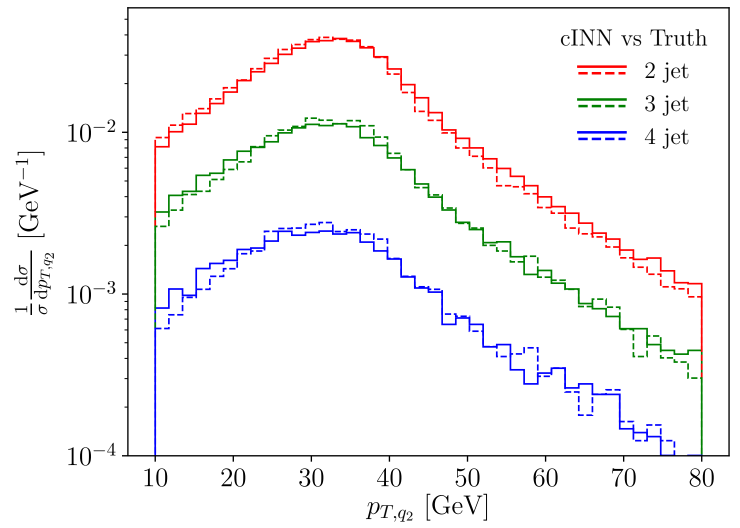
Detector simulation

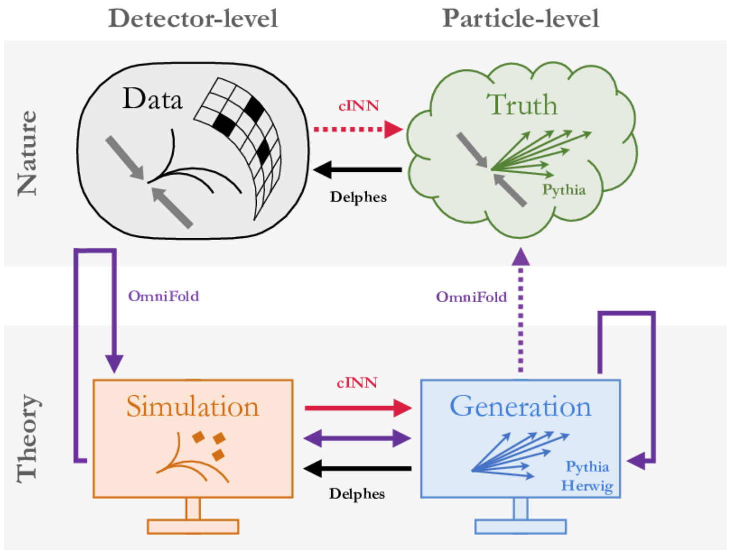




Unfolding & MEM







It is time to move from proof of concept to real applications !