

Returning CP-observables to the frames they belong

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With

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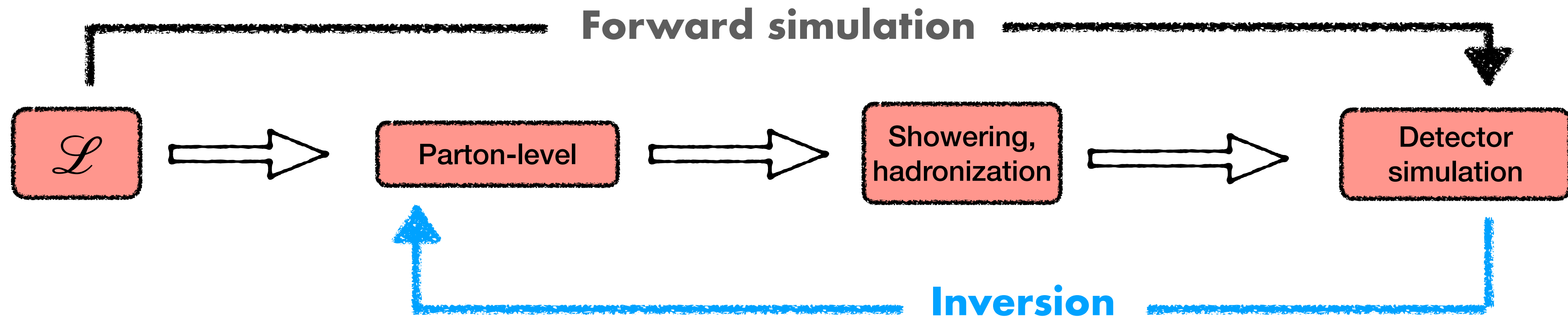
Based on
[arXiv: 2308.00027](https://arxiv.org/abs/2308.00027)

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Unfolding



- Conventional LHC analysis involves comparing measured data with MC events simulated under NP hypothesis.
 - Reconstructed LHC events present a convoluted version of the true underlying physics.
 - Forward simulation chain can be highly resource intensive.

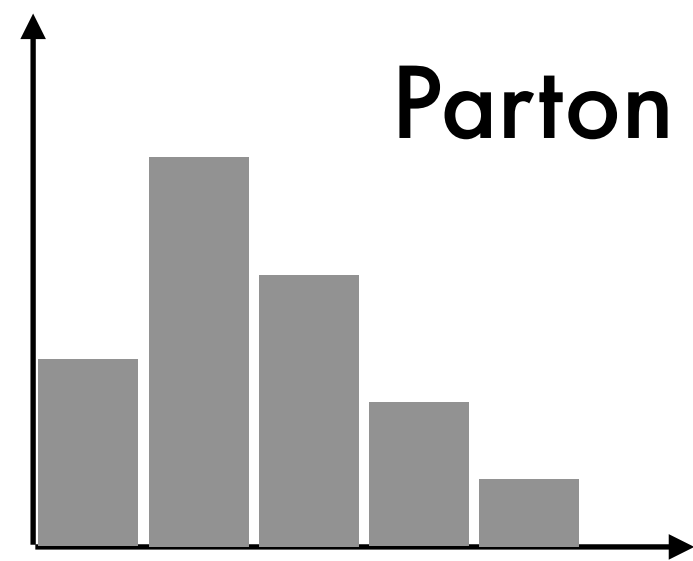
Invert simulation chain → apply on measured data → reconstruct parton-level

→ compare new physics hypotheses at the parton-level.

Unfolding

- **Bin-by-bin unfolding:**

- Correct the information in each bin using correction factor \mathcal{C}_i computed from MC data.



$$\mathcal{C}_i = N_{\text{truth},i} / N_{\text{reco},i}$$

Unfolded distribution: $x_{p,i} = x_{d,i} \times \mathcal{C}_i$



- **Matrix inversion:**

- Build response matrix $R \rightarrow$ each cell $\{i, j\}$ represents the fraction of events which have a true value in bin i but get reconstructed in bin j .

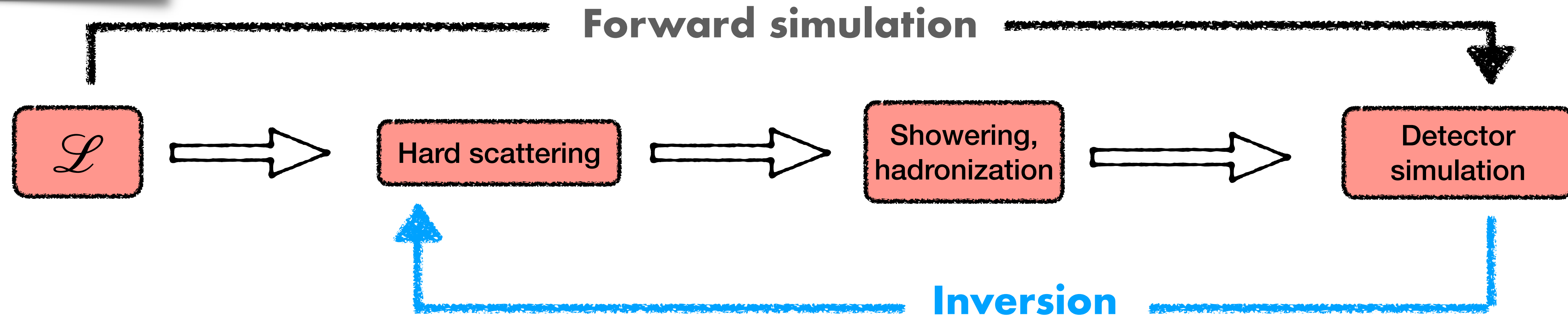
- **Iterative unfolding**

- Augment R_{ij} by correction factors computed by comparing generated with true parton level data.

❖ Bin-dependent unfolding.

❖ Dimensionality limitations.

ML-Unfolding



◆ Bin-independent

◆ Able to invert multi-dimensional d.o.f.

Possible with machine learning based generative models.

- Generative Adversarial Networks (GAN)
- Normalizing Flows (NF)
- Variational Auto Encoders (VAE)

[Bellagente, Butter, Kasieczka, Plehn, Winterhalder (2020)]

[Bellagente, Butter, Kasieczka, Plehn, Rousselot, Winterhalder, Ardizzone, Kothe (2020)]

[Andreassen, Komiske, Metodiev, Nachman, Thaler (2020)]

[Komiske, McCormack, Nachman (2021)]

GANs

In GANs, the generator and discriminator network competes against each other.

[Bellagente, Butter, Kasieczka, Plehn, Winterhalder(2019)]

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G

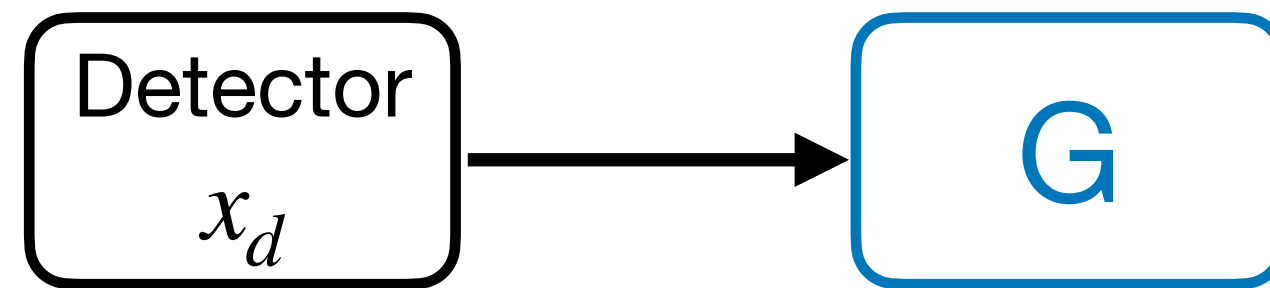
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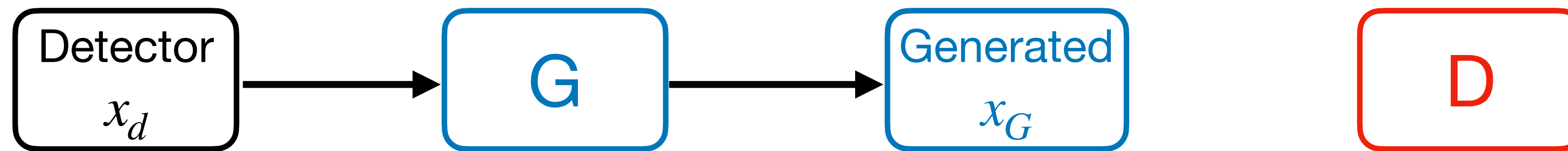


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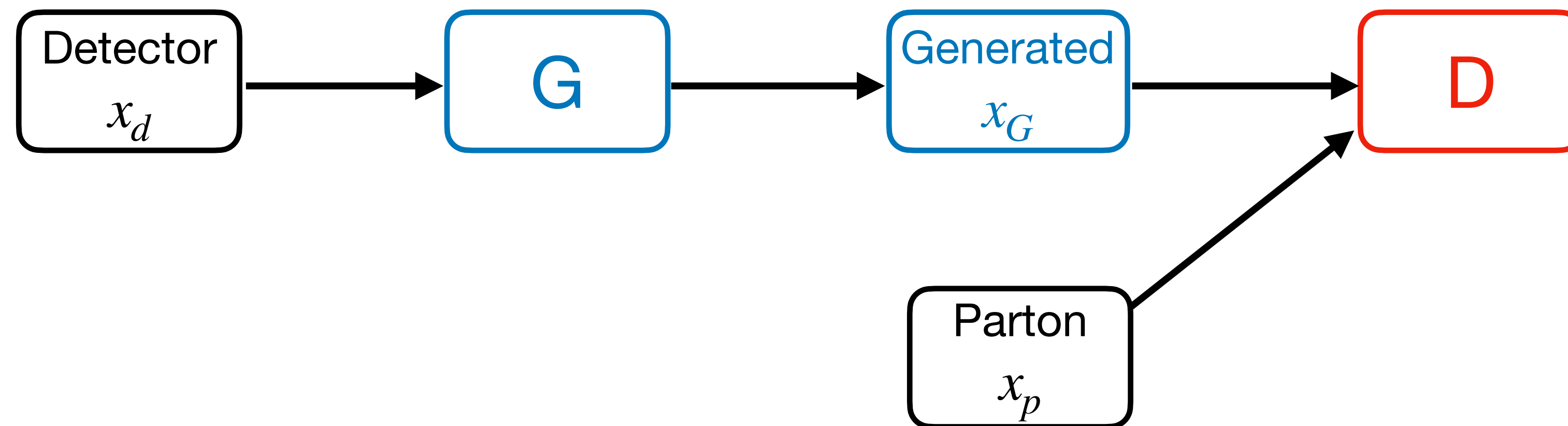


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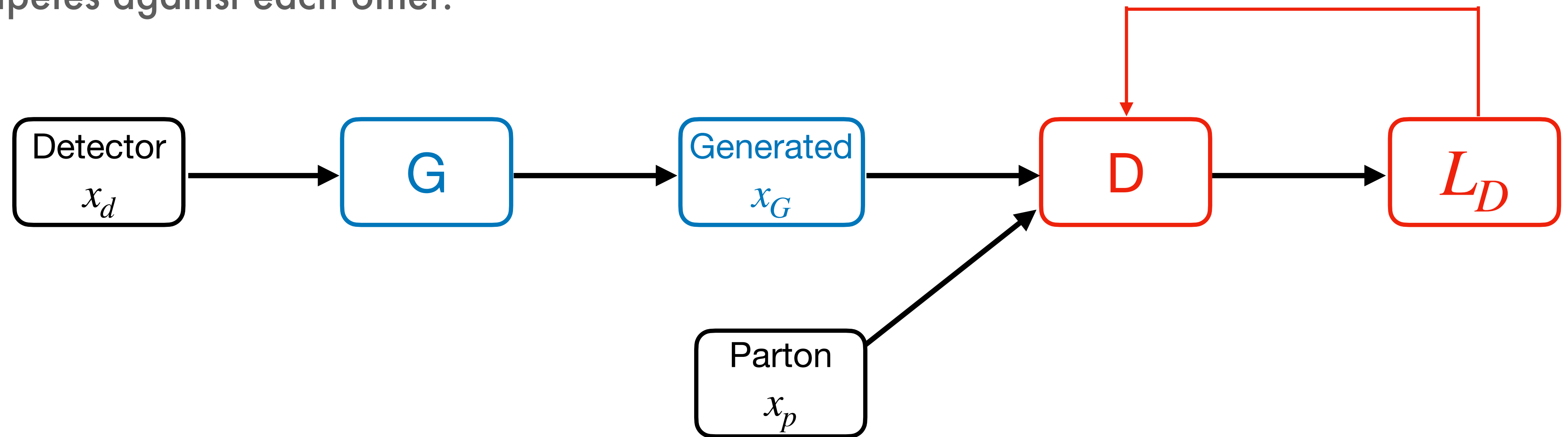
$$D(x_p) \rightarrow 1, \quad D(x_G) \rightarrow 0$$

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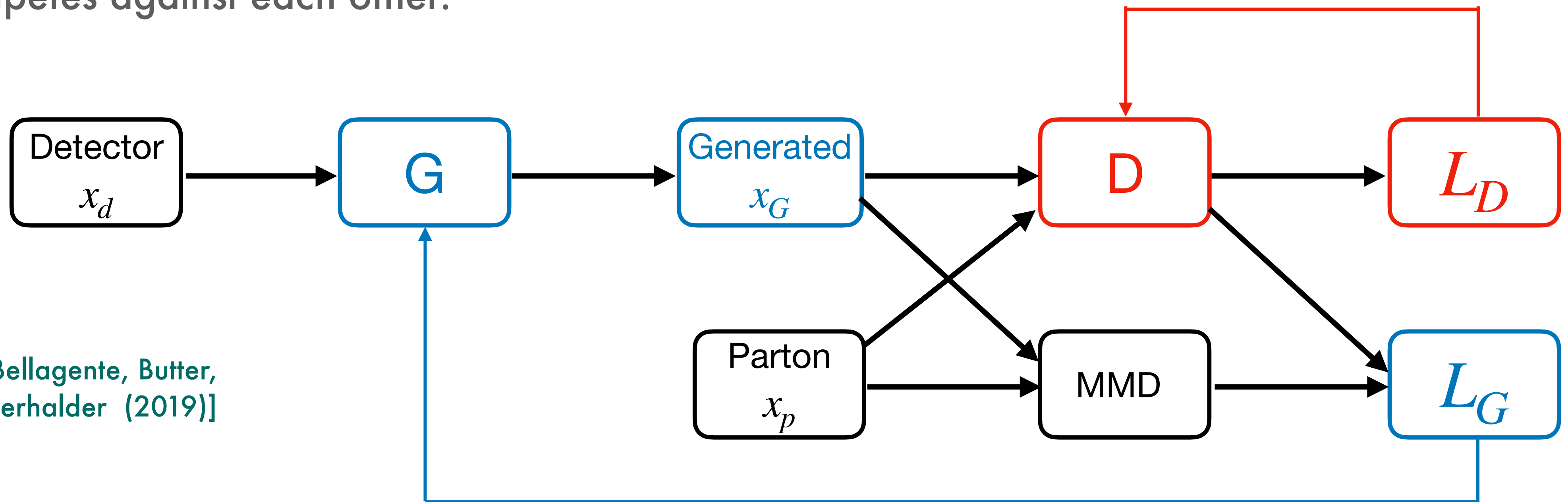
$$L_D = \langle -\log D(x) \rangle_{x \sim P_p} + \langle -\log(1 - D(x)) \rangle_{x \sim P_G}$$

GANs

In GANs, the generator and discriminator network competes against each other.

[Bellagente, Butter, Kasieczka, Plehn, Winterhalder(2019)]

[Butter, Plehn, Winterhalder(2019)]



[Image adopted from Bellagente, Butter, Kasieczka, Plehn, Winterhalder (2019)]

- Discriminator works to distinguish generated data $\{x_G\}$ from truth data $\{x_p\}$. [$D(x_p) \rightarrow 1, D(x_G) \rightarrow 0$]

- Generator works to fool the discriminator such that $D(x_G) \rightarrow 1$.

$$L_D = \langle -\log D(x) \rangle_{x \sim P_p} + \langle -\log(1 - D(x)) \rangle_{x \sim P_G}$$

$$L_G = \langle -\log D(x) \rangle_{x \sim P_G}$$

$$D(x_p) \rightarrow 1, \quad D(x_G) \rightarrow 0$$

Naive GAN unfolding

$$pp \rightarrow ZW \rightarrow (Z \rightarrow \ell^+ \ell^-)(W \rightarrow jj)$$

Training data

$$p_{T,j} > 25 \text{ GeV}, |\eta_j| < 2.5$$

2 ℓ + 2 j exclusive
@ detector level

Parton-level

Detector-level

- Targeted loss terms required for sharp kinematic features.
- Fails if training and test data to not statistically similar.

Test data

2 ℓ + 2 j exclusive @ detector level

$$30 \text{ GeV} < p_{T,j_1} < 60 \text{ GeV},$$

$$30 \text{ GeV} < p_{T,j_2} < 50 \text{ GeV}$$

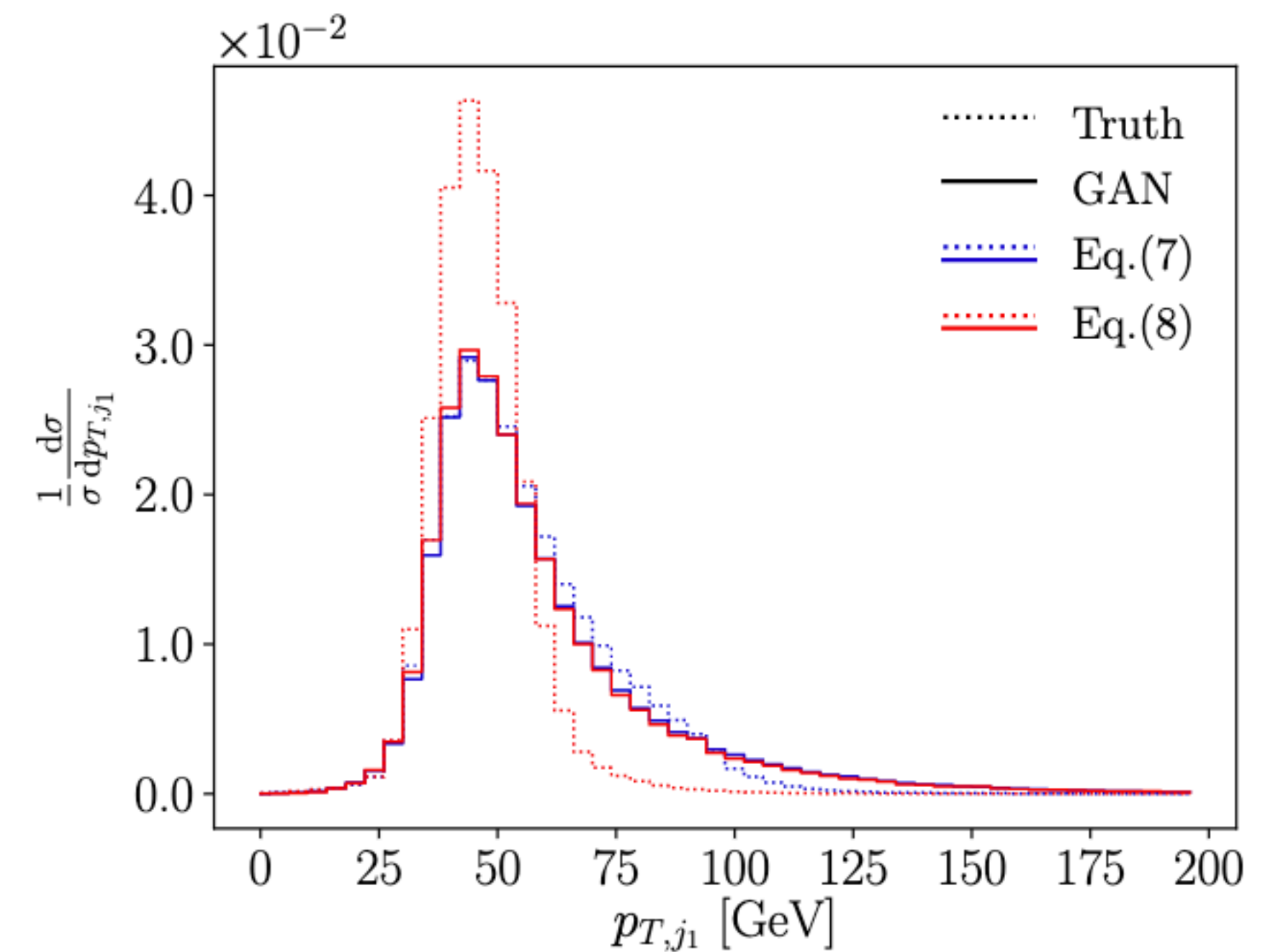
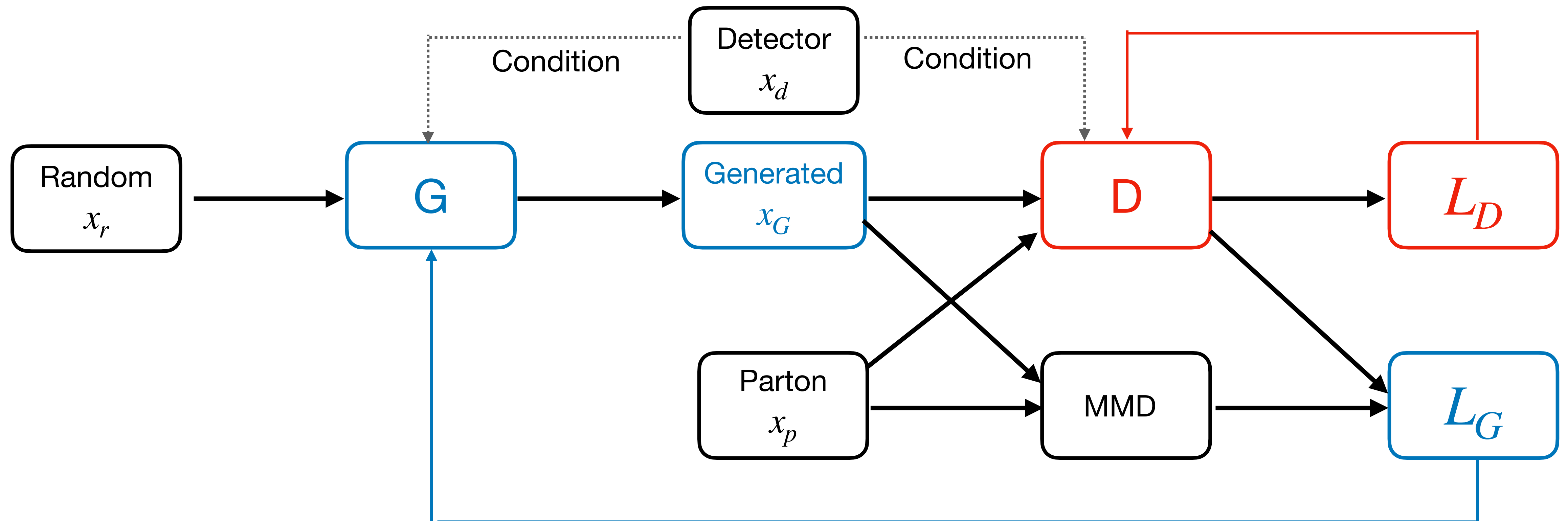


Figure taken from Bellagente, Butter, Kasieczka, Plehn, Winterhalder(2019)

Way-forward: FCGAN

[Image adopted from Bellagente, Butter, Kasieczka, Plehn, Winterhalder (2019)]



FCGAN

$$L_D^{FC} = \langle -\log D(x, y) \rangle_{x \sim P_p, y \sim P_d} + \langle -\log(1 - D(x, y)) \rangle_{x \sim P_G, y \sim P_d}$$

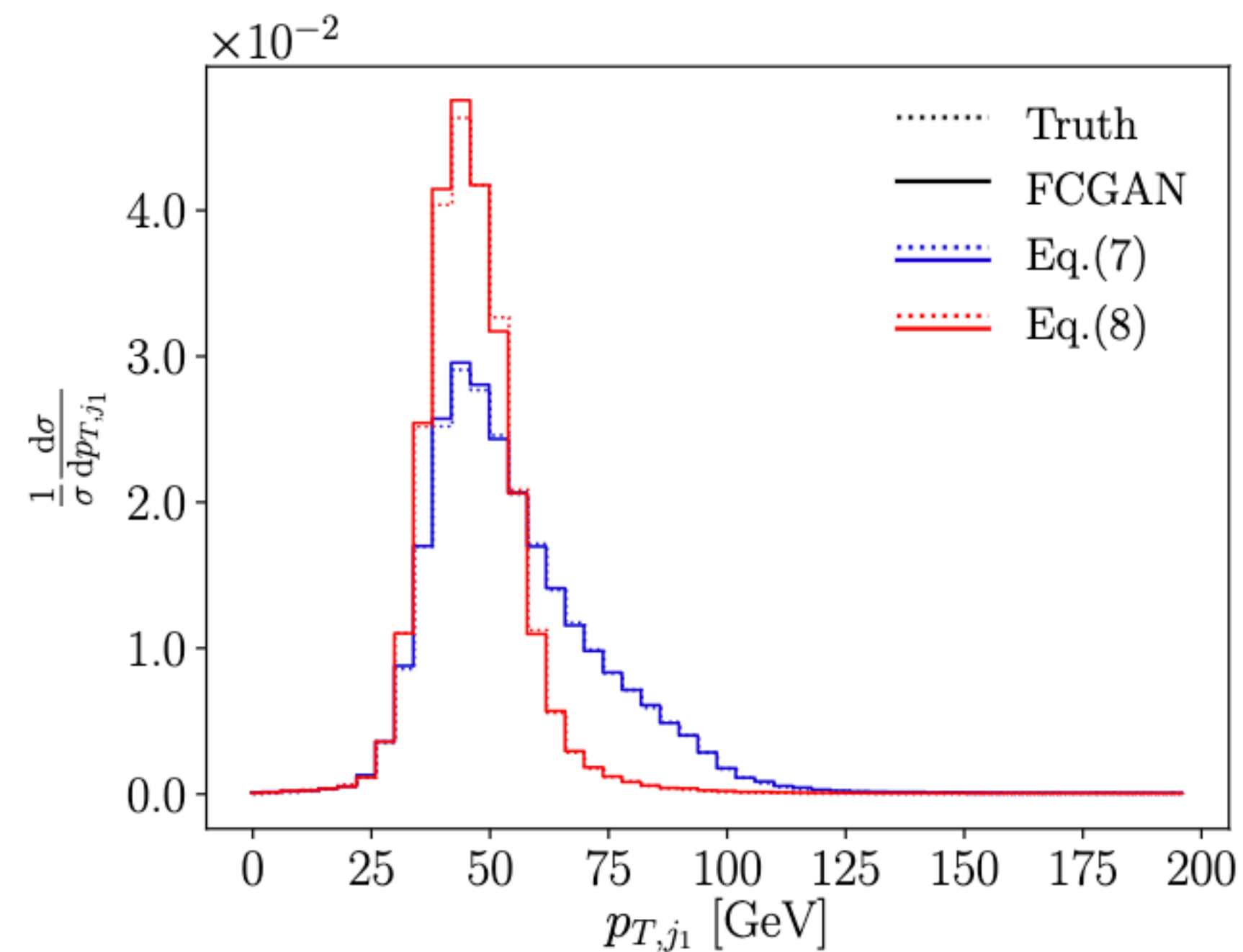
$$L_G = \langle -\log D(x, y) \rangle_{x \sim P_G, y \sim P_d}$$

- Event-by-event matching \rightarrow exploit the pairing information between parton and detector level.
- Trained network can be applied to statistically different regions of phase space.

Test data

$2\ell + 2j$ exclusive @ detector level

$30 \text{ GeV} < p_{T,j_1} < 60 \text{ GeV}, 30 \text{ GeV} < p_{T,j_2} < 50 \text{ GeV},$
($\sim 14\%$ of events)



[Image adopted from Bellagente, Butter, Kasieczka, Plehn, Winterhalder (2019)]

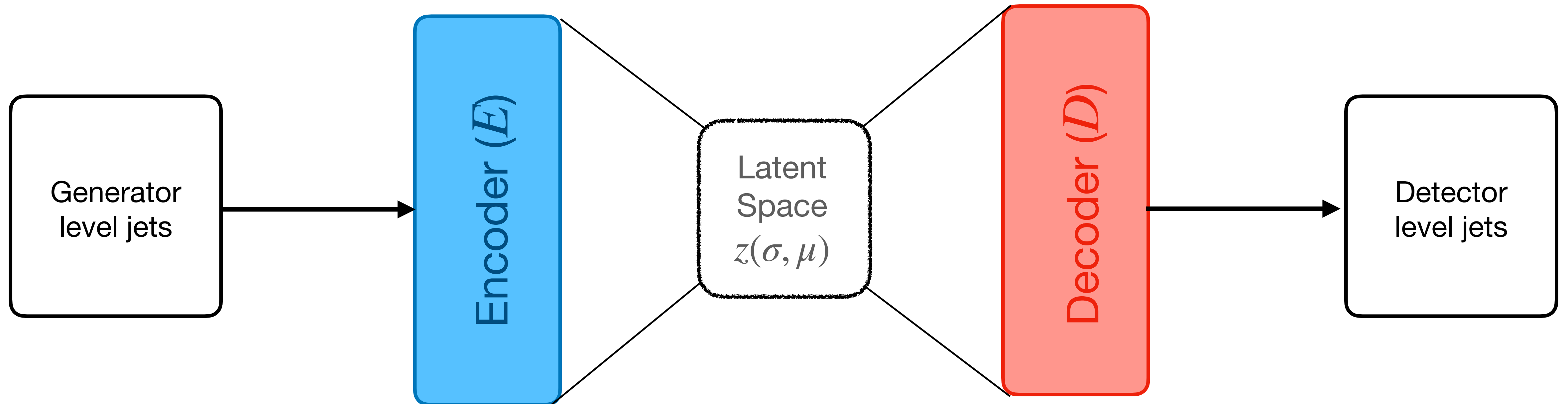
\rightarrow **Fails with harsher cuts !**

Variational Auto Encoders

→ Regress detector response function starting from a generator-level jet

[Touranakou, Chernyavskaya, Duarte, Gunopulos, Kansal, Orzari, Pierini, Tomei, Vlimant (2022)]

[Otten, Caron, Swart, Beekveld, Hendriks, Leeuwen, Podareanu, Austri, Verheyen (2019)]



$$L = ||y - D(E(x))||^2 + \eta KL(p(z|x) || q(Z))$$

Reconstruction Loss KL divergence term

[Ianazi, Sato, Ambrozewicz, Blin, Melnitchouk, Battaglieri, Liu, Li (2021)]

Variational Auto Encoders

→ Regress detector response function starting from a generator-level jet

[Touranakou, Chernyavskaya, Duarte, Gunopulos, Kansal, Orzari, Pierini, Tomei, Vlimant (2022)]

Process: $pp \rightarrow WW \rightarrow (W \rightarrow jj)(W \rightarrow jj)$

Training data

Jet constituents: $p_T > 250 \text{ MeV}, |\eta| < 3.2$

Jets (anti- k_T with $\Delta R = 0.5$): $p_T > 200 \text{ GeV}, |\eta| < 2.5$

Input-target jet matched
by minimizing ΔR

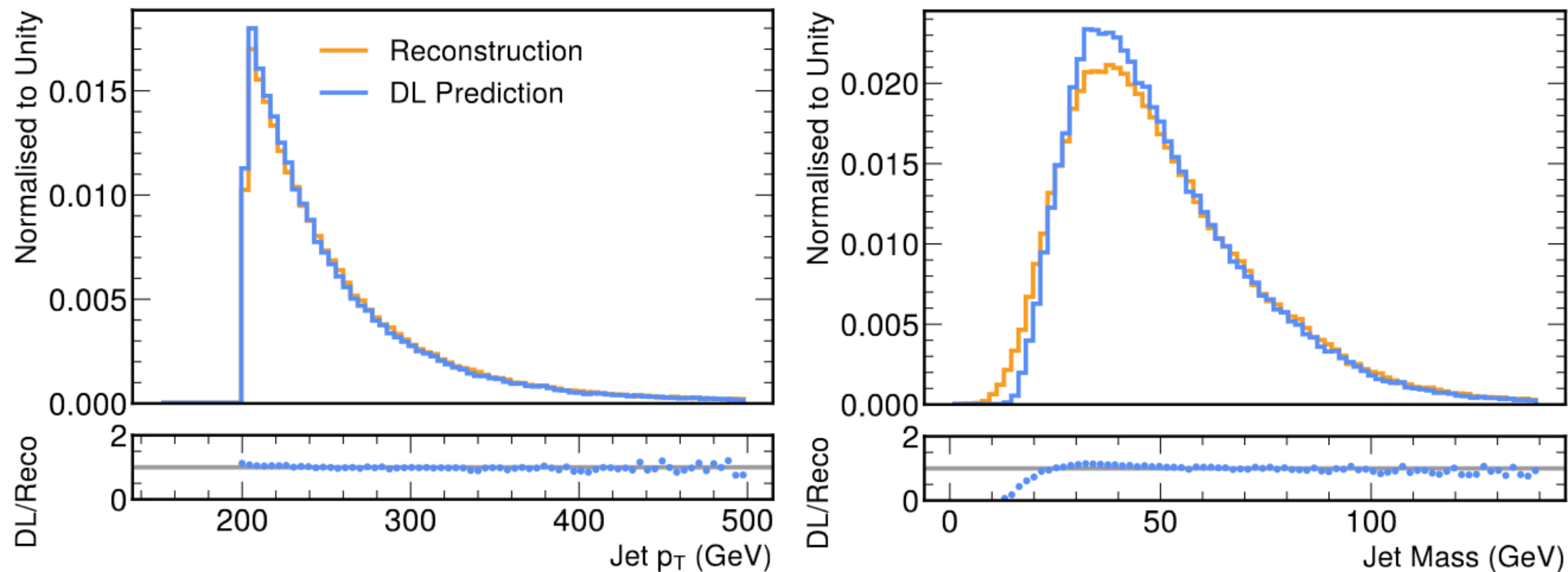
Generator-level

Detector-level

Variational Auto Encoders

Process: $pp \rightarrow WW \rightarrow (W \rightarrow jj)(W \rightarrow jj)$

$$\text{Loss } L \propto \beta D_{KL}^i + (1 - \beta)(L_R^i + \alpha_m (m_{jet}^i - \tilde{m}_{jet}^i)^2 + \alpha_{p_T} (p_T^i - \tilde{p}_T^i)^2)$$



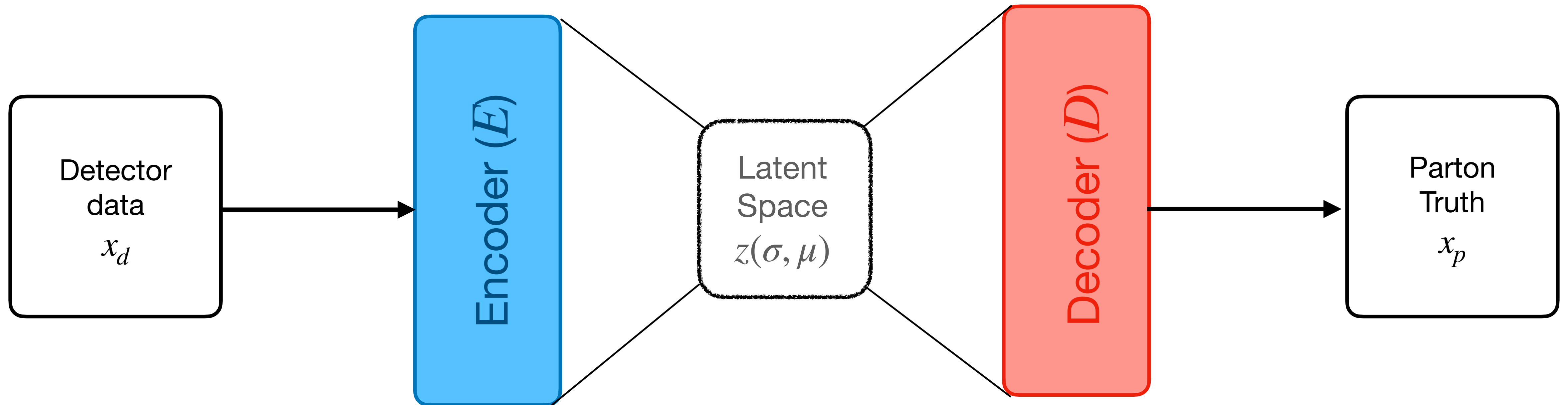
Figures taken from Touranakou, Chernyavskaya, Duarte, Gunopulos, Kansal, Orzari, Pierini, Tomei, Vlimant (2022)

Good agreement between reco and predicted distributions, but jet substructure quantities not well reproduced.

Variational Auto Encoders

☑ Unfolding

→ Map detector data to the parton level phase space



- The Encoder maps the input detector data d to a more tractable latent space $z = E(d)$ while preserving the essential features.
- The decoder maps z to the parton level $p' = D(z) = E(l(d))$.

Normalizing flows

☑ Exact likelihood estimation

☑ Invertibility :

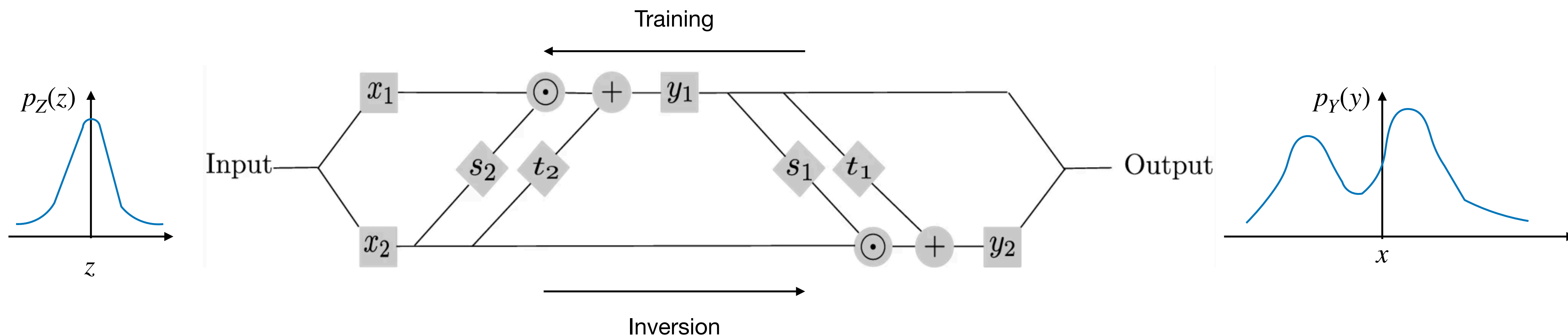
- ▶ **NF**: capable of bi-directional mapping w/o information loss.
- ▶ **VAEs**: not strictly invertible due to stochasticity of the latent space.
- ▶ **FCGANs**: focus on generation (sharper data), and invertibility is not strictly defined.

☑ Flexibility:

- ◎ **NF** can model intricate distributions without making strict assumptions.
- ◎ **VAEs** assume a **Gaussian latent space** → may not always capture the complexity of the distributions.
- ◎ **GANs** focus on generating data that matches the target distribution → no explicit latent mapping and less statistical robustness.

Normalizing flows

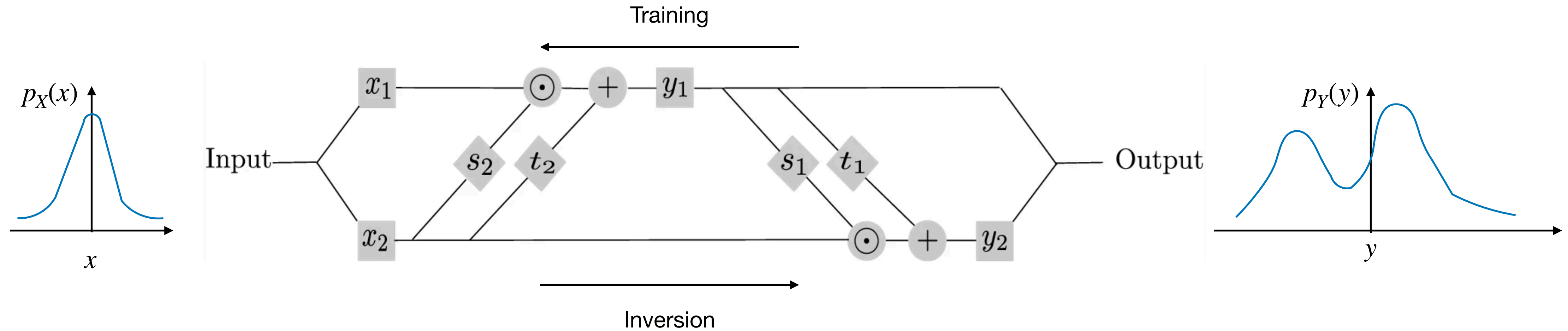
- Series of bijective layers that transform complex (Y) to simple probability distributions (Z).
- Learns both directions of the mapping in parallel \rightarrow bijectivity encoded in the same network.
- Building blocks \rightarrow Invertible coupling layers. [Dinh, Krueger, Bengio (2016), Dinh, Sohl-Dickstein, Bengio (2016)]



[Image adapted from Nguyen, Ardizzone, Kothe (2019) and talk by A. Butter at Pheno-2022]

Normalizing flows

[Image adapted from Nguyen, Ardizzone, Kothe (2019)
and talk by A. Butter at Pheno-2022]



- In the coupling layers, the coupling functions s_2 and t_2 take x_2 as input, and scale/translate x_1 .

- Fully invertible coupling layer $\rightarrow [x_1, x_2]$ can be reconstructed given $[y_1, y_2]$

Forward pass:

$$y_1 = x_1 \odot e^{s_2(x_2)} + t_2(x_2)$$

$$y_2 = x_2 \odot e^{s_1(y_1)} + t_1(y_1)$$

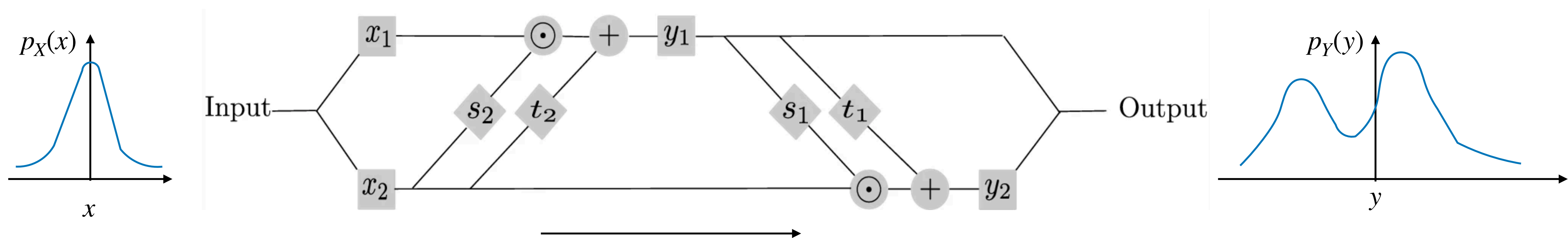
Inverse transformations:

$$x_1 = (y_1 - t_2(x_2)) \odot e^{-s_2(x_2)}$$

$$x_2 = (y_2 - t_1(y_1)) \odot e^{-s_2(y_1)}$$

Normalizing flows

[Image adapted from Nguyen, Ardizzone, Kothe (2019) and talk by A. Butter at Pheno-2022]



Forward pass:

$$y_1 = x_1 \odot e^{s_2(x_2)} + t_2(x_2)$$

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$$x_1 = (y_1 - t_2(x_2)) \odot e^{-s_2(x_2)}$$

$$x_2 = (y_2 - t_1(y_1)) \odot e^{-s_1(y_1)}$$

For a coupling block transformation $f(x) \sim y$

tractable Jacobian $J_f(x) : \frac{\partial f(x)}{\partial x} = \begin{bmatrix} e^{s_2(x_2)} & \text{finite} \\ 0 & e^{s_1(y_1)} \end{bmatrix}$

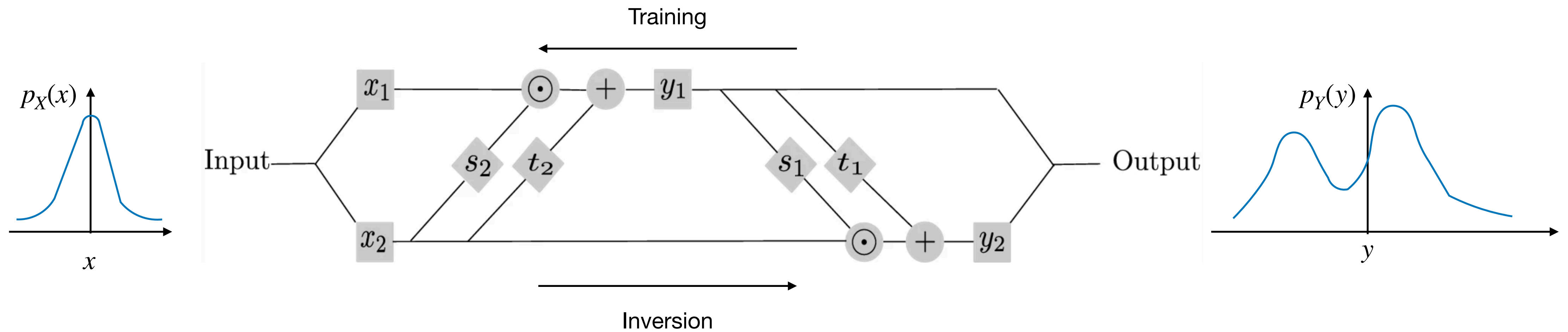
→ rule of change of variables

$$p_Y(x_d) = p_Z(x_p) \times |\det(J_f(x_p))|^{-1}$$

→ ensures bijective transformations and exact likelihood estimation

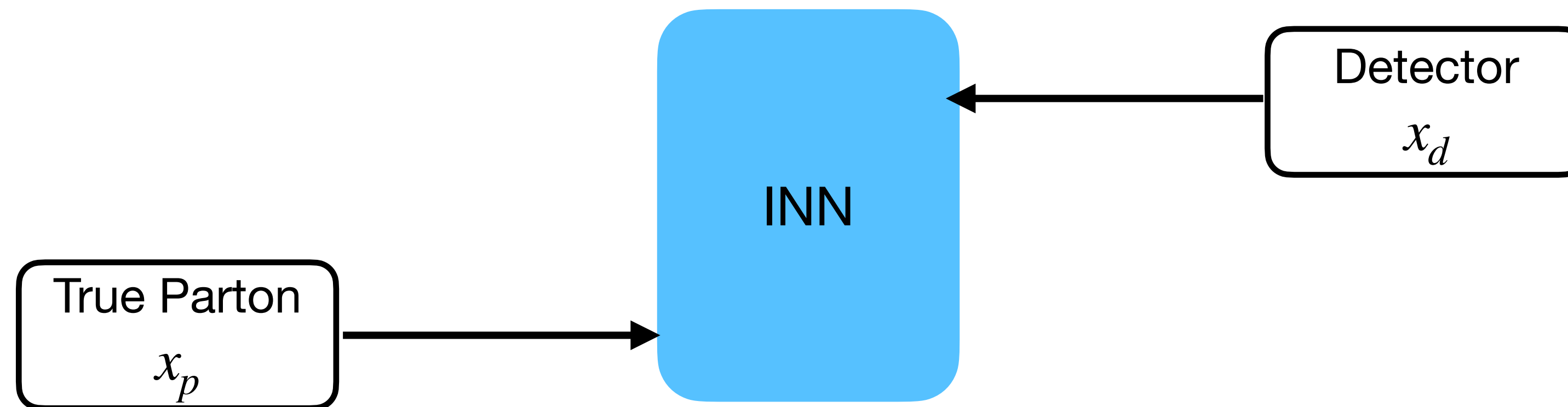
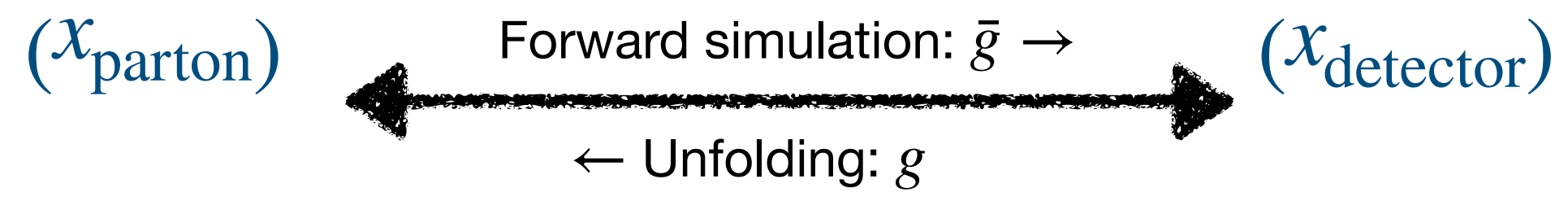
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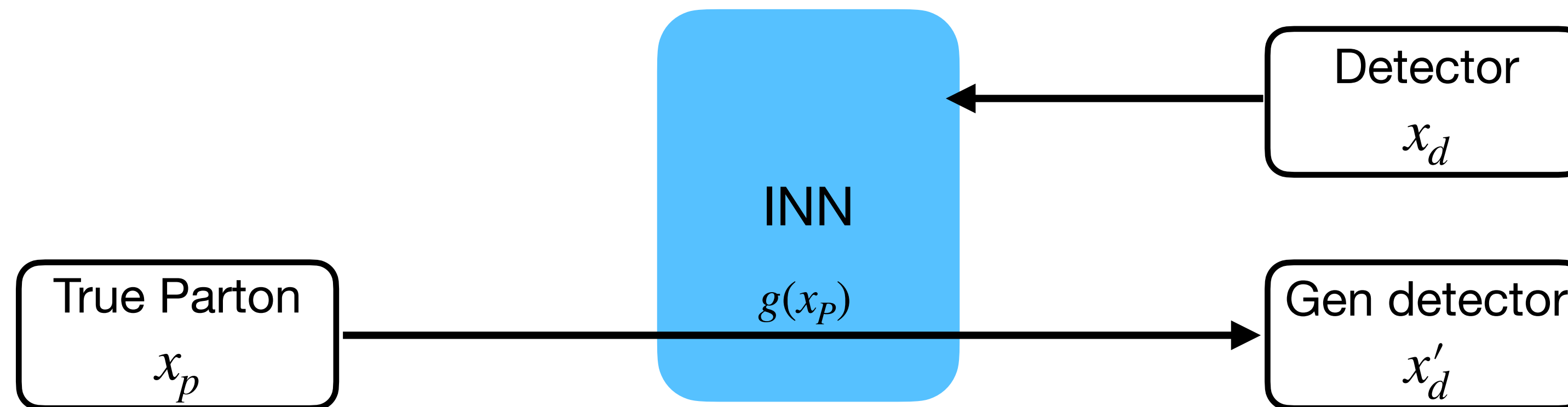
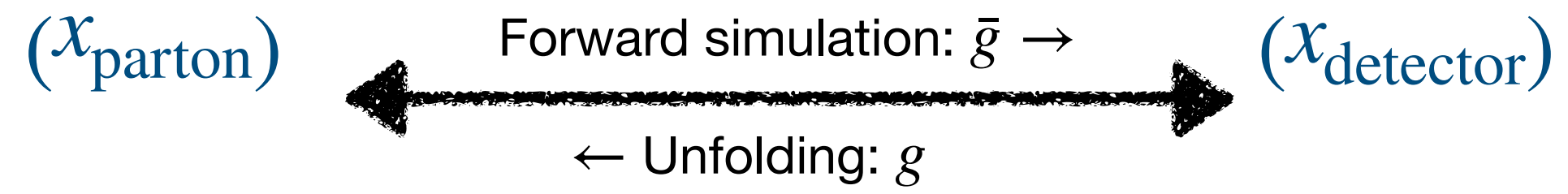


- Coupling layers stacked together → **Invertible Neural Network (INN)**.
- Typically, DNNs suffer an inherent information loss in the forward direction, making the inverse mapping ambiguous → **Not an issue with INNs**.

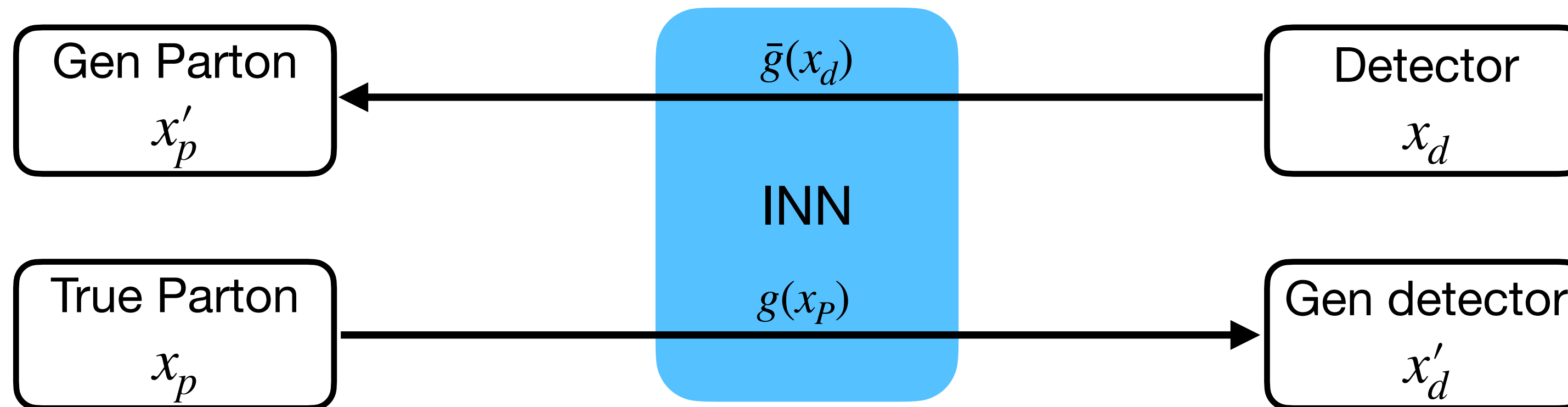
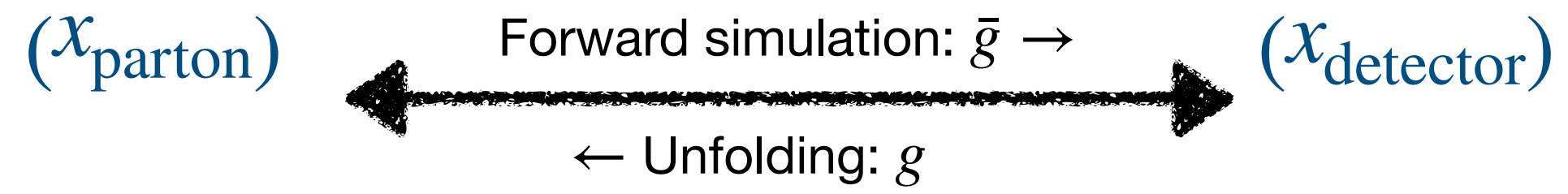
Naive INN unfolding



Naive INN unfolding



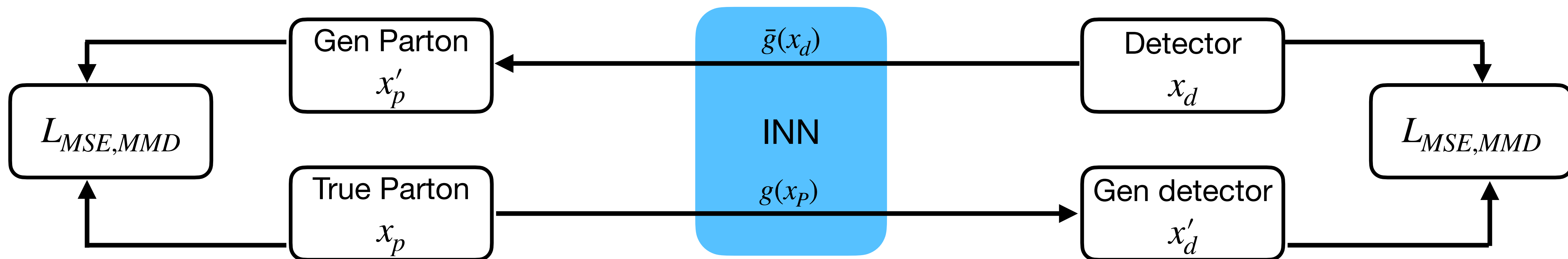
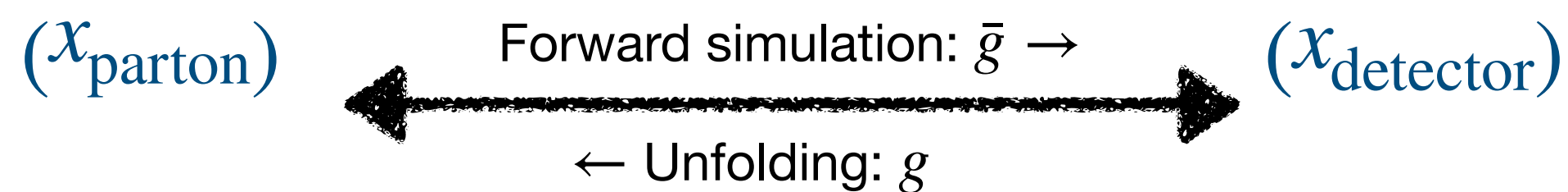
Naive INN unfolding



Naive INN unfolding

Process: $pp \rightarrow ZW \rightarrow (Z \rightarrow \ell^+ \ell^-)(W \rightarrow jj)$

[Figure adopted from Bellagente, Butter, Kasieczka, Plehn, Rousselot, Winterhalder, Ardigzone, Kothe (2020)]

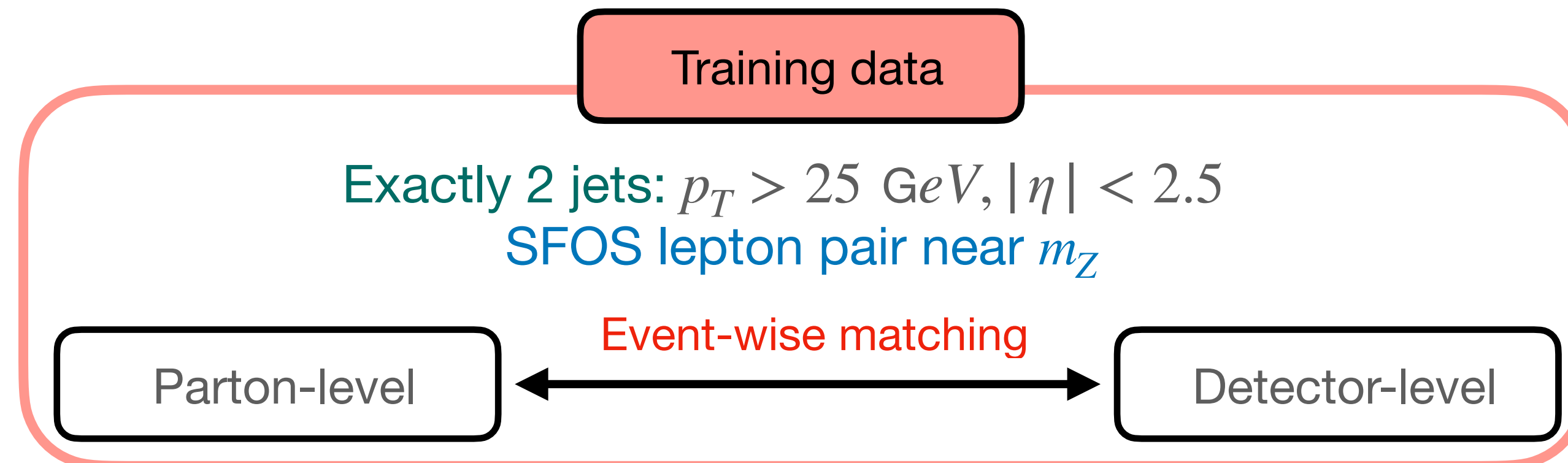
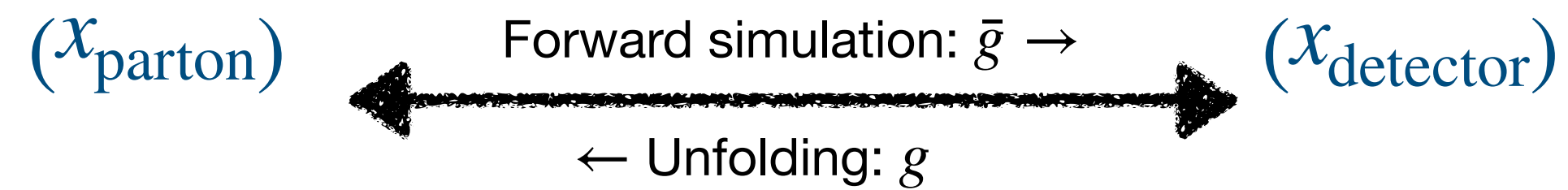


Loss: $L_{MSE}(x_p) + L_{MSE}(x_d) + L_{MMD}$

Naive INN unfolding

[Bellagente, Butter, Kasieczka, Plehn, Rousselot, Winterhalder, Ardizzone, Kothe (2020)]

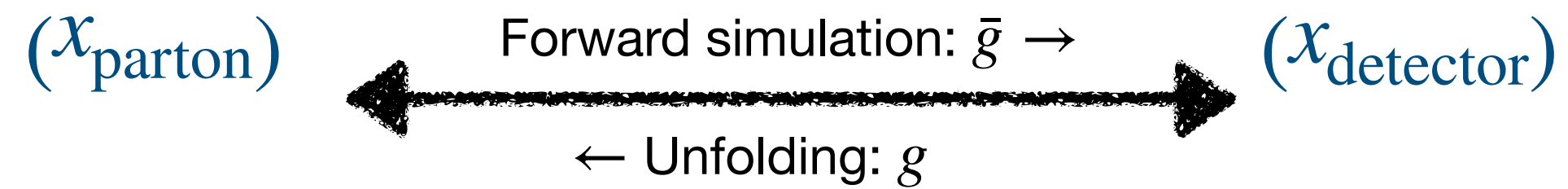
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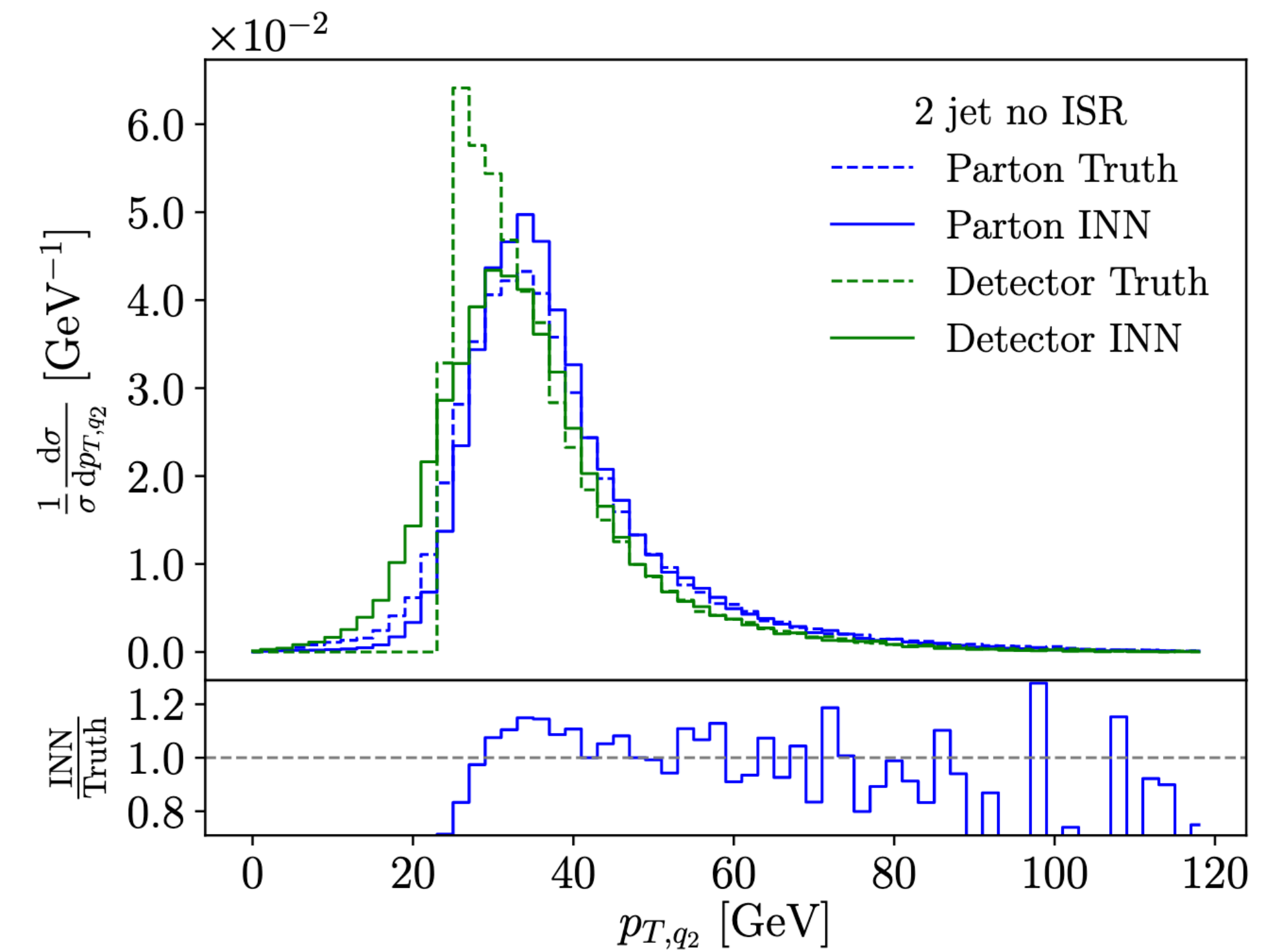
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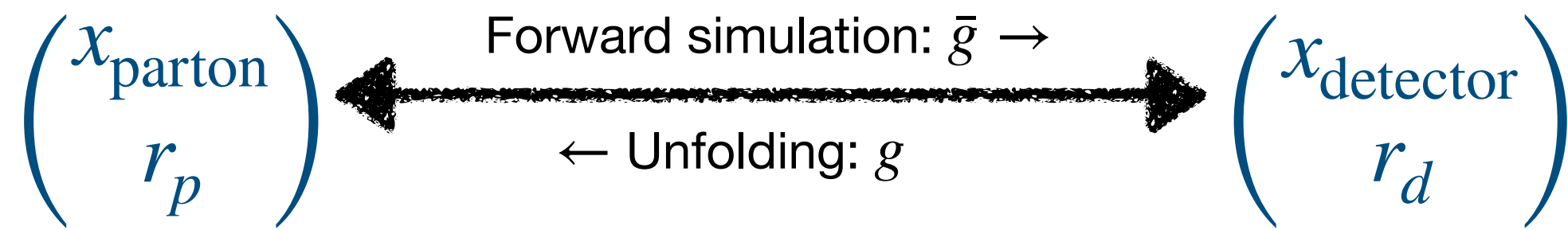
[Figure taken from Bellagente, Butter, Kasieczka, Plehn, Rousselot, Winterhalder, Ardigzone, Kothe (2020)]



- Differences between generated and parton truth deviate in the soft p_{T,j_2} region and tails.
- Typically inefficient in the inversion of features not included in event parametrization.
- Dimensionality limitations.

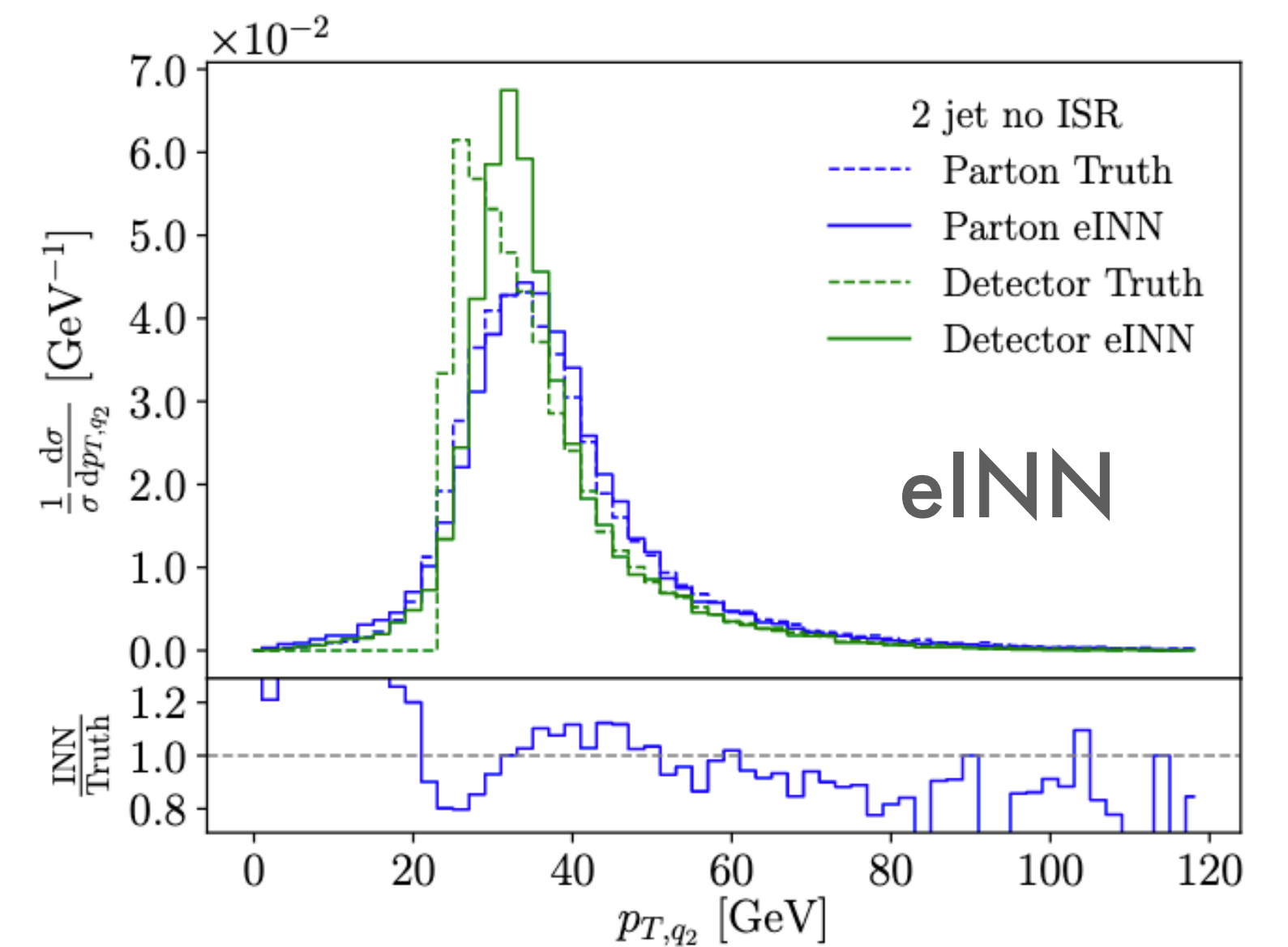
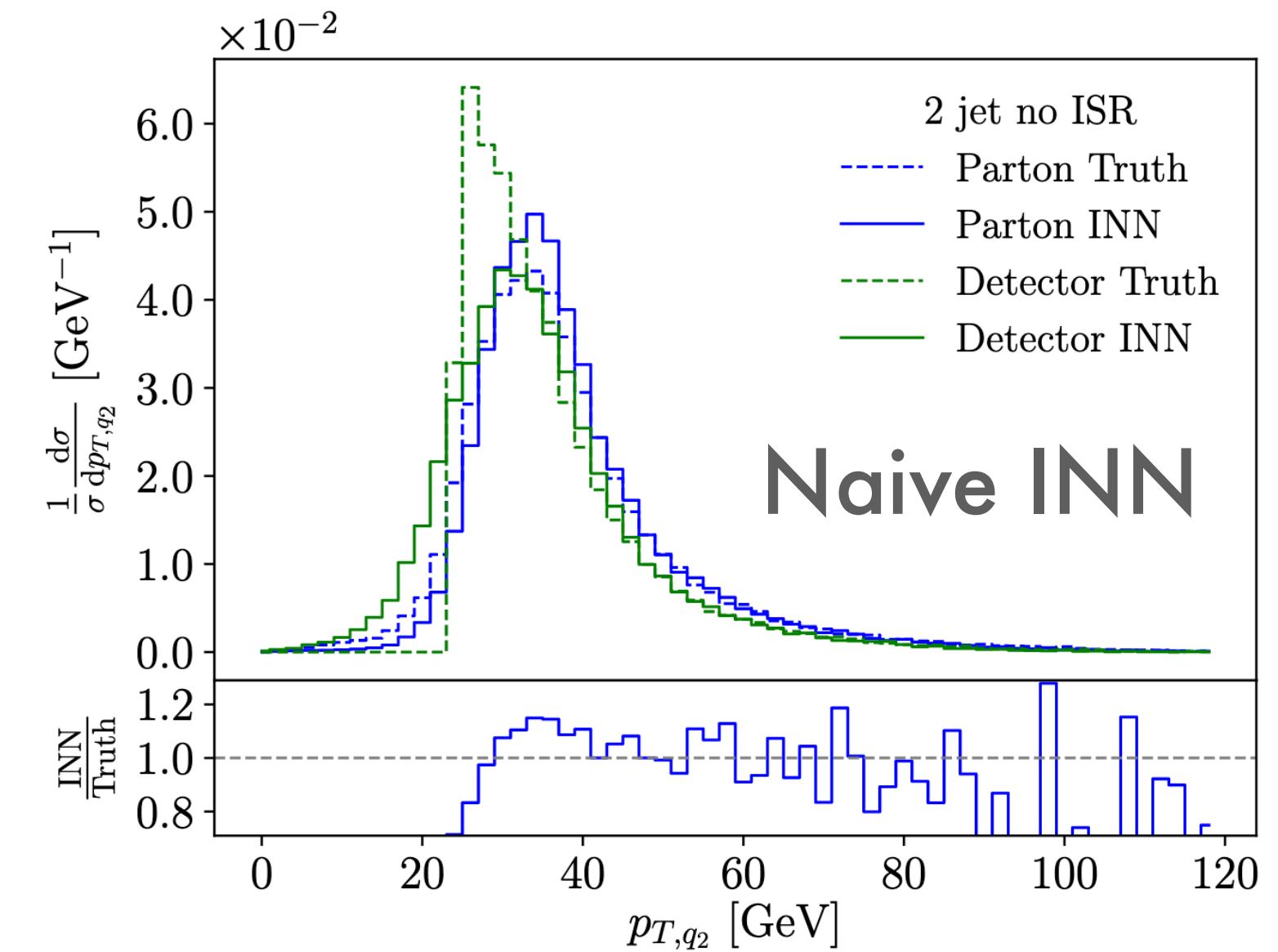


Noise-extended INN



- Allows mapping between unequal degrees of freedom at the parton and detector level.
- MMD terms included for each observable and gaussian input \rightarrow improves unfolding in the low and high p_T regions.

Process: $pp \rightarrow ZW \rightarrow (Z \rightarrow \ell^+ \ell^-)(W \rightarrow jj)$



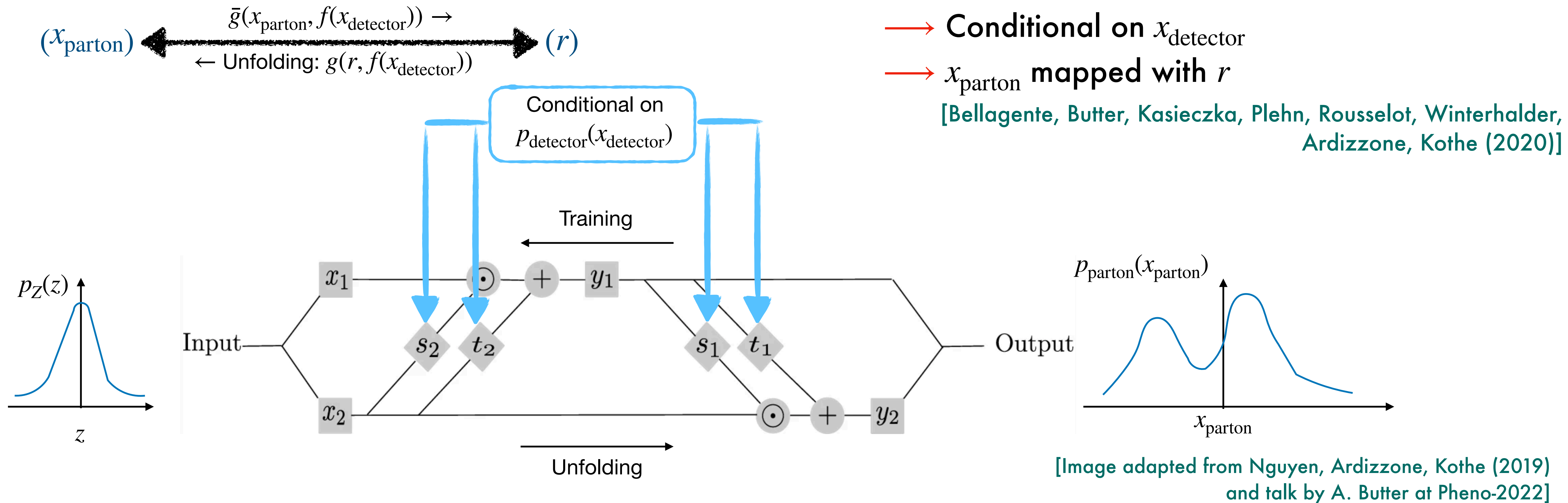
Noise-extended INN: Limitations and Challenges

- Inclusive detector level information requires using large number of random variables.
- Calibration of weights associated to different loss terms.
- Combination of several loss terms pose training challenges.

→ Upgrade to conditional INN

Conditional INN

- Generate probability distributions at the parton-level, given detector-level events x_{detector}



Target phase space for unfolding can be chosen flexibly to include:

- QCD jet radiation
- Particle decays

Unfolding semileptonic $t\bar{t}h$ events

$$pp \rightarrow t\bar{t}h \rightarrow (t \rightarrow \ell \nu b)(\bar{t} \rightarrow jj\bar{b})(h \rightarrow \gamma\gamma)$$

➔ Parton-level:

$$1\ell + 2b + 2\gamma + \nu + 2j$$

➔ Detector-level:

$$1\ell + 2b + 2\gamma + MET + \leq 6 \text{ jets inclusive}$$

Acceptance cuts

$$|\eta_b| < 4, \quad |\eta_j| < 5, \quad |\eta_\ell| < 4, \quad |\eta_\gamma| < 4$$

$$p_{T,b} > 25 \text{ GeV}, \quad p_{T,j} > 25 \text{ GeV}, \quad p_{T,\ell} > 15 \text{ GeV}, \quad p_{T,\gamma} > 15 \text{ GeV}$$

Challenges:

- ★ Can the unfolding model correctly reconstruct the two hard jets at the parton level from a variable number of jets at the detector level?
- ★ How well can the dedicated BSM observables be reconstructed?
- ★ How model-dependent is the training?

Event parametrization

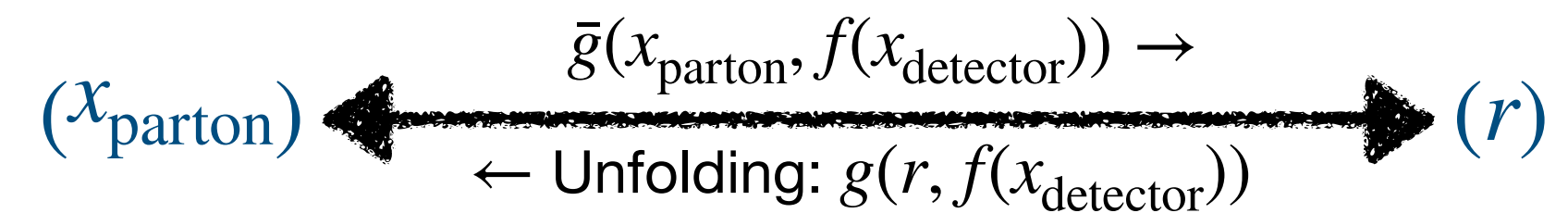
- Event information at the parton level can be parametrised through the 4-momentum of the final state particles → may include redundant d.o.f.
- **Reconstruction of sharp kinematic features like mass peaks can be challenging:**
 - ✓ Can be improved by adding targeted maximum mean discrepancy loss:
 - ✓ **Affects only the target distributions** [Butter, Plehn, Winterhalder (2019)]
 - ✓ **Avoids large model dependence** [Bellagente, Butter, Kasieczka, Plehn, Rousselot, Winterhalder, Ardizzone, Kothe (2020)]
 - ✗ **Complications in training and performance limitations.**

Alternative approach:

→ directly learn invariant mass features and important observable with appropriate phase-space parametrization.

→ may provide direct access to the most important BSM observables.

Conditional INN



- We use the Bayesian version of cINN [Butter, Heimes, Hummerich, Krebs, Plehn, Rousselot, Vent (2021)]
 - ▶ Stable network predictions
 - ▶ Allows the estimation of training-related uncertainties.

- Degrees of freedom:

Parton-level: $(t \rightarrow \ell \nu b)(\bar{t} \rightarrow jj\bar{b})h$
 22 d.o.f.

Detector-level:

46 d.o.f.

$1\ell + 2b + 2\gamma + MET + \leq 6$ jets inclusive

A natural parametrization involving top mass:

$$\left\{ m_t, p_{T,t}, \eta_t, \phi_t, m_W, \eta_W^t, \phi_W^t, \eta_{\ell,u}^W, \phi_{\ell,u}^W \right\}$$

- Alternatively, redefine the parton level parametrization including the important CP observables

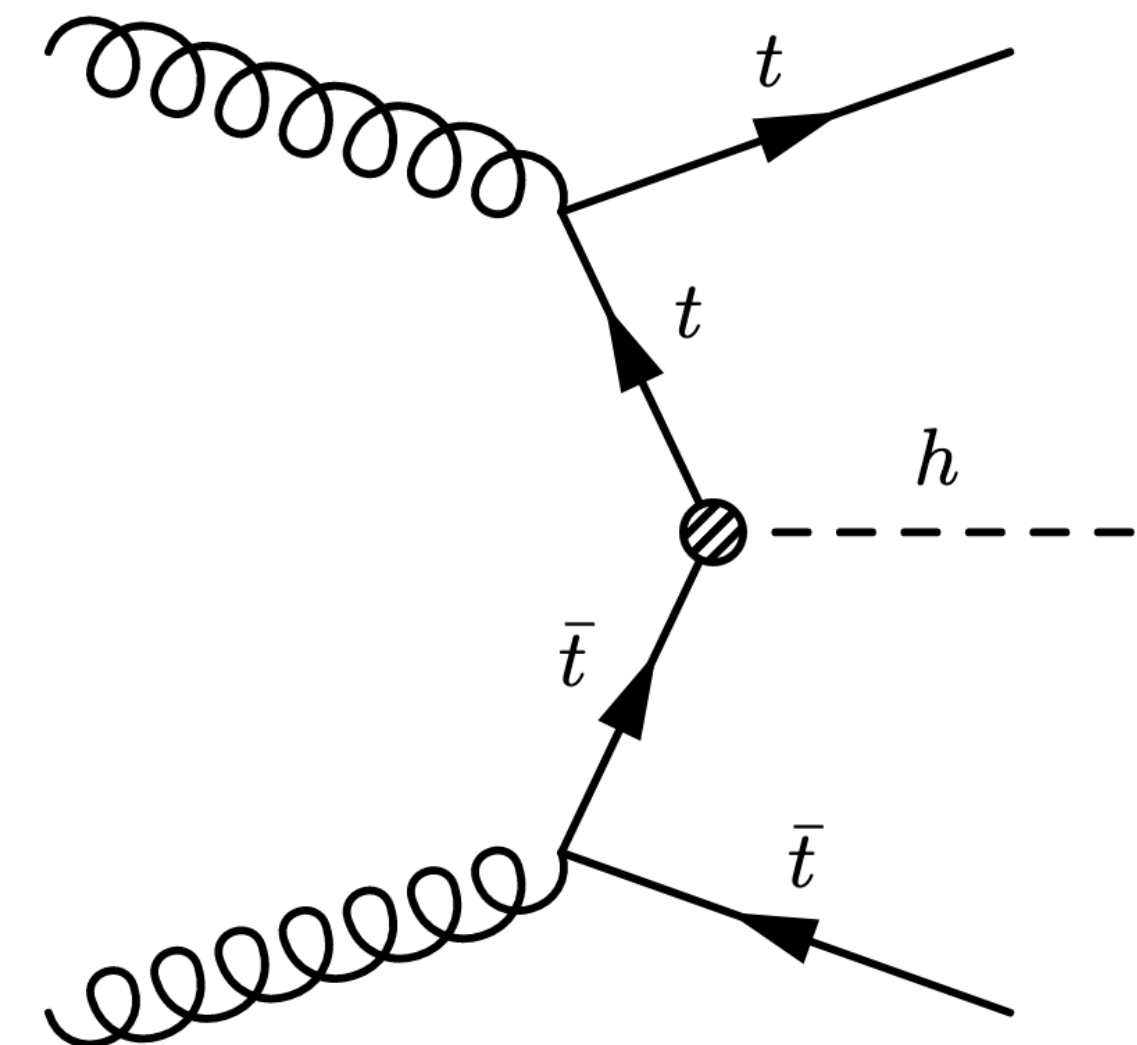
$$\begin{aligned} & \vec{p}_{t\bar{t}}, m_{t_\ell}, |\vec{p}_{t_\ell}^{\text{CS}}|, \theta_{t_\ell}^{\text{CS}}, \phi_{t_\ell}^{\text{CS}}, m_{t_h}, \\ & \text{sign}(\Delta\phi_{\ell\nu}^{t\bar{t}}) m_{W_\ell}, |\vec{p}_\ell^{t\bar{t}}|, \theta_\ell^{t\bar{t}}, \phi_\ell^{t\bar{t}}, |\vec{p}_\nu^{t\bar{t}}| \\ & \text{sign}(\Delta\phi_{du}^{t\bar{t}}) m_{W_h}, |\vec{p}_d^{t\bar{t}}|, \theta_d^{t\bar{t}}, \Delta\phi_{\ell d}^{t\bar{t}}, |\vec{p}_u^{t\bar{t}}| \end{aligned}$$

CP measurement in Higgs-top interactions

- New sources of CPV interactions can explain the matter-antimatter asymmetry in the universe.
- One such scenario: CP violation in the Higgs sector.
- CPV in hVV interactions is extensively tested at the LHC.

[See for instance: G. Aad et al. (1506.05669), G. Aad et al. (1602.04516), A. M. Sirunyan et al. (1707.00541), A. M. Sirunyan et al. (1903.06973), A. M. Sirunyan et al. (1901.00174), G. Aad et al. (2002.05315), Bernreuther, Gonzalez, Wiebusch (2010), Englert, Goncalves, Mawatari, Plehn (2012), Djouadi, Godbole, Mellado, Mohan (2013), Anderson, Bolognesi, Caola, Gao et al. (2013)]

- CPV in hff couplings manifest at tree-level:
→ desirable choice: $ht\bar{t}$



Direct probes at the LHC

$$\mathcal{L} = -\frac{m_t}{v}\kappa_t h\bar{t}(\cos\alpha + i\gamma_5 \sin\alpha)t$$

SM: $(\kappa_t, \alpha) = (1, 0)$

- $pp \rightarrow h$ (+ jets): indirect constraints.

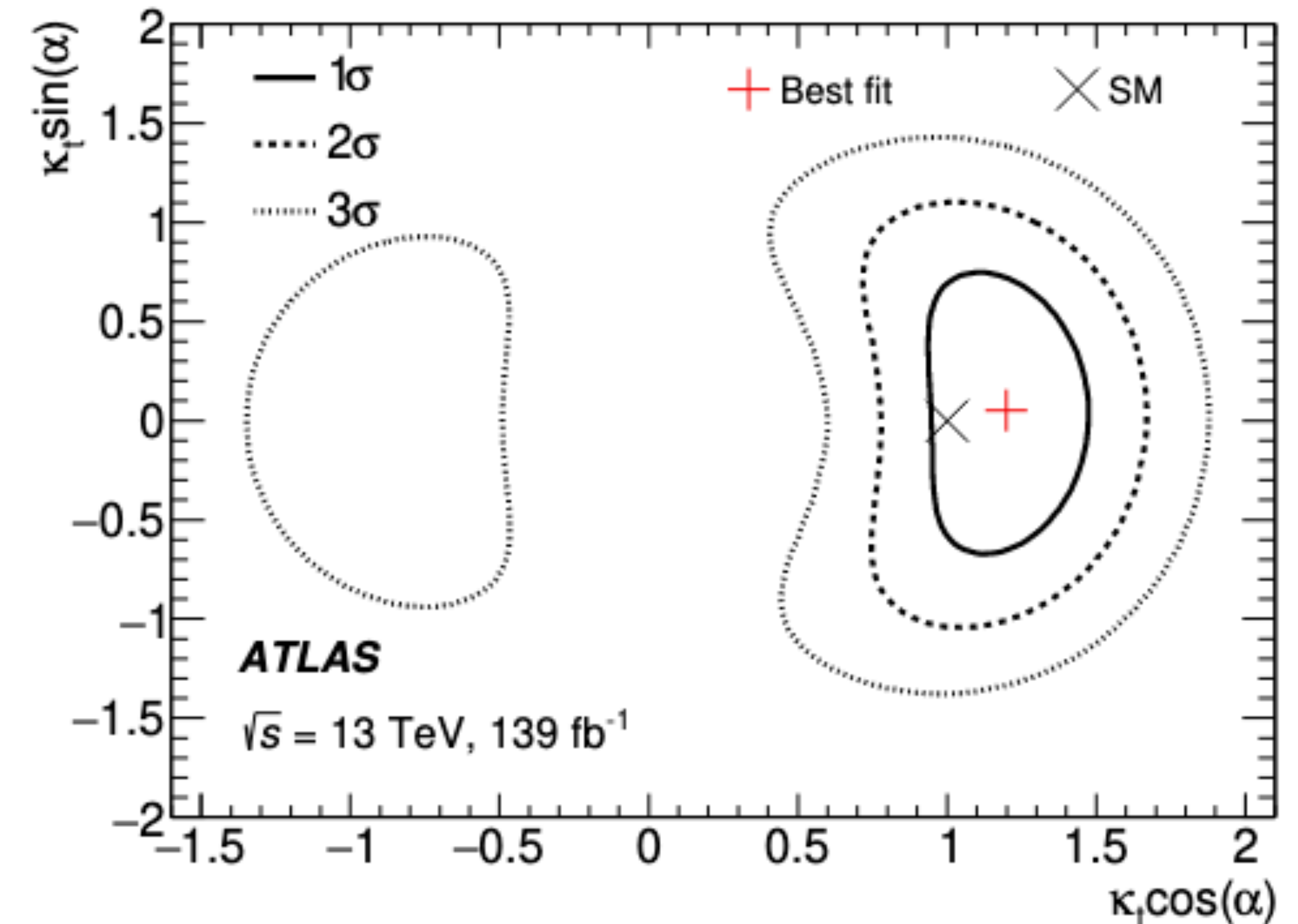
[Duca, Kilgore, Oleari, Schmidt, Zeppenfeld (2001), Klamke, Zeppenfeld (2007), Grojean et al. (2013), Dolan, Harris, Jankowiak, Spannowsky (2014)]

- $pp \rightarrow t\bar{t}h$ stands out as the viable direct probe:

- ◆ *Small rate at the LHC and complex topology.*

- ◆ **Silver Lining:** Observation at 5.2σ by ATLAS [2004.04545] and 6.6σ by CMS [2003.10866]

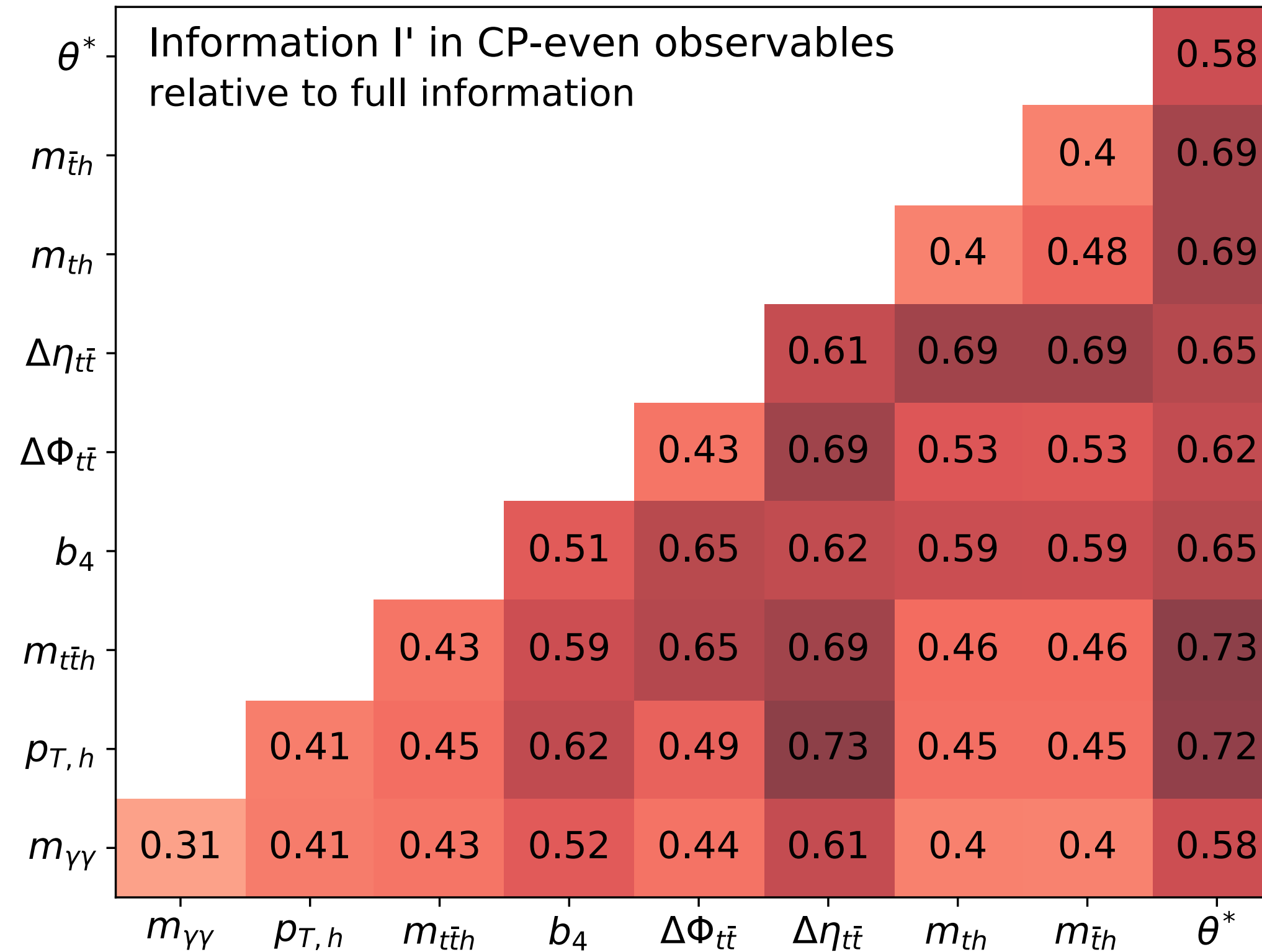
- **Current limits:** $|\alpha| < 43^\circ$ (ATLAS) and $|\alpha| < 55^\circ$ (CMS), at 95 % CL.



Improved statistics @ HL-LHC paves the pathway for precision studies.

$t\bar{t}(h \rightarrow \gamma\gamma)$ @ HL-LHC

Importance matrix at the **non-linear level**



[RKB, Goncalves, Kling (2021)]

Sensitive to non-linear new physics effects.

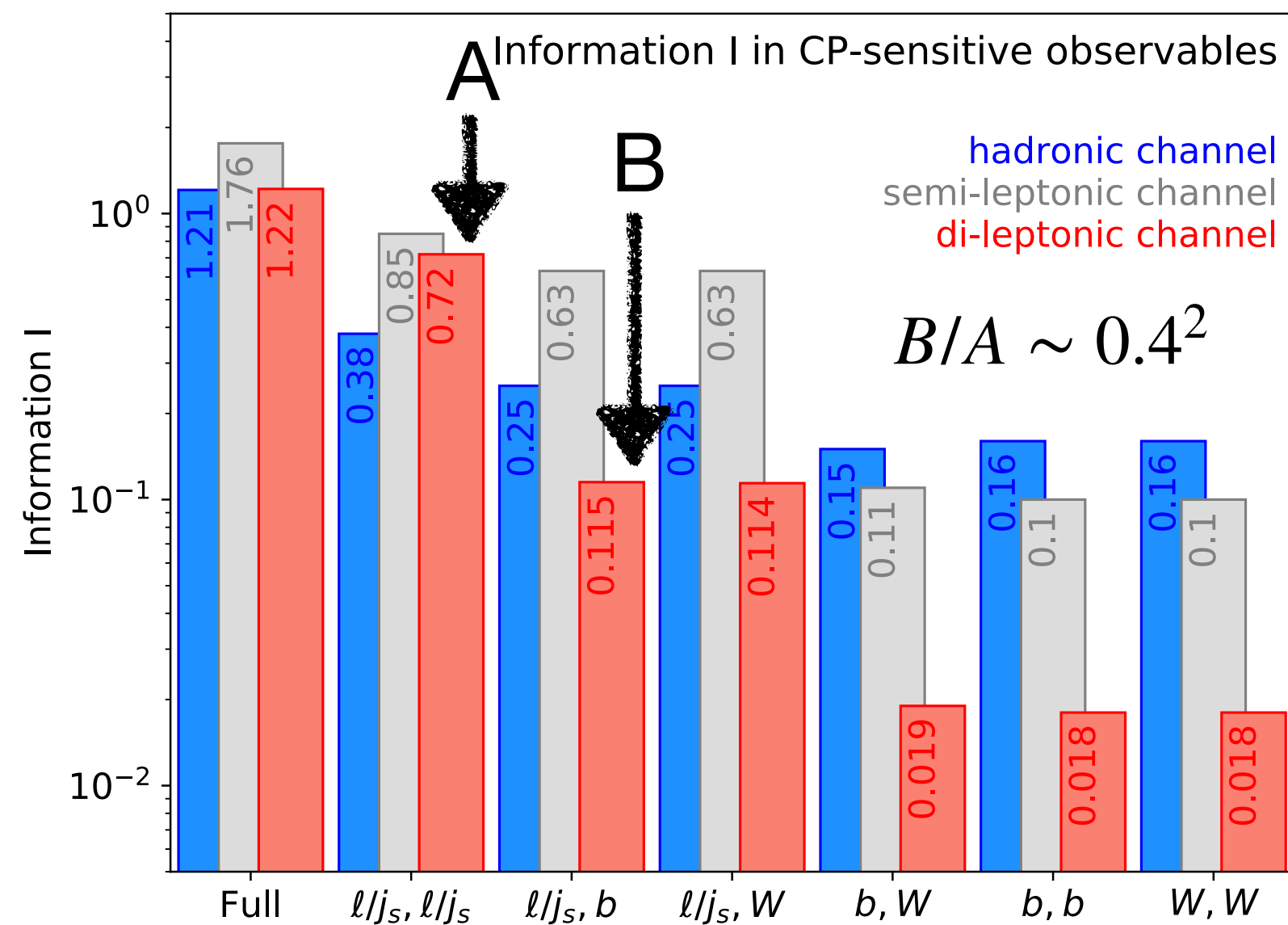
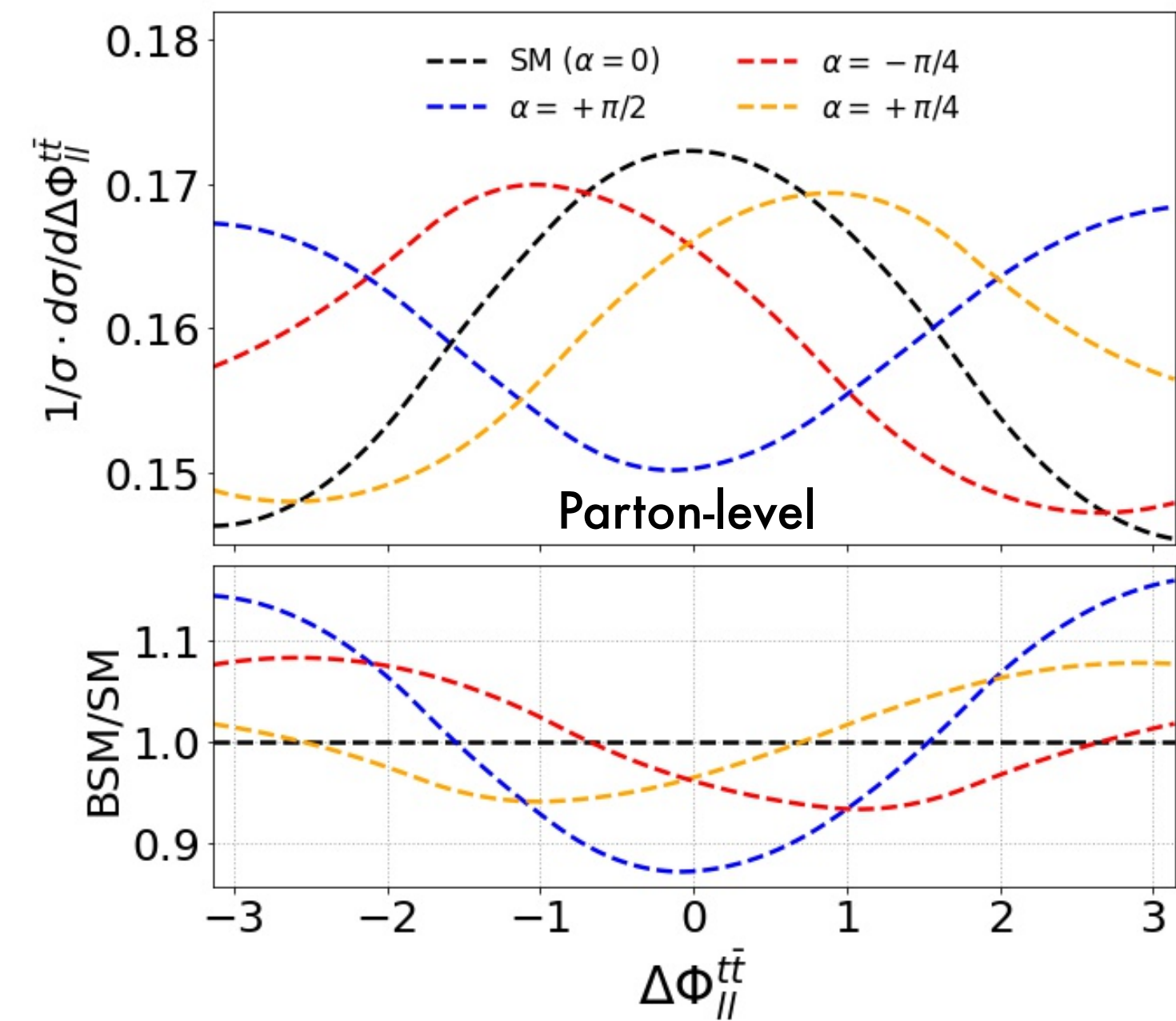
CP-odd observables

- Short lifetime for t (10^{-25} s) \rightarrow Spin correlations can be traced back from their decay products.

- CP-odd observables constructed from antisymmetric tensor products

$$\epsilon(p_t, p_{\bar{t}}, p_i, p_j) \sim \epsilon_{\mu\nu\rho\sigma} p_t^\mu p_{\bar{t}}^\nu p_i^\rho p_j^\sigma:$$

$$\Delta\phi_{ij}^{t\bar{t}} = \text{sgn} \left[\vec{p}_t \cdot (\vec{p}_i \times \vec{p}_j) \right] \arccos \left[\frac{\vec{p}_t \times \vec{p}_i}{|\vec{p}_t \times \vec{p}_i|} \cdot \frac{\vec{p}_t \times \vec{p}_j}{|\vec{p}_t \times \vec{p}_j|} \right]$$



← Spin correlations scale with the spin analysing power β_i .

[Mileo, Kiers, Szykman, Crane, Gegner (2016); Goncalves, Kong, Kim (2018)]; RKB, Goncalves, Kling (2021)]

$$\frac{1}{\Gamma} \frac{d\Gamma}{d \cos \xi_i} = \frac{1}{2} (1 + \beta_i P_t \cos \xi_i) \quad \left| \quad \text{Fisher Info} = \mathbb{E} \left[\frac{\partial \log p(x | \kappa_t, \alpha)}{\partial \alpha} \frac{\partial \log p(x | \kappa_t, \alpha)}{\partial \alpha} \right] \right.$$

- Kinematic reconstruction efficiency is limited at the detector level

Use Machine learning techniques to maximize the extraction of NP information from CP observables.

[RKB, Goncalves, Kling (2021)]

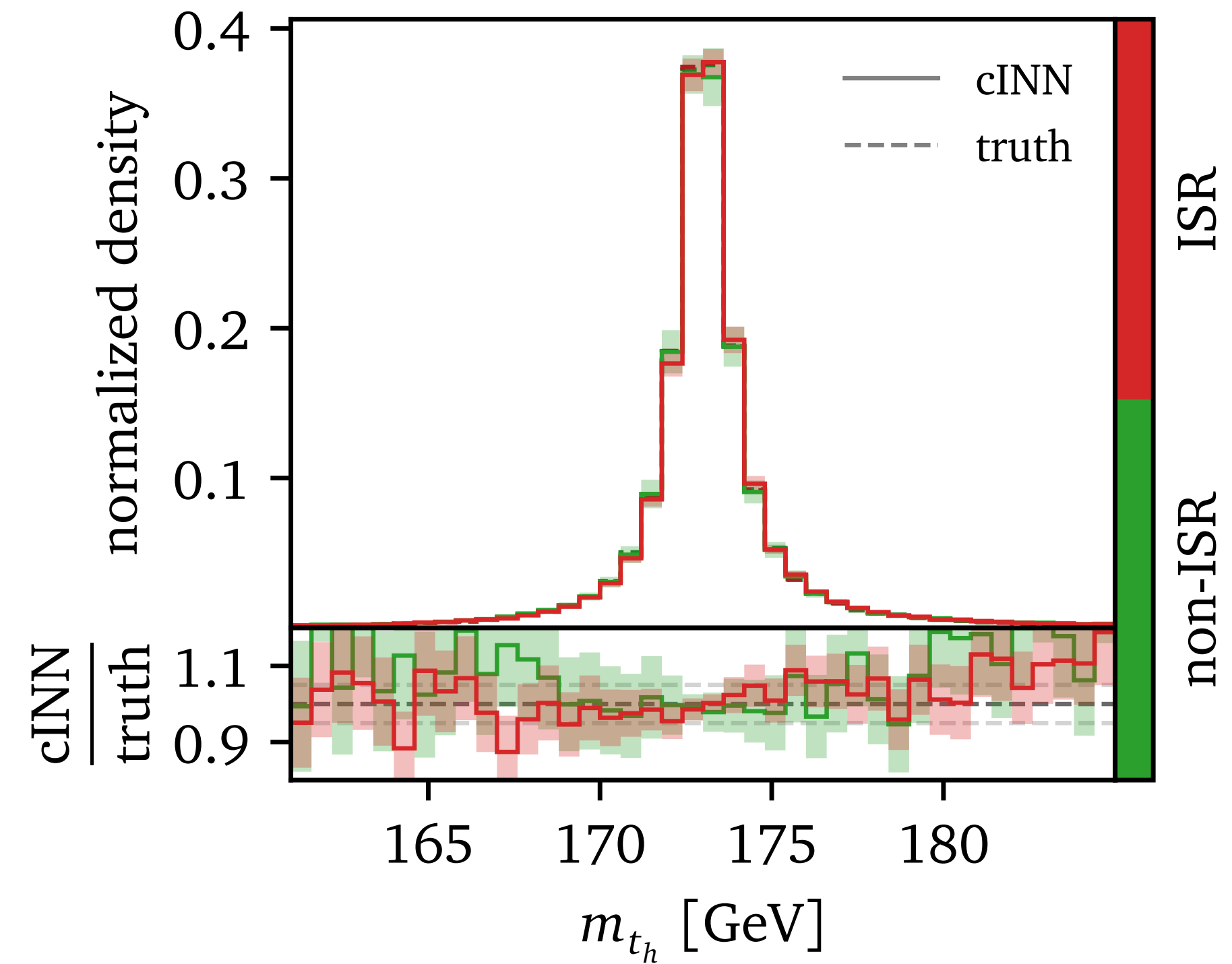
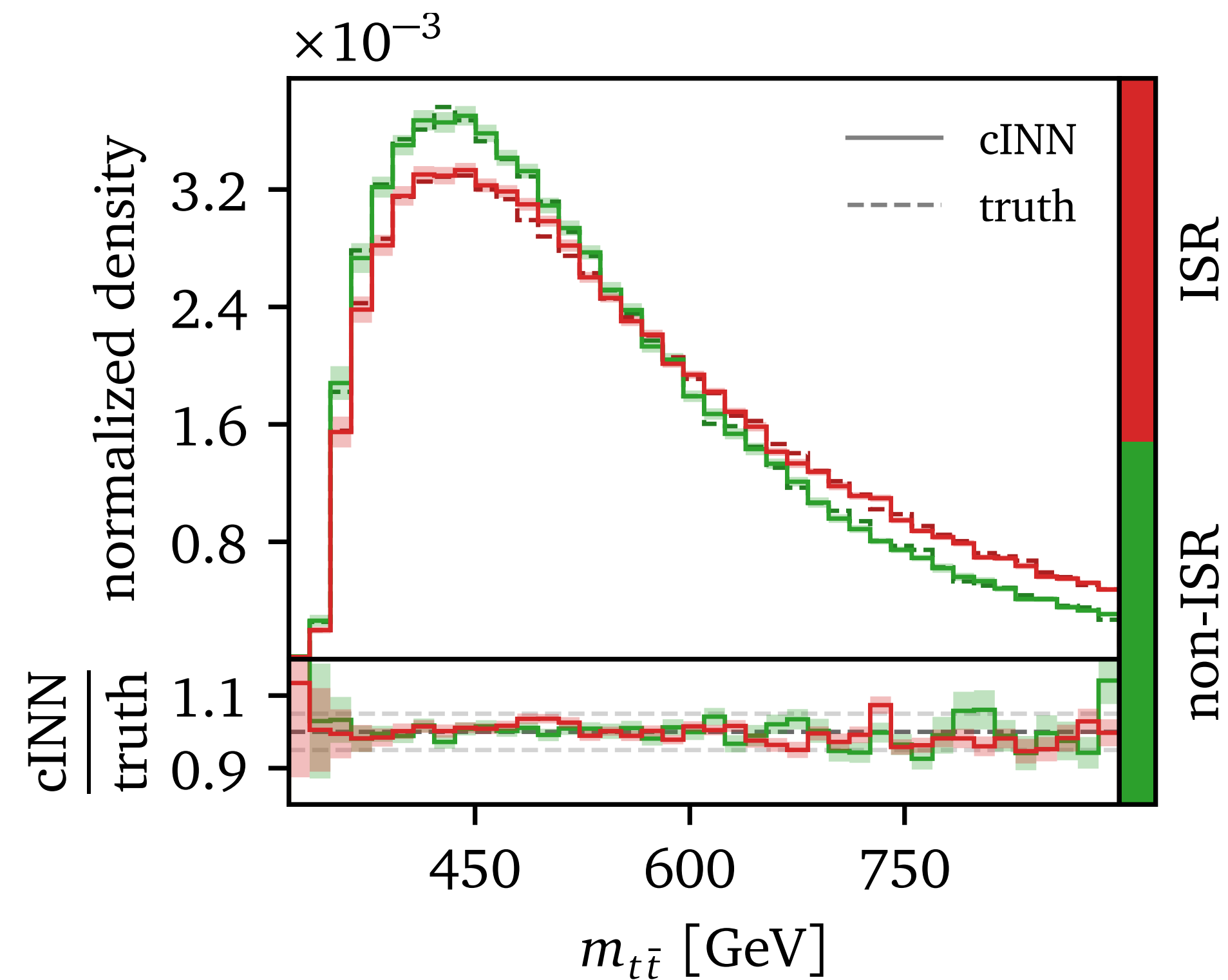
Back to results from unfolding with cINN...

Challenges:

- ★ Can the unfolding model correctly reconstruct the two hard jets at the parton level from a variable number of jets at the detector level?
- ★ How well can the dedicated BSM observables be reconstructed?
- ★ How model-dependent is the training?

Jet combinatorics

Parton level truth and unfolded top invariant masses m_{t_ℓ} and m_{t_h}



★ Unfolded distributions in good agreement with parton level truth despite added combinatorial ambiguity at the detector level.

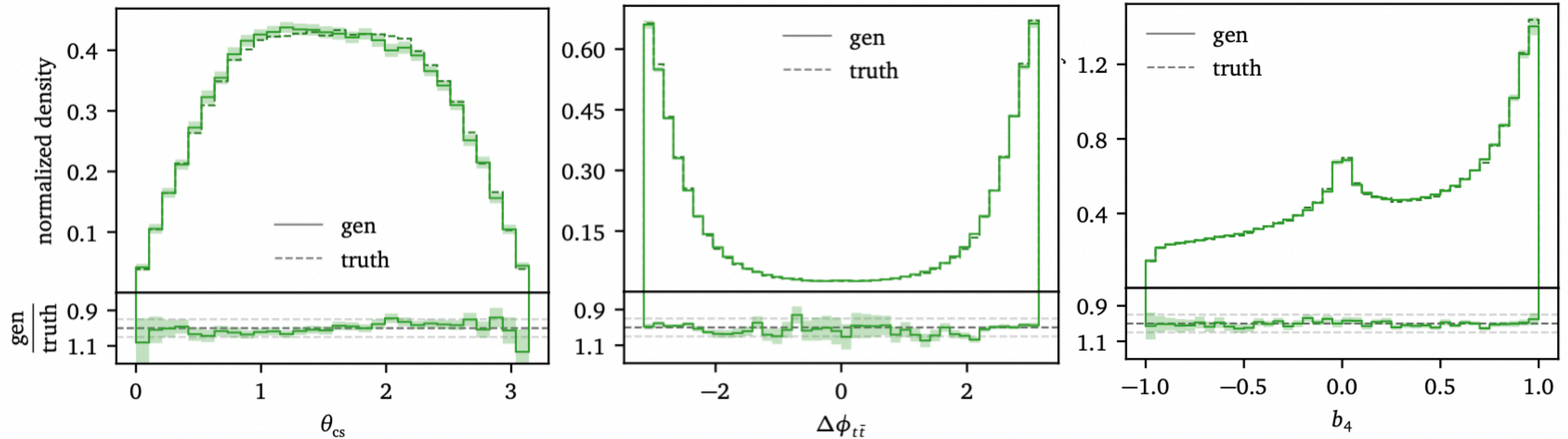
Back to results from unfolding with cINN...

Challenges:

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Reconstruction of dedicated observables

Parton level truth and unfolded SM for θ_{CS} , $\Delta\phi_{t\bar{t}}$ and b_4 .



- ★ Unfolded distributions in close agreement with truth:
 - ✓ Close agreement even for observables not included in event parametrization.
 - ✓ Full phase space reconstruction.
- ★ Potential differences from the truth are covered by the uncertainty estimates of the Bayesian network.

Back to results from unfolding with cINN...

Challenges:

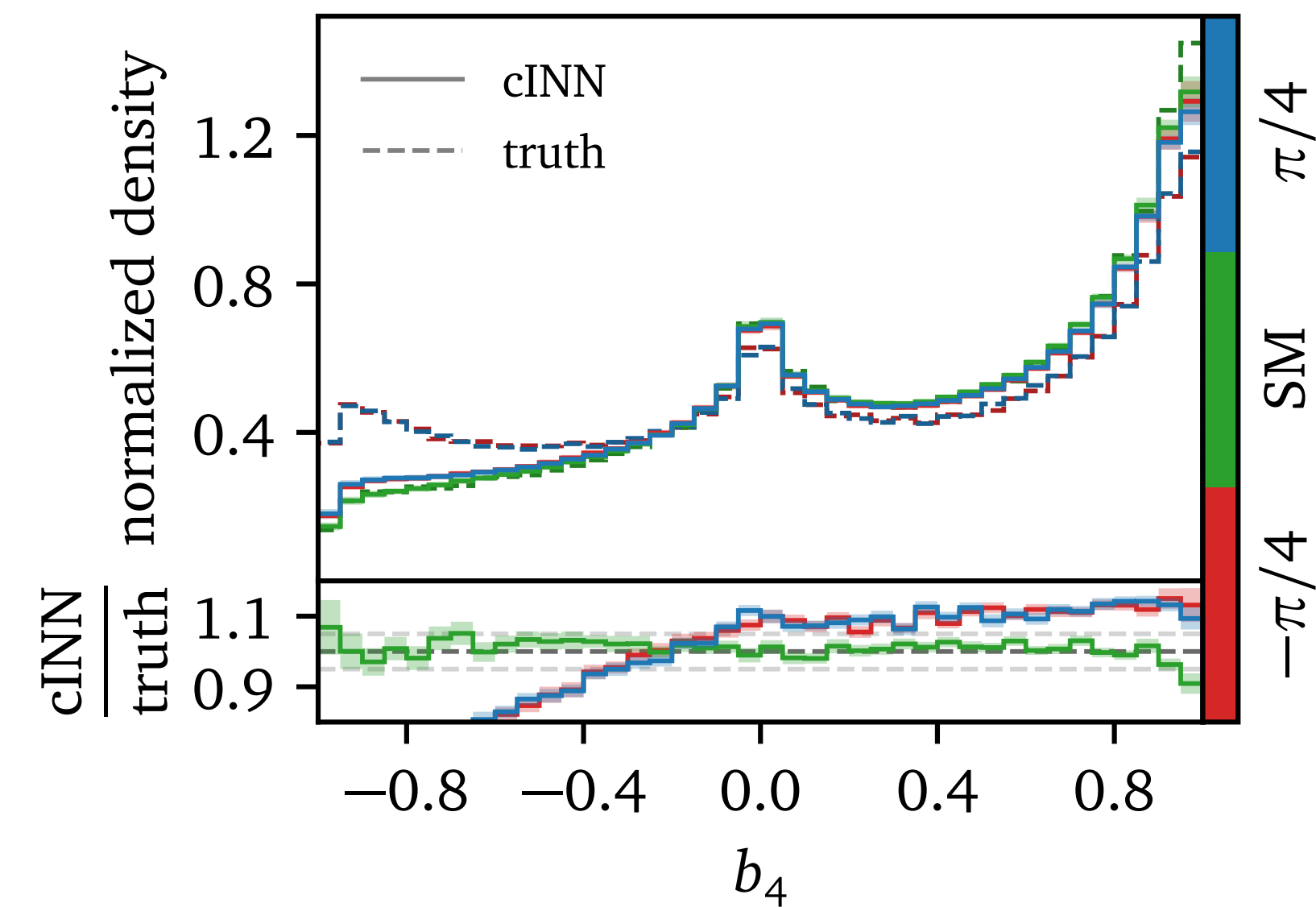
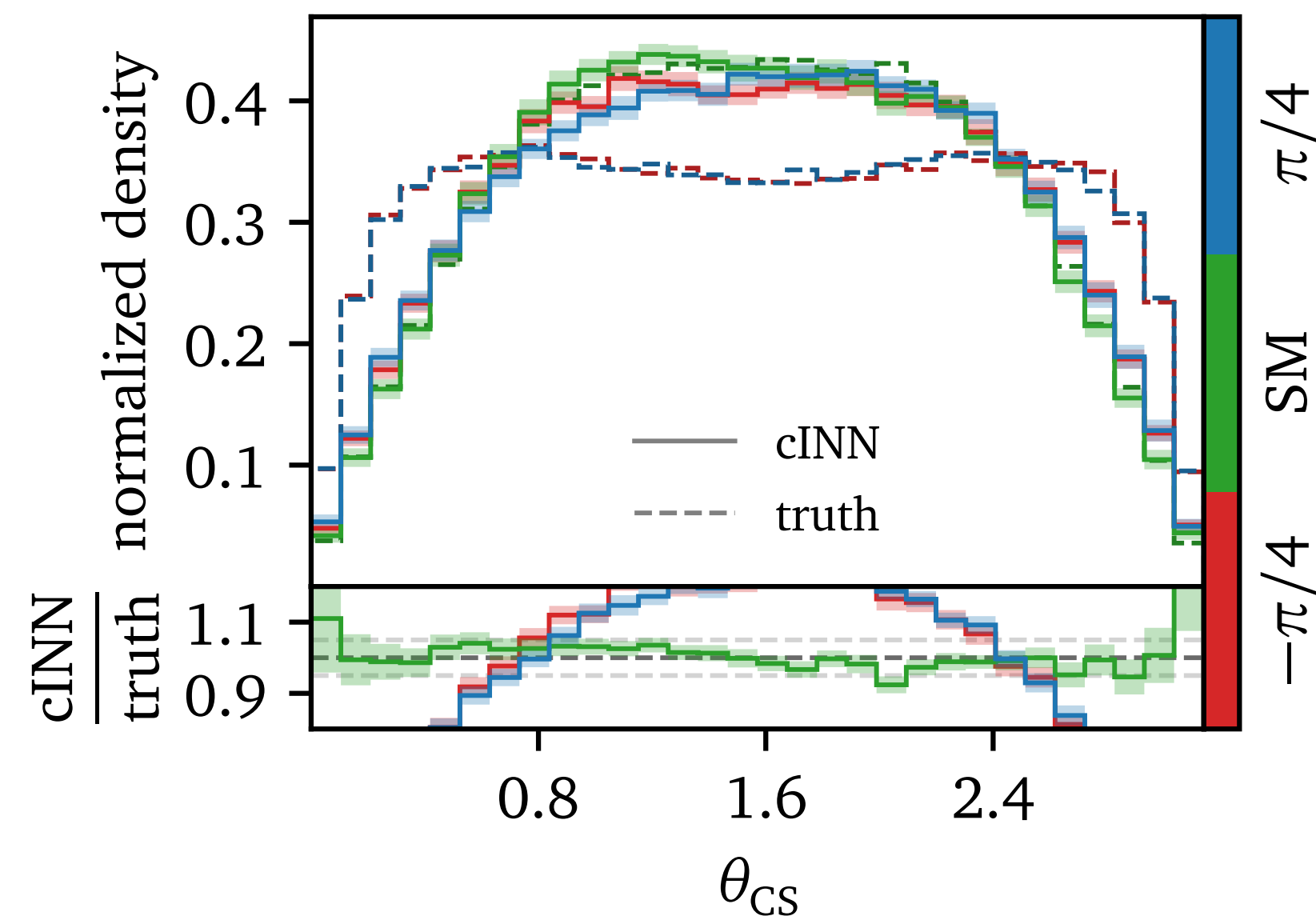
- ★ Can the unfolding model correctly reconstruct the two hard jets at the parton level from a variable number of jets at the detector level?
- ★ How well can the dedicated BSM observables be reconstructed?
- ★ How model-dependent is the training?

Model dependence

Unfolding SM events using networks trained on events with different amounts of CP-violation.

We train 3 networks on $\alpha = +\pi/4, -\pi/4$ and SM, respectively

Unfold SM dataset



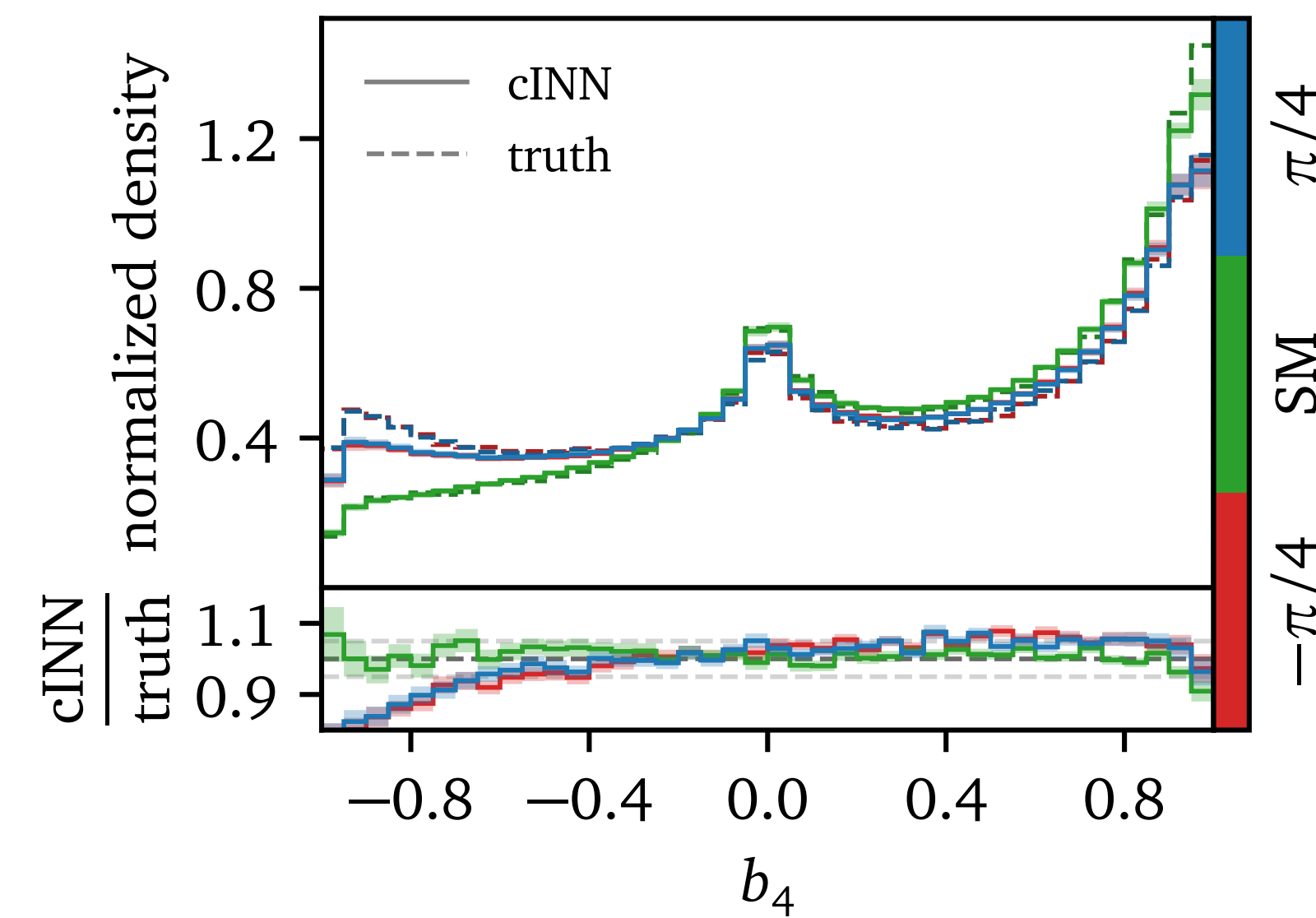
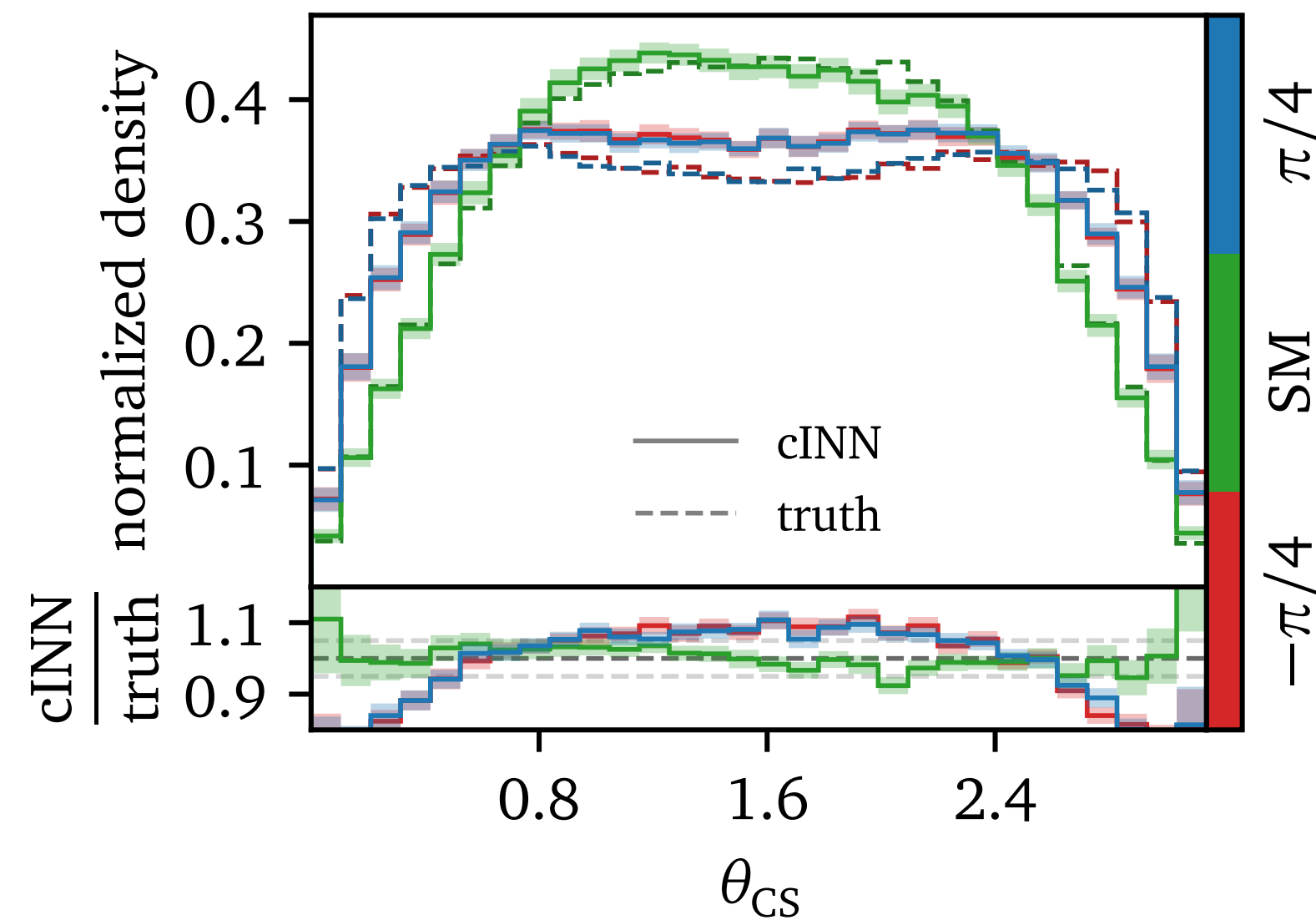
- ★ Networks trained on $\alpha = \pi/4$ and $-\pi/4$ show only a slight bias towards broader θ_{CS} and flatter b_4 distributions.
- ★ $\sim 10 - 20\%$ bias \rightarrow much smaller than the changes at parton truth from varying α .

Model dependence

Unfolding events with CP-violation using a network trained on SM events.

Train network on *SM* dataset

Unfold $\alpha = +\pi/4, -\pi/4$ and *SM* dataset



★ Again, the effect of bias is much smaller than the effect of α on the data.

Outlook

- Generative unfolding makes it possible to invert high-dimensional distributions and full phase-space reconstruction.
- The trained cINN behaves as an efficient kinematic reconstruction algorithm capable of tackling complex reconstruction challenges.
- The trained unfolding network was able to
 - extract various CP observables at the parton level with appropriate phase space parametrization.
 - resolve jet combinatorial ambiguity.
 - absolve any large model-dependence.
- While this study is clearly not the last word on this analysis technique, it presents a promising outlook for an experimental study, with a proper treatment of statistical limitations, continuum backgrounds, calibration, and iterative improvements of the unfolding network.

Thank you