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SEIT 1386

France-Berkeley PHYSTAT Conference on Unfolding
10.06.2024

Generative Unfolding

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Nathan Huetsch

Huetsch et al. 2404.18807
The Landscape of Unfolding with Machine Learning

Simulation chain — Inversion

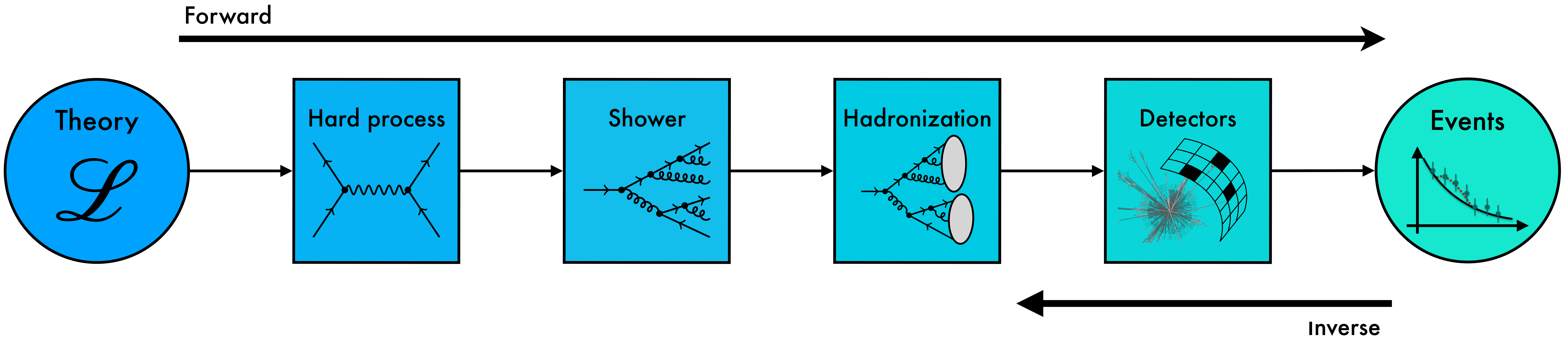


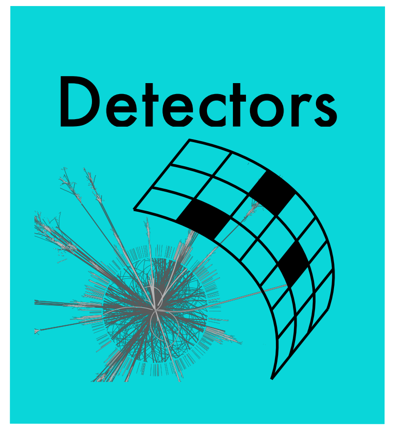
Figure from A. Butter et al.: arXiv:2203.07460, R. Winterhalder

Probabilistic transfer

Transfer probability

$$p(x_{rec} | x_{gen})$$

x_{gen}



x_{rec}

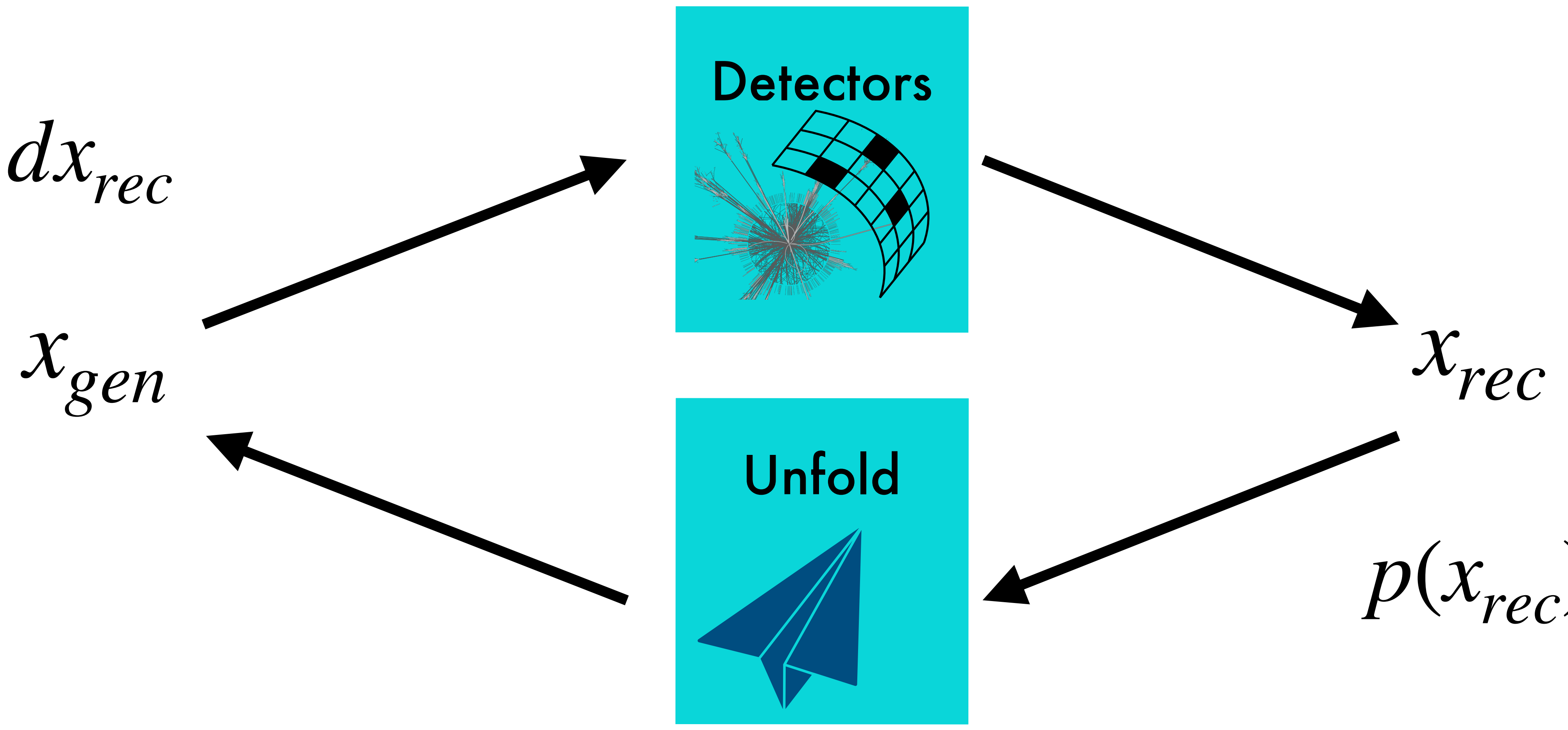
$$p(x_{rec}) = \int p(x_{gen}) p(x_{rec} | x_{gen}) \, dx_{gen}$$

Generative unfolding

Transfer probability

$$p(x_{rec} | x_{gen})$$

$$p(x_{gen}) = \int p(x_{rec}) p(x_{gen} | x_{rec}) \, dx_{rec}$$



$$p(x_{rec}) = \int p(x_{gen}) p(x_{rec} | x_{gen}) \, dx_{gen}$$

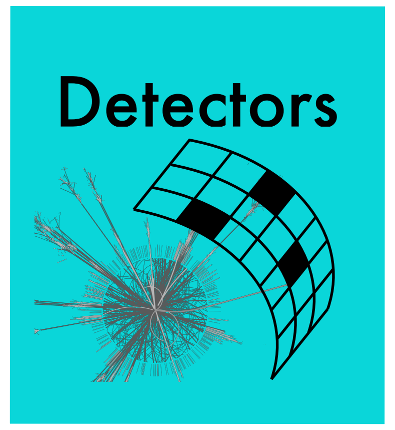
$$p(x_{gen} | x_{rec})$$

Unfolding probability

Generative unfolding

Transfer probability ← **Encoded implicitly in detector simulation**

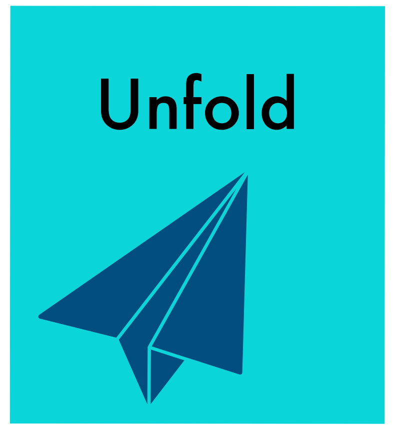
$$p(x_{rec}|x_{gen})$$



$$p(x_{gen}) = \int p(x_{rec})p(x_{gen}|x_{rec})\, dx_{rec}$$

x_{gen}

x_{rec}

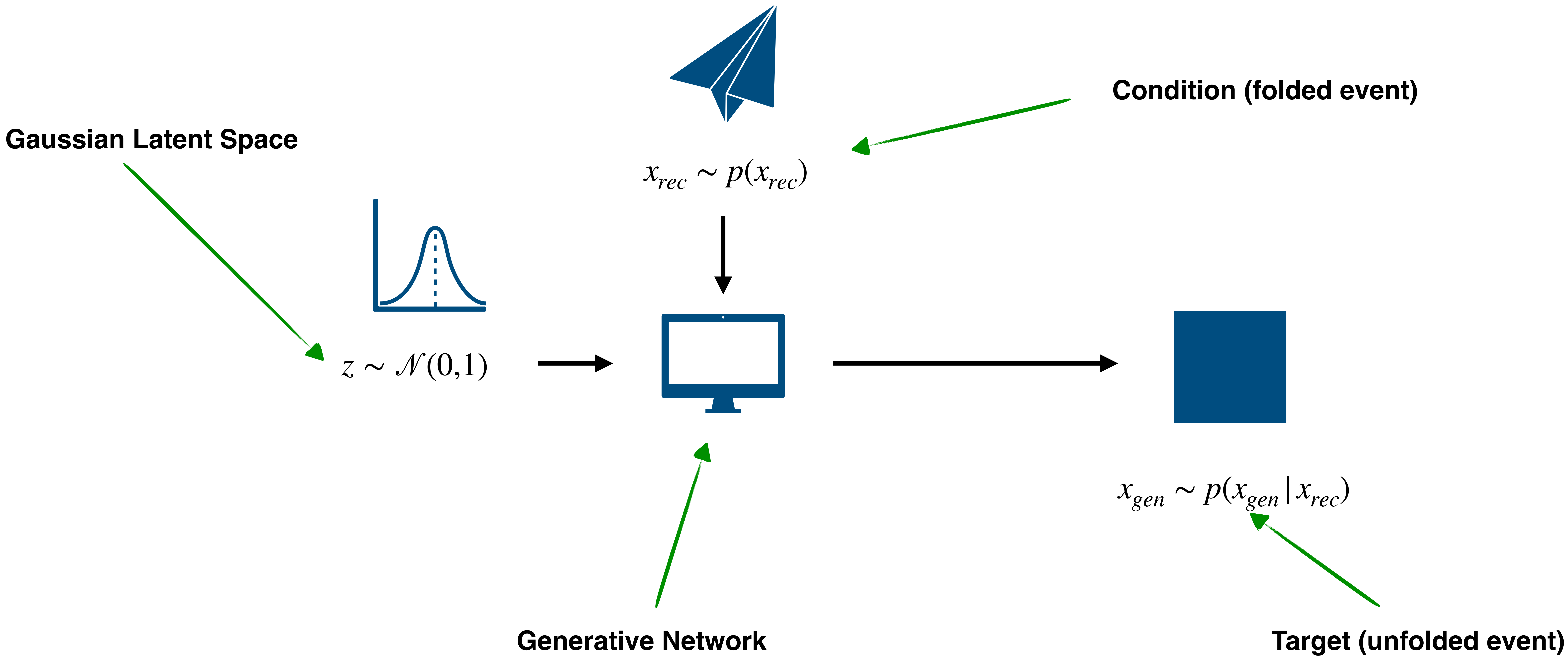


$$p(x_{rec}) = \int p(x_{gen})p(x_{rec}|x_{gen})\, dx_{gen}$$

$$p(x_{gen}|x_{rec})$$

Unfolding probability ← **Encoded in neural network trained on simulation**

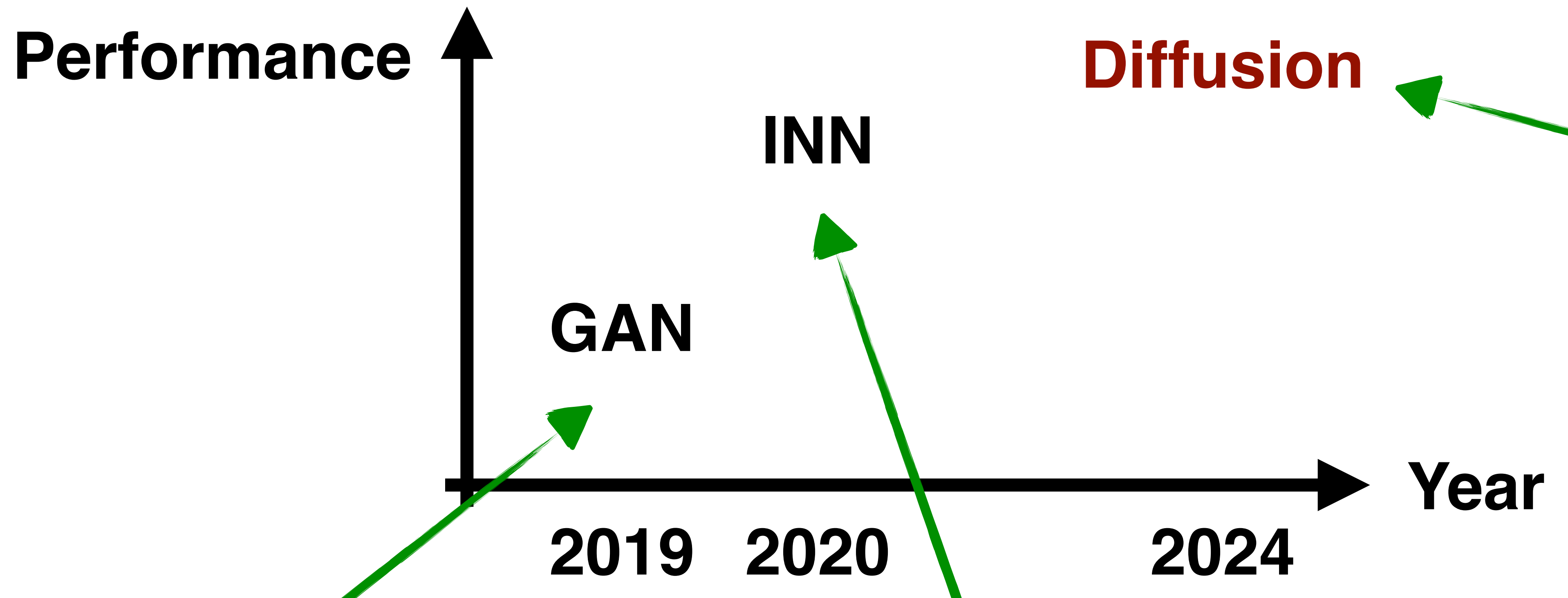
Conditional generative networks



Slide Credit: Sofia Palacios Schweitzer

Conditional generative networks

Which generative Network?



Bellagente et al.
arXiv:1912.00477

Bellagente et al.
arXiv:2006.06685

CFM
Huetsch et al.
arXiv:2404.18807

VLD
Shmakov et al.
arXiv: 2305.10399
arXiv: 2404.14332

DDPM
Pazos et al.
arXiv: 2406.01507

Talks on thursday!

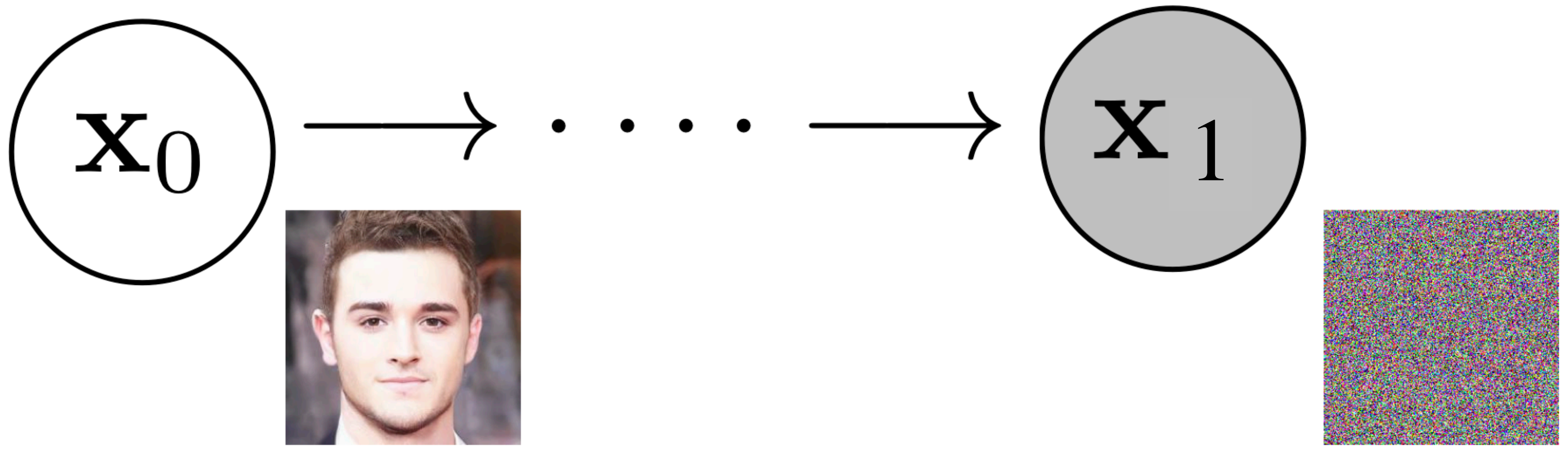
Flow Matching (Lipman et al. 2210.02747)

Phase Space

$x_0 \sim p_0(x_0)$

Latent Space

$x_1 \sim p_1(x_1)(= \mathcal{N}(0,1))$



Continuous time evolution **t**

Evolution governed by $v \equiv \dfrac{dx}{dt}$

Slide Credit: Sofia Palacios Schweitzer

Figure from J.Ho et al.: arXiv:2006.11239

Flow Matching (Lipman et al. 2210.02747)

Phase Space
$t = 0$

Individual Samples
$x_0 = x_{gen} \sim p_0(x_0)$

Density:
$p_0(x) = p(x_{gen})$

$$\frac{dx_t}{dt} = v_\theta(x_t\,,\,t)$$

$$\frac{\partial p(x,t)}{\partial t} + \nabla_x\left[p(x,t)v_\theta(x,t)\right] = 0$$

Latent Space
$t = 1$

Individual Samples
$x_1 = \epsilon \sim p_1(x_1)$

Density:
$p_1(x) = \mathcal{N}(0,1)$

Flow Matching (Lipman et al. 2210.02747)

$x_{rec} \sim p(x_{rec})$

Phase Space

$t = 0$

Individual Samples

$x_0 = x_{gen} \sim p_0(x_0)$

Density:

$p_0(x) = p(x_{gen} | x_{rec})$

$$\frac{dx_t}{dt} = v_\theta(x_t\,,\, t \,|\, x_{rec})$$

$$\frac{\partial p(x, t \,|\, x_{rec})}{\partial t} + \nabla_x \left[p(x, t \,|\, x_{rec}) v_\theta(x, t \,|\, x_{rec}) \right] = 0$$

Latent Space

$t = 1$

Individual Samples

$x_1 = \epsilon \sim p_1(x_1)$

Density:

$p_1(x) = \mathcal{N}(0,1)$

Z + jet results

$pp \rightarrow Z+$ jets events following Andreassen et al. arXiv: 1911.09107

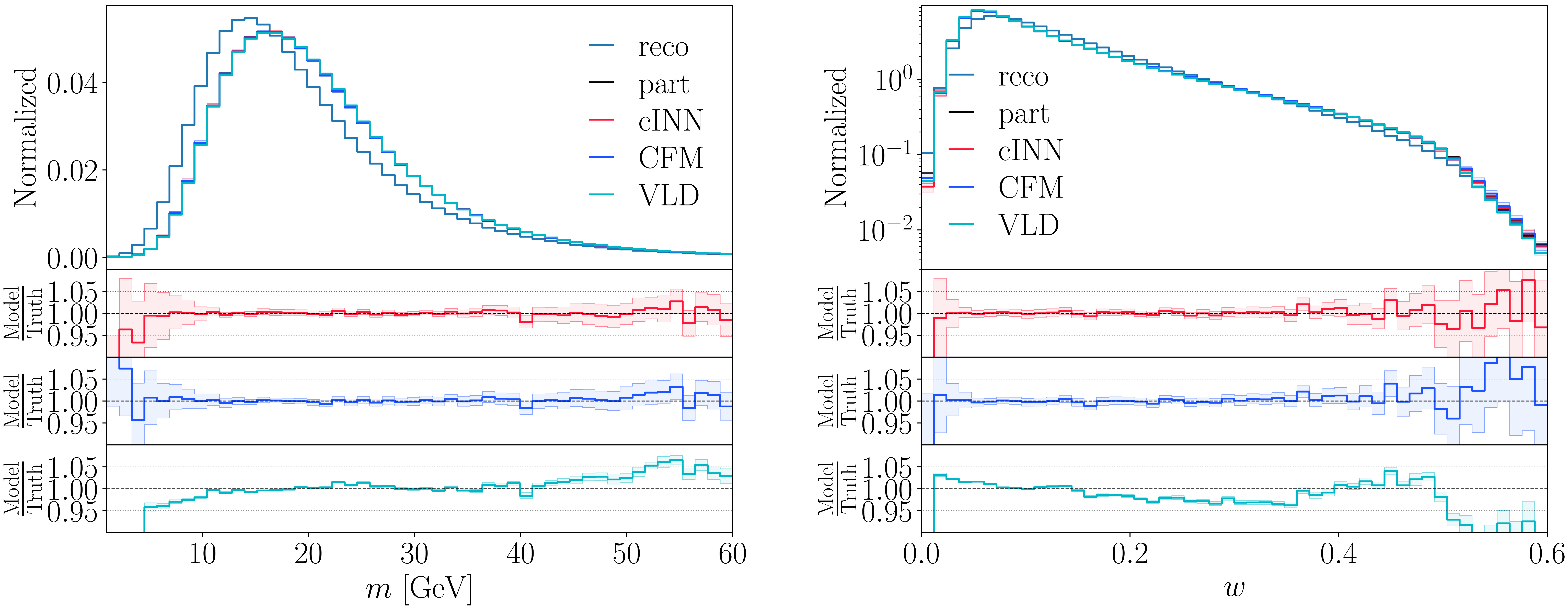
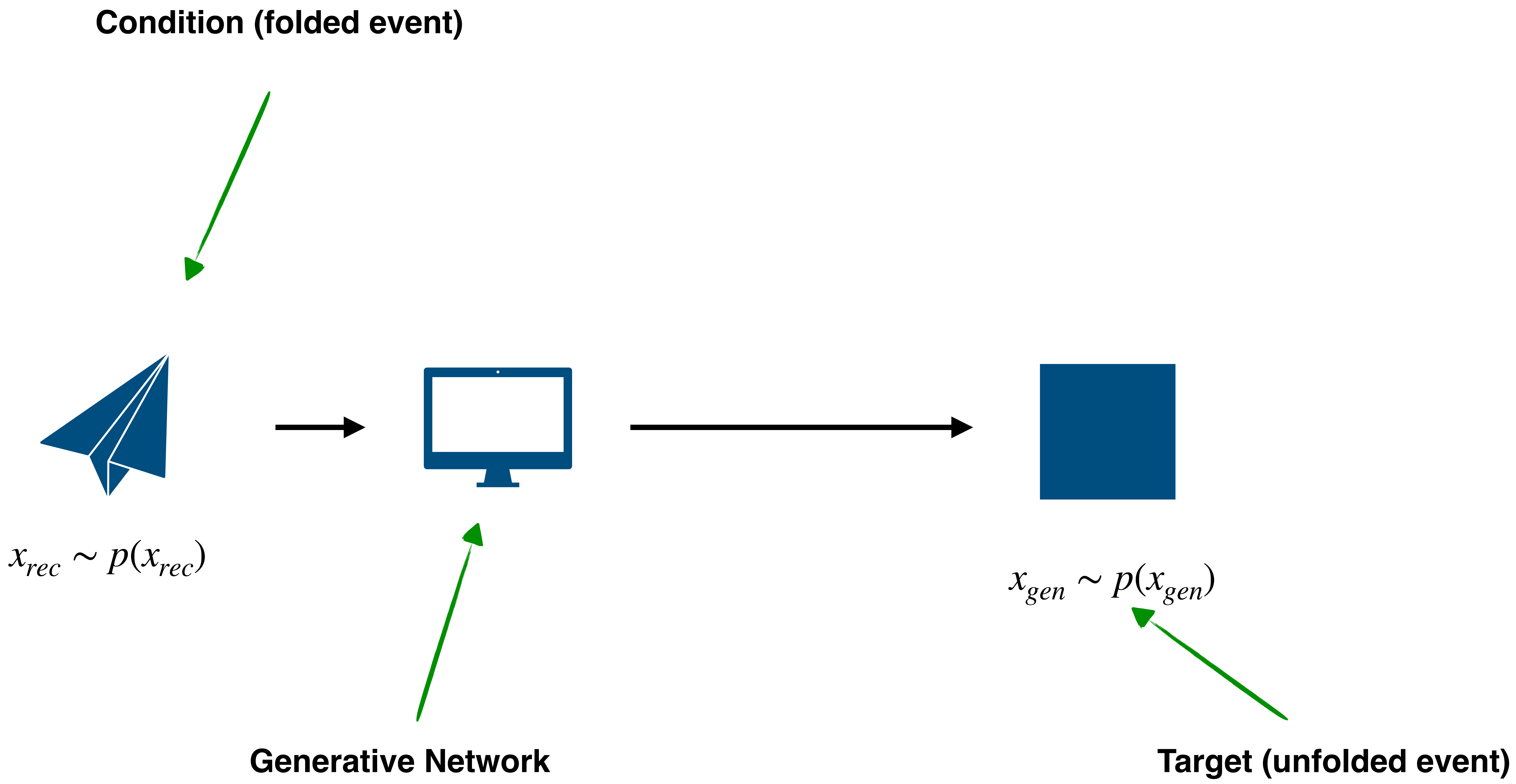
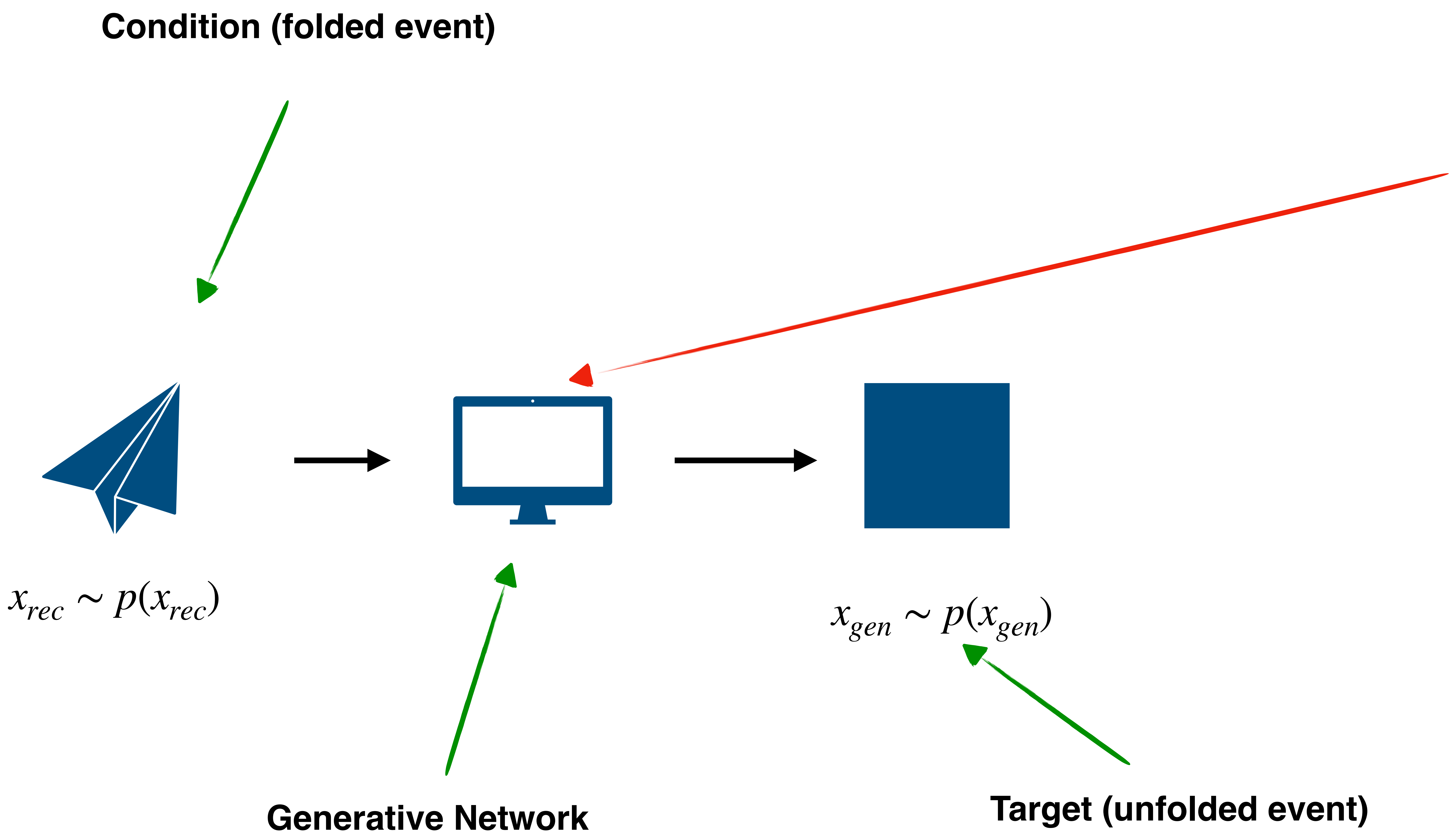


Figure from Huetsch et. al: arXiv:2404.18807

Distribution mapping



Distribution mapping



Schroedinger Bridge

Diefenbacher et al.
arXiv:2308.12351

Direct Diffusion

Butter et al.
arXiv:2311.17175
Huetsch et al.
arXiv:2404.18807

Z + jet results

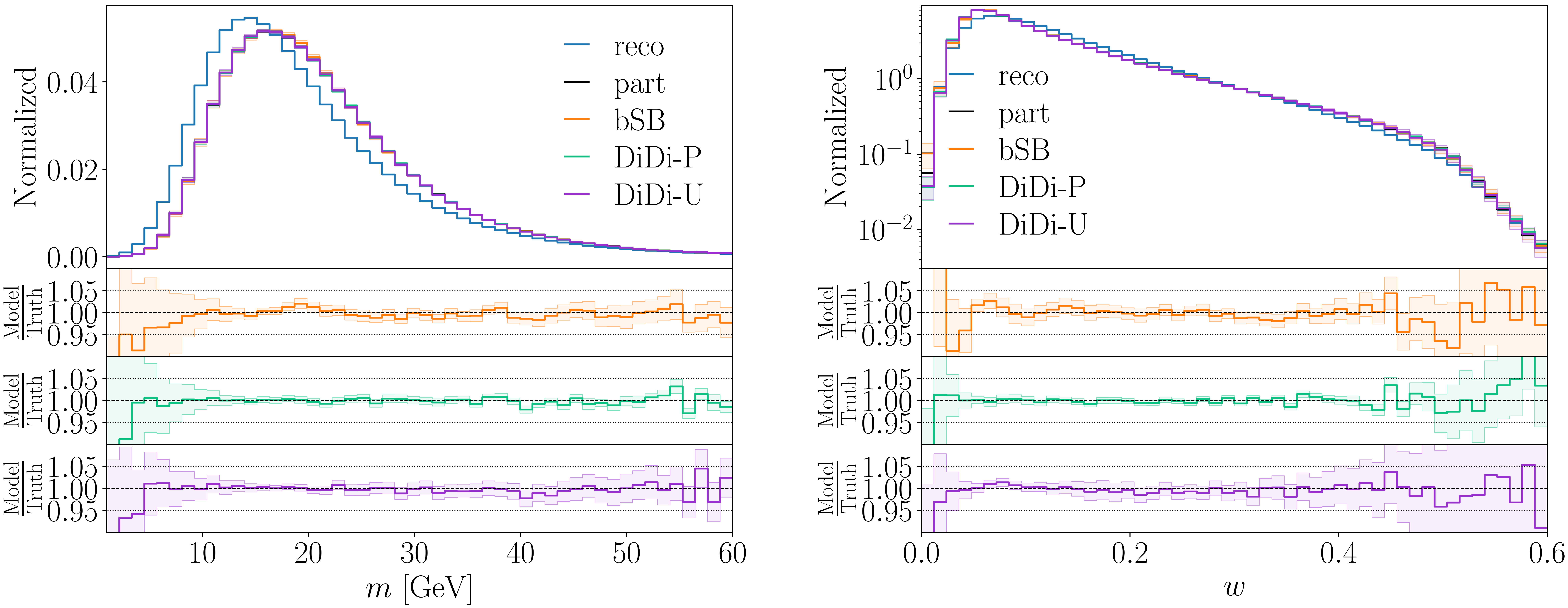


Figure from Huetsch et. al: arXiv:2404.18807

Z + jet migration

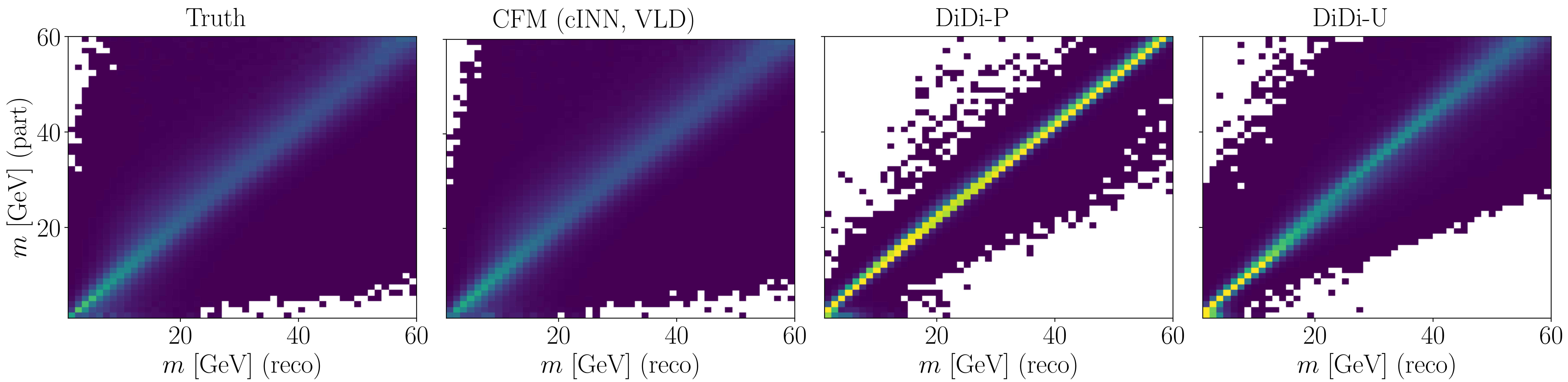


Figure from Huetsch et. al: arXiv:2404.18807

Parton-level unfolding — $t\bar{t}$ decay

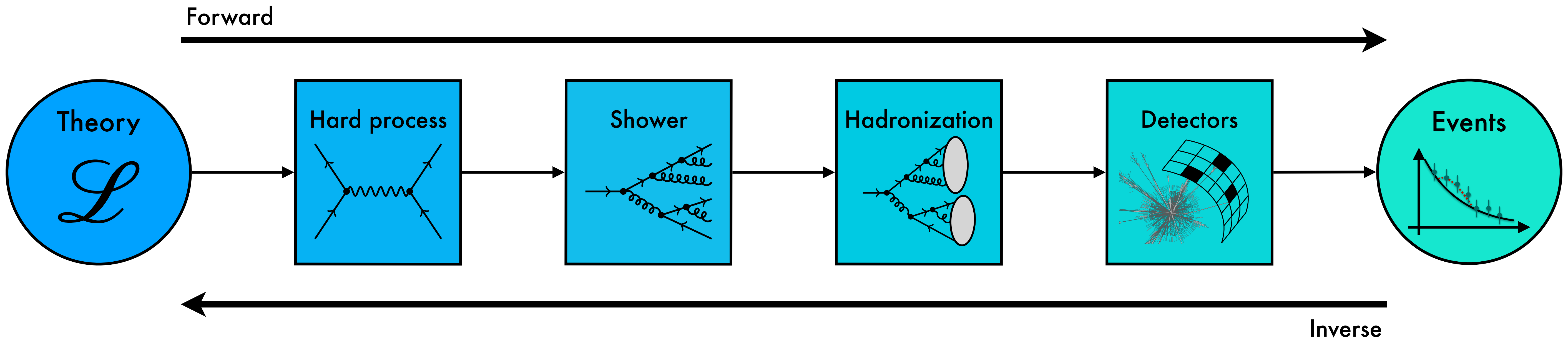
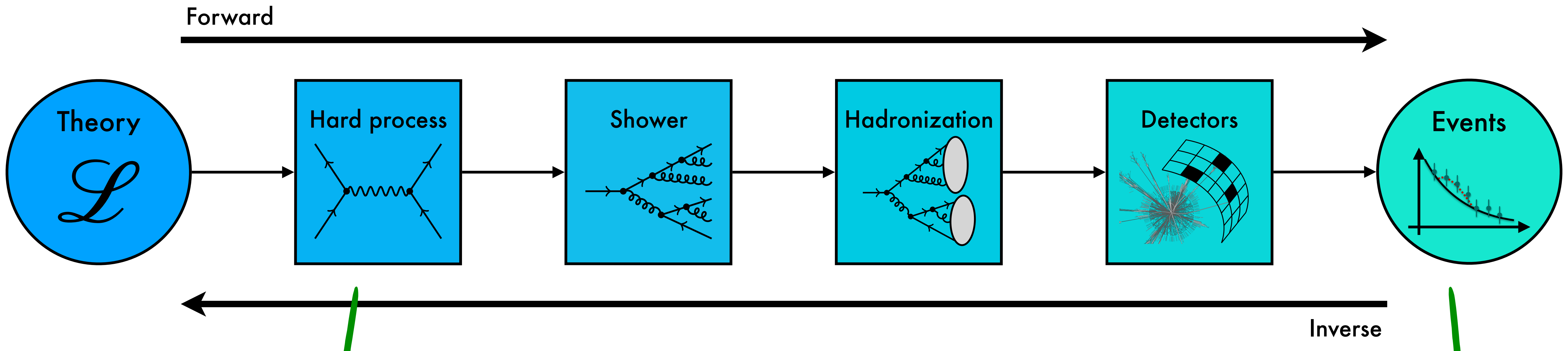
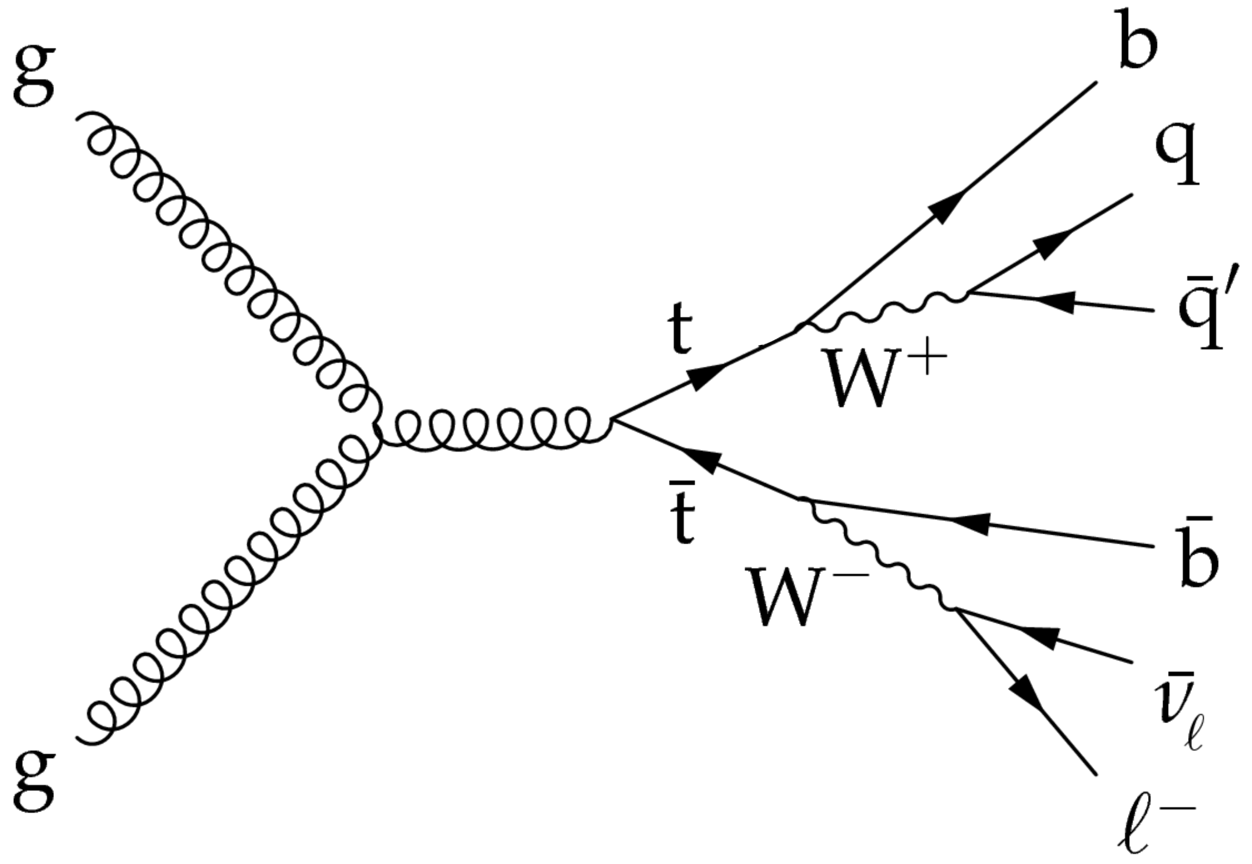


Figure top from A. Butter et al.: arXiv:2203.07460, R. Winterhalder

Parton-level unfolding — $t\bar{t}$ decay



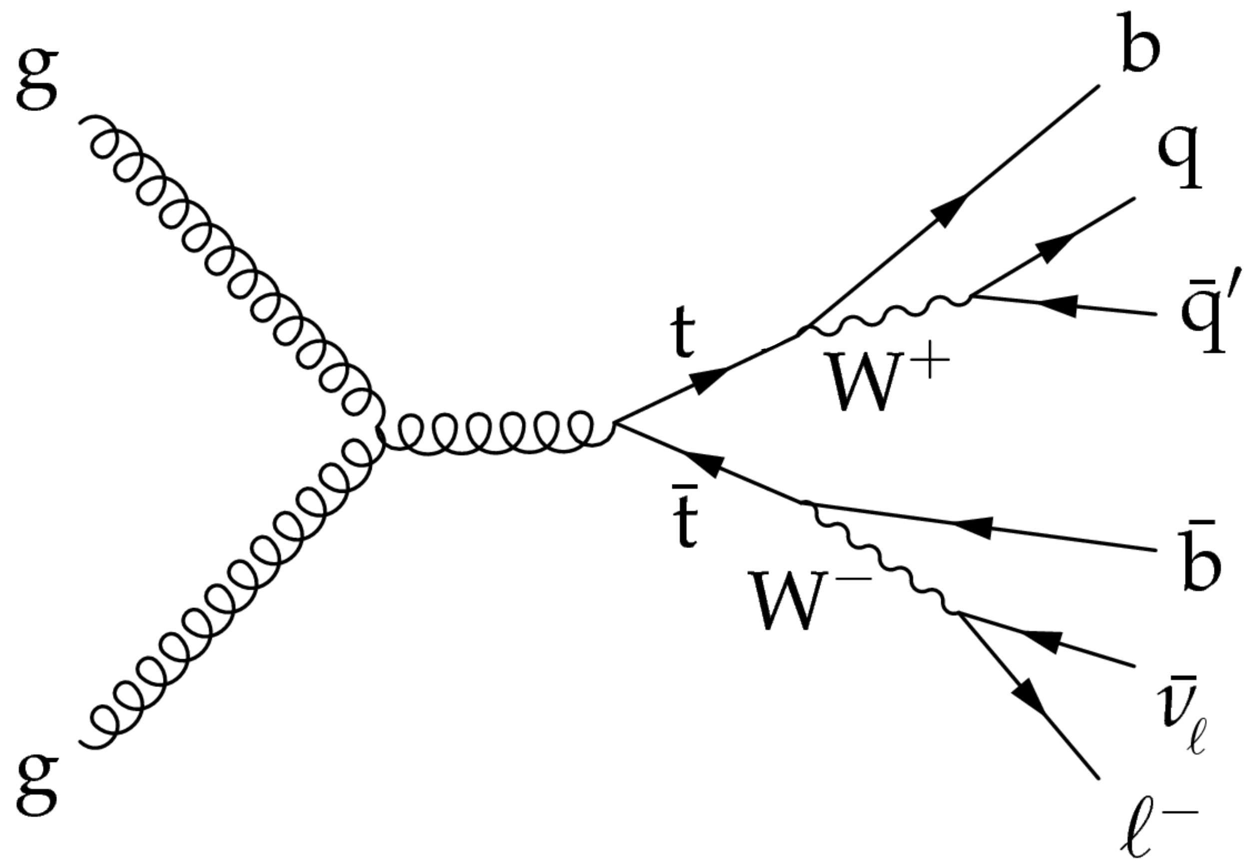
$$q\bar{q}/gg \to t\bar{t} \to (b\ell^-\bar{\nu}_\ell)\,(\bar{b}qq) \longrightarrow \ell^-\bar{\nu}_\ell\{j\}$$



Following
Shmakov et al.
arXiv: 2305.10399

Figure top from A. Butter et al.: arXiv:2203.07460, R. Winterhalder

Parton-level unfolding — $t\bar{t}$ decay



→ $\ell^+\nu_\ell\{j\}$

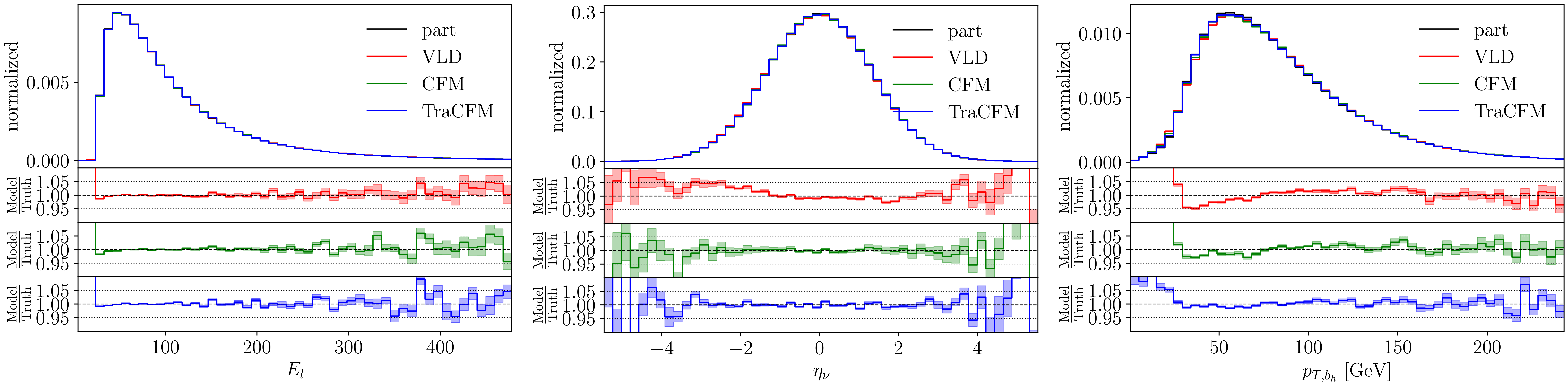
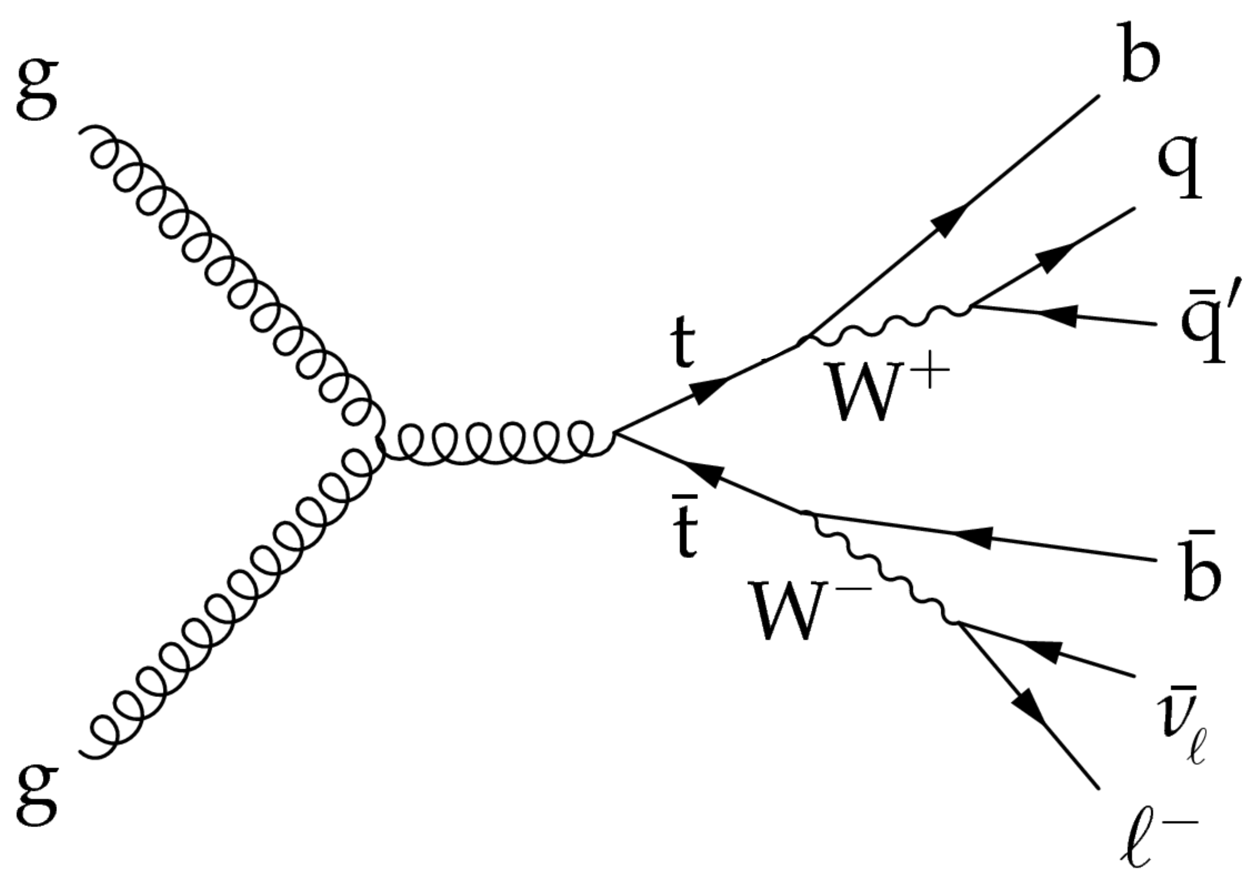


Figure from Huetsch et. al: arXiv:2404.18807

Parton-level unfolding — $t\bar{t}$ decay



$\ell^+\nu_\ell\{j\}$

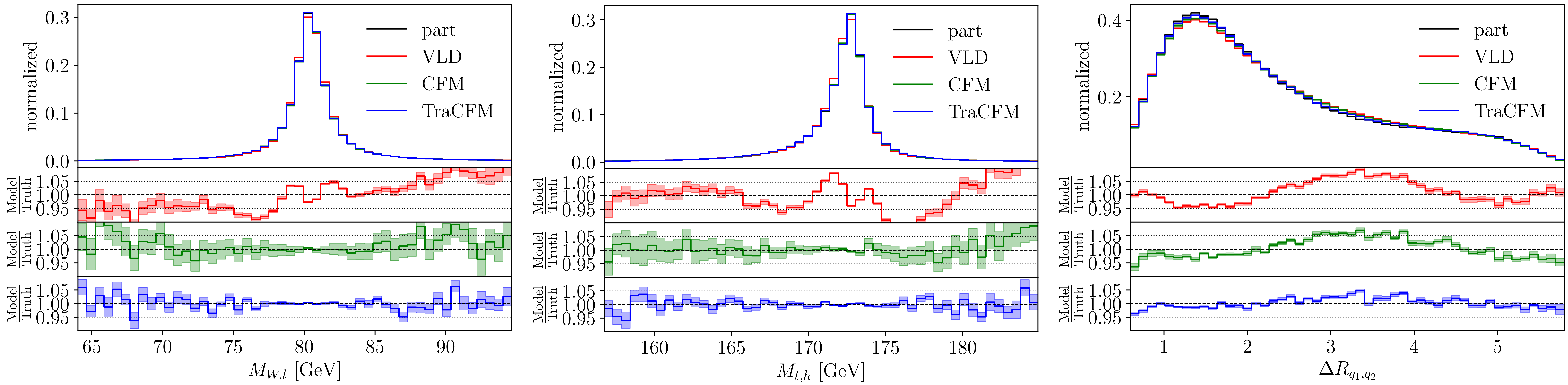
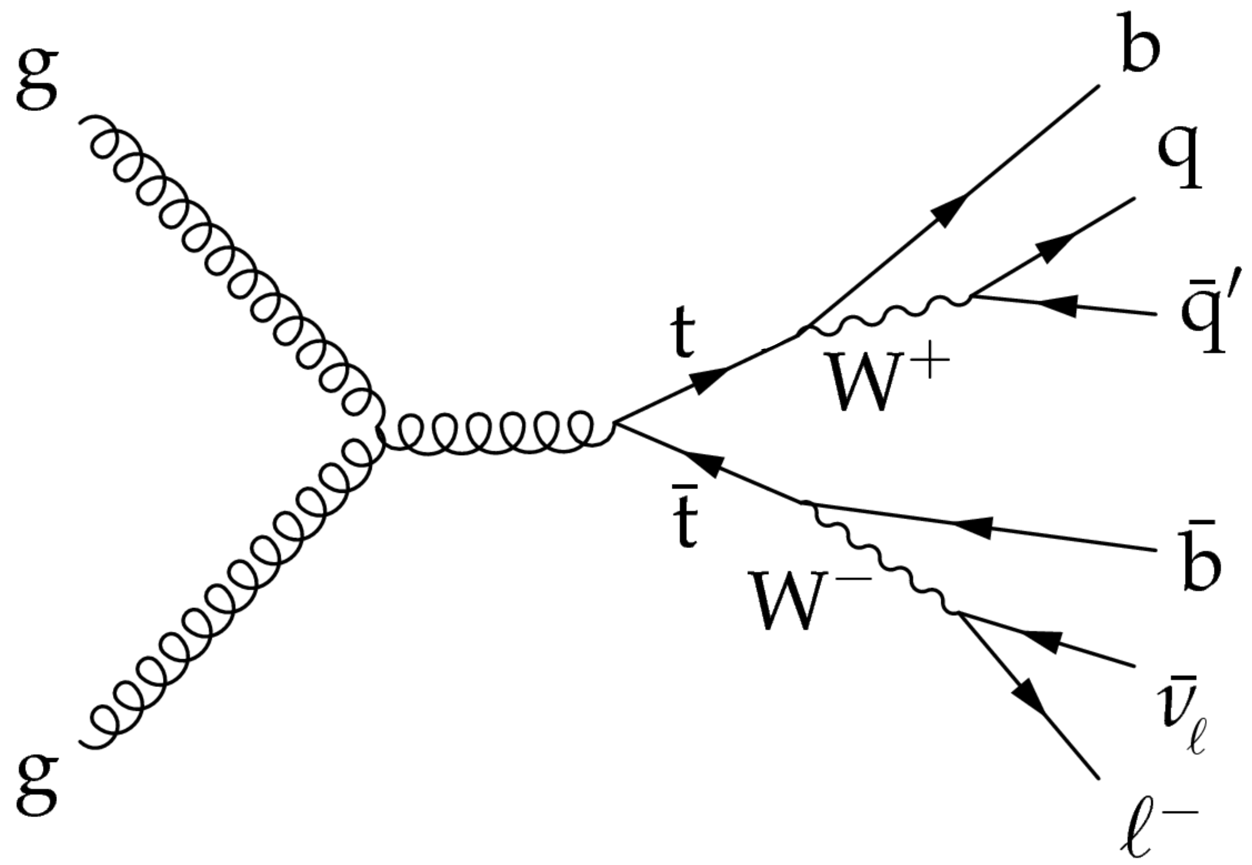


Figure from Huetsch et. al: arXiv:2404.18807

Parton-level unfolding — $t\bar{t}$ decay



$\longrightarrow \quad \ell^+ \nu_\ell \{j\}$

Train a classifier classifier between $p_{gen}(x)$ and $p_{unfold}(x)$

It learns the likelihood ratio

$$w(x) = \frac{p_{gen}(x)}{p_{unfold}(x)}$$

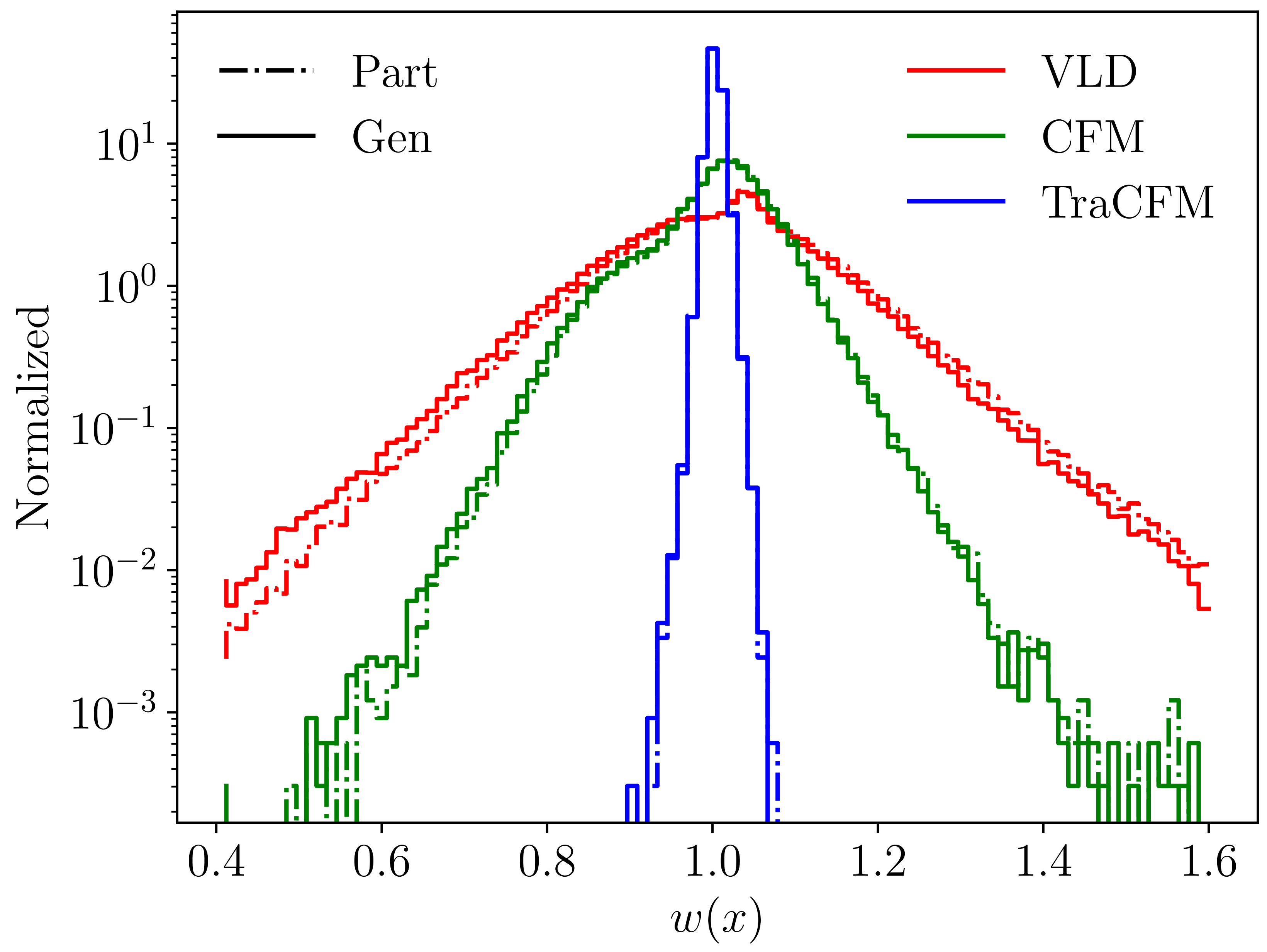


Figure from Huetsch et. al: arXiv:2404.18807

What about model dependence?

Prior

$$p(x_{gen}|x_{rec}) = \frac{p(x_{rec}|x_{gen})p(x_{gen})}{p(x_{rec})}$$

What about model dependence?

This problem is common to a long list of unfolding methods, with and without ML

Solution: Follow an iterative approach where we update our prior after each iteration

The same is done in Iterative Bayesian Unfolding, RooUnfold

Prior

$$p(x_{gen}|x_{rec}) = \frac{p(x_{rec}|x_{gen})p(x_{gen})}{p(x_{rec})}$$

$$p_{unfold}(x_{gen}) = \int p_{data}(x_{rec})p(x_{gen}|x_{rec})\, dx_{rec}$$

Use as new prior and start over

Iterative generative unfolding

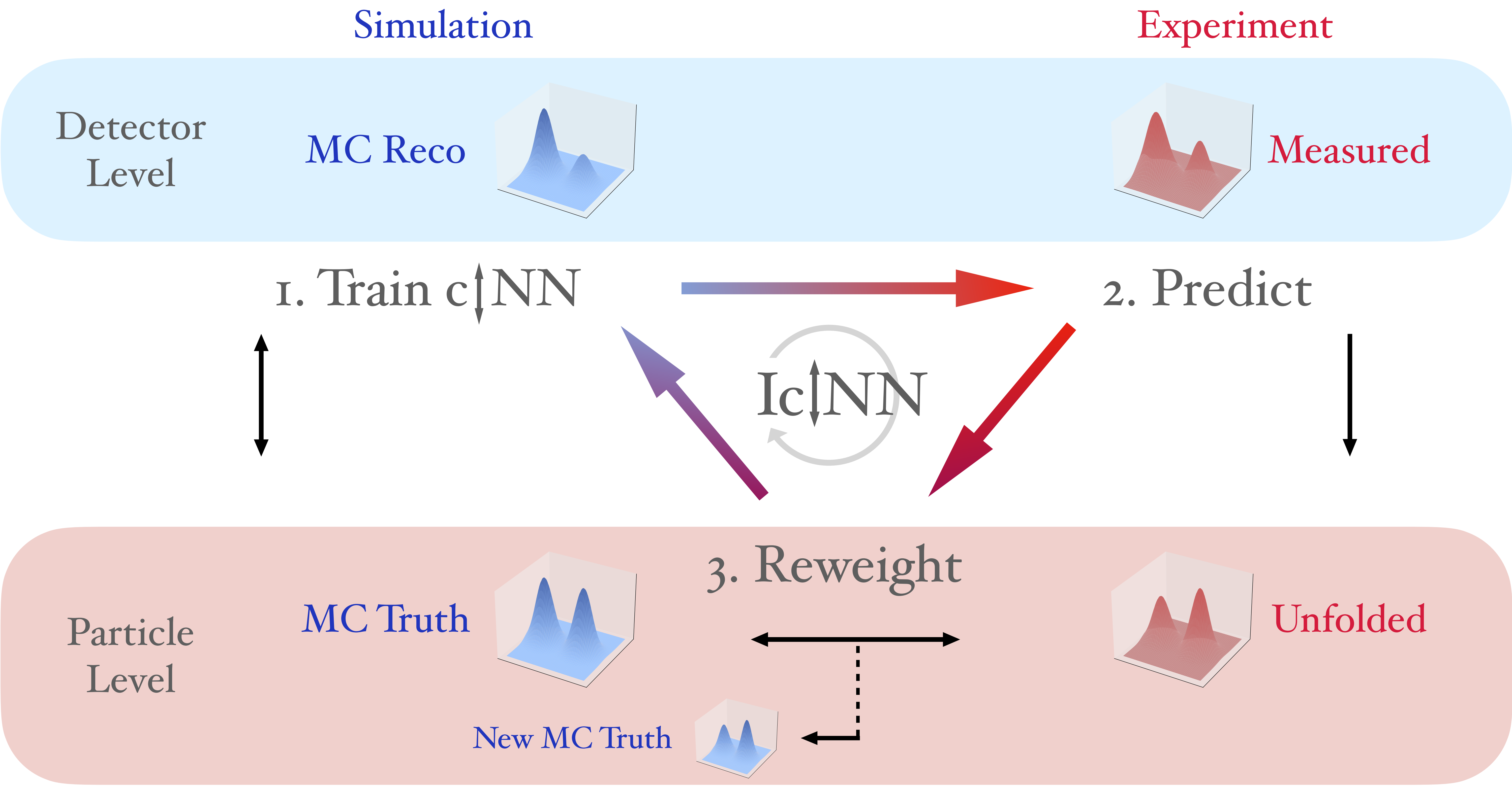
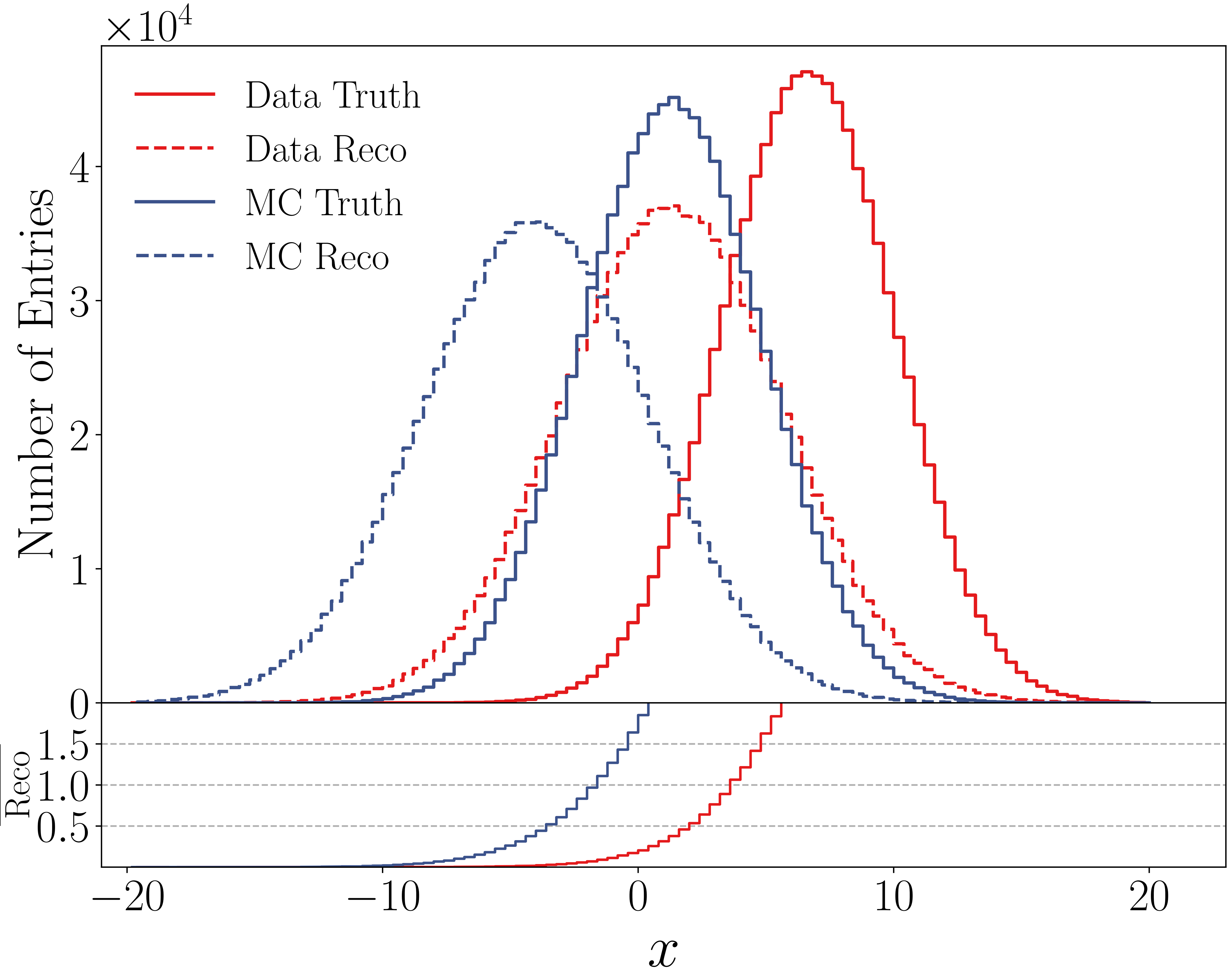
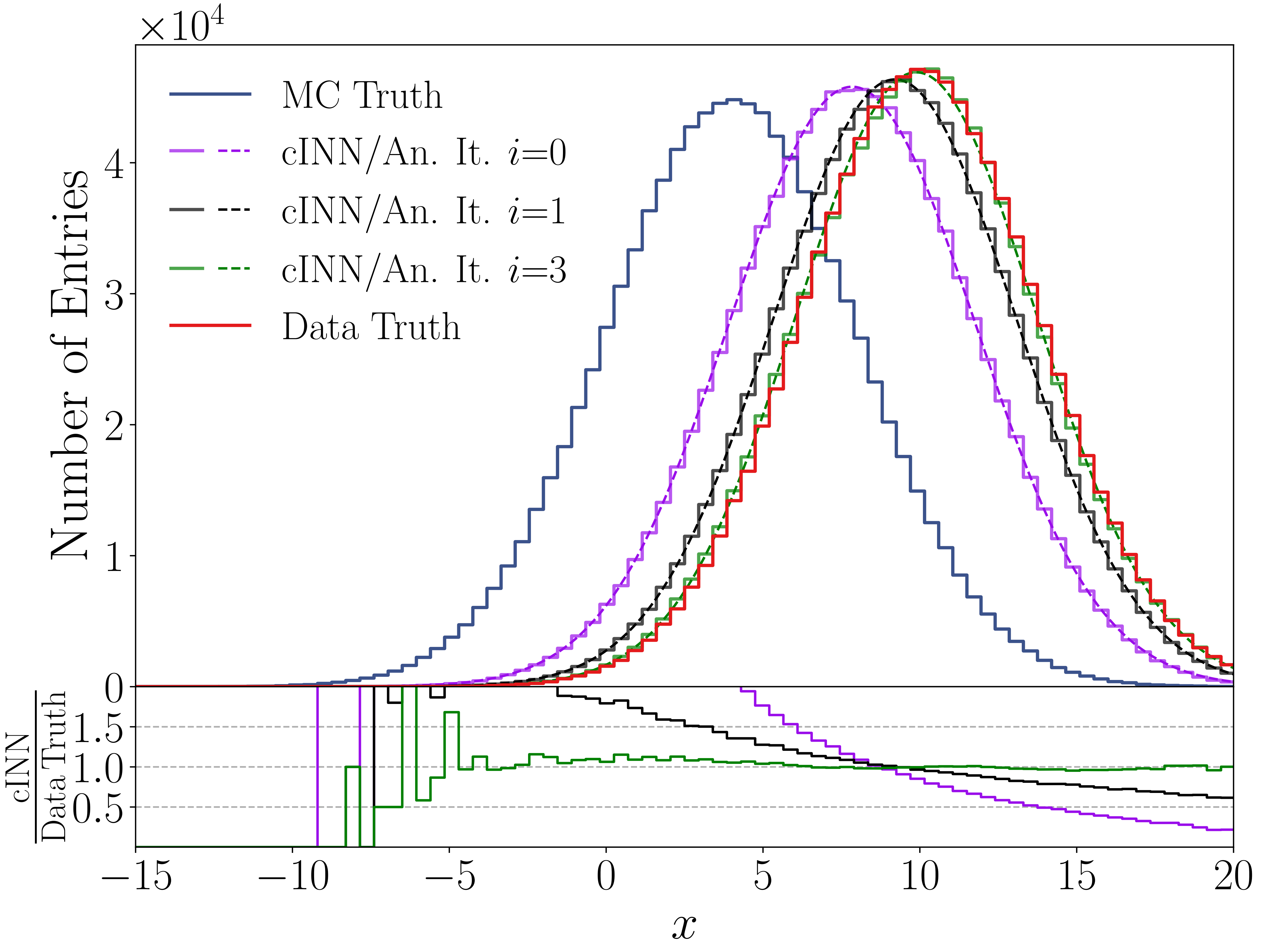


Figure from Backes et al.: arXiv:2212.08674

Iterative generative unfolding



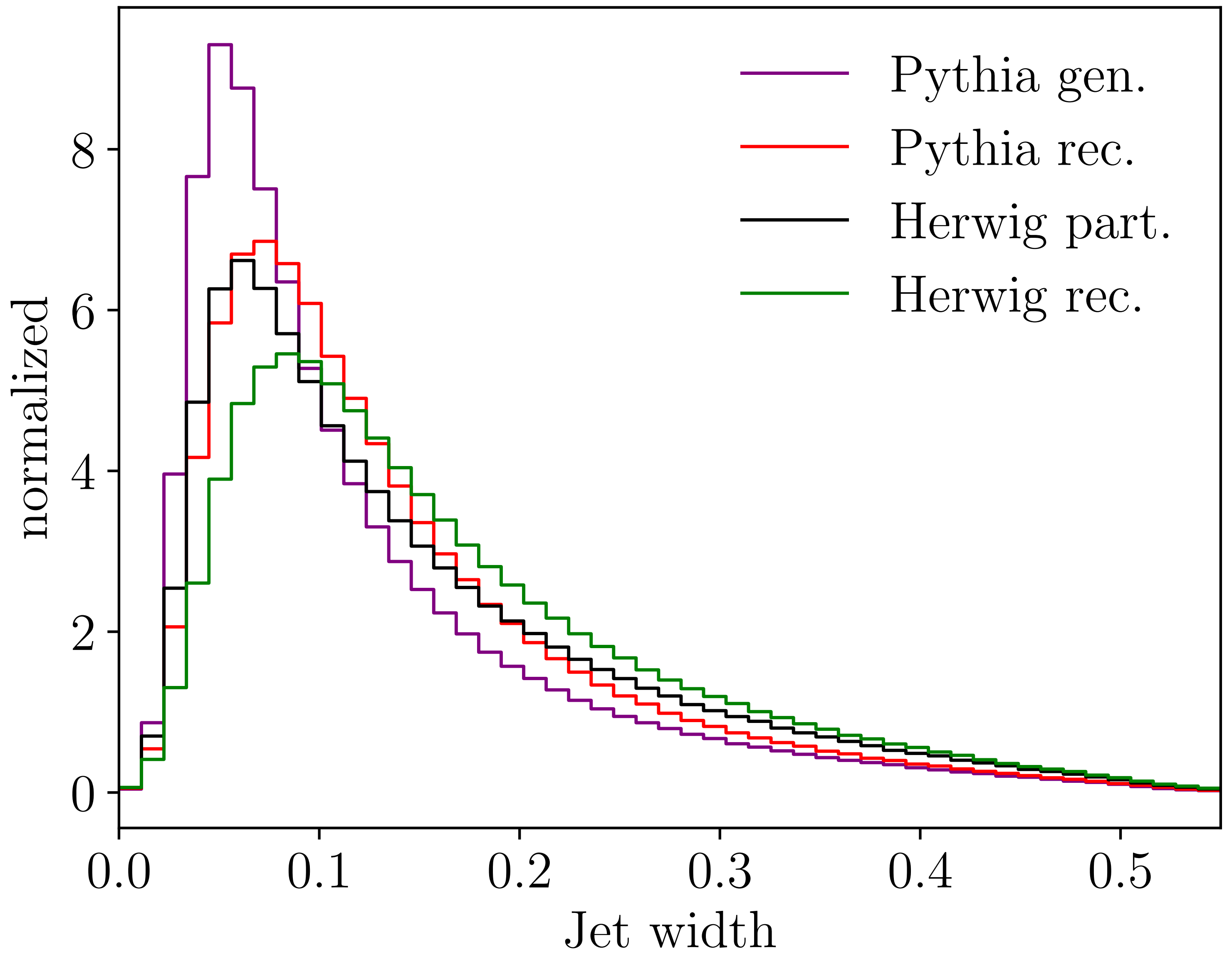


Figures from Backes et al.: arXiv:2212.08674

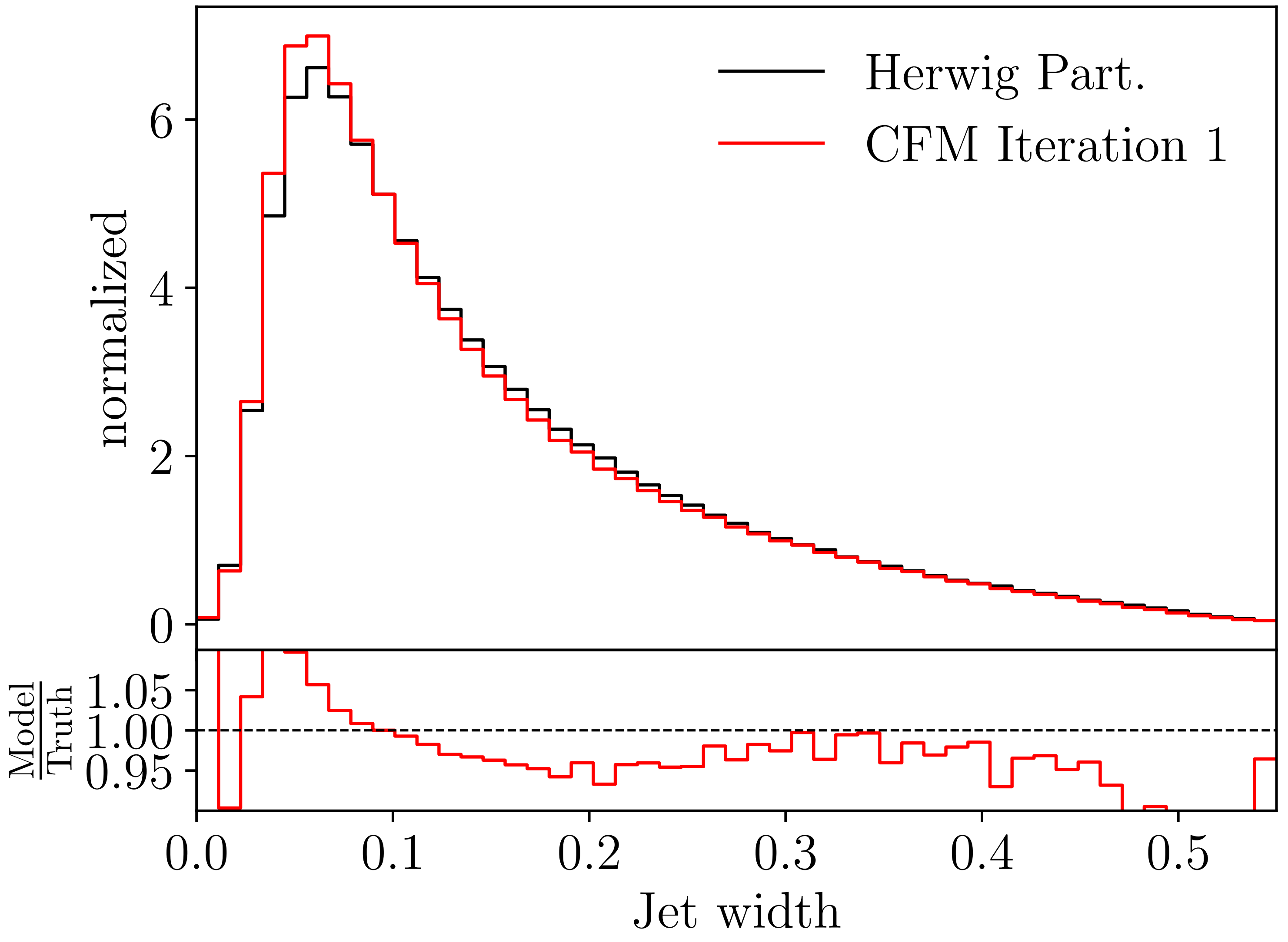
Z+jets: Pythia vs Herwig simulation

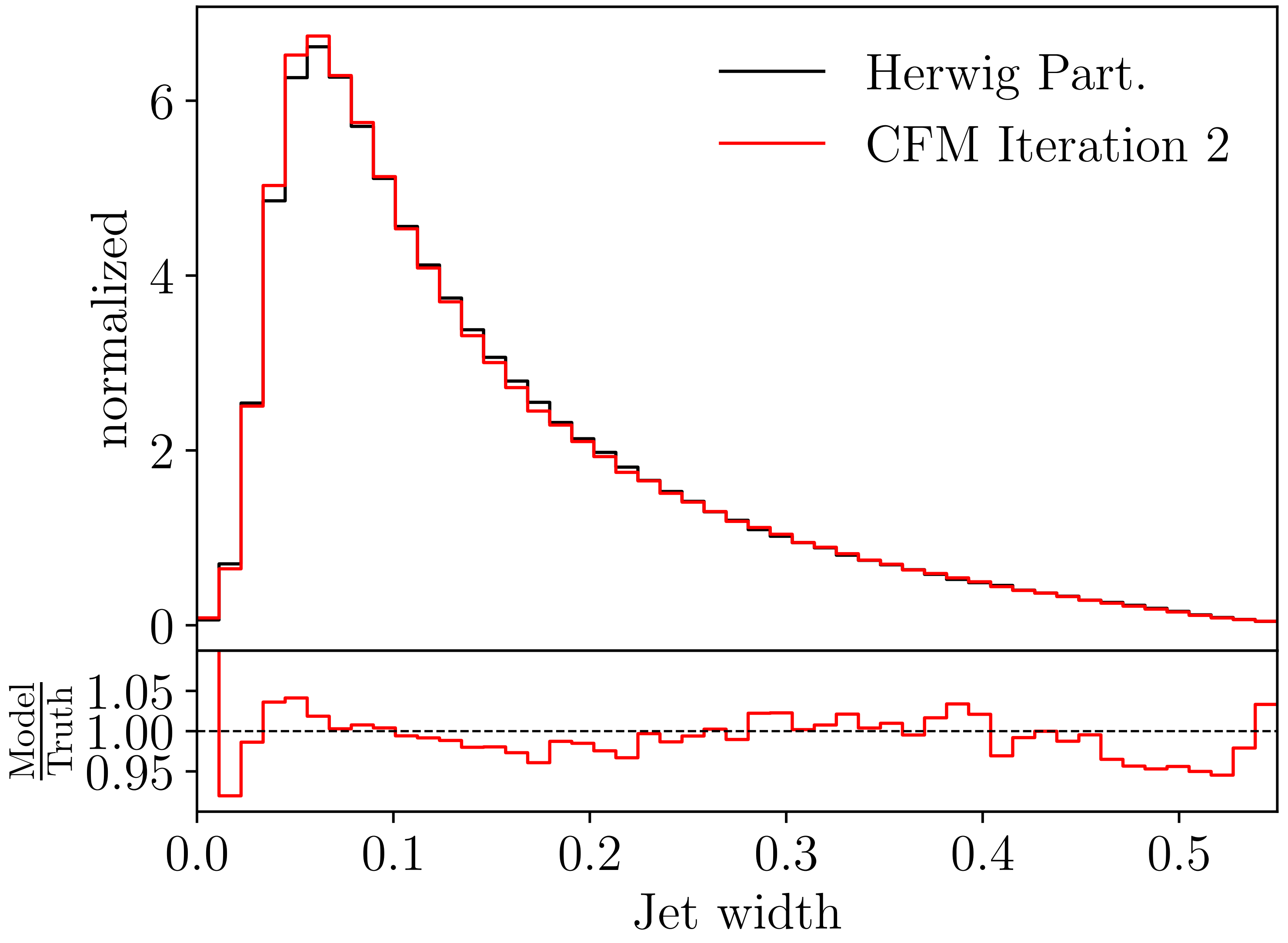
Use Pythia simulation as MC

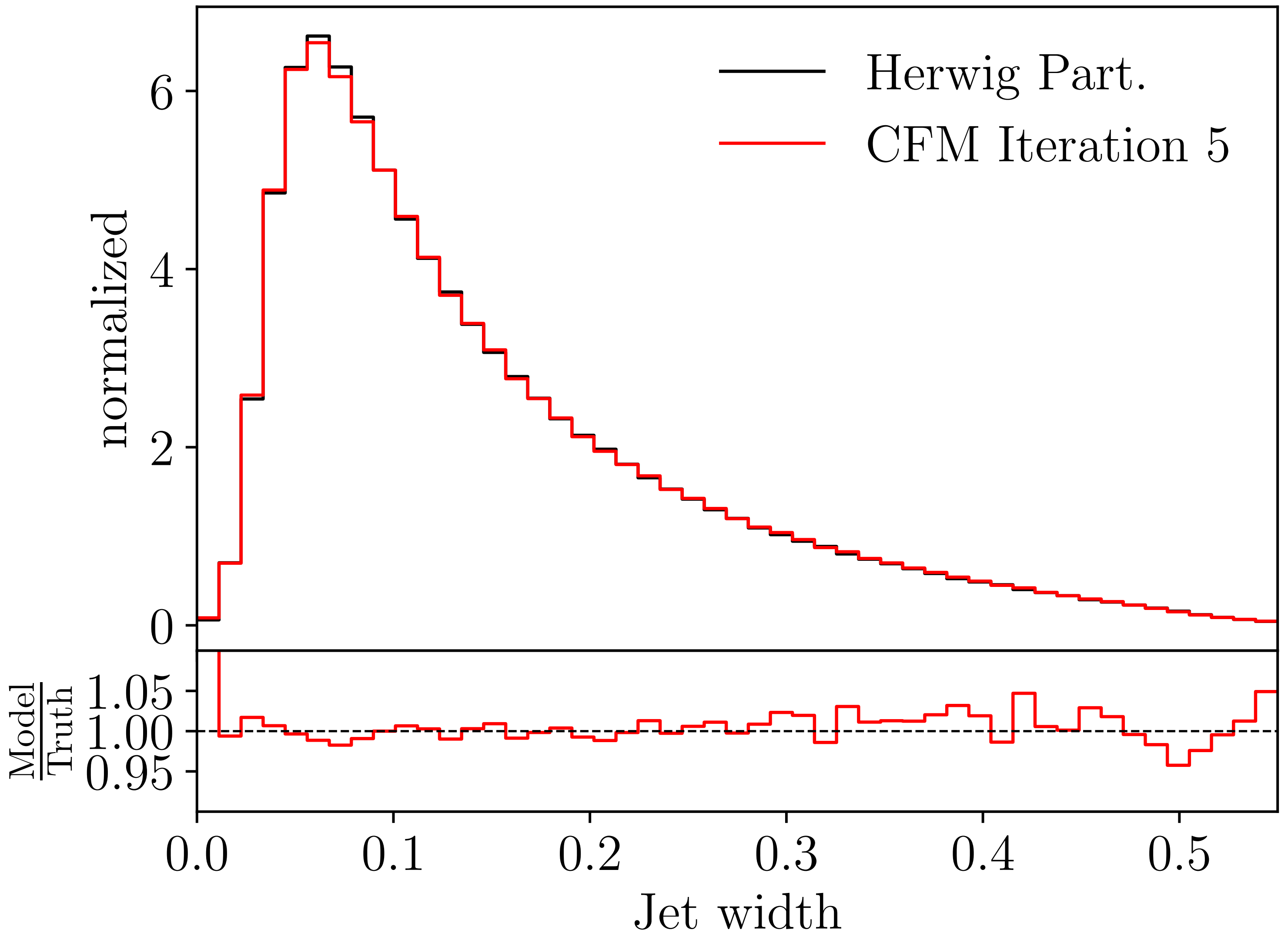
Use Herwig simulation as Data



Following
Andreassen et al.
arXiv: 1911.09107



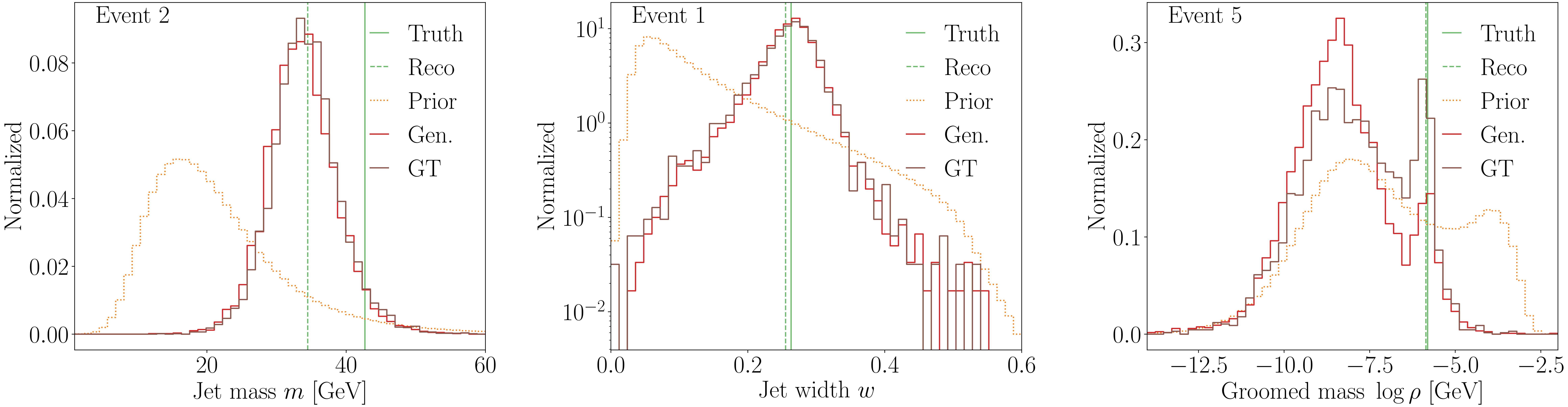




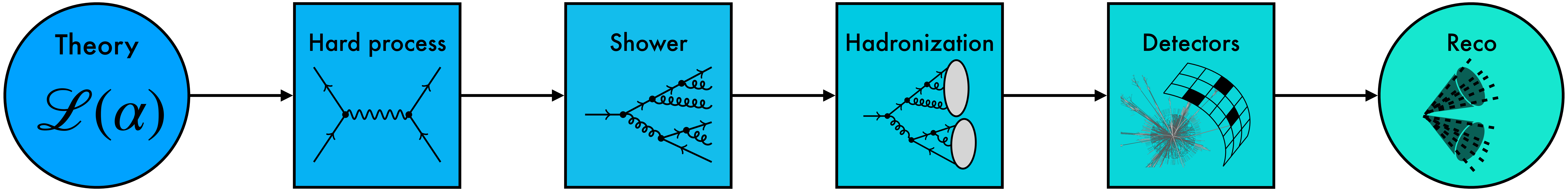
Single-event posteriors

Our network learned the posterior distribution $p(x_{gen} \mid x_{rec})$

We can sample from this for a single reco event to map out the posterior



Making use of single-event posteriors



$$\int dx_{hard} \quad p(x_{hard}\,|\,\alpha) \quad \underbrace{p(x_{reco}\,|\,x_{hard})} \quad = \; p(x_{reco}\,|\,\alpha)$$

We want to explicitly calculate reco-level likelihoods for our observed data given some theory hypothesis $\mathscr{L}(\alpha)$

Let us say we somehow now the transfer probability $p(x_{reco}\,|\,x_{hard})$ and can efficiently calculate it

How can we solve the difficult high-dimensional integral precisely and efficiently?

Figure adapted from A. Butter et al.: arXiv:2203.07460

Making use of single-event posteriors

Challenging

$$\int dx_{hard}\ p(x_{hard}|\alpha)\ p(x_{reco}|x_{hard}) \ = \ p(x_{reco}|\alpha)$$

$$= \left\langle \frac{1}{q(x_{hard}} p(x_{hard}|\alpha)\ p(x_{reco}|x_{hard})\ ) \right\rangle_{x_{hard} \sim q}$$

Integral becomes trivial if : $q(x_{hard}|x_{reco}, \alpha) = p(x_{hard}|x_{reco}, \alpha)$

This is exactly our unfolding network !

For details see Butter at al. 2210.00019, Heimel et al. 2310.07752

Conclusion

Generative Unfolding works !

Conditional Networks and Distribution Mapping both achieve percent-level precision

Conditional Networks learn the true migration encoded in the detector simulation. Distribution Mapping Networks learn a simple optimal-transport based mapping

Conditional Generative Unfolding enables probabilistic inversion of simulation chain

Prior dependence is a solvable problem

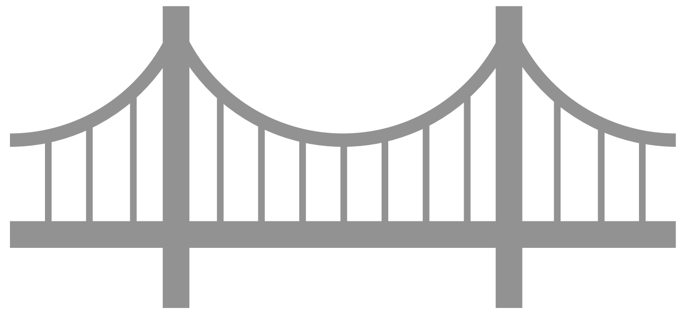
Conditional Generative Models map out the single-event posterior distributions

2404.18807

SciPost Physics Submission

The Landscape of Unfolding with Machine Learning

Nathan Huetsch[1], Javier Mariño Villadamigo[1], Alexander Shmakov[2], Sascha Diefenbacher[3], Vinicius Mikuni[3], Theo Heimel[1], Michael Fenton[2], Kevin Greif[2], Benjamin Nachman[3,4], Daniel Whiteson[2], Anja Butter[1,5], and Tilman Plehn[1,6]



Further investigation of failure modes

Further investigation of uncertainties

Further investigation of background, cuts, efficiencies

Flow Matching (Lipman et al. 2210.02747)

Training

1. **Sample paired data from our simulation**

$$(x_0, c) = (x_{gen}, x_{rec}) \sim p(x_{gen}, x_{rec})$$

2. **Sample noise and a timestep**

$$x_1 = \epsilon \sim \mathcal{N}(0,1)\ ,\ t \sim \mathcal{U}([0,1])$$

3. **Calculate the trajectory**

$$x_t = (1-t)x_0 + tx_1$$

$$v_t = \frac{dx_t}{dt} = -x_0 + x_1$$

4. **Predict the velocity field**

$$\mathcal{L} = \left| v_\theta(x_t, t, c) - v_t \right|^2$$

Generation

1. **Sample a reco event from our measured data**

$$c = x_{rec} \sim p(x_{rec})$$

2. **Sample noise as initial condition**

$$x_1 = \epsilon \sim \mathcal{N}(0,1)$$

3. **Solve the ODE numerically**

$$x_0 = x_{gen} = x_1 + \int_1^0 v_\theta(x_t, t, c)\ dt$$