UNIVERSITÄT
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ZUKUNFT
SEIT 1386

ML4Jets 2024
04.11.2024

The Landscape of Unfolding with Machine Learning

Nathan Huetsch

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

Simulation chain — Forward

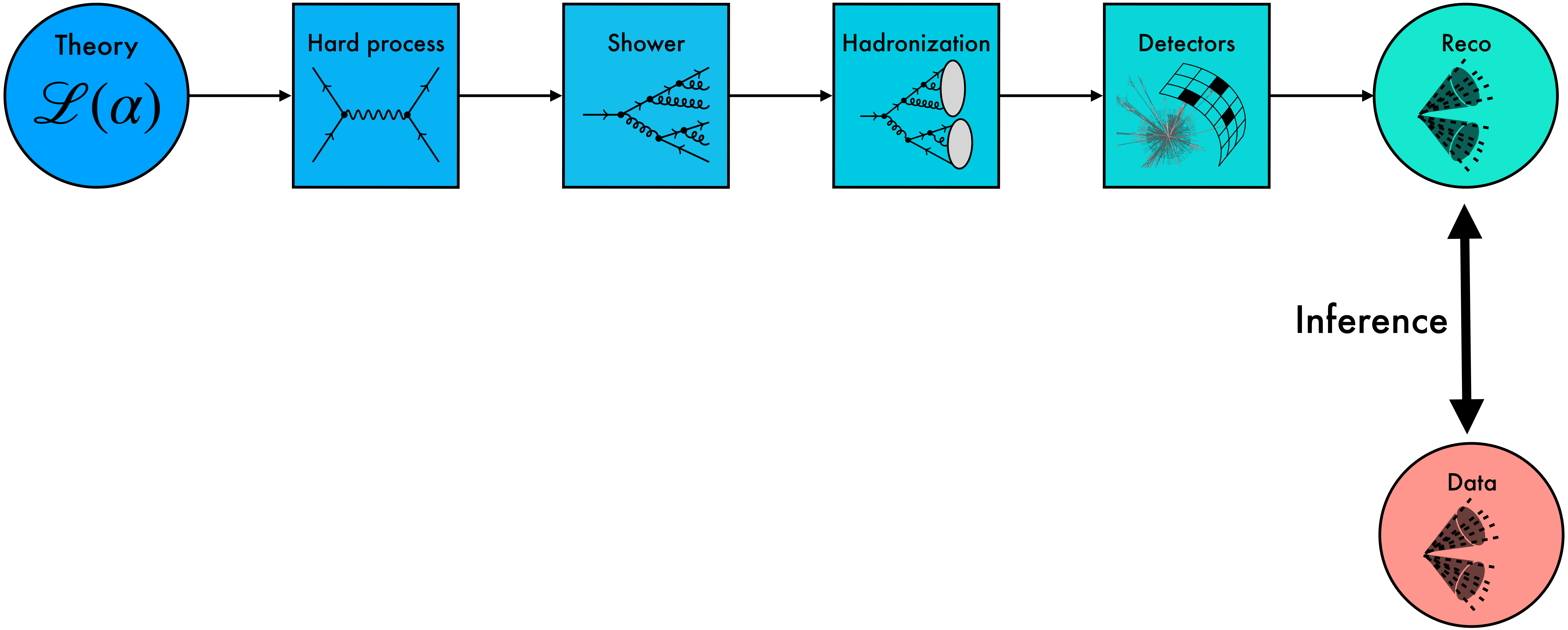


Figure adapted from R. Winterhalder

Simulation chain — Inversion

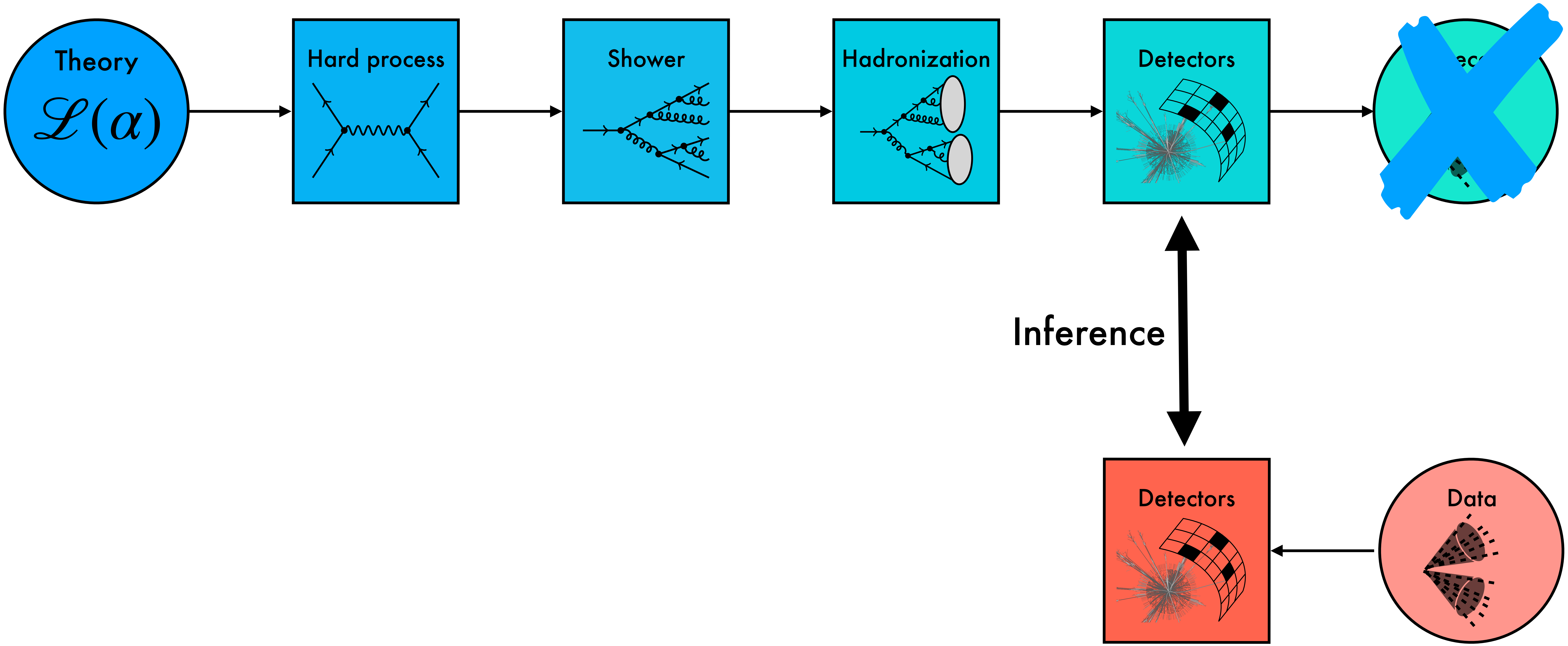


Figure adapted from R. Winterhalder

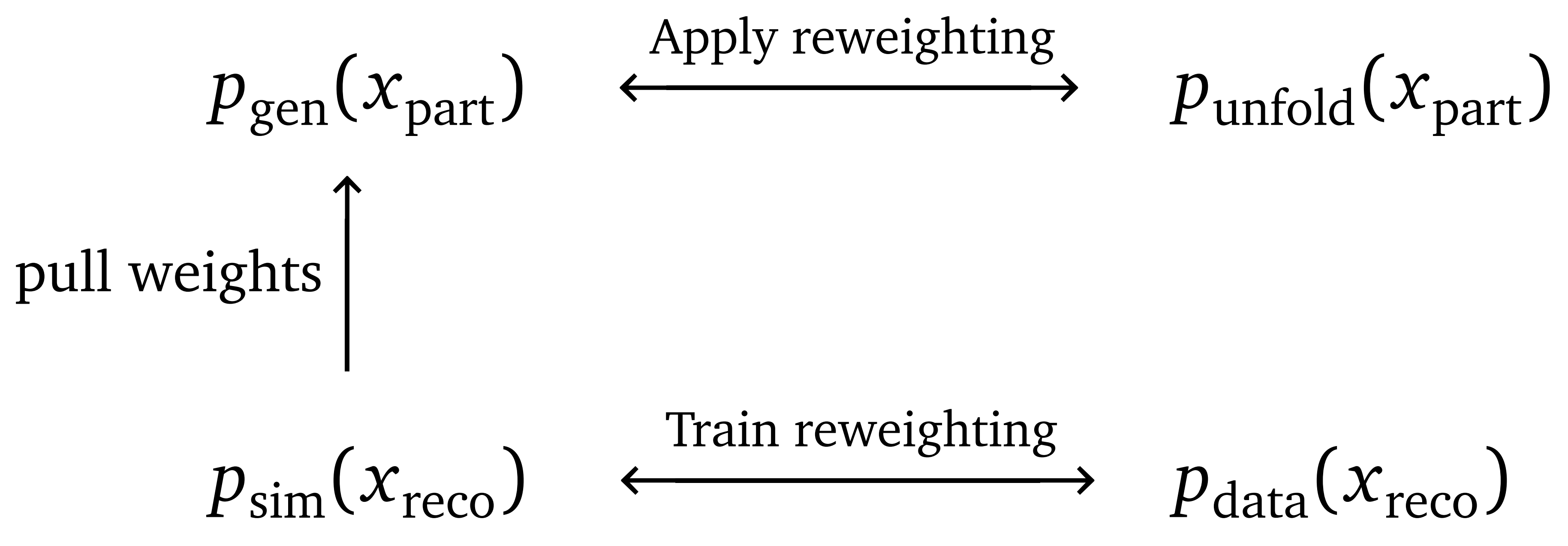
Unfolding

$$
\begin{array}{ccc}
p_{\text{gen}}(x_{\text{part}}) & \longleftrightarrow & p_{\text{unfold}}(x_{\text{part}}) \\
\text{simulation} \Big\downarrow & & \Big\uparrow \text{unfolding} \\
p_{\text{sim}}(x_{\text{reco}}) & \longleftrightarrow & p_{\text{data}}(x_{\text{reco}})
\end{array}
$$

Unfolding

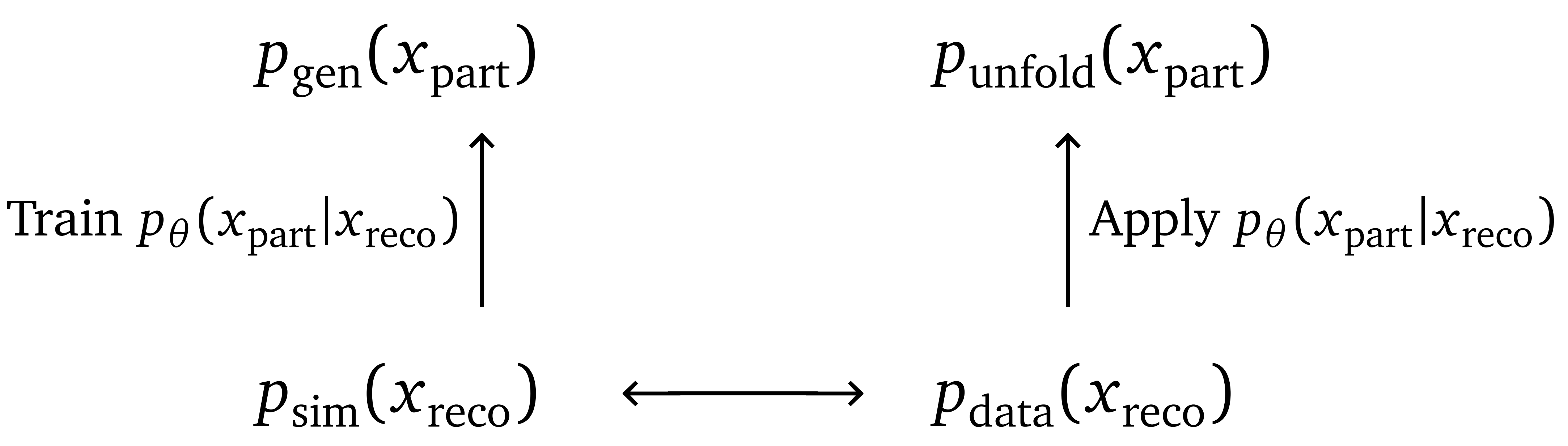
Omnifold

Andreassen et al.
arXiv:1911.09107
arXiv:2105.04448



Generative Unfolding

Bellagente et al.
arXiv:1912.00477
arXiv:2006.06685



Unfolding

Omnifold

Andreassen et al.
arXiv:1911.09107
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Thursday Afternoon !

Generative Unfolding

Bellagente et al.
arXiv:1912.00477
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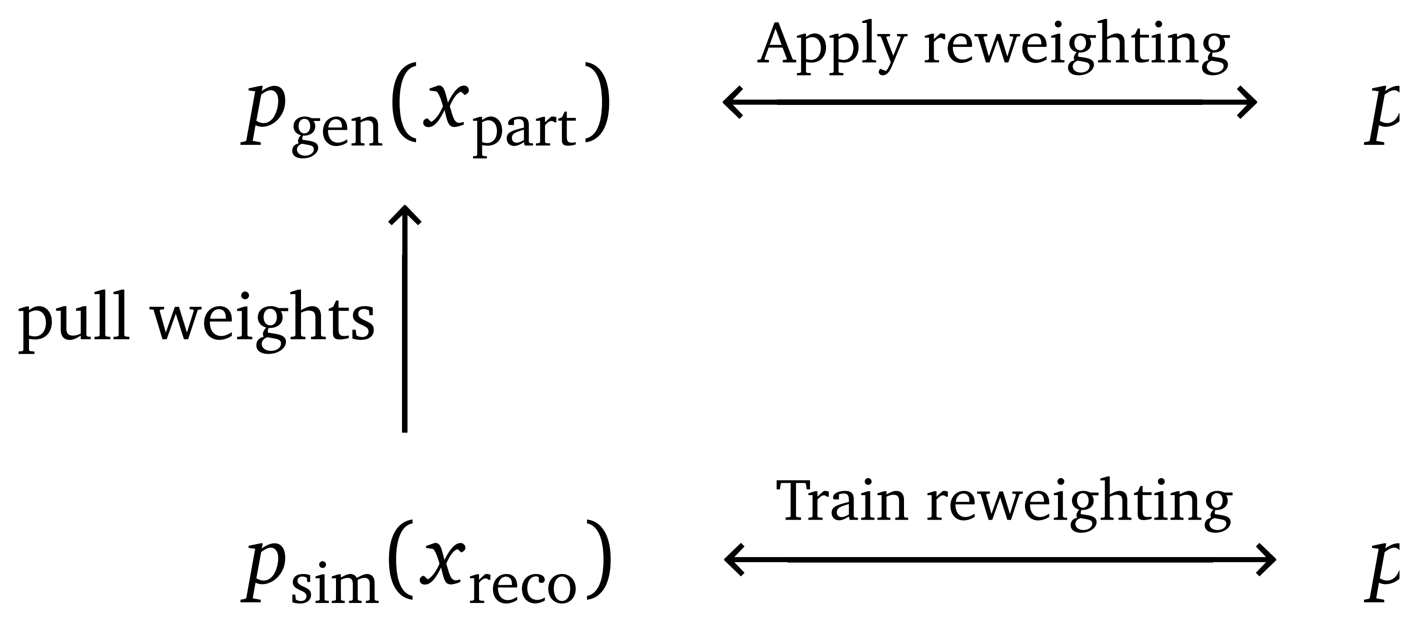
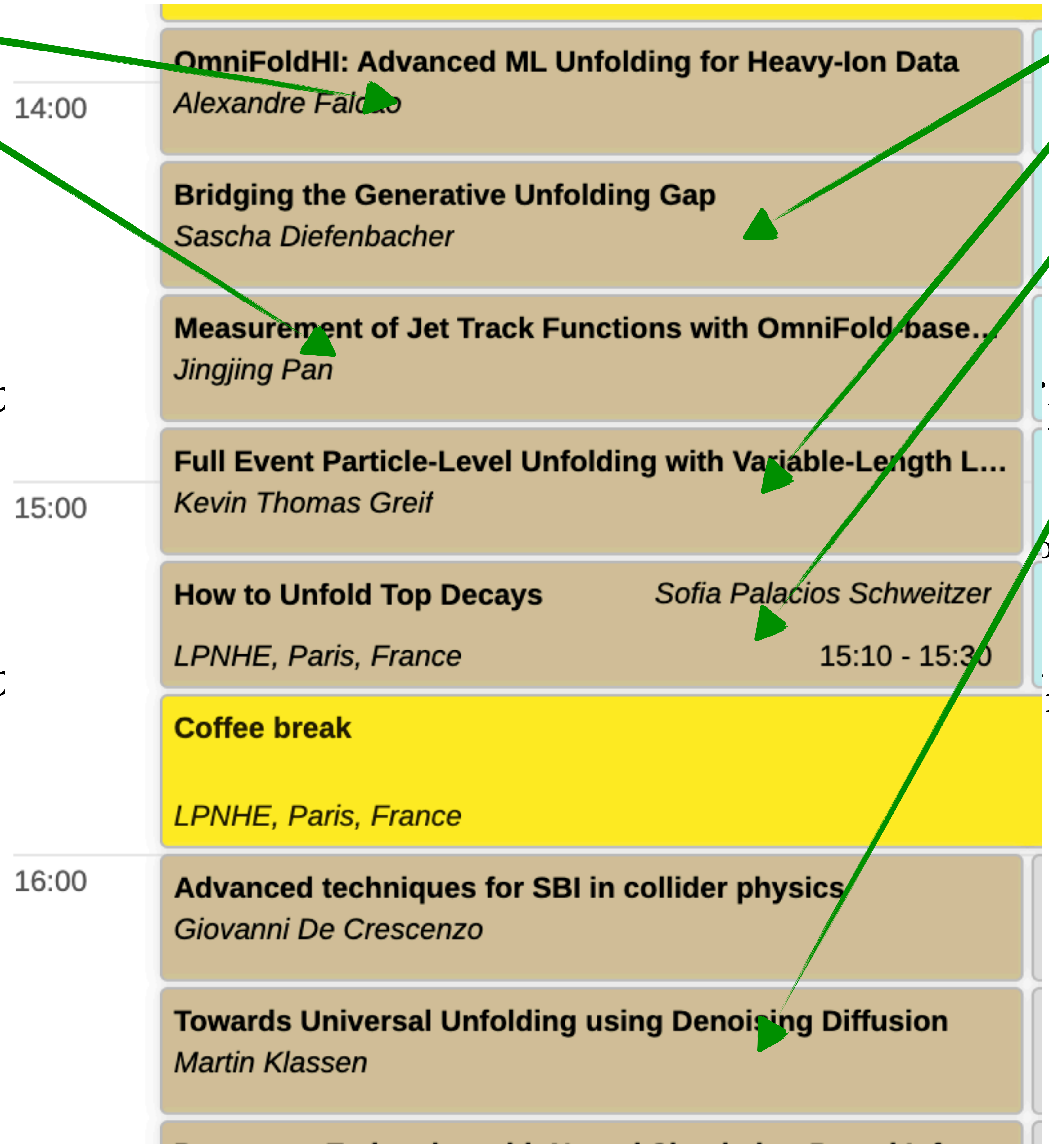
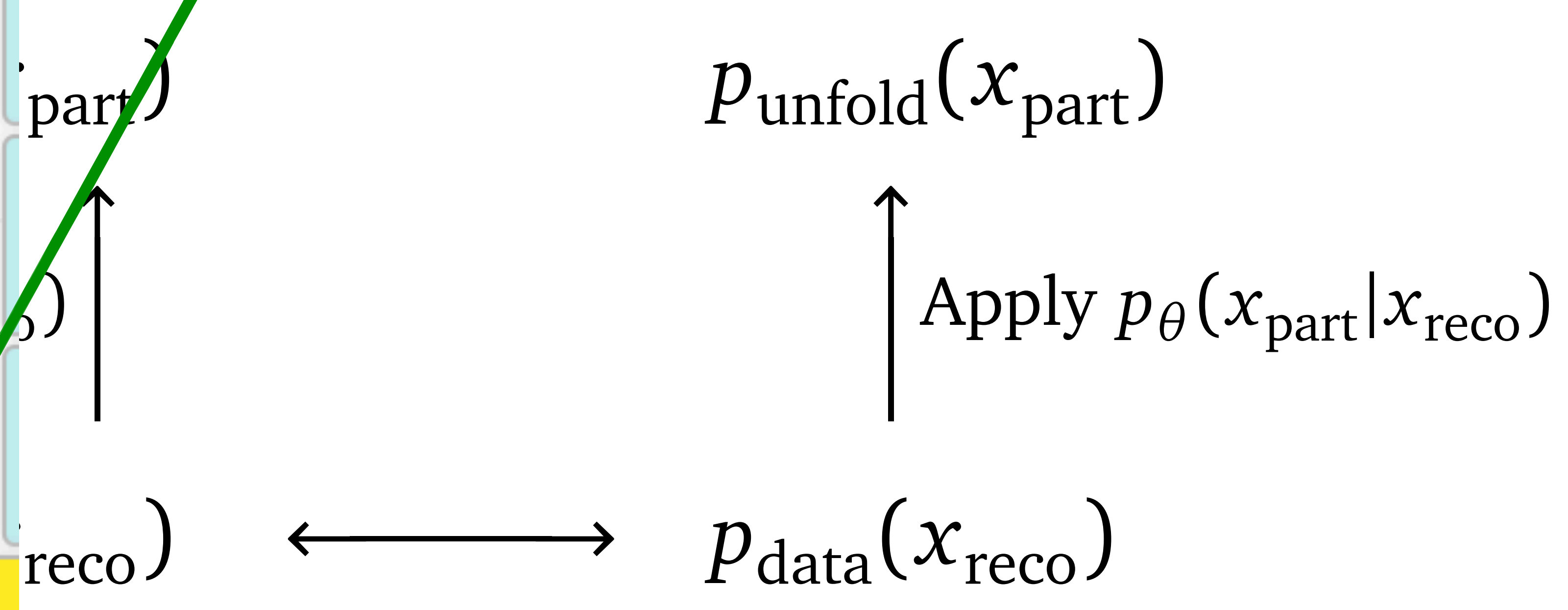




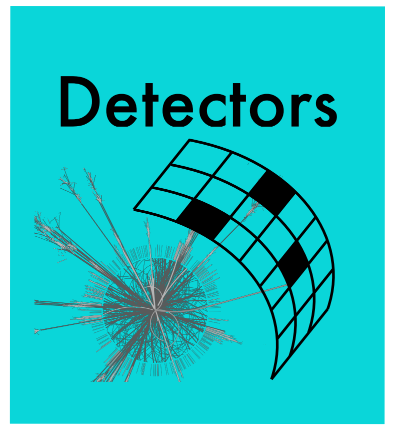


Probabilistic transfer

Transfer probability

Encoded implicitly in detector simulation

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



x_{gen}

x_{rec}

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

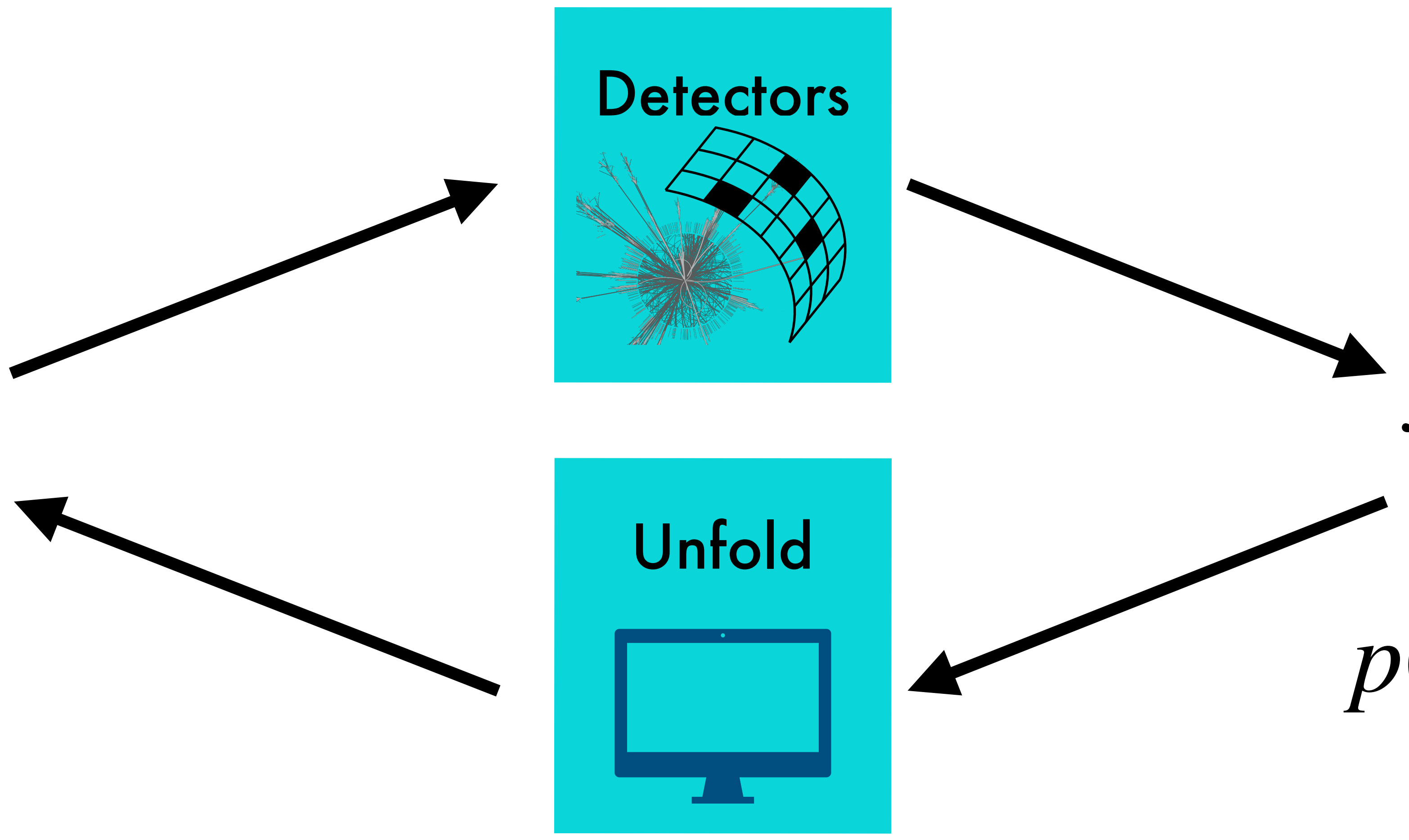
Generative unfolding

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}



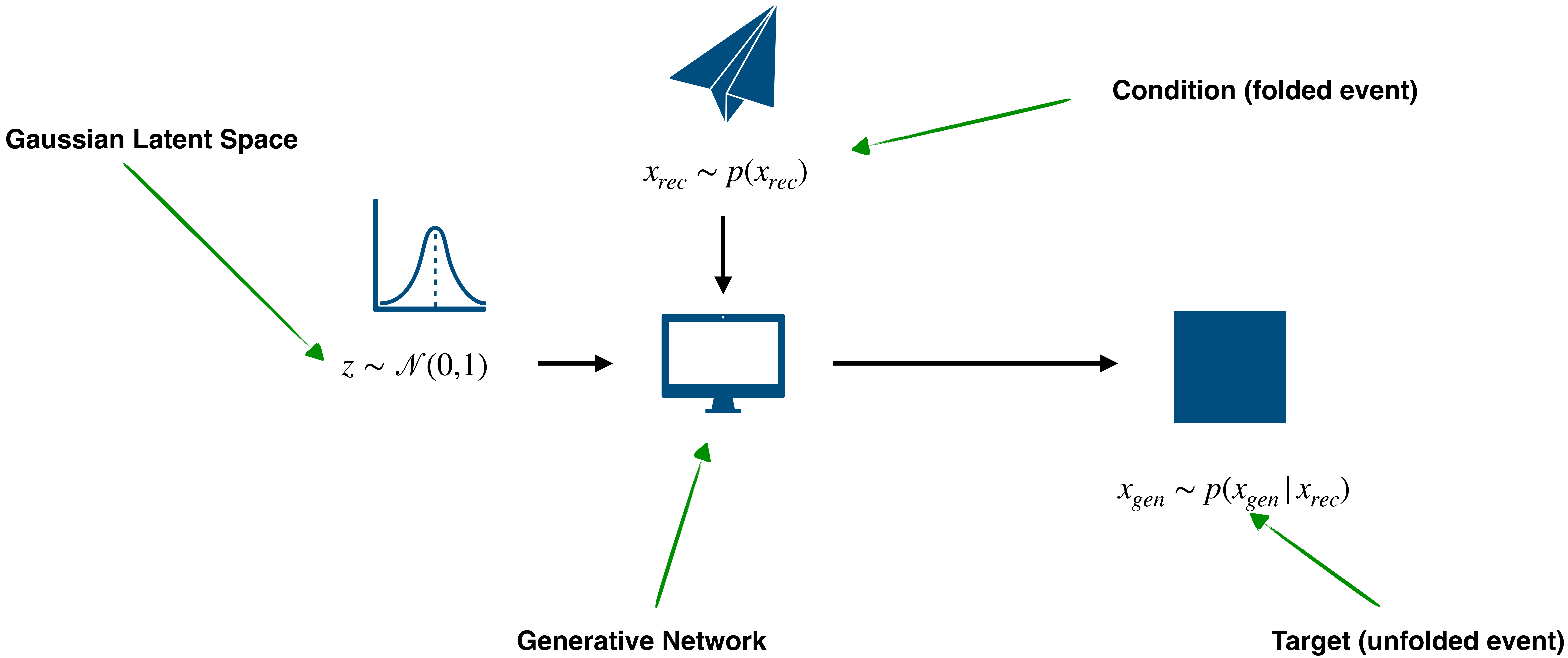
x_{rec}

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

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

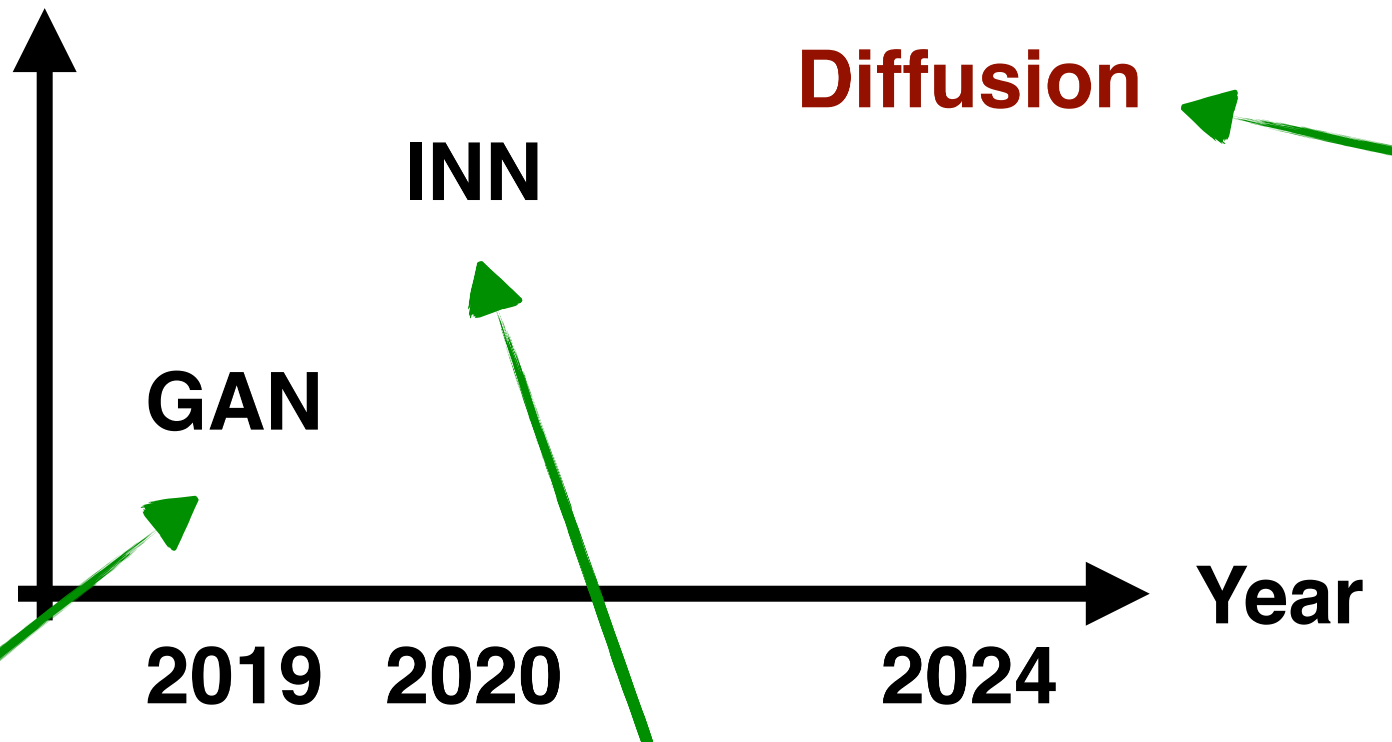
Unfolding probability ← **Encoded in neural network trained on simulation**

Conditional generative networks



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
Butter et al.
arXiv:2411. xxxxx

VLD
Shmakov et al.
arXiv: 2305.10399
arXiv: 2404.14332

DDPM
Pazos et al.
arXiv: 2406.01507

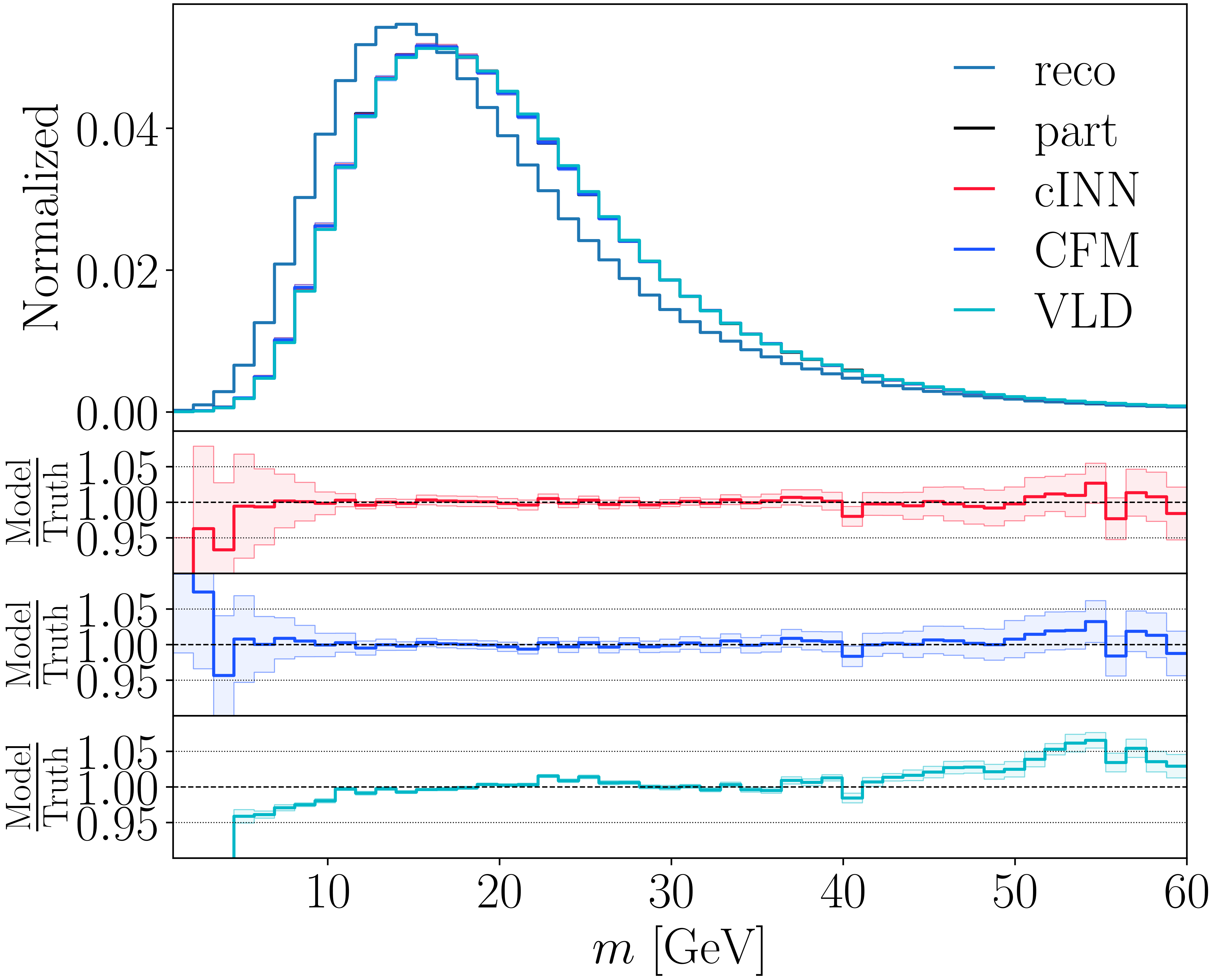
Talks on thursday!

Slide adapted from Sofia Palacios Schweitzer

6-dimensional unfolding

Z + jets events following Andreassen et al. arXiv: 1911.09107

6-dimensional phase space of jet observables



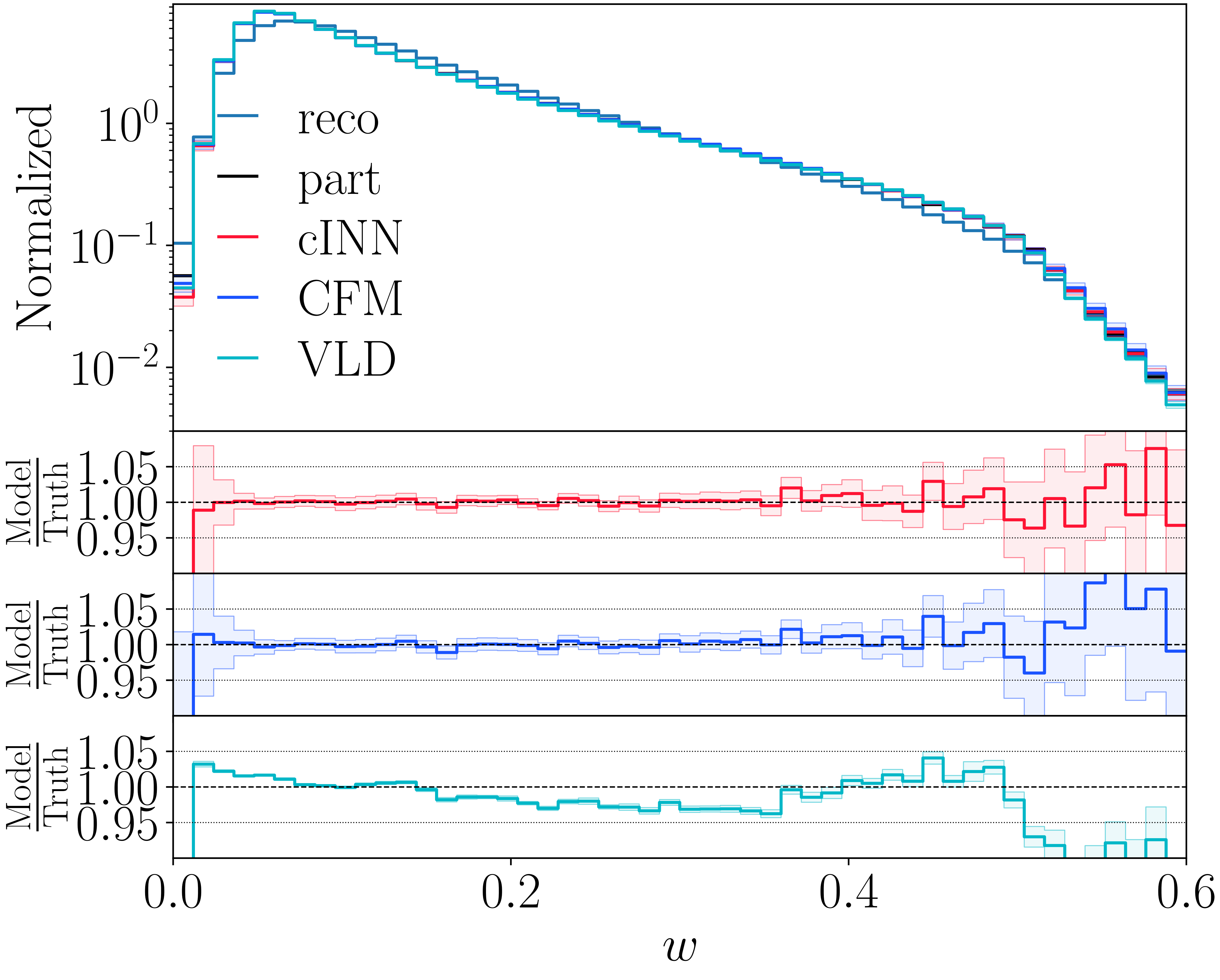


Figure from Huetsch et. al: arXiv:2404.18807

22-dimensional unfolding

Z + 2 jets events following ATLAS arXiv:2405.20041

22-dimensional phase space of μ-kinematics, jet-kinematics, jet-observables

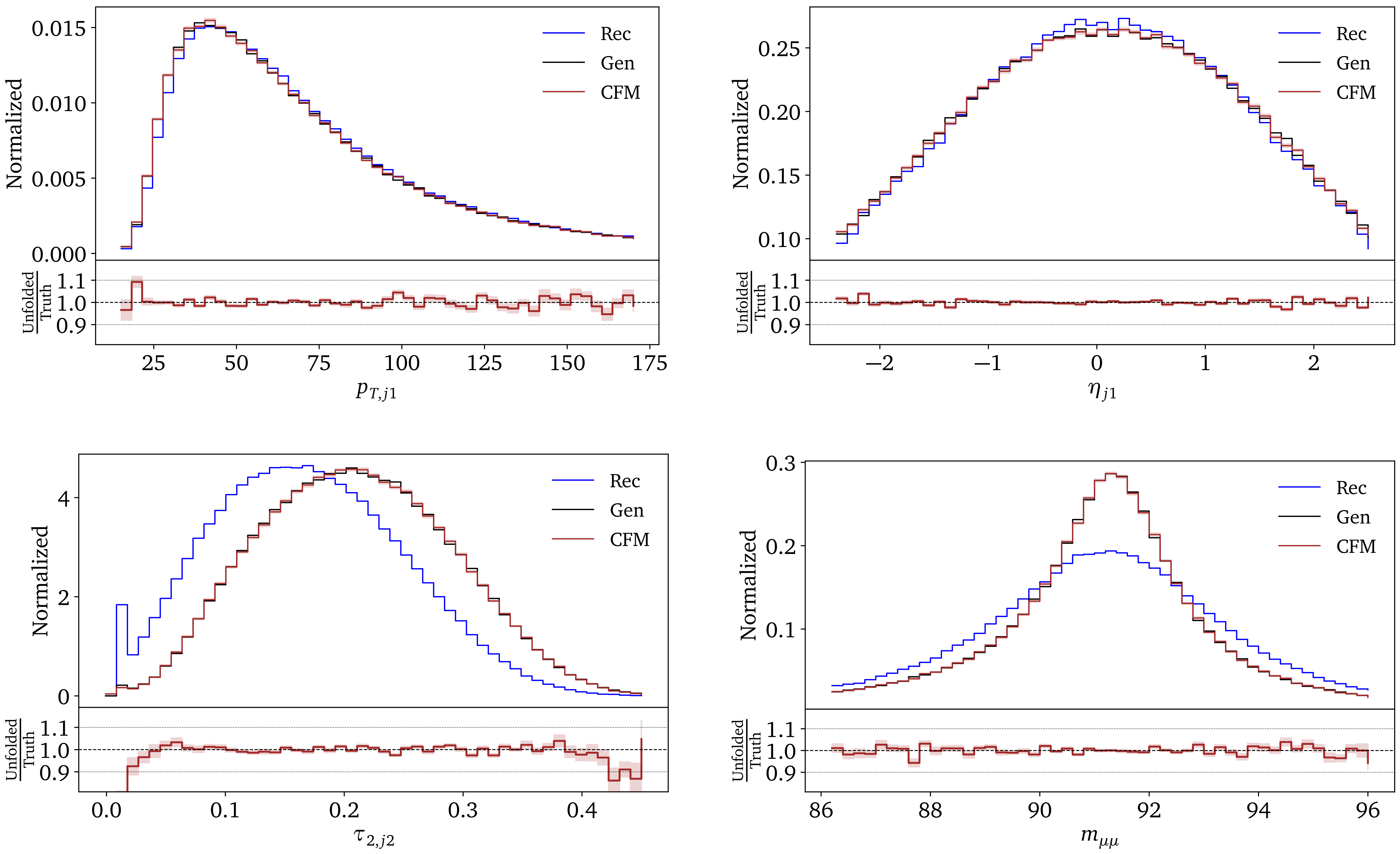


Figure adapted from Butter et. al: arXiv:2411. xxxxx

22-dimensional unfolding

Z + 2 jets events following ATLAS arXiv:2405.20041

22-dimensional phase space of μ-kinematics, jet-kinematics, jet-observables

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

It learns the likelihood ratio

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

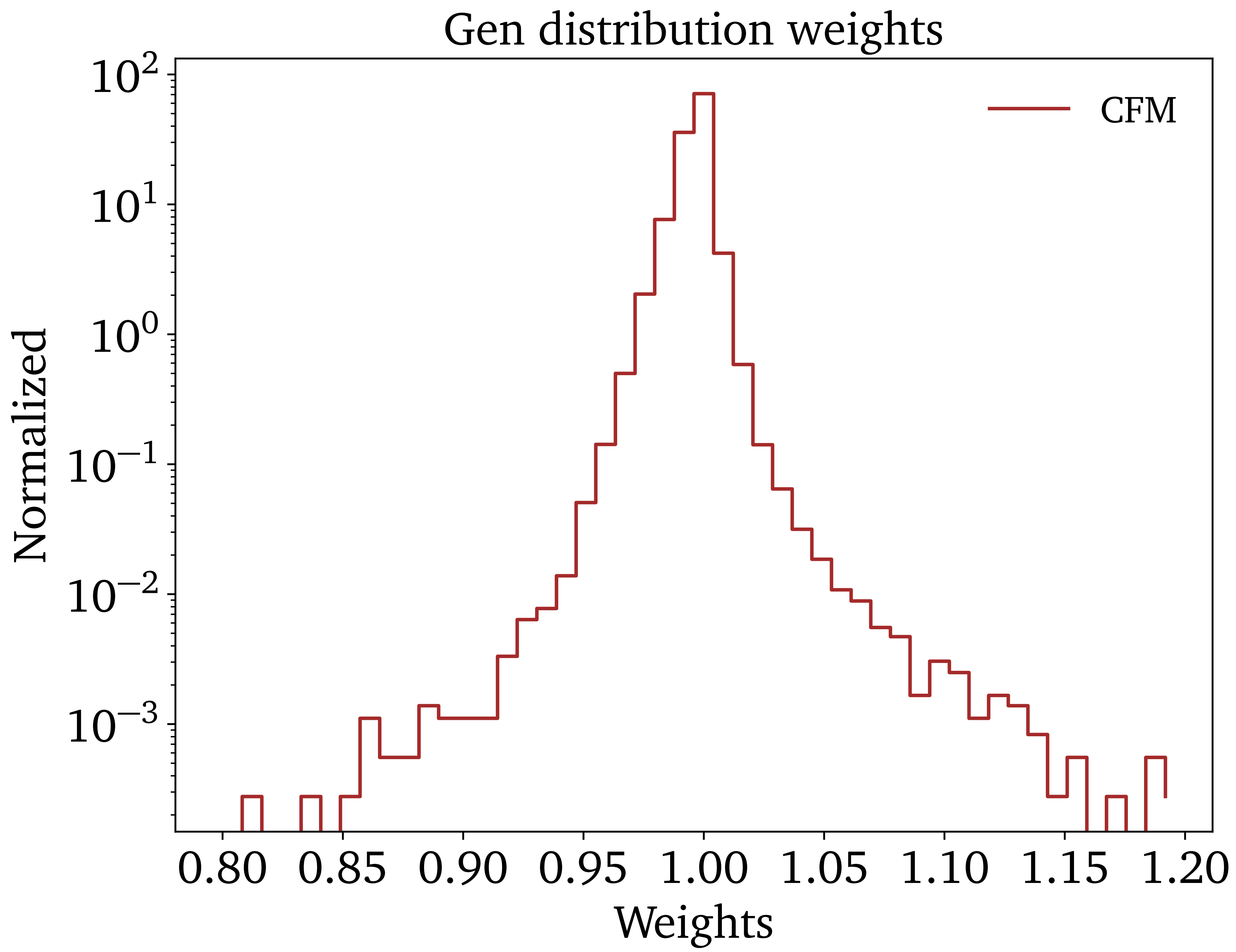


Figure adapted from Butter et. al: arXiv:2411. xxxxx

Simulation chain — Inversion

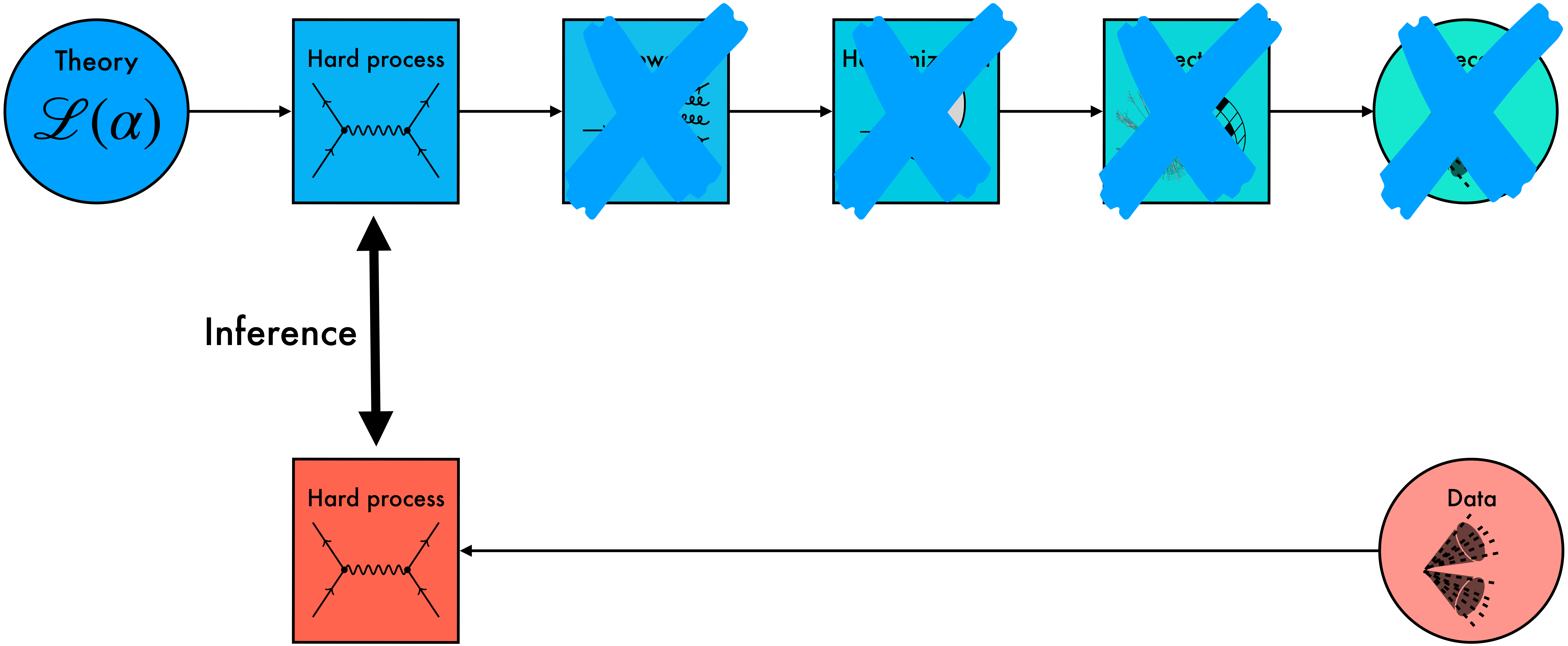
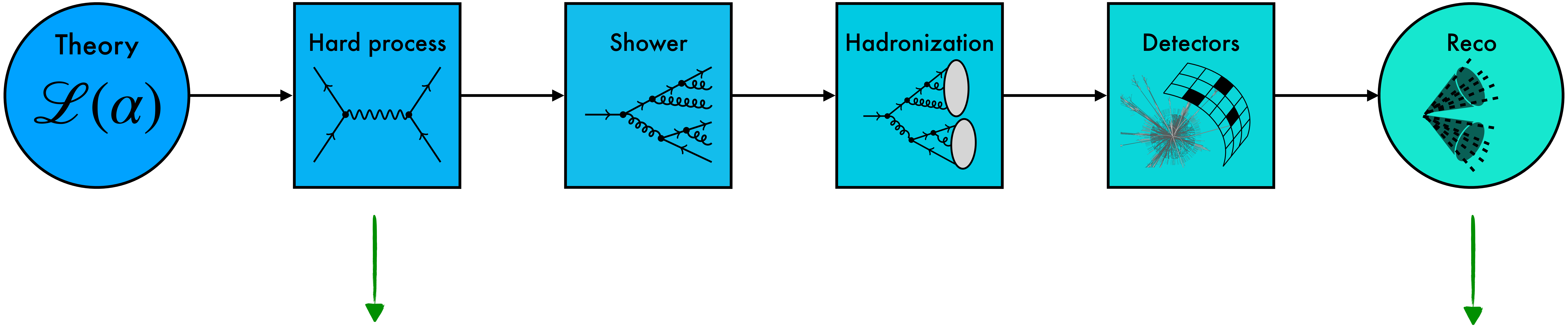


Figure adapted from R. Winterhalder

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



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

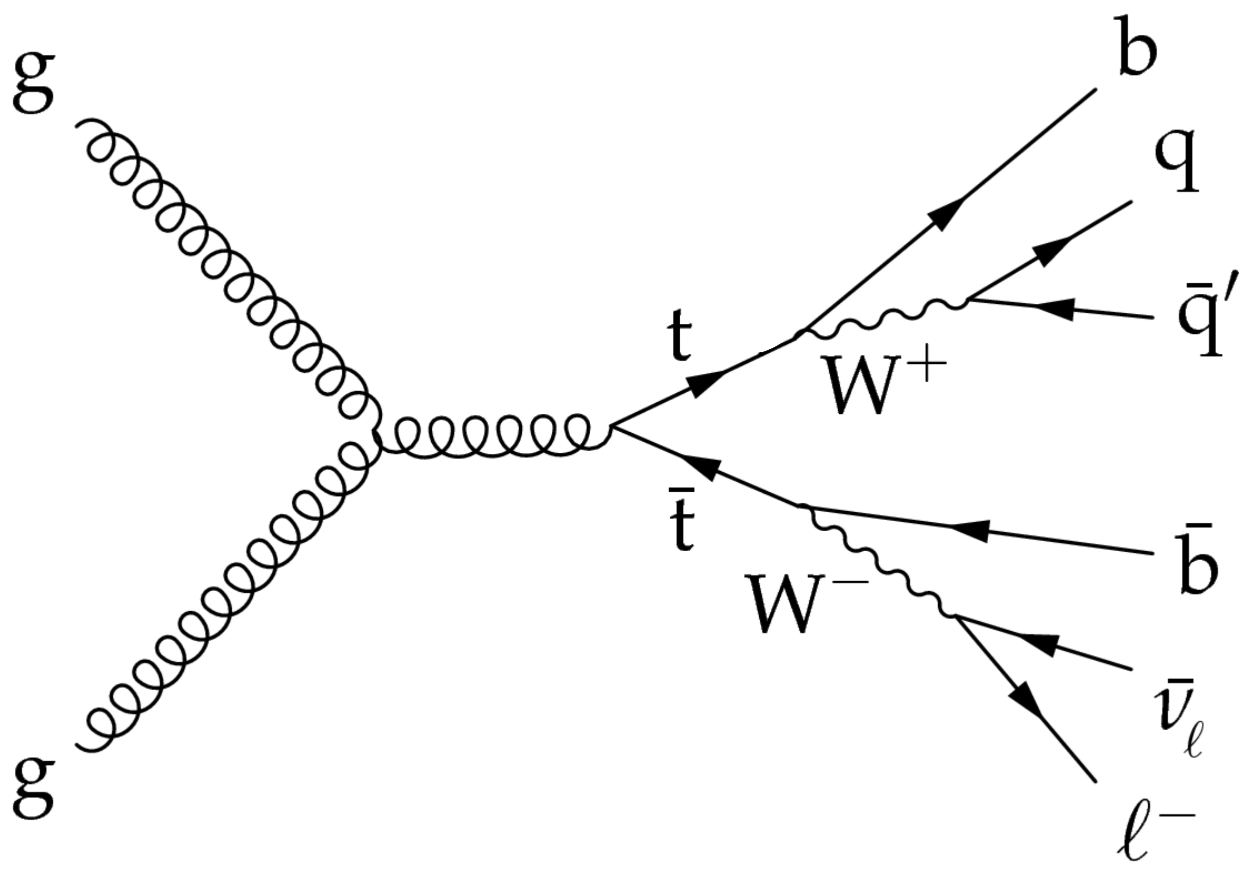
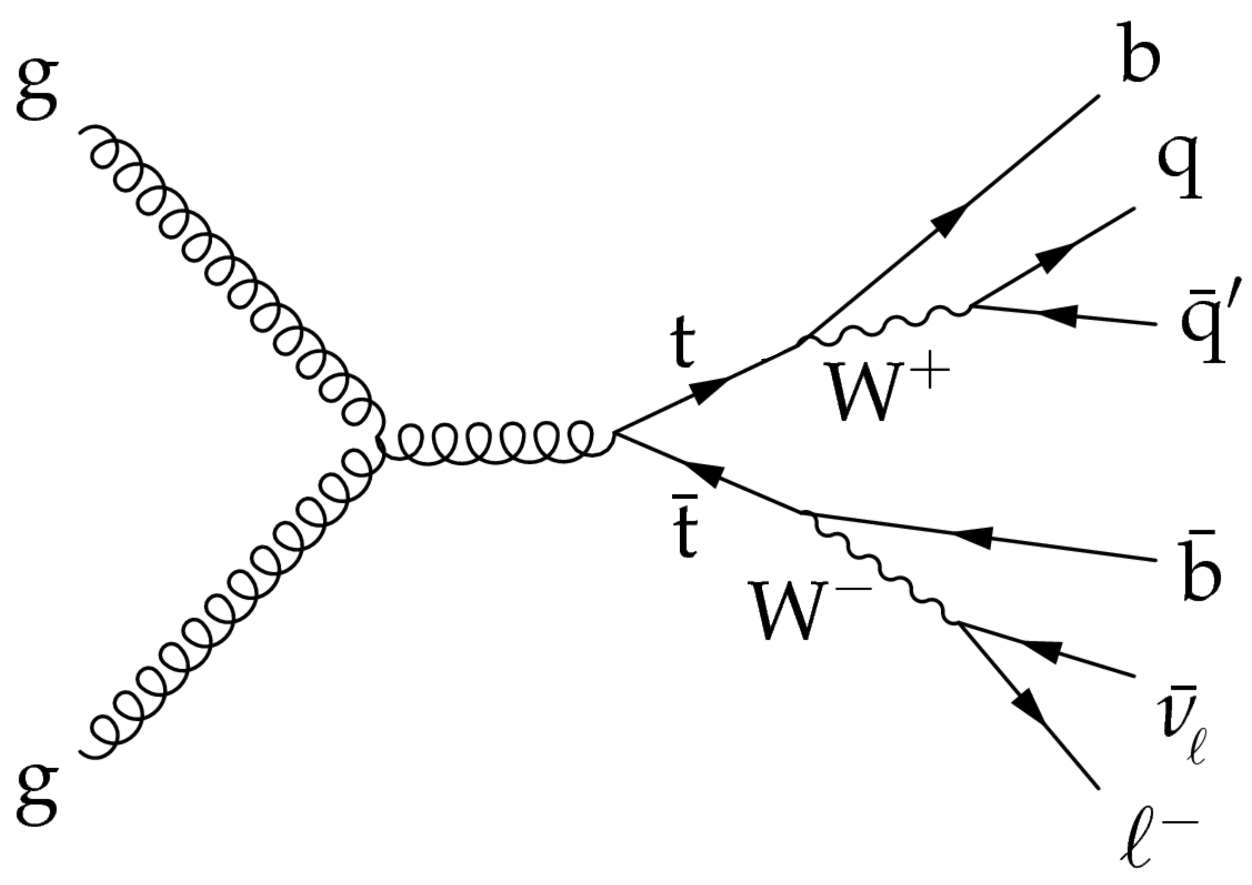


Figure on top adapted from R. Winterhalder

Dataset from Shmakov et al. arXiv: 2305.10399

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



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

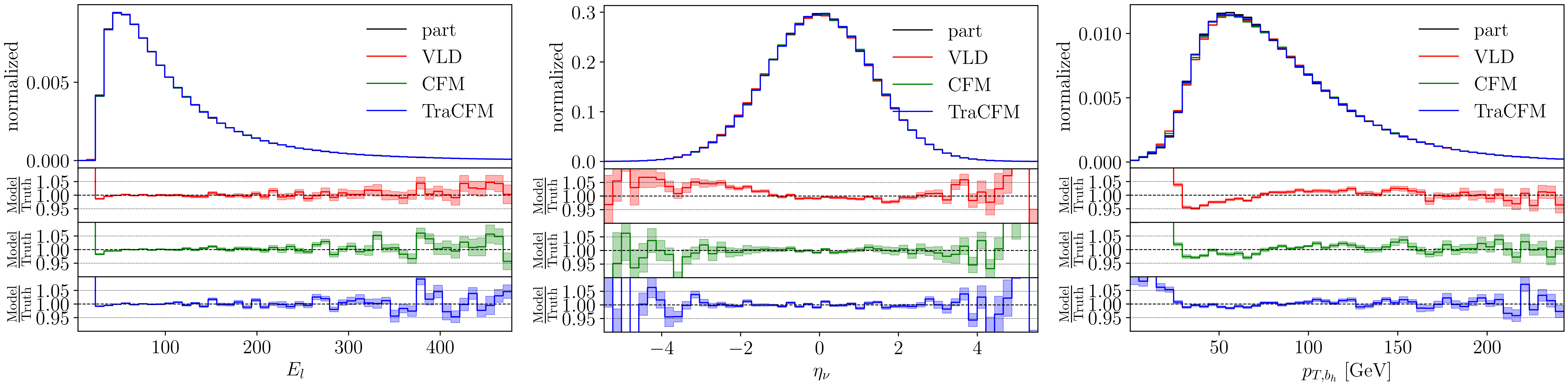
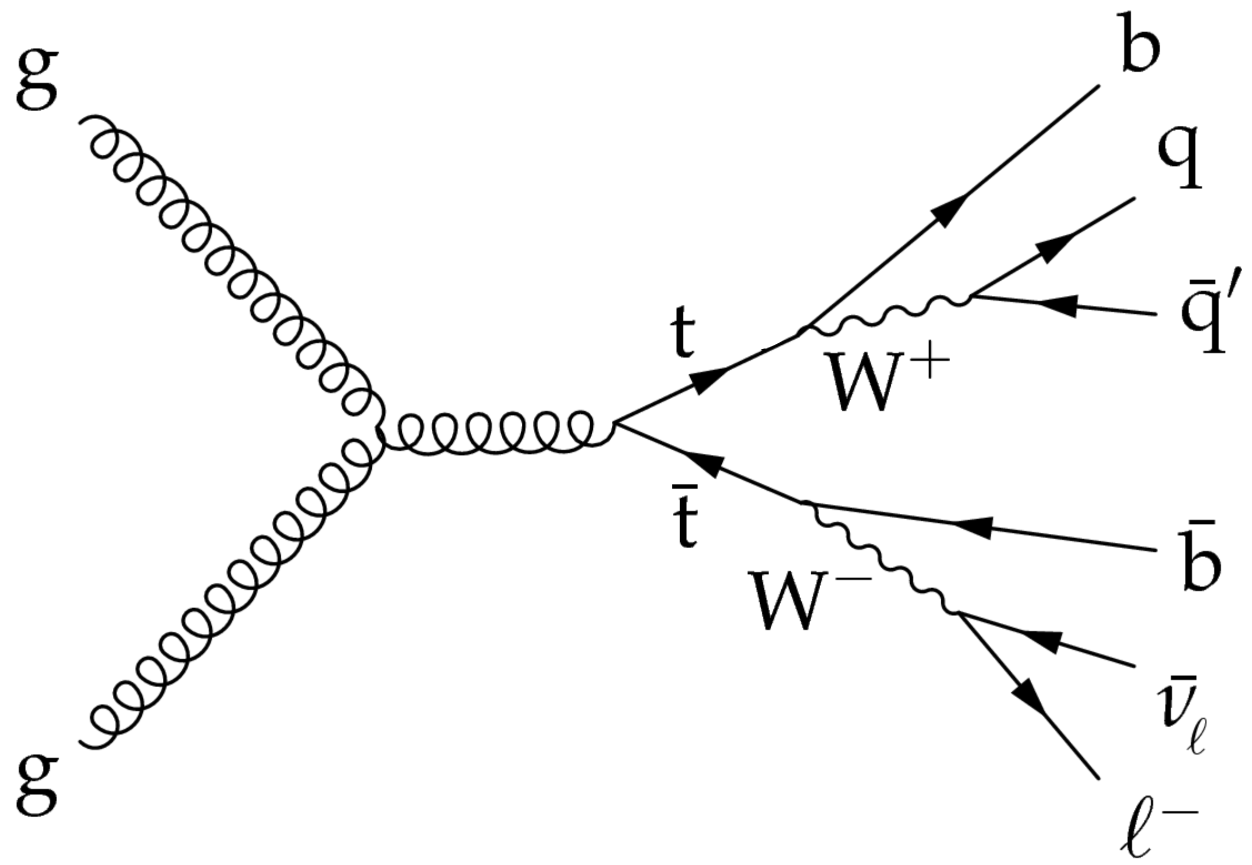


Figure from Huetsch et. al: arXiv:2404.18807

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



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

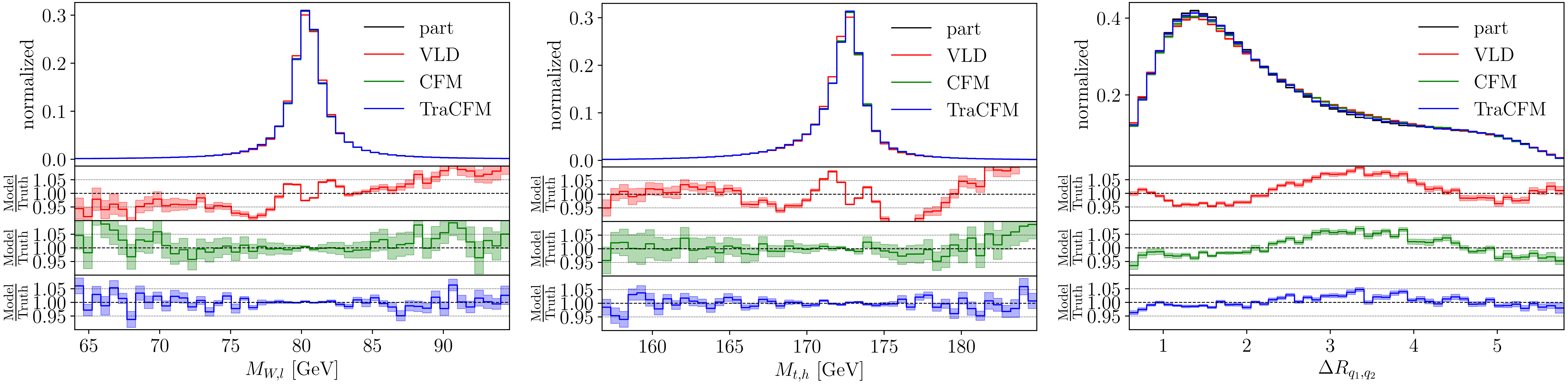
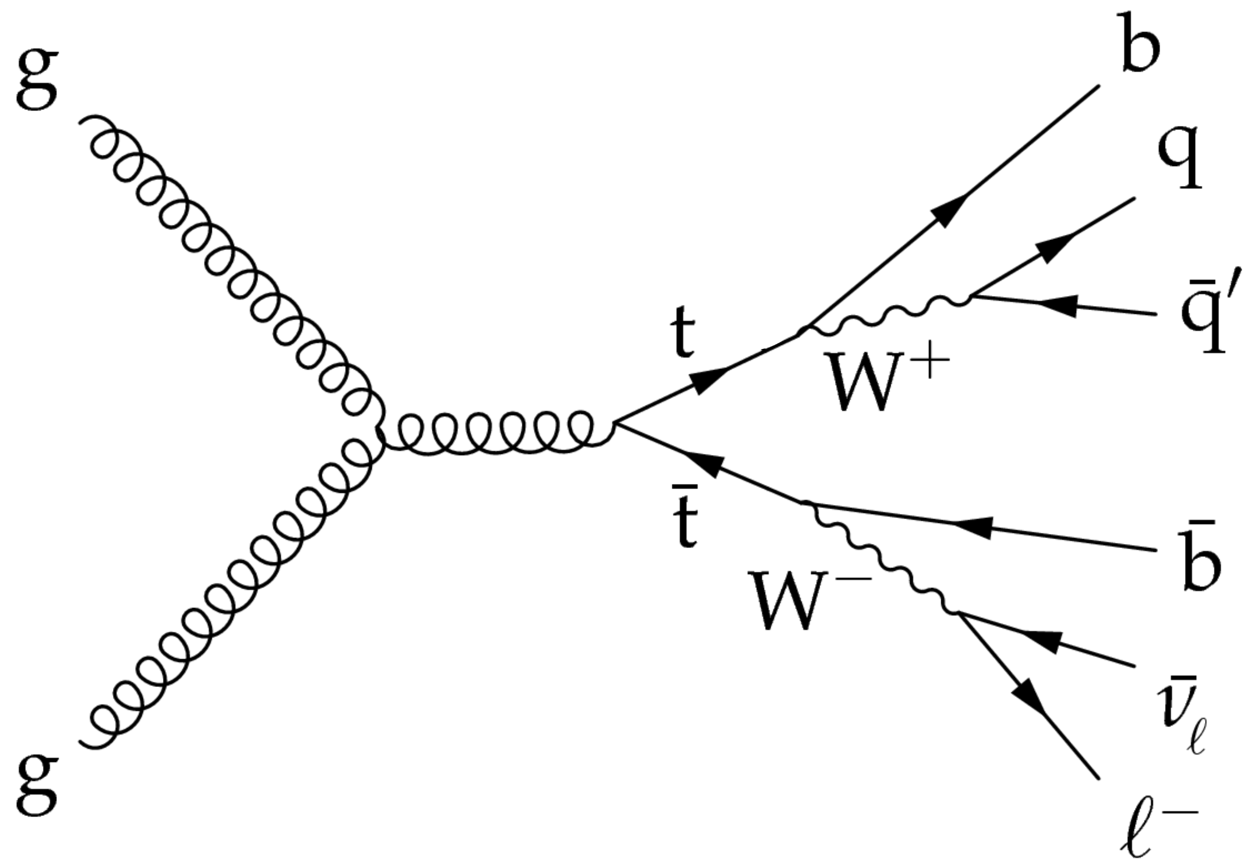


Figure from Huetsch et. al: arXiv:2404.18807

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



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

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

It learns the likelihood ratio

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

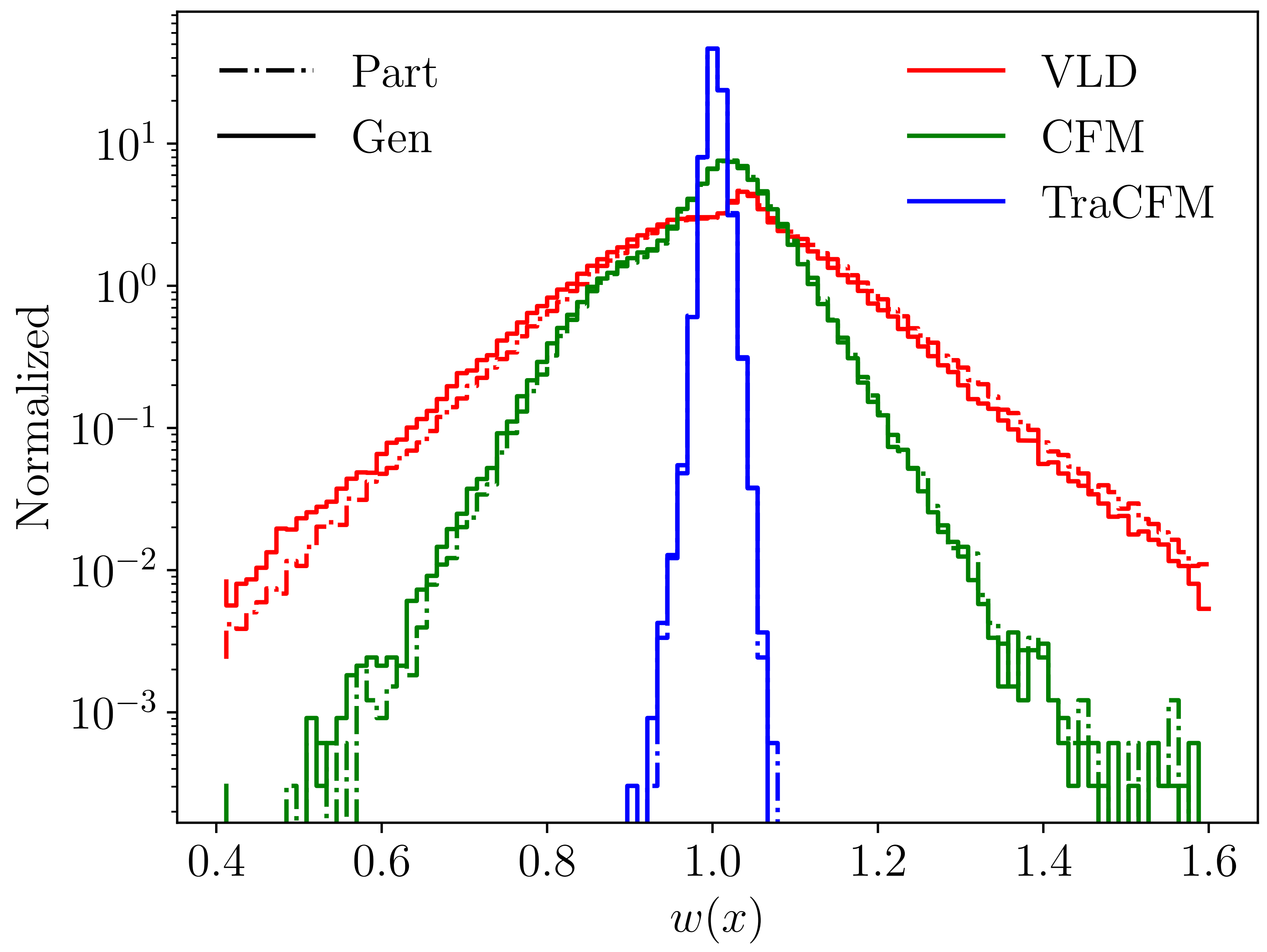
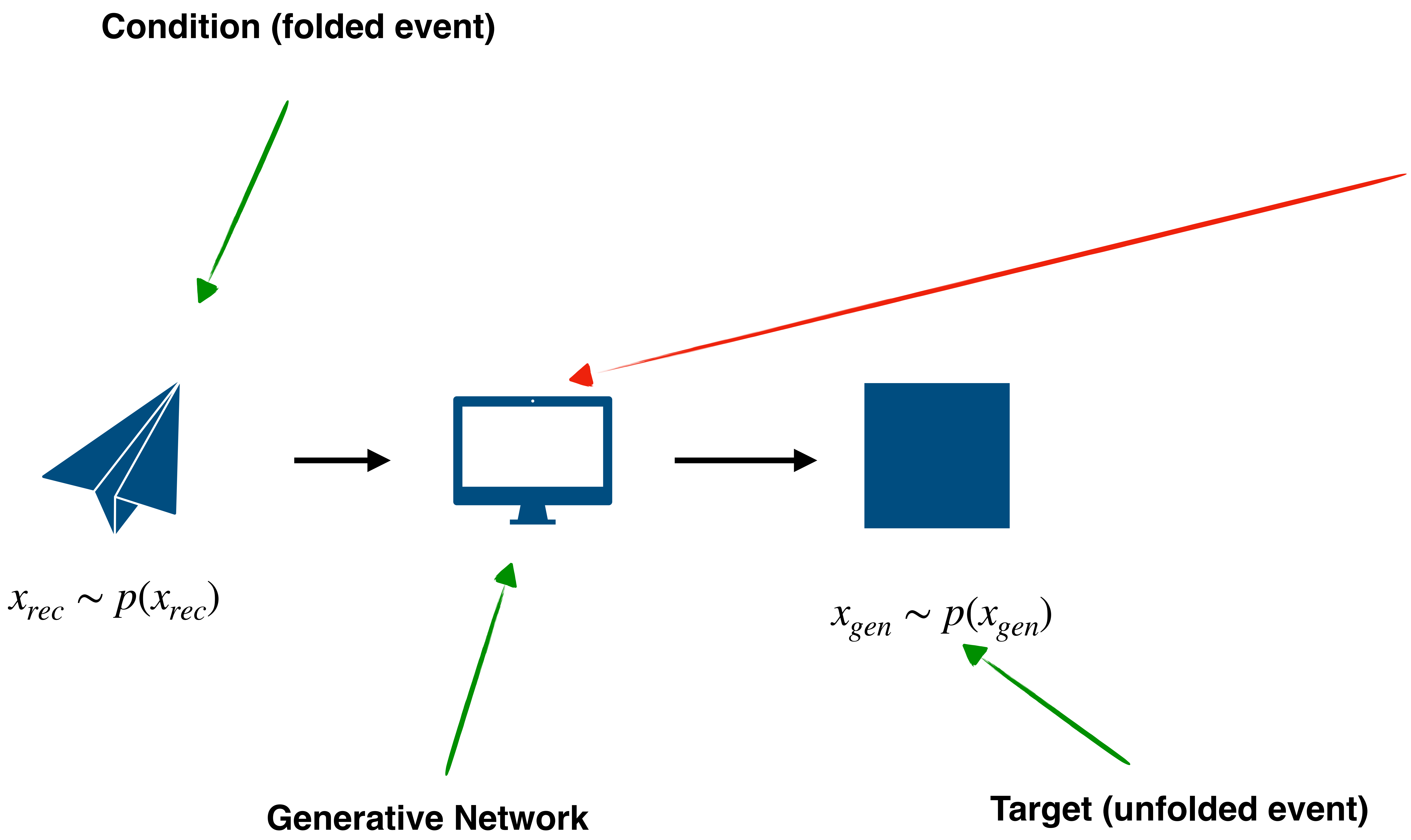


Figure from Huetsch et. al: arXiv:2404.18807

Distribution mapping



Schrödinger Bridge

Diefenbacher et al.
arXiv:2308.12351

Direct Diffusion

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

Slide adapted from Sofia Palacios Schweitzer

Z + jet results

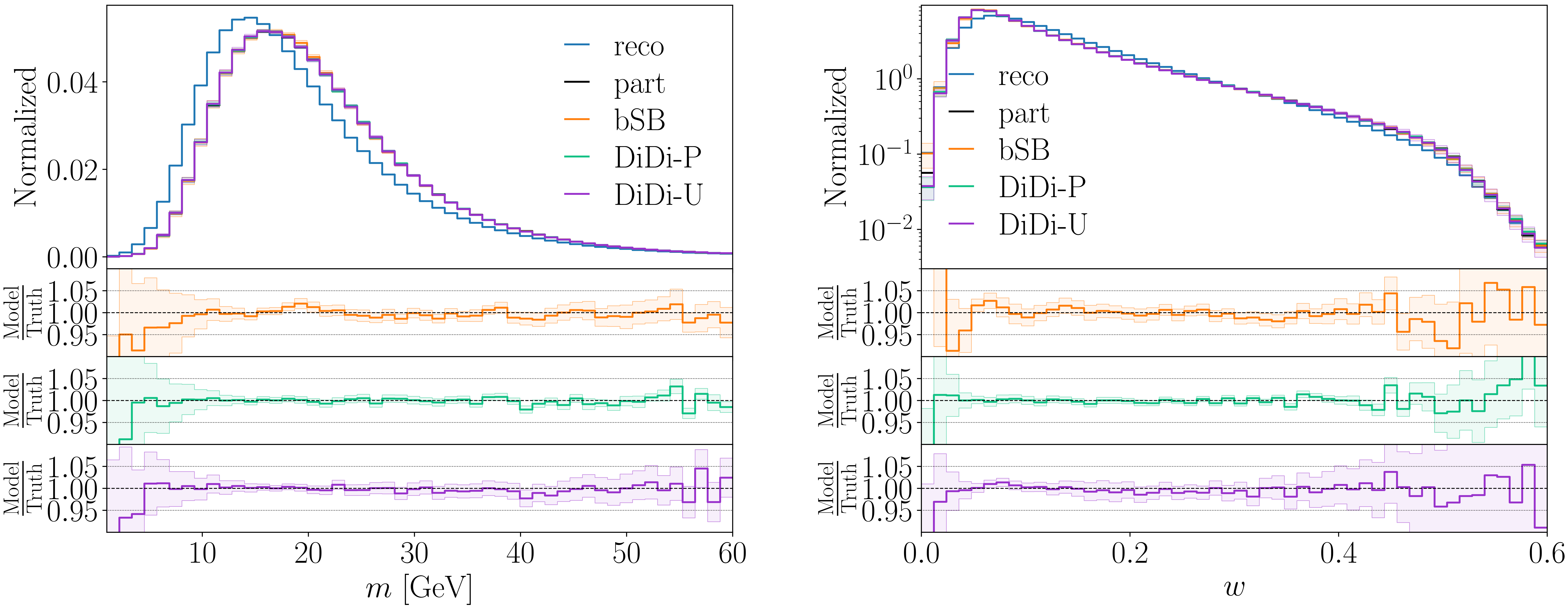


Figure from Huetsch et. al: arXiv:2404.18807

Z + jet migration

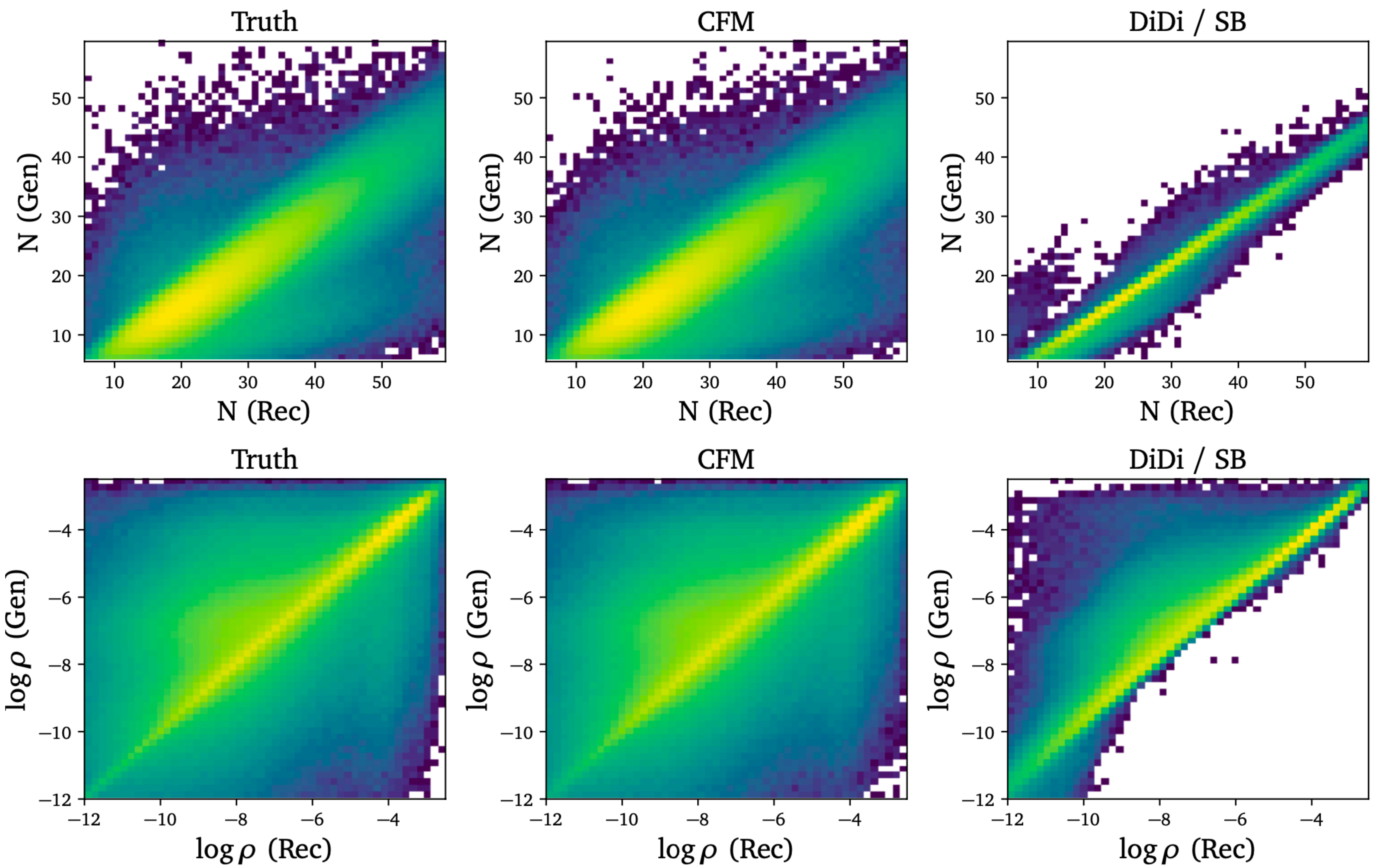
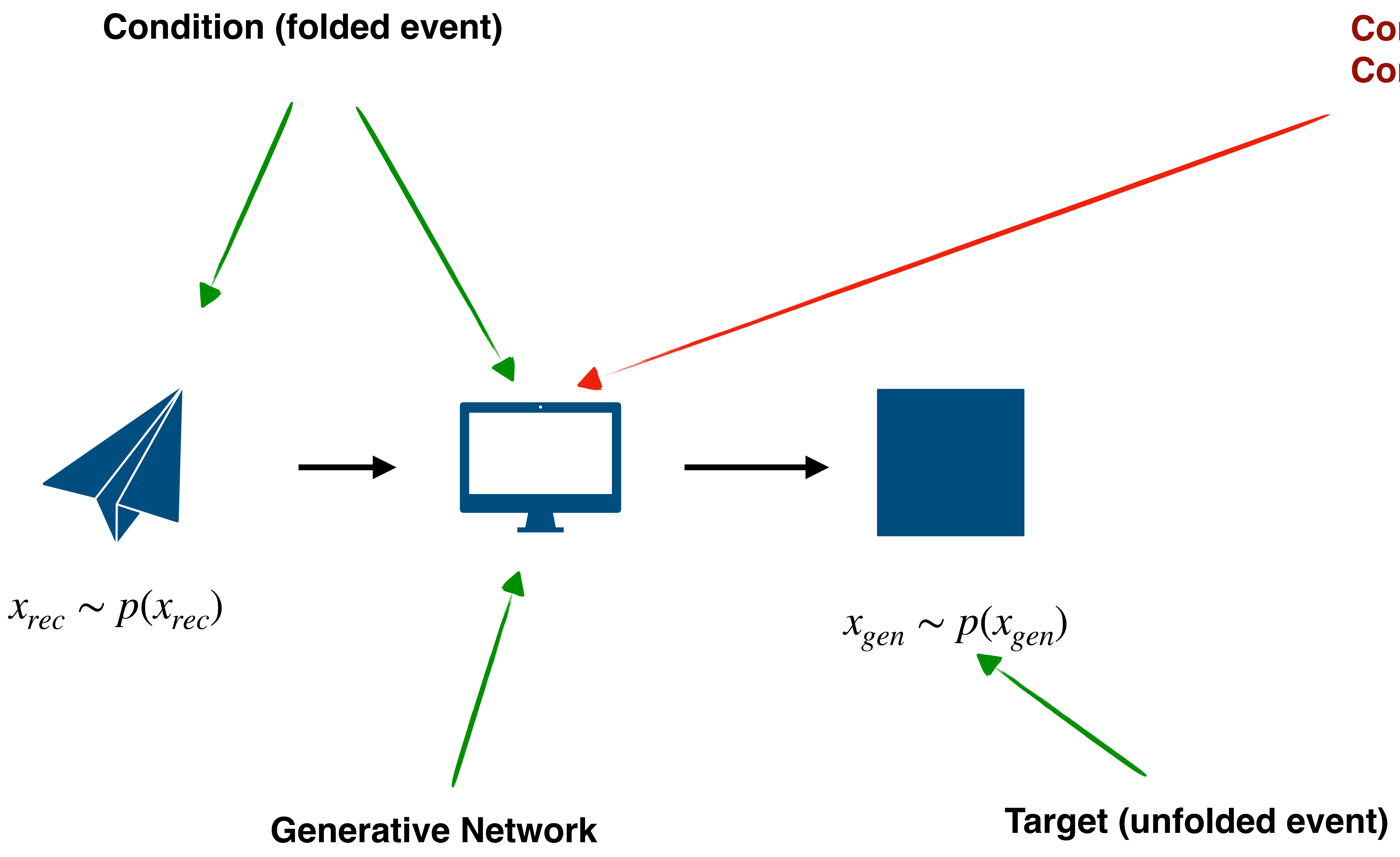


Figure adapted from Huetsch et. al: arXiv:2404.18807

Conditional distribution mapping



Conditional Direct Diffusion
Conditional Schrödinger Bridge

Butter et al.
arXiv:2411.xxxx

Talk by S. Diefenbacher
on Thursday

Slide adapted from Sofia Palacios Schweitzer

Conditional distribution mapping

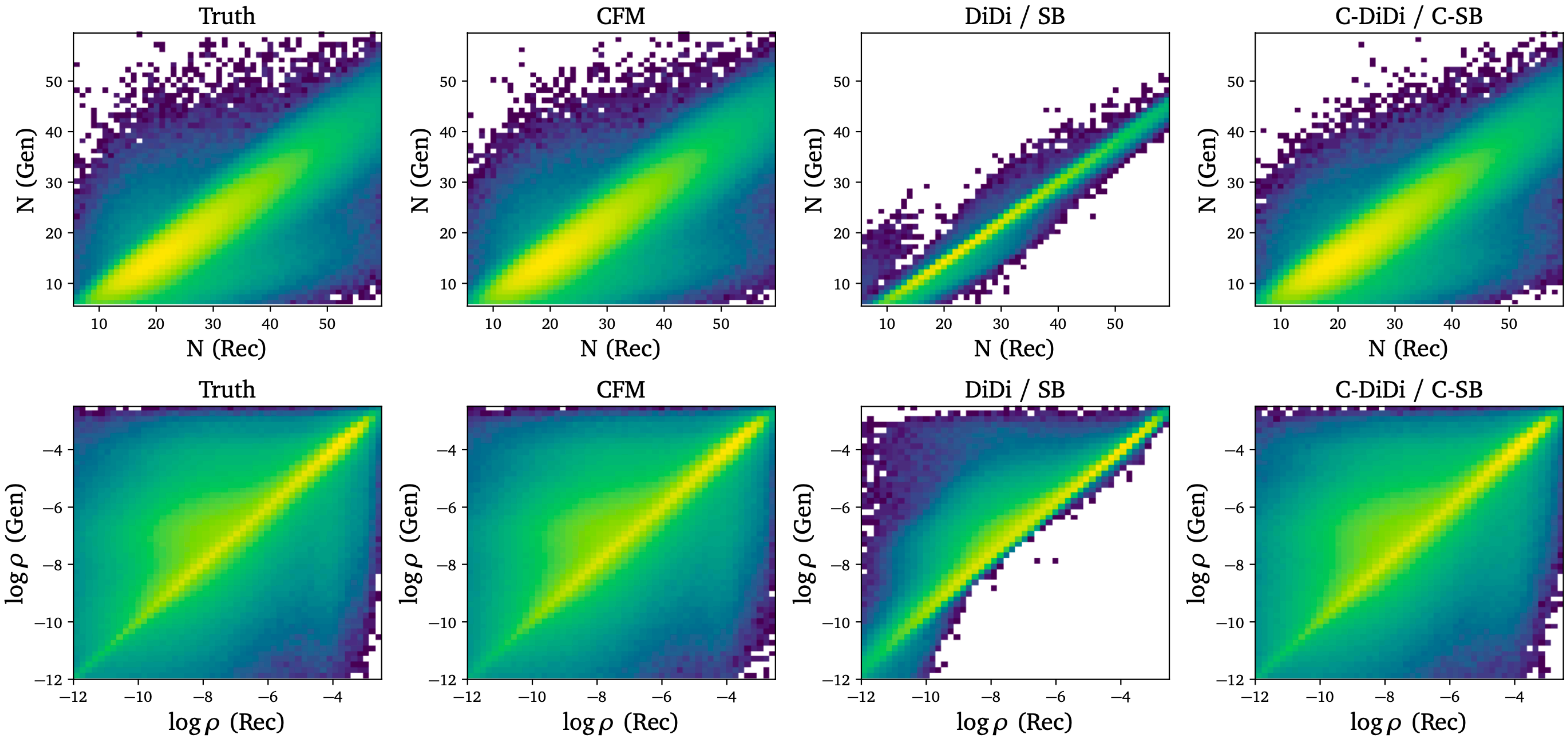


Figure adapted from Butter et. al: arXiv:2411. xxxxx

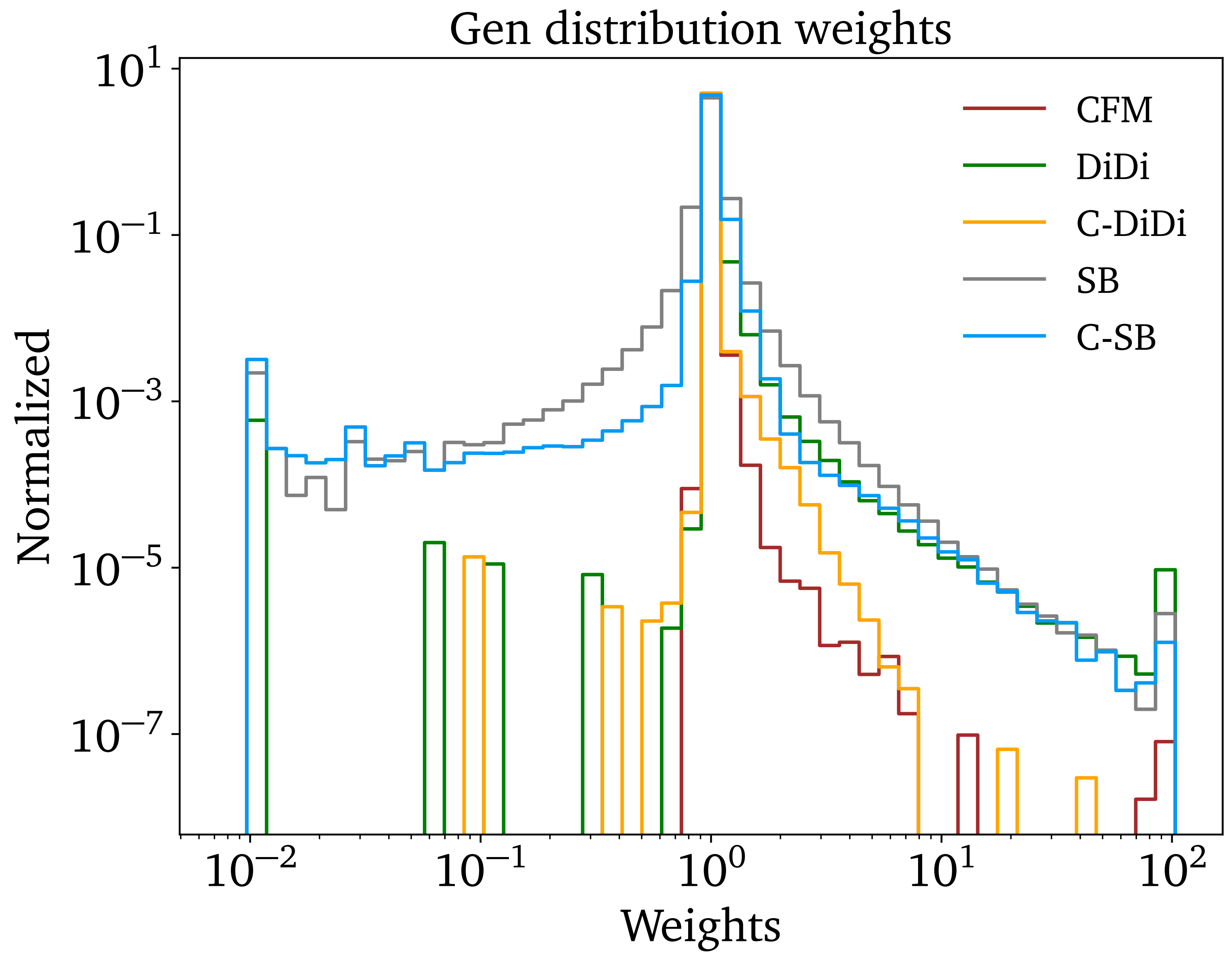
Conditional distribution mapping

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

It learns the likelihood ratio $w(x) = \dfrac{p_{gen}(x)}{p_{unfold}(x)}$

Train a classifier classifier
between $p_{true}\,(x_{rec}, x_{part})$ and $p_{model}\,(x_{rec}, x_{part})$

It learns the likelihood ratio $w(x) = \dfrac{p_{true}\,(x_{rec}, x_{part})}{p_{model}\,(x_{rec}, x_{part})}$



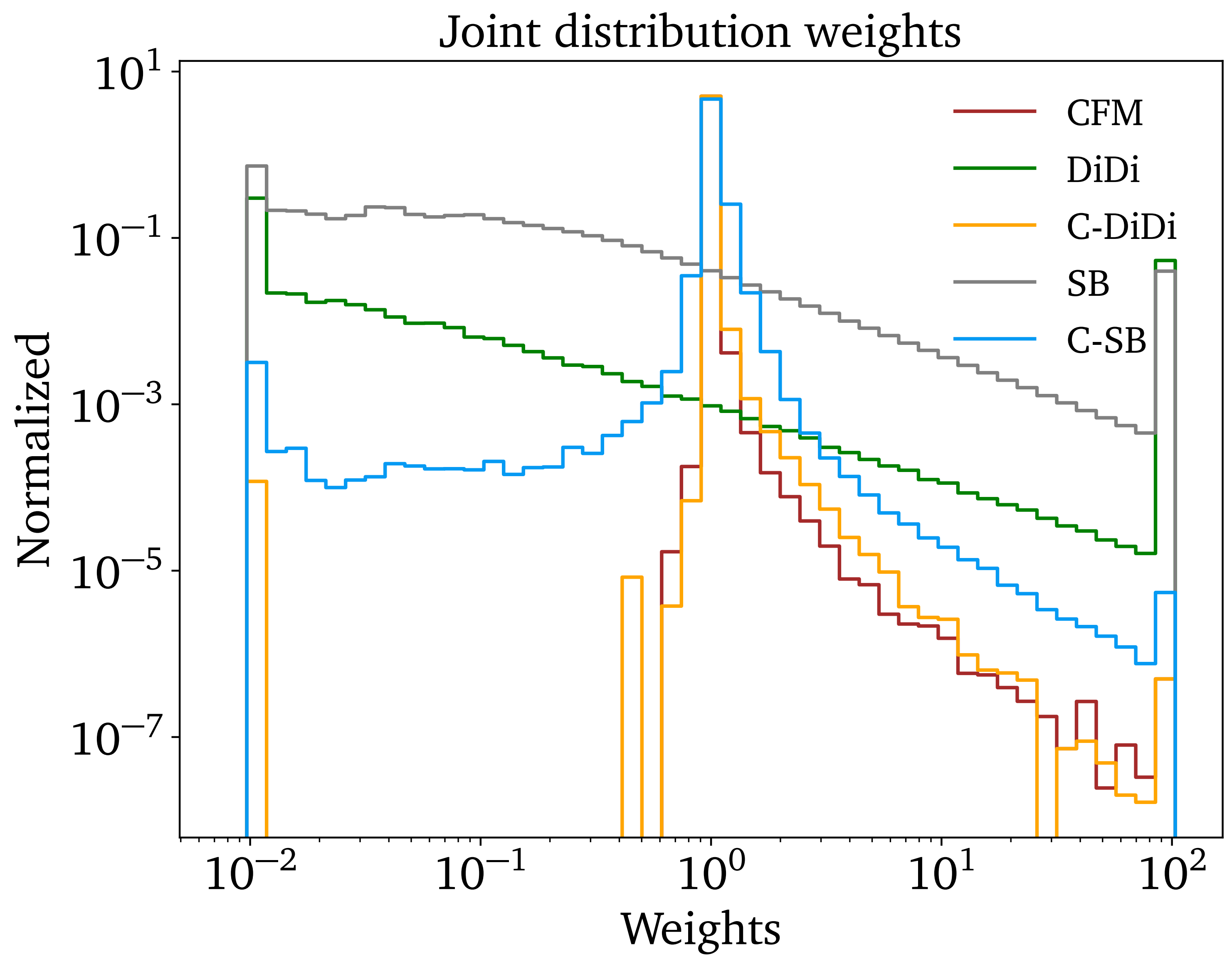


Figure from Butter et. al: arXiv:2411. xxxxx

Conclusion

ML Unfolding works ! ← ATLAS arXiv:2405.20041

Conditional Generative Unfolding enables probabilistic inversion of simulation chain

Classifier test reveals no artefacts and/or miss-modelled correlations

Distribution Mapping is a new and evolving ML-approach to generative unfolding

Further investigation of uncertainties

Application to real data ← (almost)

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]

SciPost Physics **Submission**

Generative Unfolding with Distribution Mapping

Anja Butter[1,2], Sascha Diefenbacher[3], Nathan Huetsch[1], Vinicius Mikuni[4], Benjamin Nachman[3,5], Sofia Palacios Schweitzer[1] and Tilman Plehn[1,6]

Talk by S. Diefenbacher on Thursday

How to Unfold Top Decays	*Sofia Palacios Schweitzer*
LPNHE, Paris, France	15:10 - 15:30

Generative unfolding applied to CMS full-sim

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**

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

Flow Matching (Lipman et al. 2210.02747)

Phase Space
$t = 0$

Latent Space
$t = 1$

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

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

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

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

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

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:

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

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

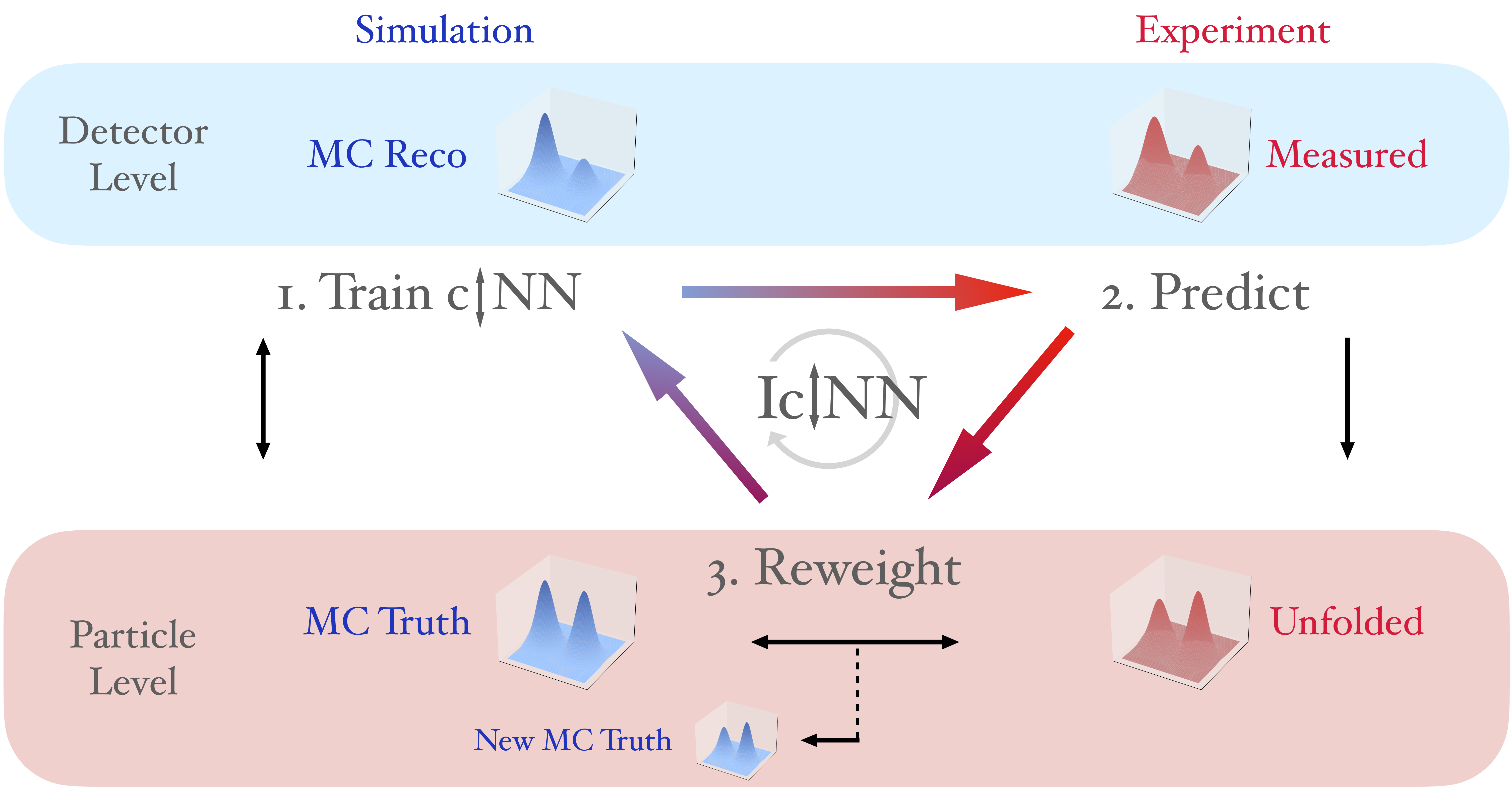
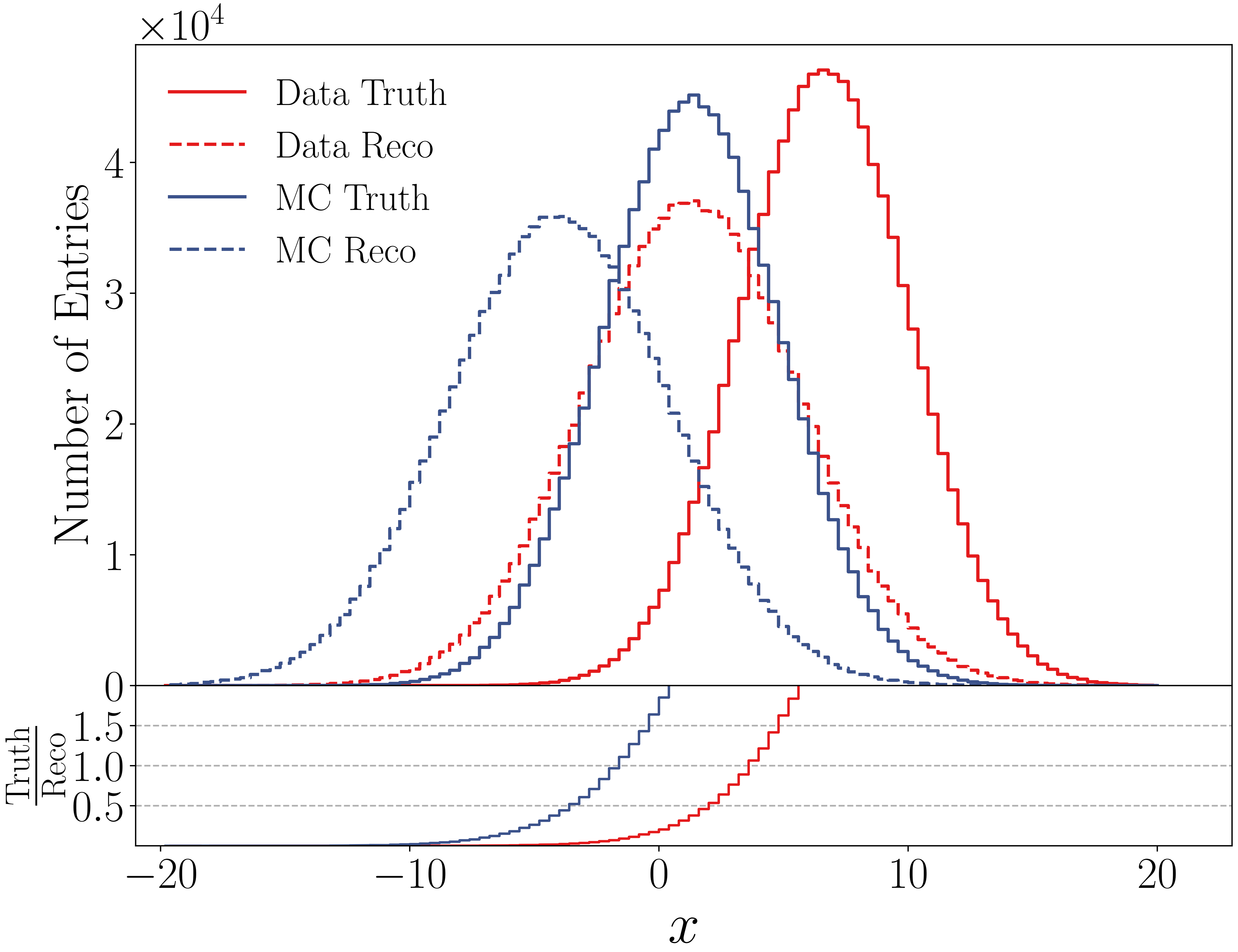
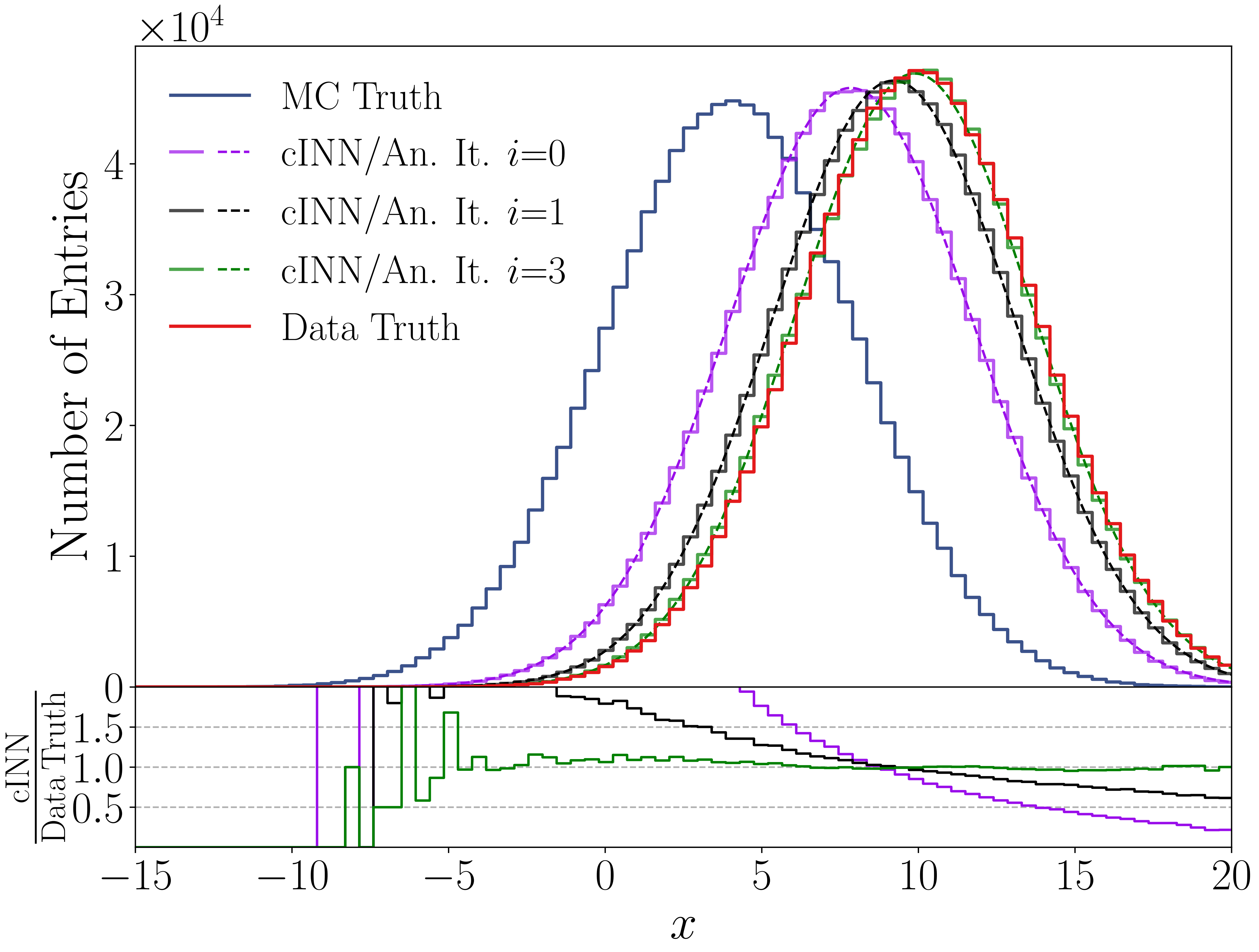


Figure from Backes et al.: arXiv:2212.08674

Iterative generative unfolding



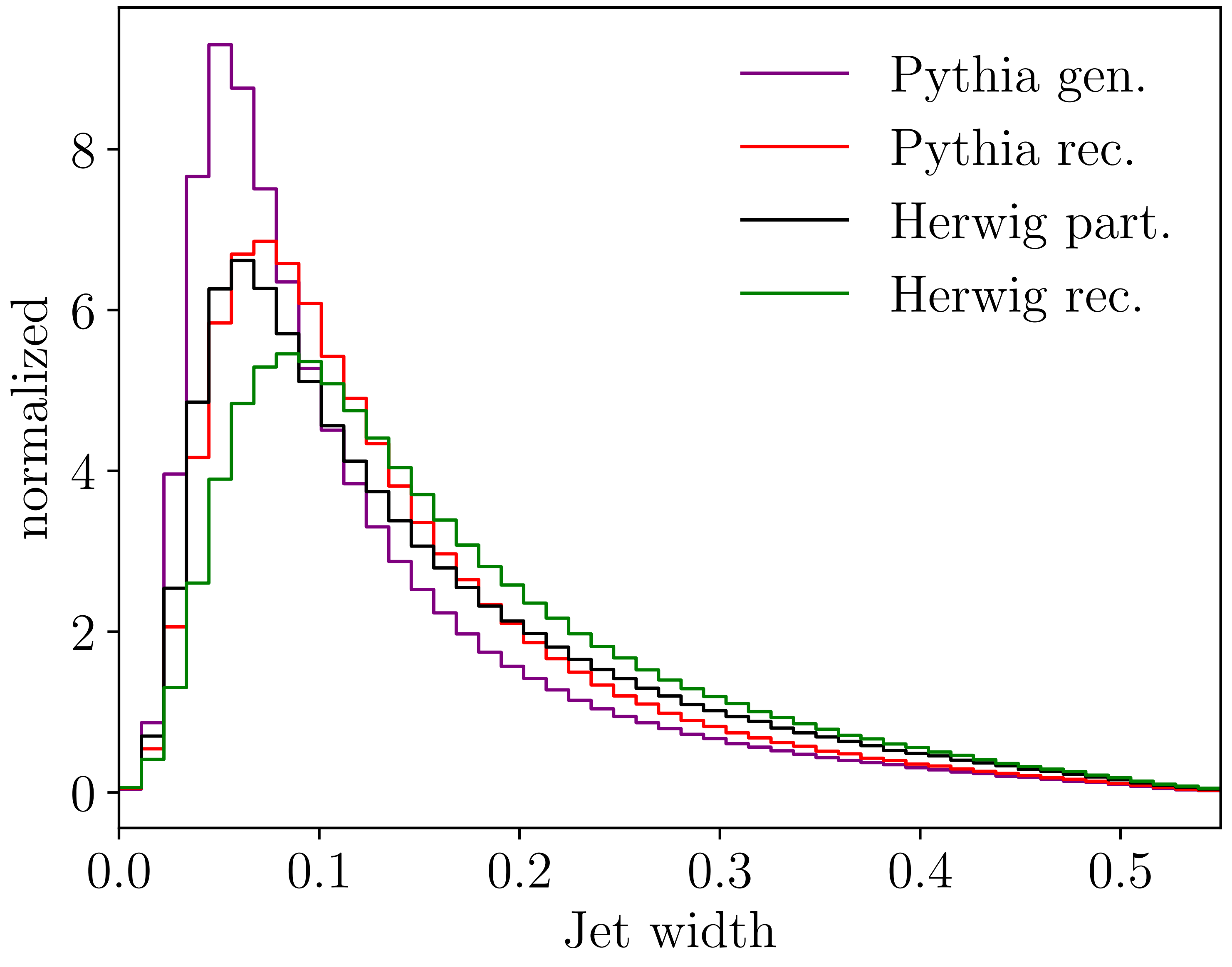


Figures from Backes et al.: arXiv:2212.08674

Z+jets: Pythia vs Herwig simulation

Use Pythia simulation as MC

Use Herwig simulation as Data



Following Andreassen et al. arXiv: 1911.09107