



UNIVERSITÄT
HEIDELBERG
ZUKUNFT
SEIT 1386

İzmir, 29.02.2024

Precision-Machine Learning for the Matrix Element Method

T. Heibel, **N. Huetsch**, R. Winterhalder, T. Plehn, A. Butter
arXiv: 2310.07752

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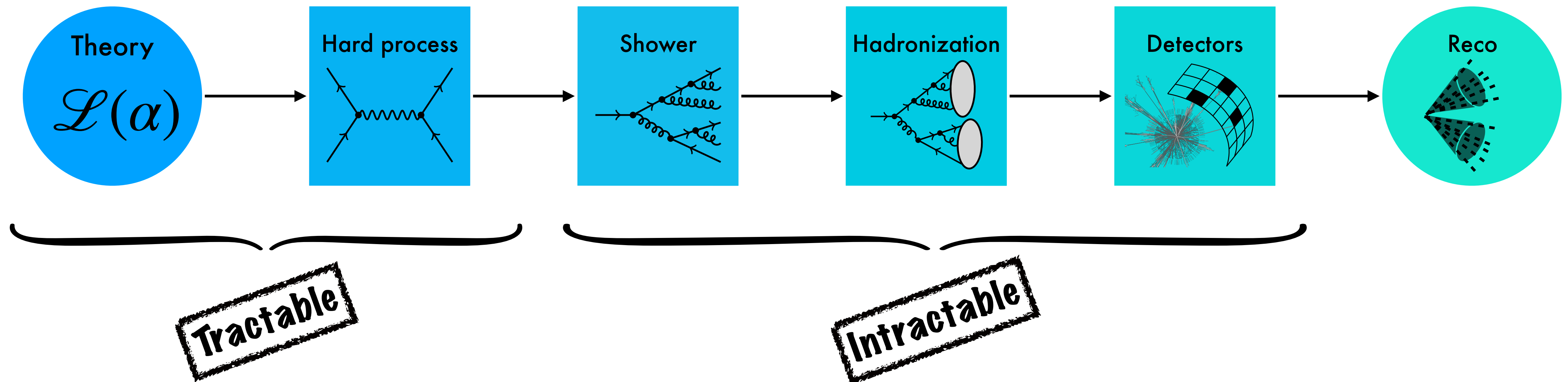


Federal Ministry
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and Research



Building on: A. Butter, T. Heibel, T. Martini, S. Peitzsch, T. Plehn: arXiv:2210.00019

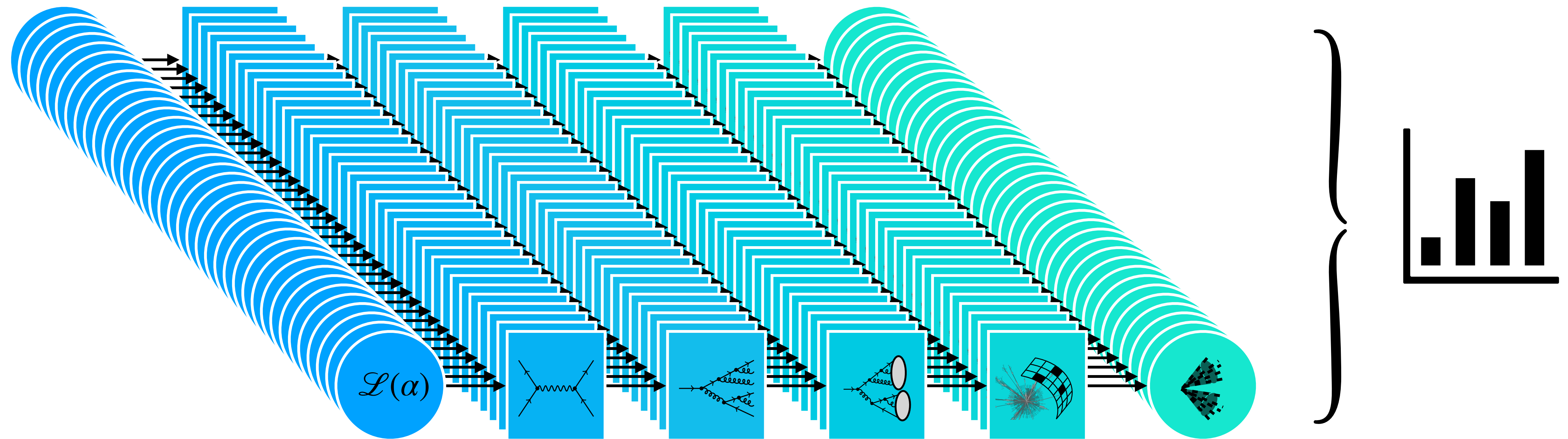
From Theory to Experiment in LHC Physics



In HEP we can never analytically calculate what we measure

We rely on simulations to connect theory and experiment

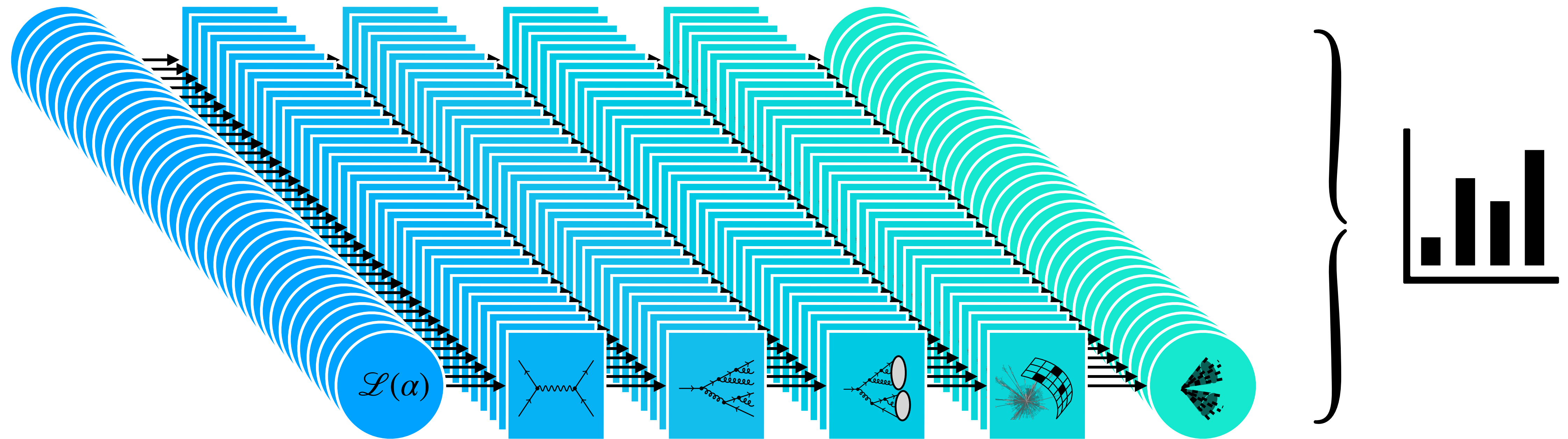
From Theory to Experiment in LHC Physics



Event samples are combined into observable histogram

Simulated and measured histograms are compared

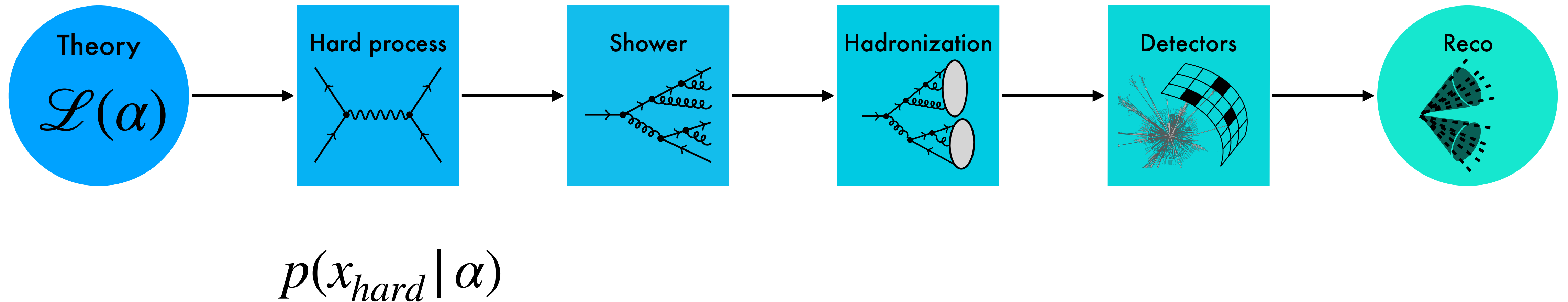
From Theory to Experiment in LHC Physics



We lose a lot of information doing this!

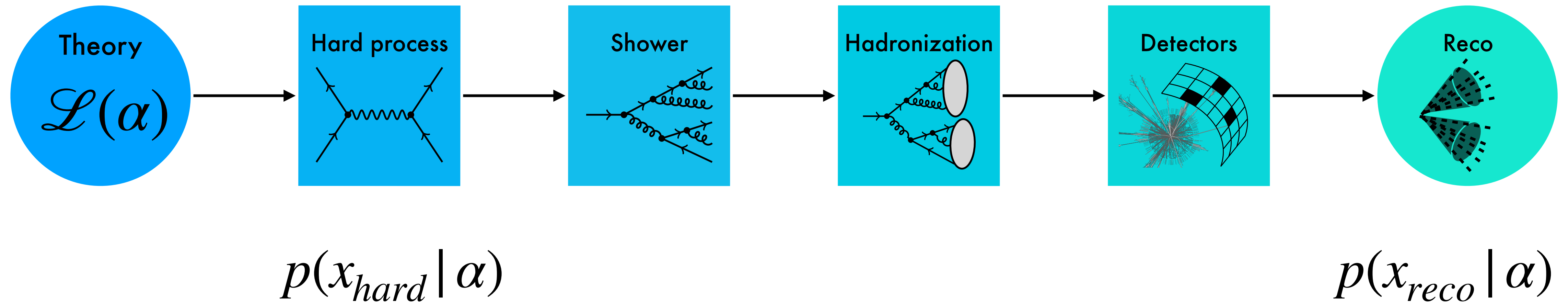
What if we could go for the likelihood instead?

Going for the likelihood



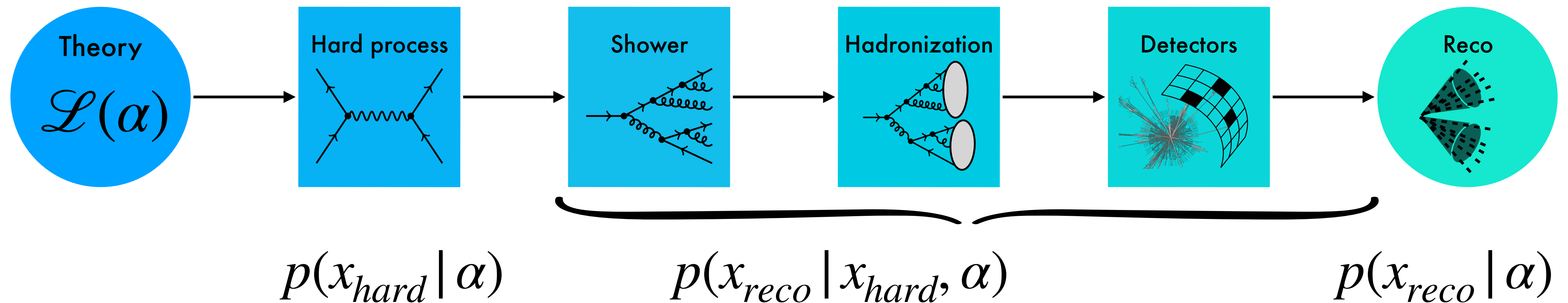
Hard-scattering level likelihood known via differential cross-section $p(x_{hard} | \alpha) = \frac{1}{\sigma(\alpha)} \frac{d\sigma(\alpha)}{dx_{hard}}$

Going for the likelihood



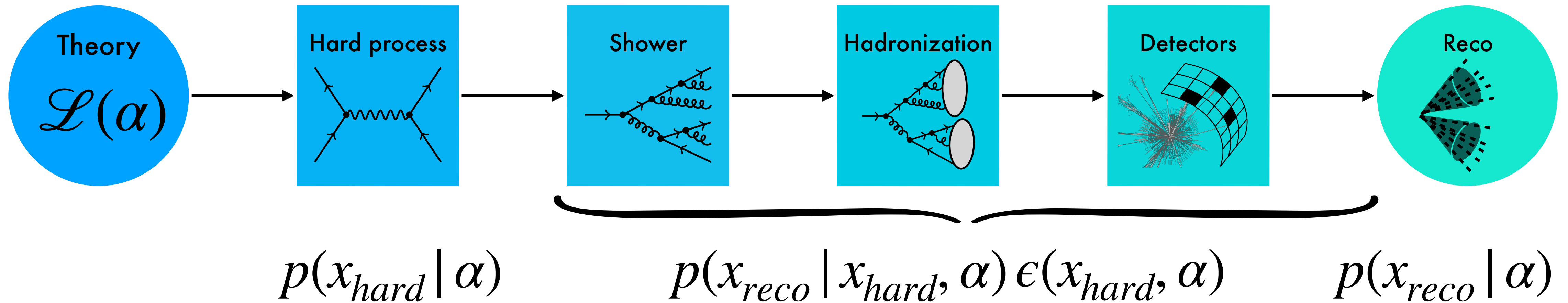
Need access to the likelihood at reconstruction level!

Going for the likelihood



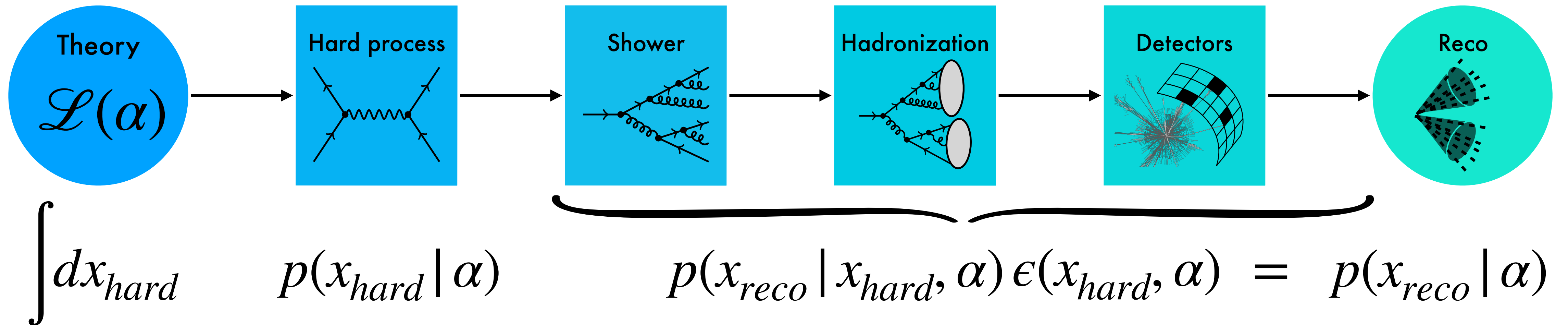
Hard-scattering and reconstruction linked by forward transfer probability

Going for the likelihood



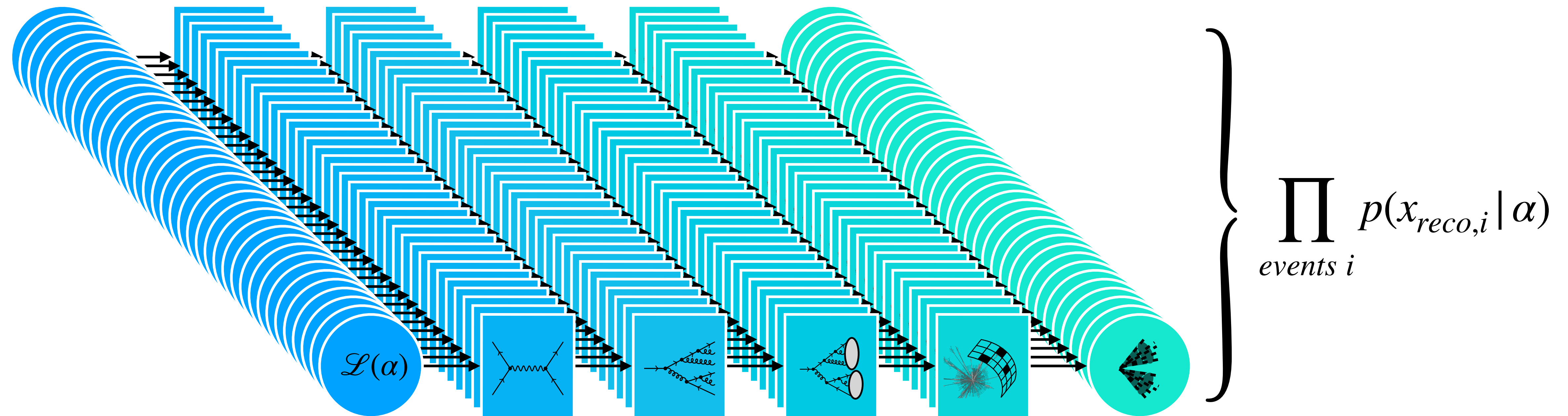
Include an efficiency term to account for acceptance of events

Going for the likelihood



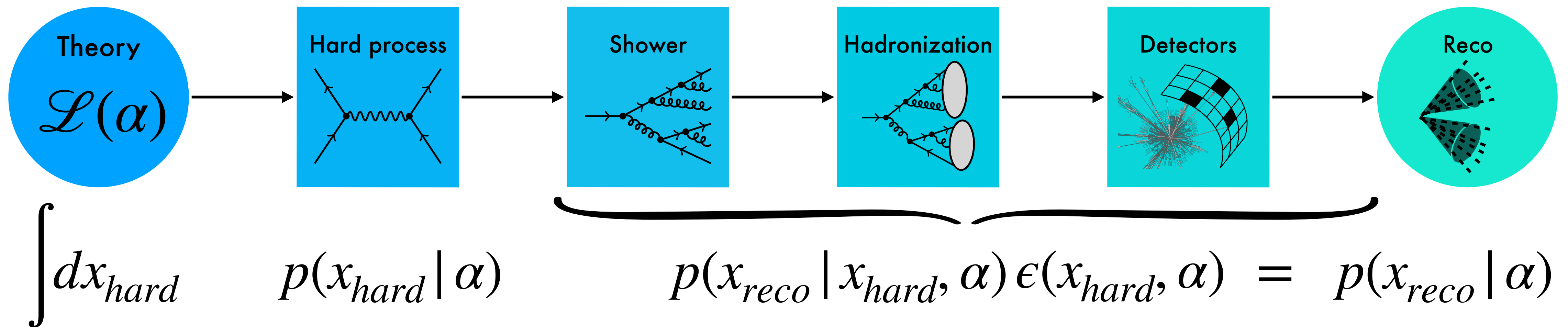
Integrate over all possible hard-scattering configurations

Going for the likelihood



Event likelihoods are combined into sample likelihoods

The Matrix Element Method



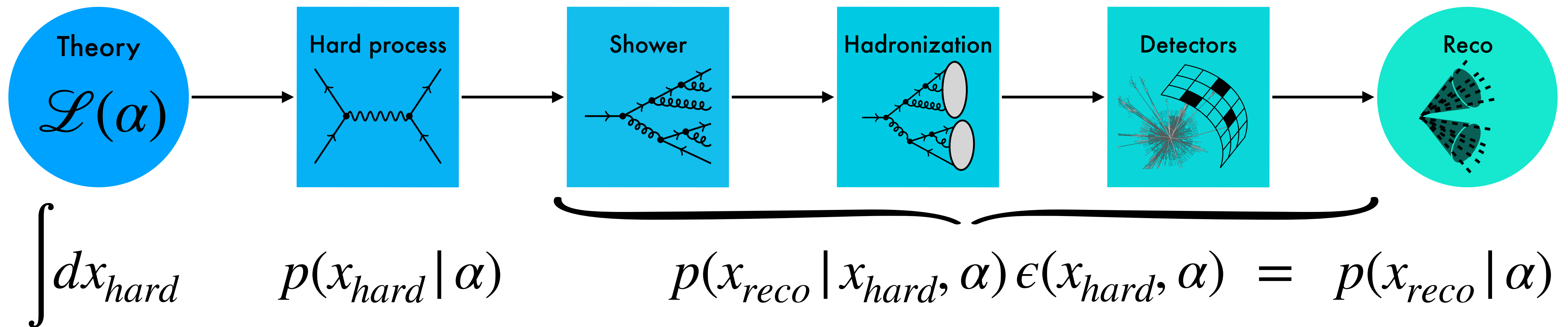
+++ Unbinned and multivariate by design

+++ Optimal use of information derived from Neyman-Pearson lemma

— — Transfer probability and efficiency not known

— — Integral numerically very challenging

The Matrix Element Method



+++ Unbinned and multivariate by design

+++ Optimal use of information derived from Neyman-Pearson lemma

— — ~~Transfer probability and efficiency not known~~ **USE MACHINE LEARNING**

— — ~~Integral numerically very challenging~~ **USE MACHINE LEARNING**

The Transfer Network

$$\int dx_{hard} p(x_{hard} | \alpha) \overset{\text{Intractable}}{p(x_{reco} | x_{hard}, \alpha)} \epsilon(x_{hard}, \alpha) = p(x_{reco} | \alpha)$$

The Transfer Network

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

Intractable

The Transfer Network

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

Intractable

Transfer probability is analytically intractable

Transfer can be simulated to generate paired data x_{hard}, x_{reco}



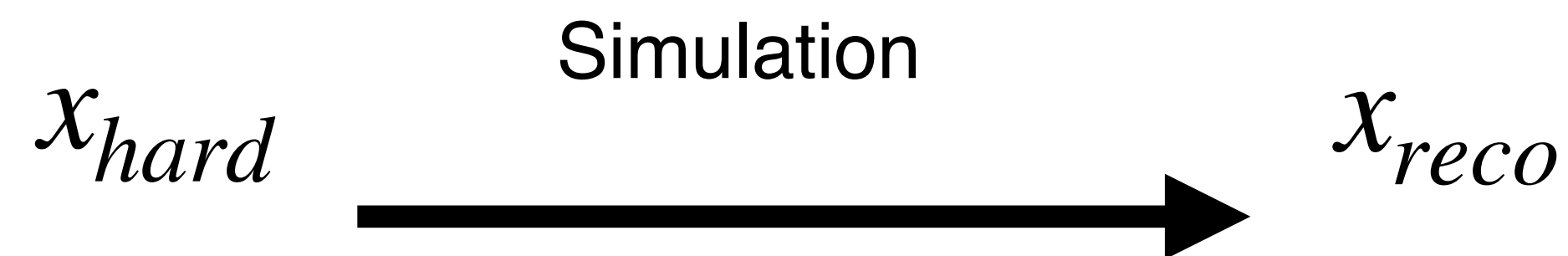
The Transfer Network

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

Intractable

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Transfer can be simulated to generate paired data x_{hard}, x_{reco}



➔ Conditional Generative Neural Network to encode the transfer probability

The Acceptance Network

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

The term $\epsilon(x_{hard}, \alpha)$ is highlighted with a red box and labeled "Unknown".

The Acceptance Network

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

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The term $\epsilon(x_{hard})$ is highlighted with a red box and labeled "Unknown".

Need to encode the efficiency at hard-scattering level

Transfer can be simulated to generate labeled data $x_{hard} \rightarrow x_{reco}(x_{hard}) \rightarrow \left. \begin{array}{l} \checkmark \\ \times \end{array} \right\}$

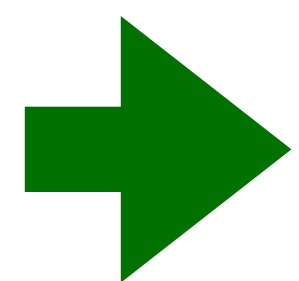
The Acceptance Network

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

Unknown

Need to encode the efficiency at hard-scattering level

Transfer can be simulated to generate labeled data $x_{hard} \rightarrow x_{reco}(x_{hard}) \rightarrow \left\{ \begin{array}{l} \checkmark \\ \times \end{array} \right.$



Classifier Neural Network to encode the acceptance probability

The Sampling Network

Challenging

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

The Sampling Network

Challenging

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

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

The Sampling Network

Challenging

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

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

The Sampling Network

Challenging

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

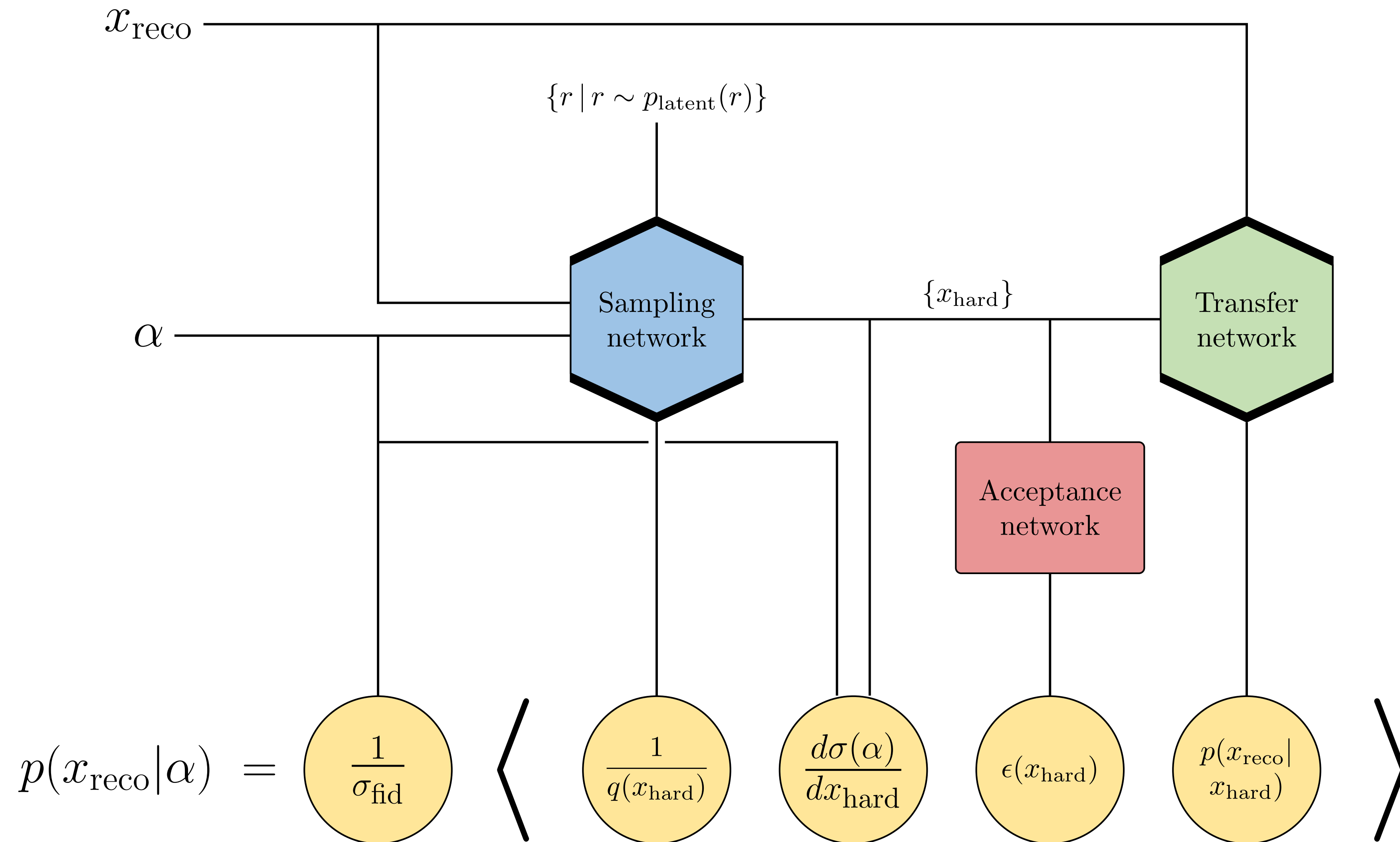
$$= \left\langle \frac{1}{q(x_{hard} | x_{reco}, \alpha)} p(x_{hard} | \alpha) p(x_{reco} | x_{hard}) \epsilon(x_{hard}) \right\rangle_{x_{hard} \sim q}$$

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

Generative Neural Network to encode sampling distribution

$$r \sim p_{latent}(r) \longleftrightarrow x_{hard}(r) \sim q_{\phi}(x_{hard} | x_{reco}, \alpha)$$

Machine-learned MEM



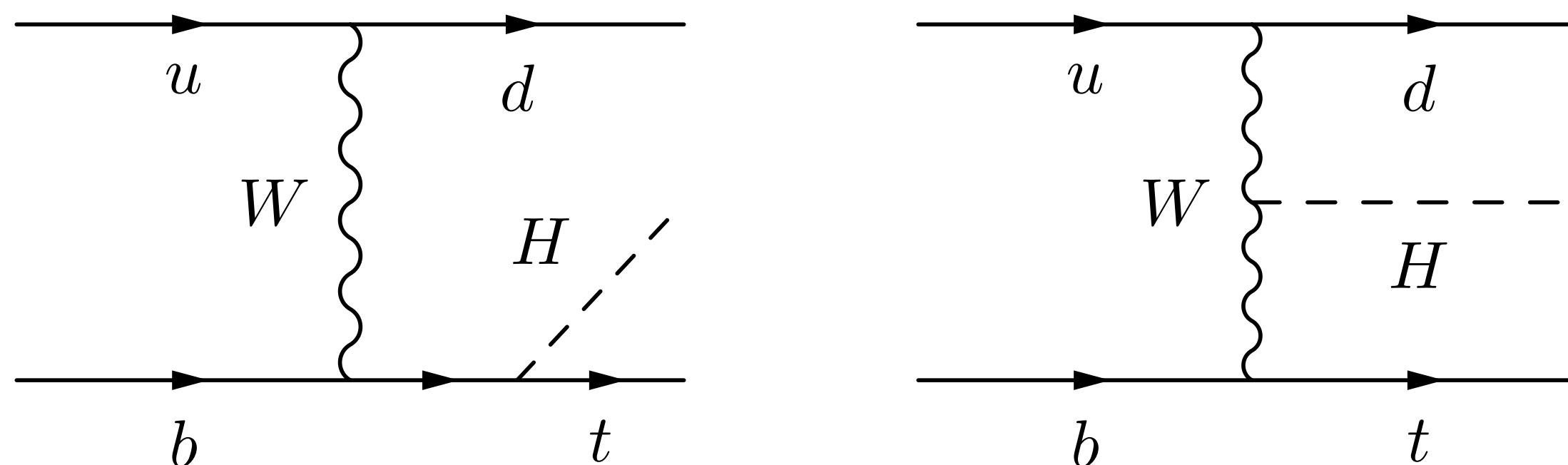
The physics example

The problem: Measuring a CP-phase in the top Yukawa coupling

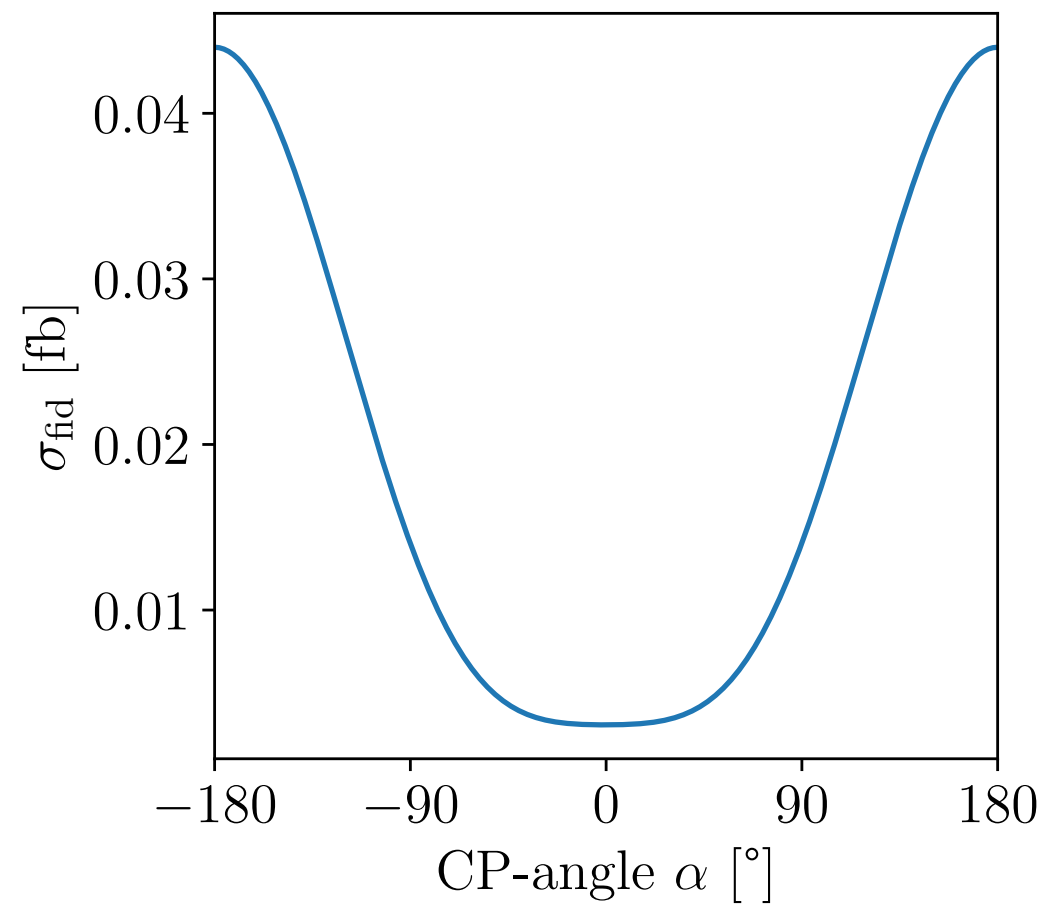
$$\mathcal{L}_{t\bar{t}H}(\alpha) = -\frac{y_t}{\sqrt{2}} \left[\cos \alpha \bar{t}t + \frac{2}{3}i \sin \alpha \bar{t}\gamma_5 t \right] H$$

The process: Associated single-top and Higgs production

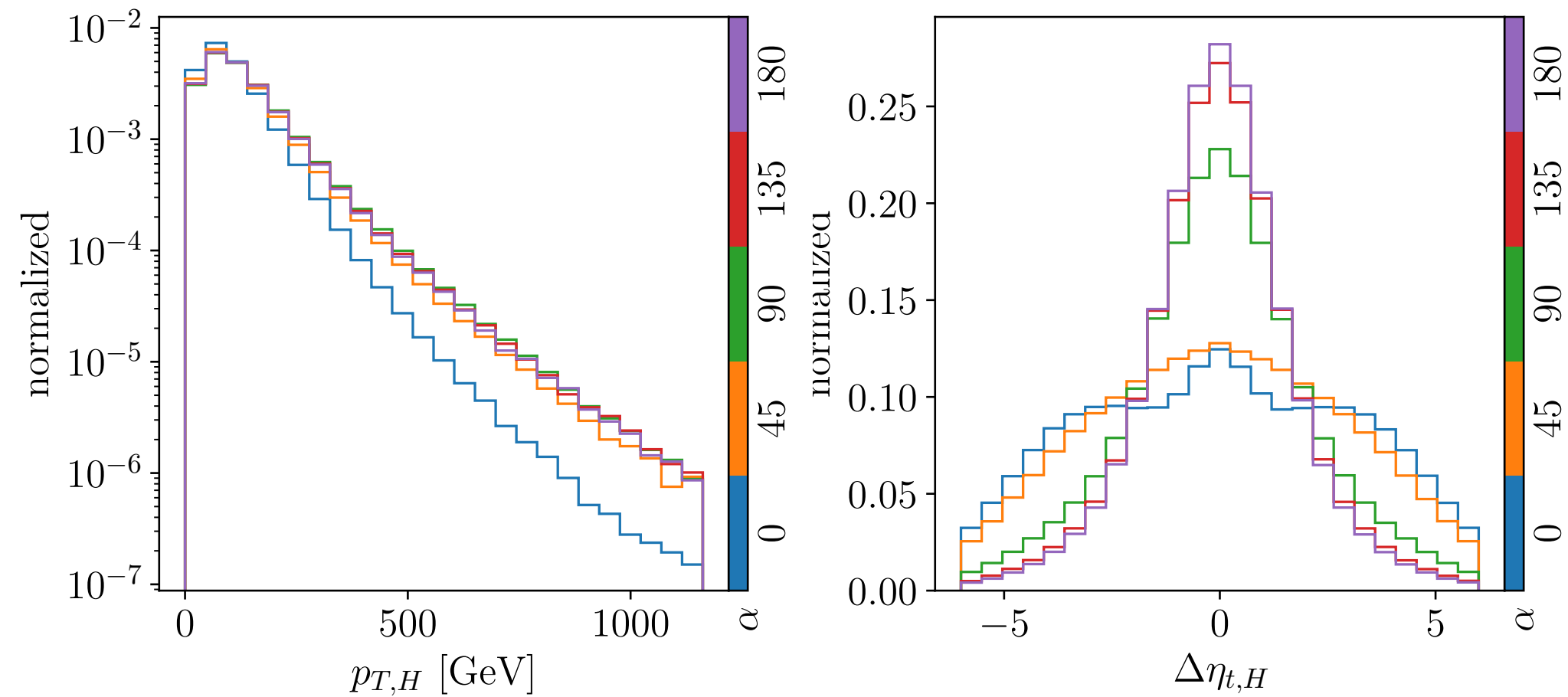
$$pp \rightarrow tHj \rightarrow (bjj) (\gamma\gamma) j + \text{ISR Jets}$$



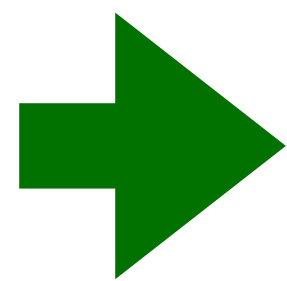
Why MEM here?



Cross-section very small and insensitive to variations in α



Hard-scattering $p(x_{\text{hard}} | \alpha)$ kinematics are sensitive



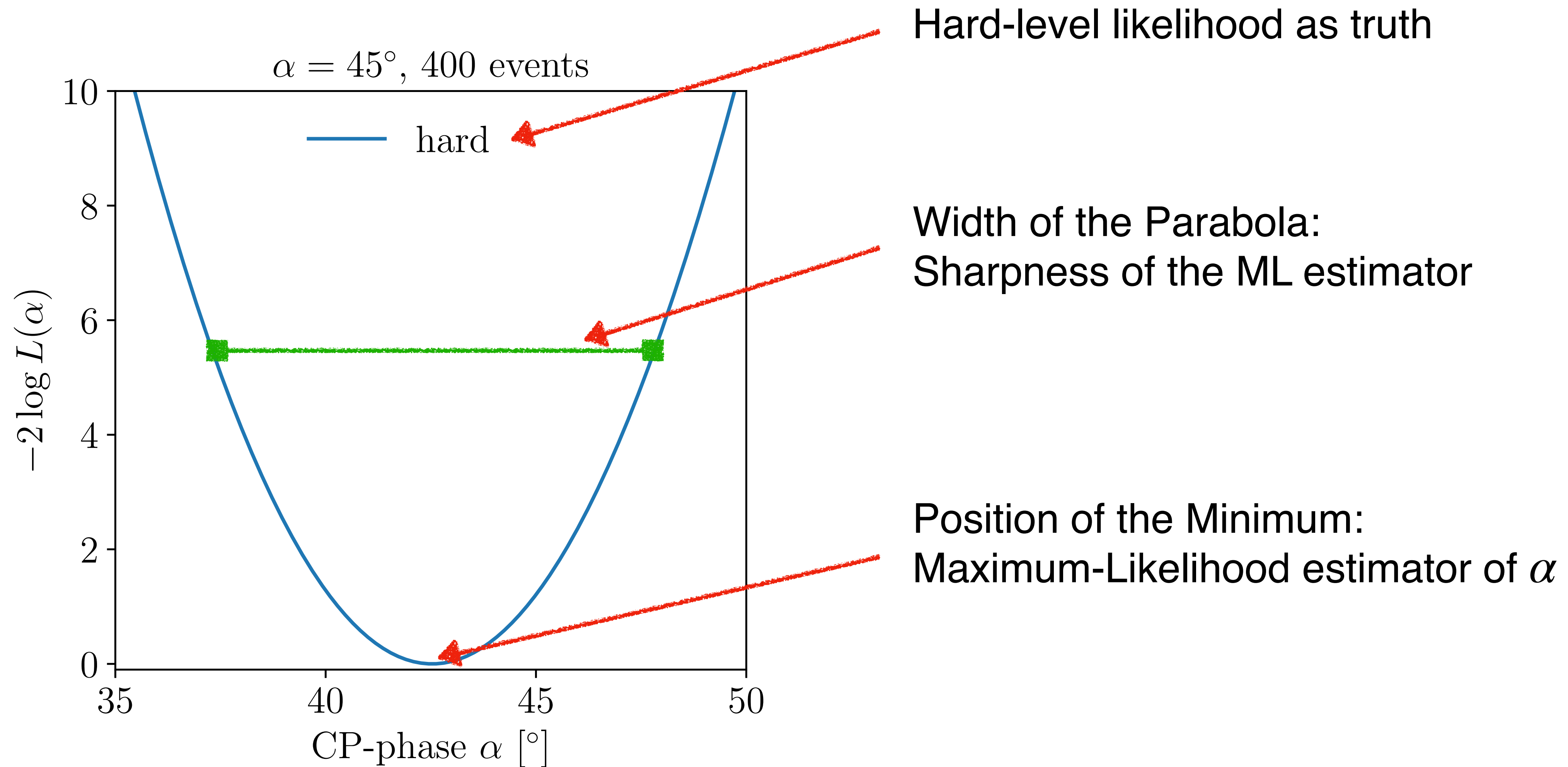
Ideal use case for the Matrix Element Method

The workflow

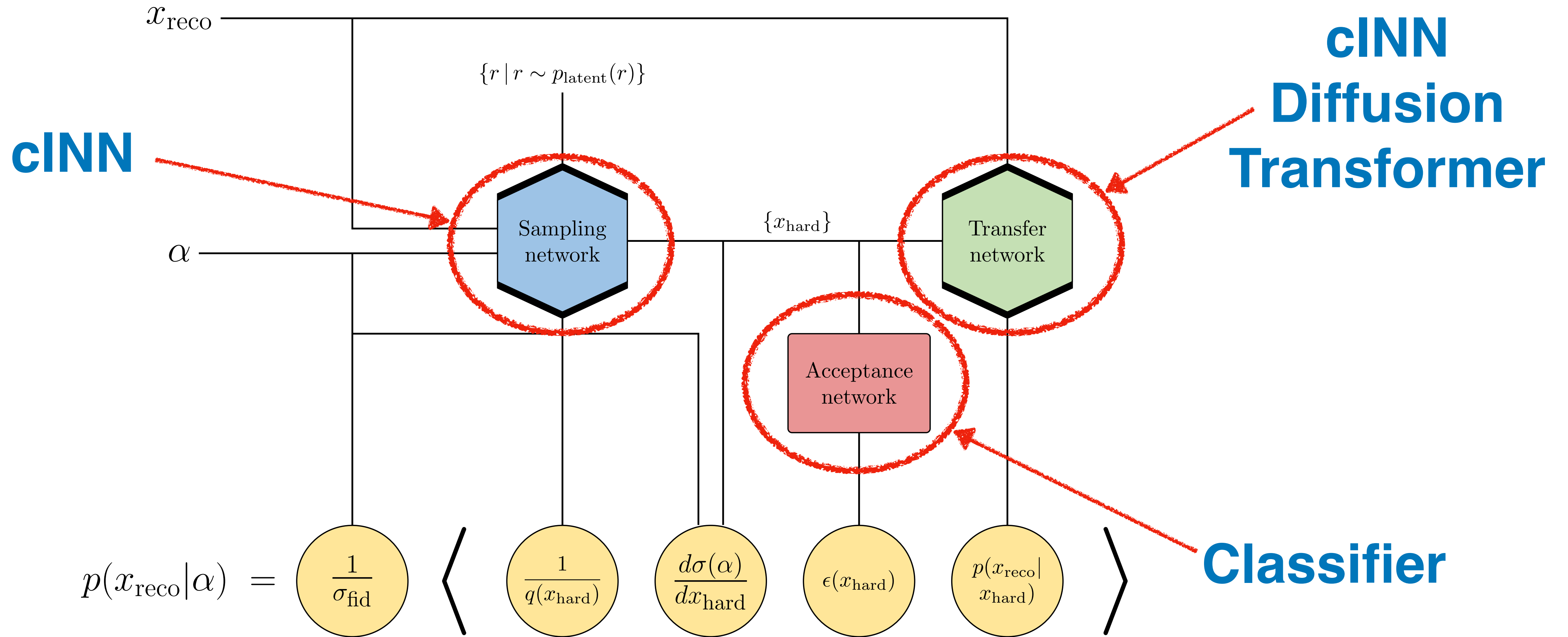
- 1) Start from Lagrangian $\mathcal{L}_{t\bar{t}H}(\alpha)$ and process $pp \rightarrow tHj \rightarrow (bjj) (\gamma\gamma) j + \text{ISR Jets}$
- 2) Simulate hard-scattering events $p(x_{hard} | \alpha)$ for a range of parameter values
- 3) Simulate transfer $x_{hard} \rightarrow x_{reco}$ to obtain paired data $(\alpha, x_{hard}, x_{reco})$
- 4) Train the networks: transfer $p(x_{reco} | x_{hard})$, efficiency $\epsilon(x_{hard})$, sampling $q(x_{hard} | x_{reco}, \alpha)$
- 5) Solve the **MEM integral** for each data sample

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

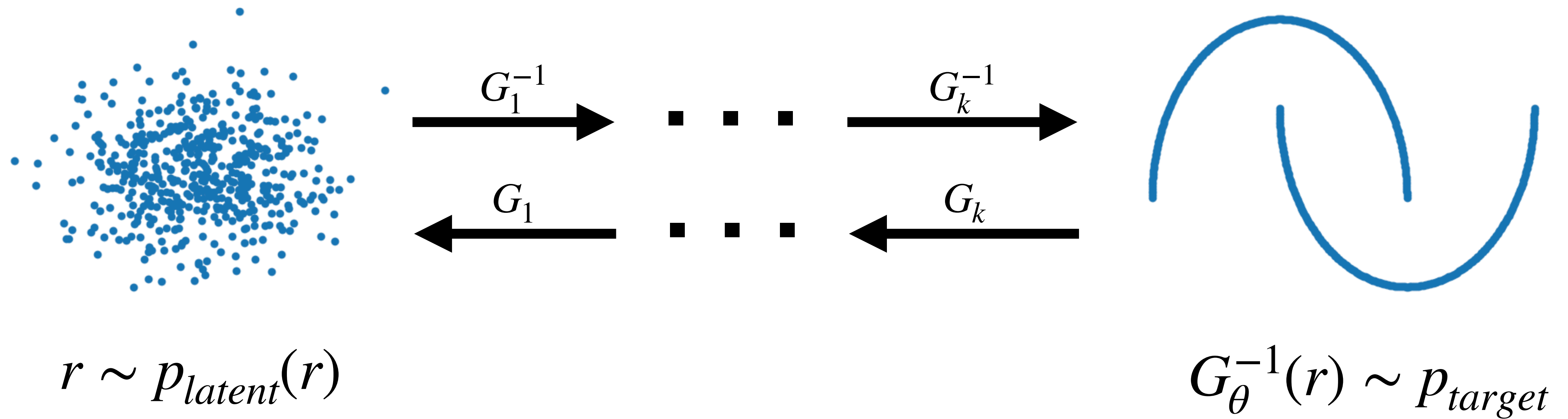
What do results look like?



Machine-learned MEM

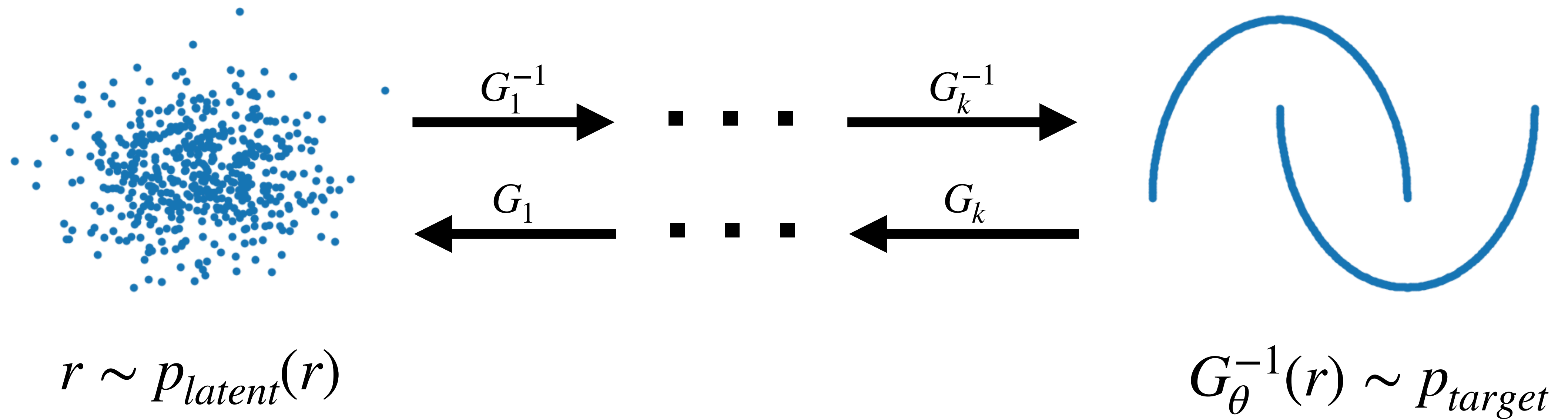


Invertible Neural Networks (or Normalizing Flows)



Invertible mapping between data and latent space

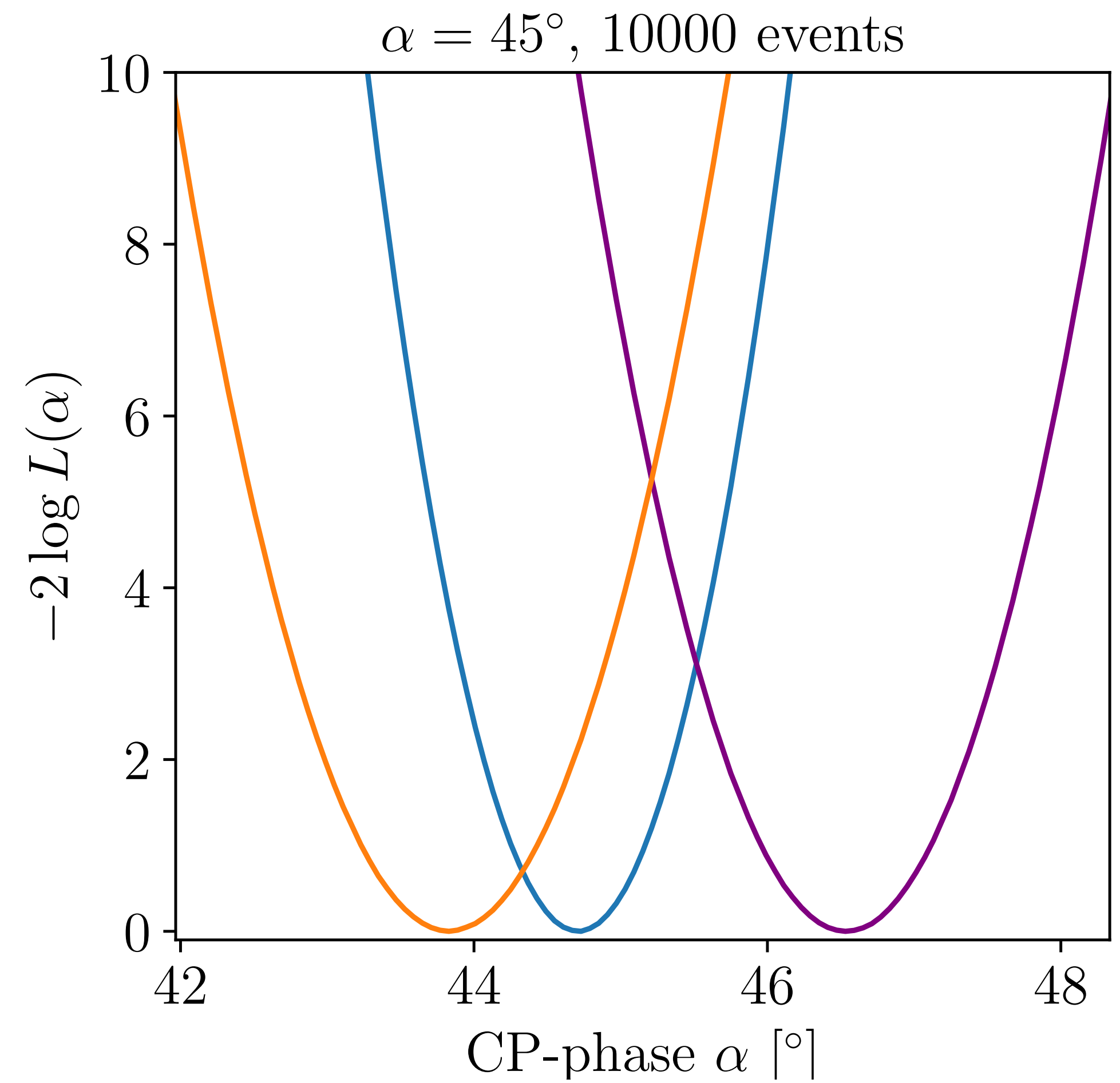
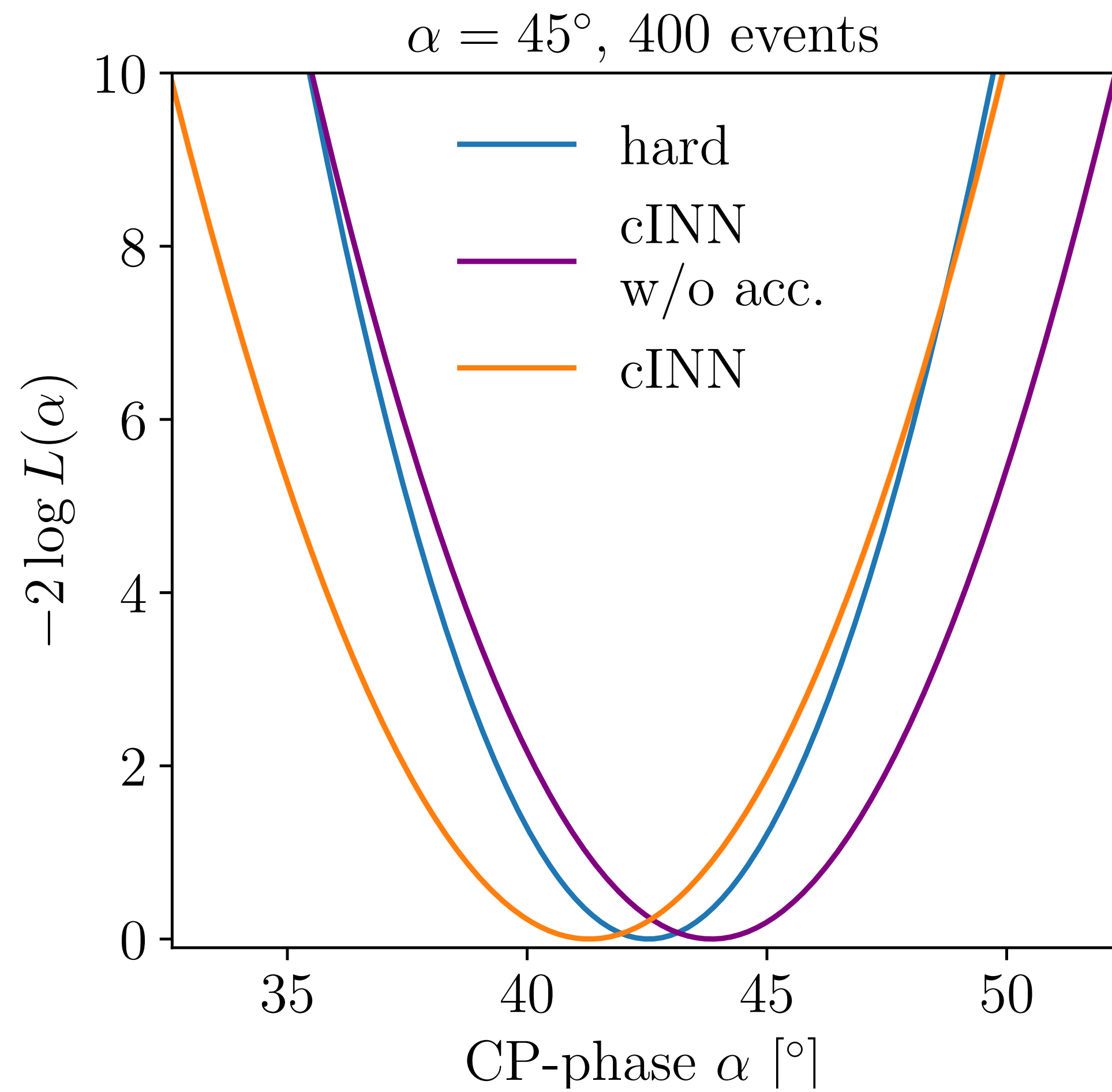
Invertible Neural Networks (or Normalizing Flows)



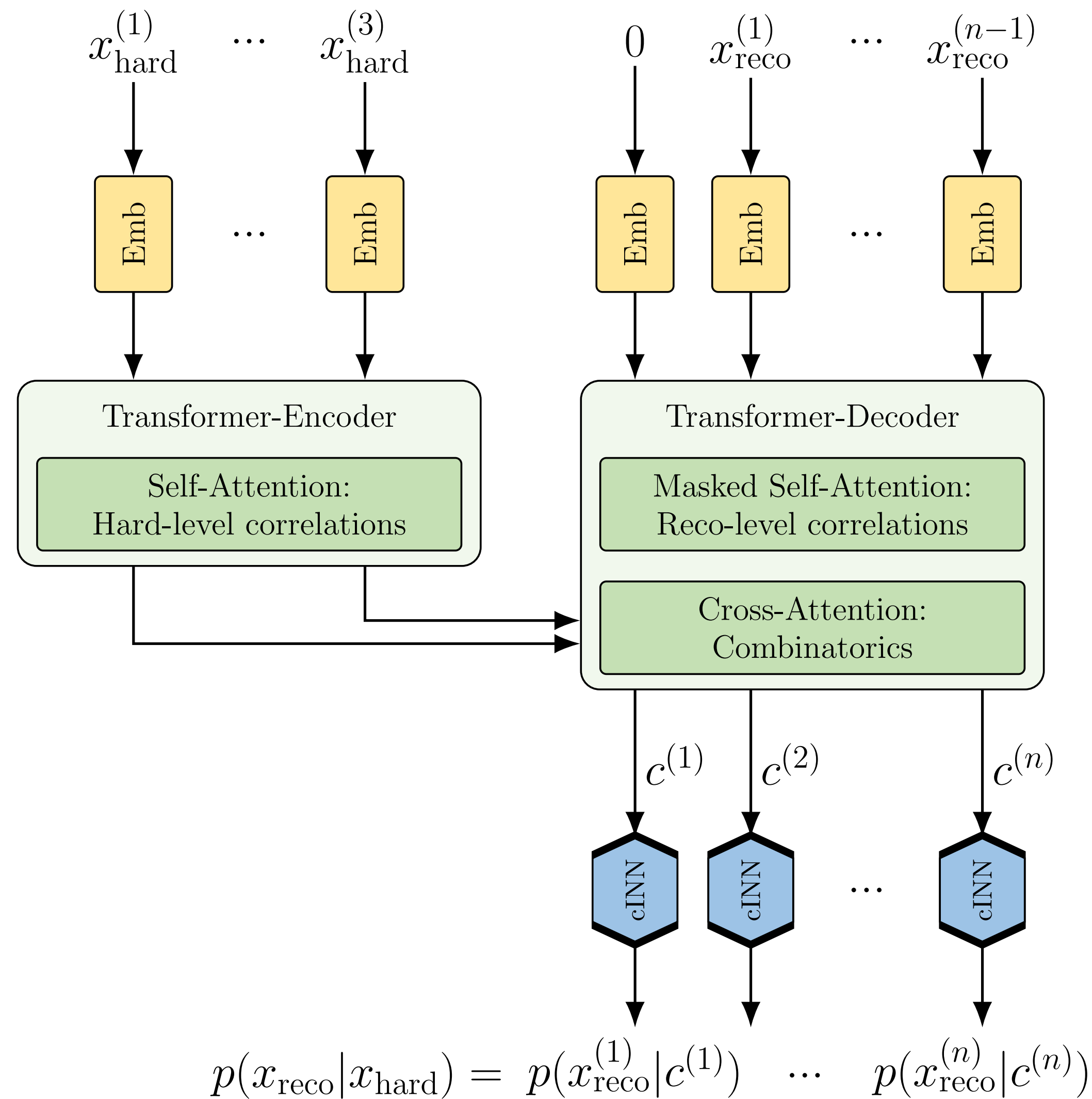
Invertible mapping between data and latent space

$$p_{\theta}(x) = p_{latent}(G_{\theta}(x)) \underbrace{\left| \det J_{G_{\theta}} \right|}_{\left| \det J_{G_1} \right| \left| \det J_{G_2} \right| \dots \left| \det J_{G_k} \right|}$$

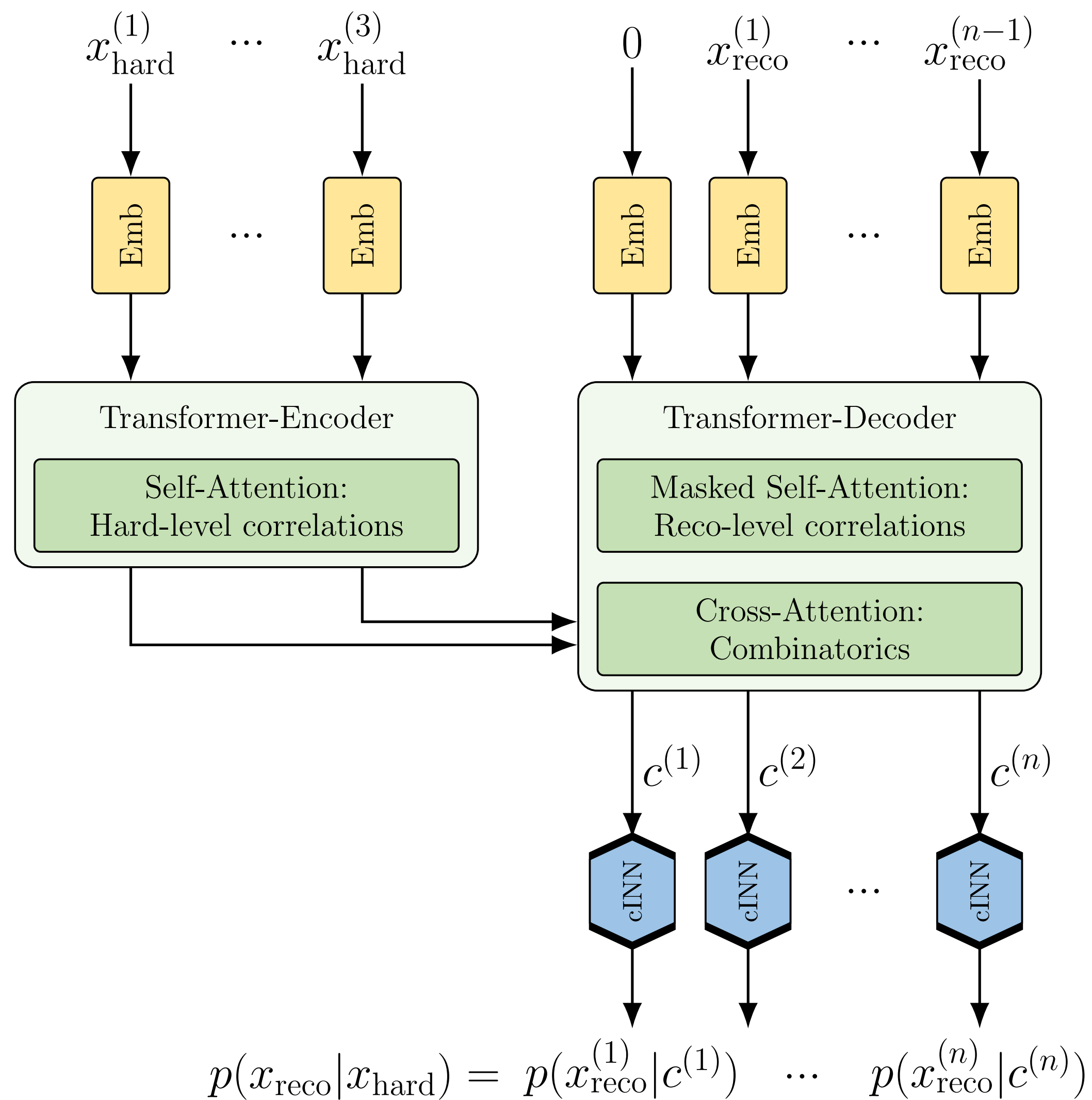
Transfer-cINN Results



The Transformer (Transfer-Transformer)



The Transfermer (Transfer-Transformer)



Why a Transformer here?

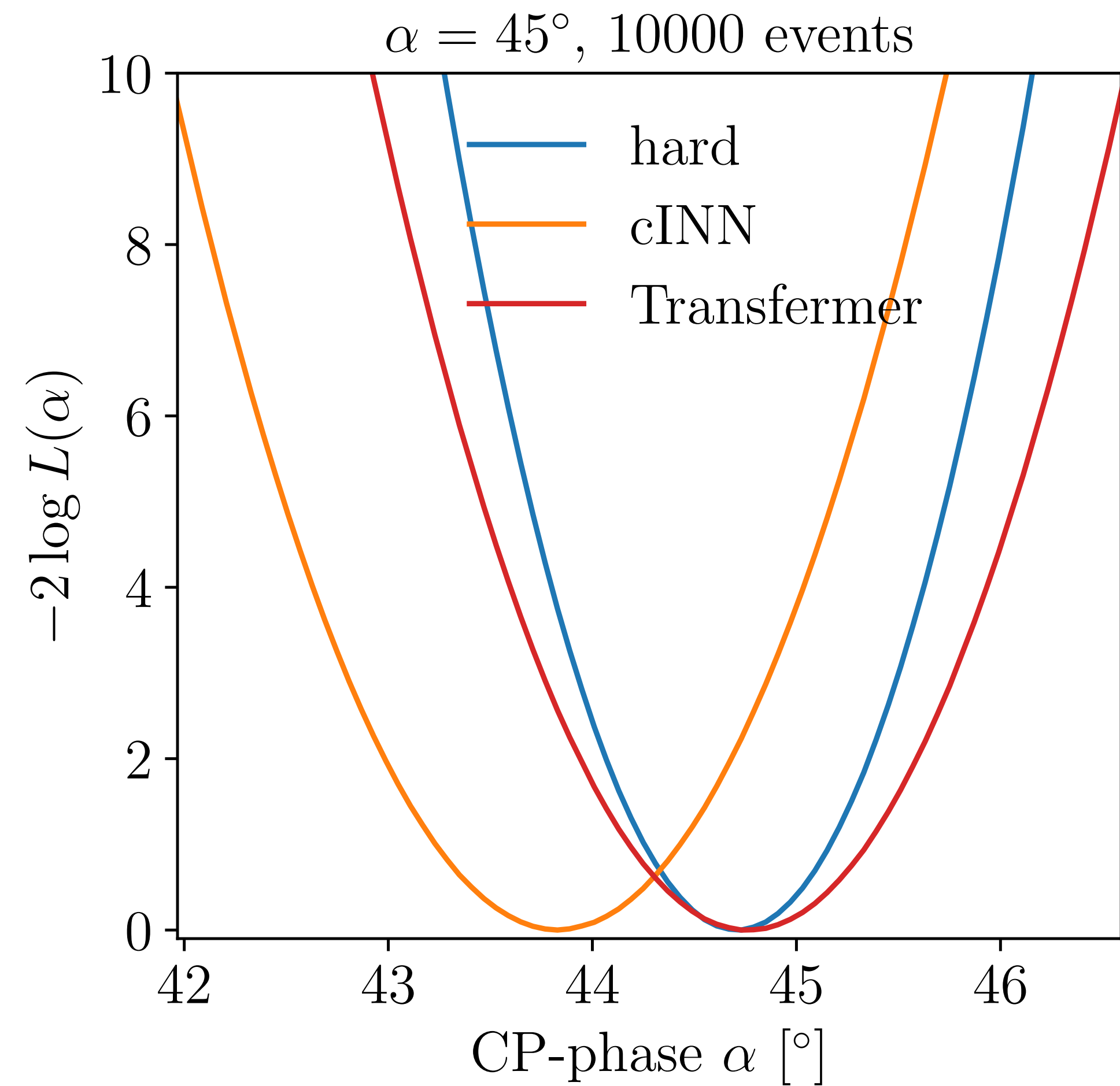
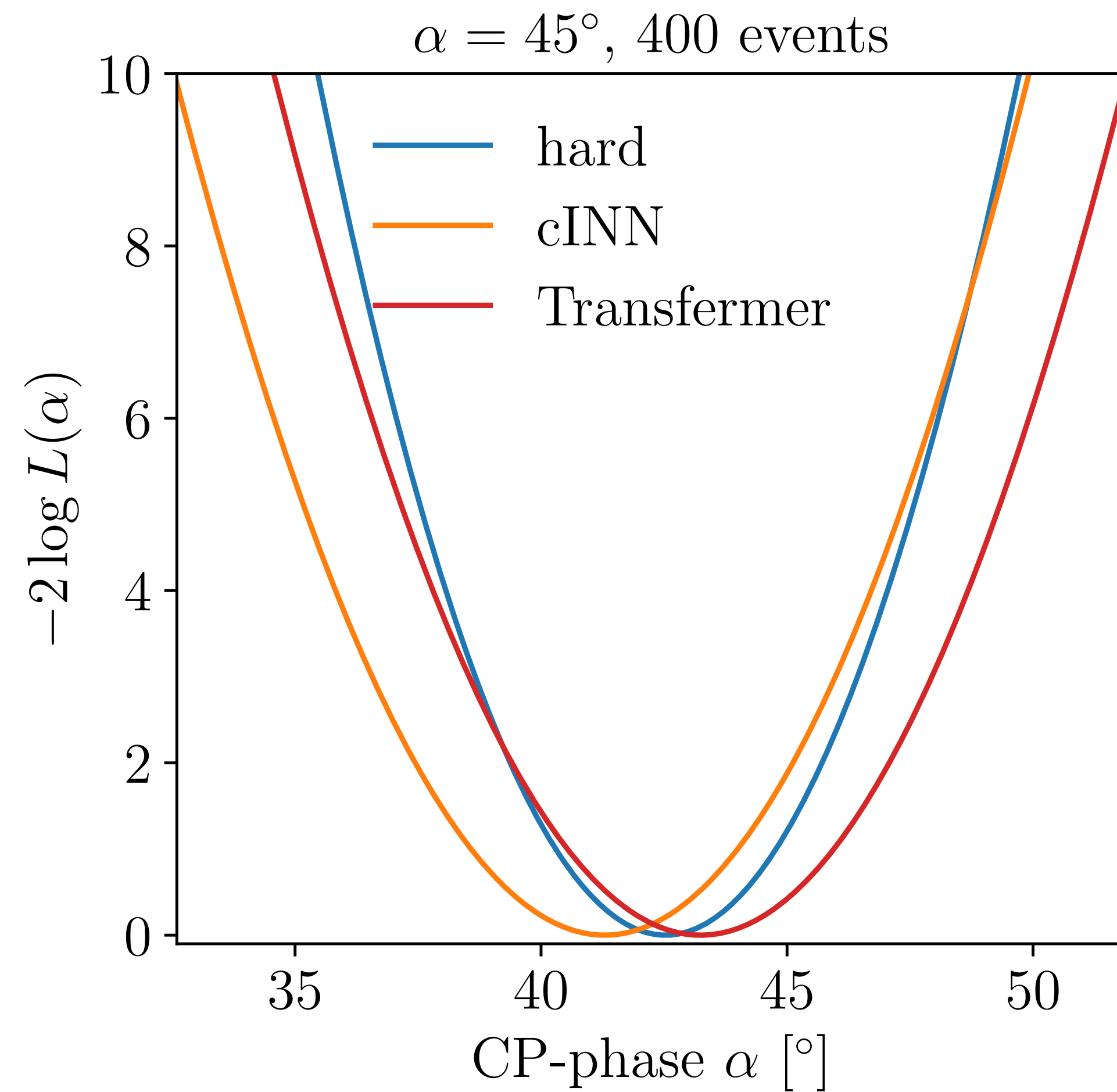
1. Jet combinatorics

$$pp \rightarrow tHj \rightarrow (bjj) (\gamma\gamma) j + \text{ISR Jets}$$

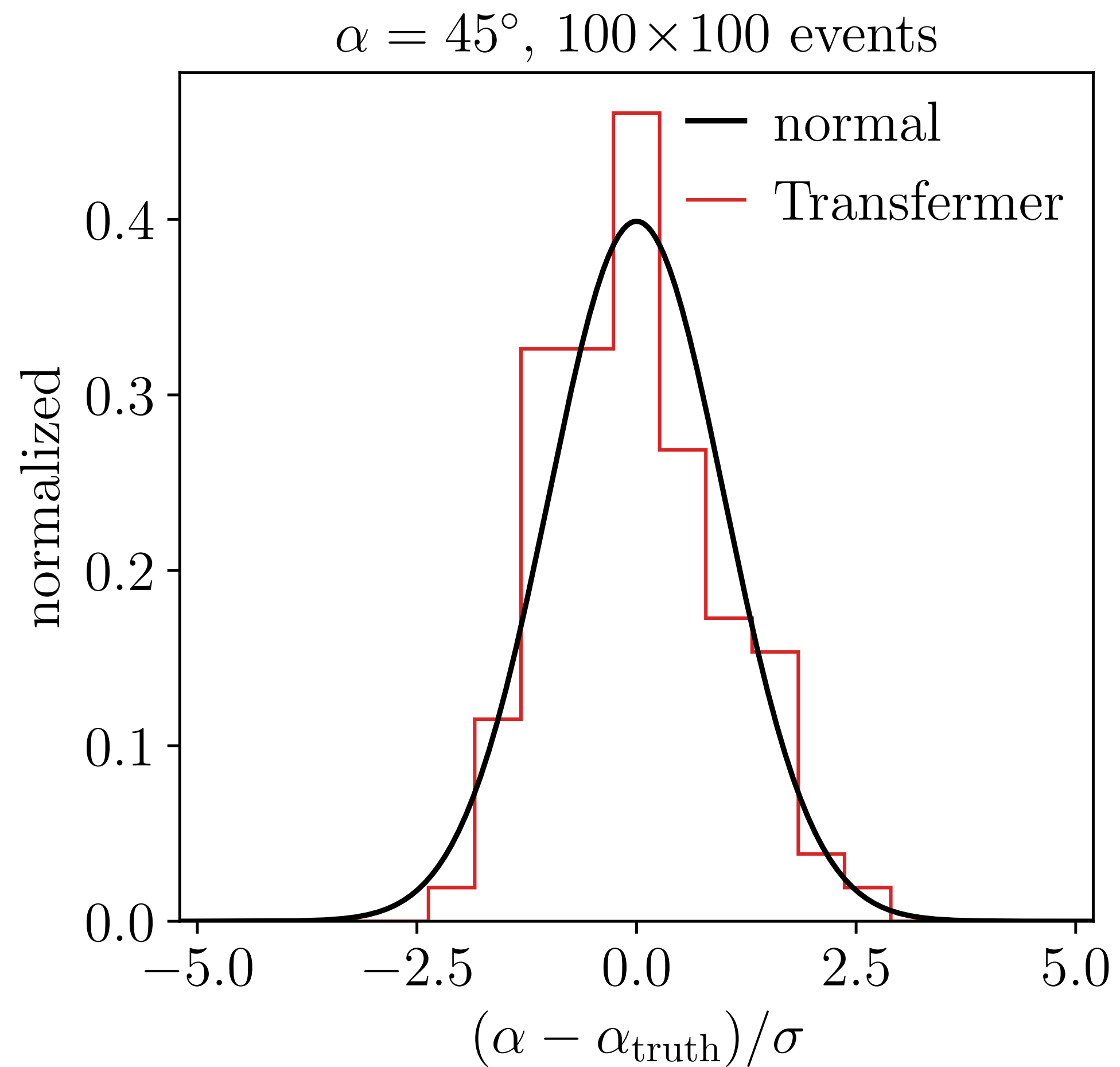
2. Can handle varying particle multiplicity

→ NLO

Transfermer Results



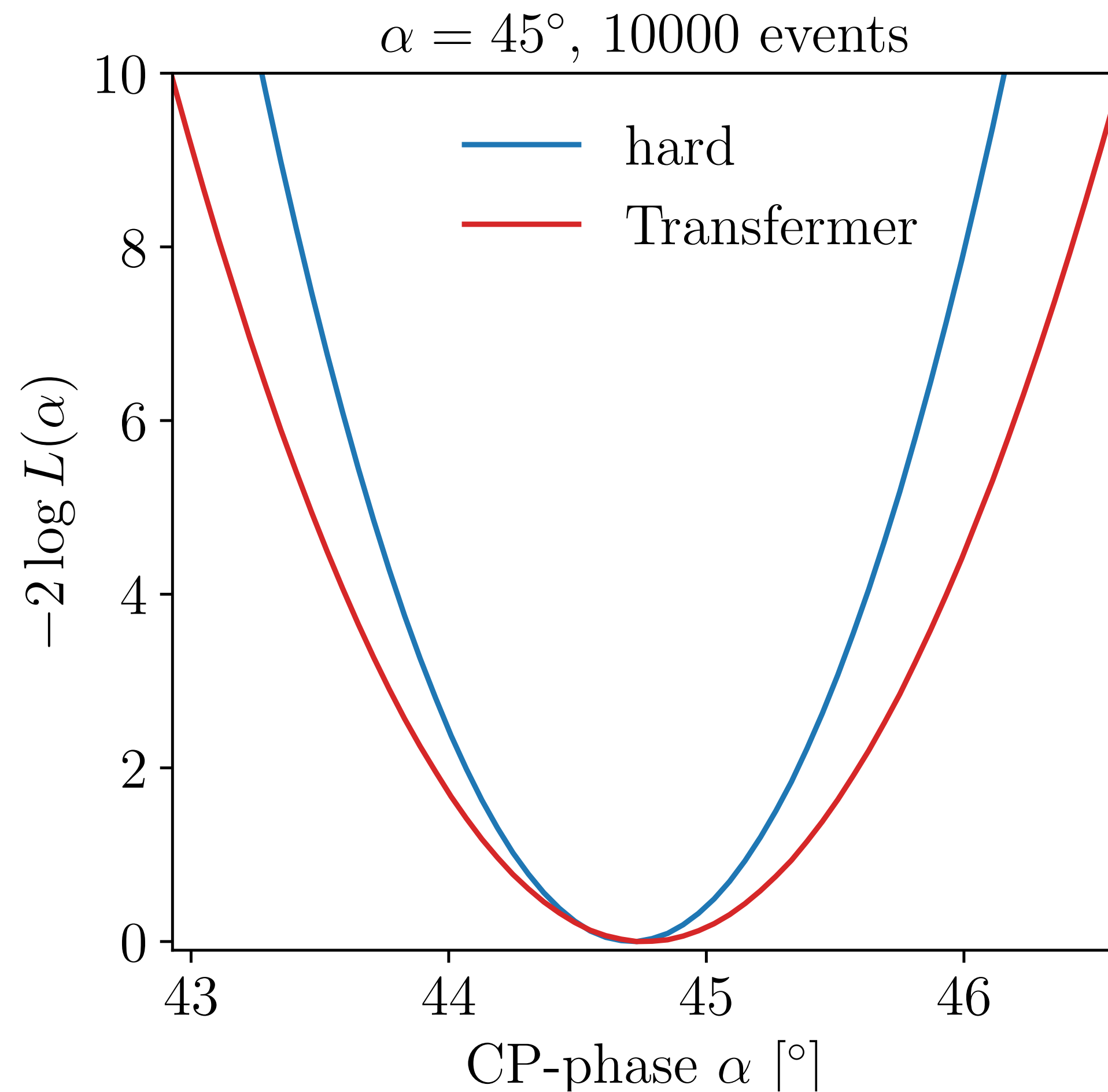
Estimating Calibration



Divide the 10k events into 100 samples of 100 events

Look at this distribution of the minima around the true α

Estimating Uncertainty



Estimate uncertainty using replicas:

Integration uncertainty:

Resample the MC points using bootstrapping

Network uncertainty:

Use Bayesian NN and resample for each replica

Summary and Outlook

SciPost Physics

2310.07752

Submission

Precision-Machine Learning for the Matrix Element Method

Theo Heindel¹, Nathan Huetsch¹, Ramon Winterhalder²,
Tilman Plehn¹, and Anja Butter^{1,3}

¹ Institut für Theoretische Physik, Universität Heidelberg, Germany

² CP3, Université catholique de Louvain, Louvain-la-Neuve, Belgium

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Three network setup makes the **MEM tractable**

- 1) **Transfer-Network** encoding the transfer probability $p(x_{reco} | x_{hard})$
- 2) **Acceptance-Network** encoding the efficiency $\epsilon(x_{hard})$
- 3) **Sampling-Network** encoding the proposal distribution $q(x_{hard})$

Pipeline gives **precise** and **well-calibrated** results

Bootstrapping and **Bayesian NNs** to estimate **uncertainties**

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Three network setup makes the **MEM tractable**

- 1) **Transfer-Network** encoding the transfer probability $p(x_{reco} | x_{hard})$
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Method gives **precise** and **well-calibrated** results

Bootstrapping and **Bayesian NNs** to estimate **uncertainties**

NLO

Model dependence

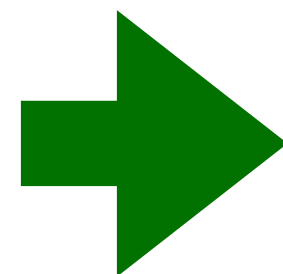
Theory \neq Practice

Improving integration convergence

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

1

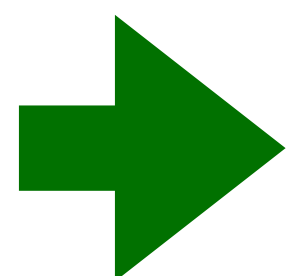
In practice $p_{\theta}(x_{reco} | x_{hard}) \neq p(x_{reco} | x_{hard})$



Train Sampling Network on trained Transfer Probability

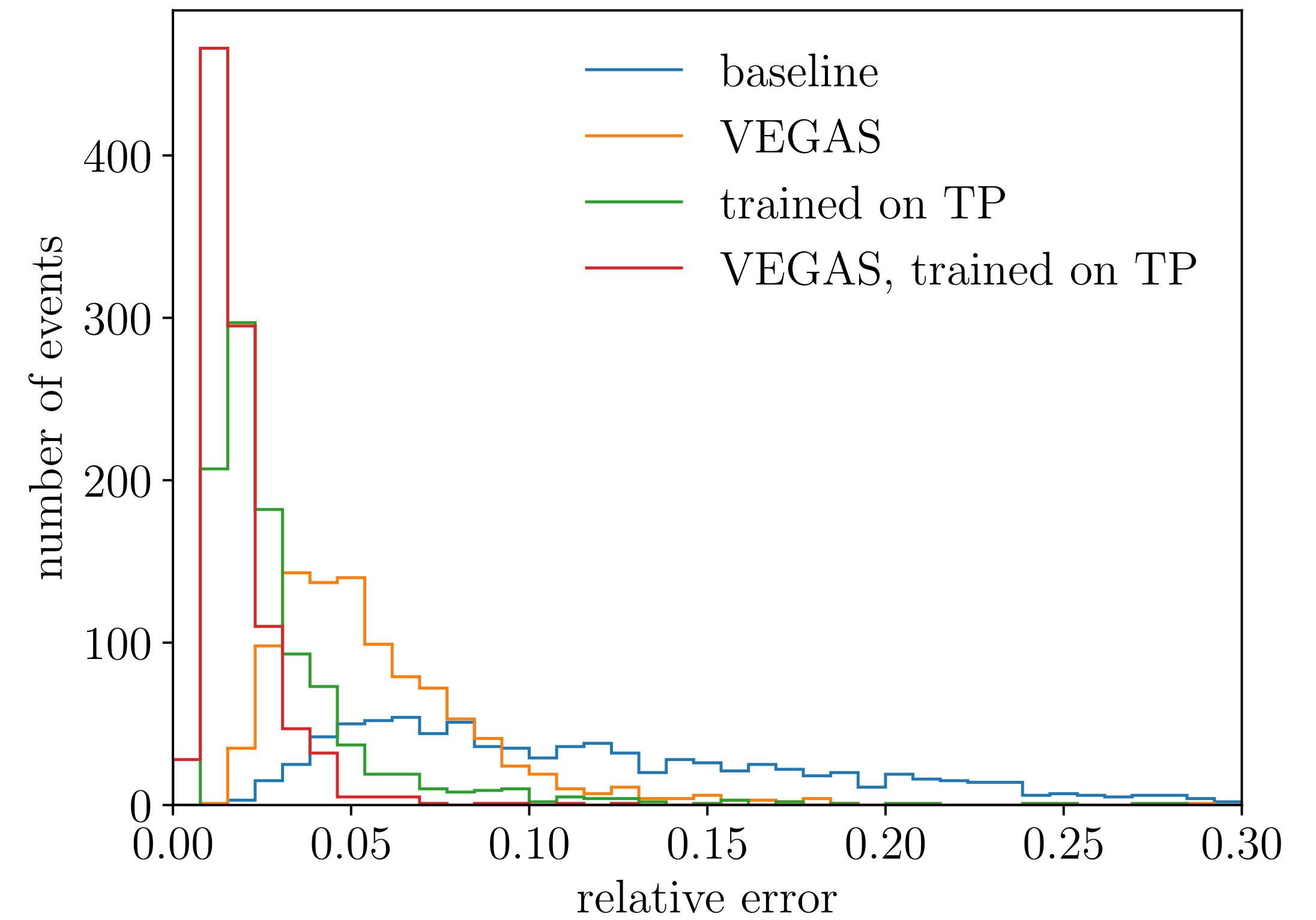
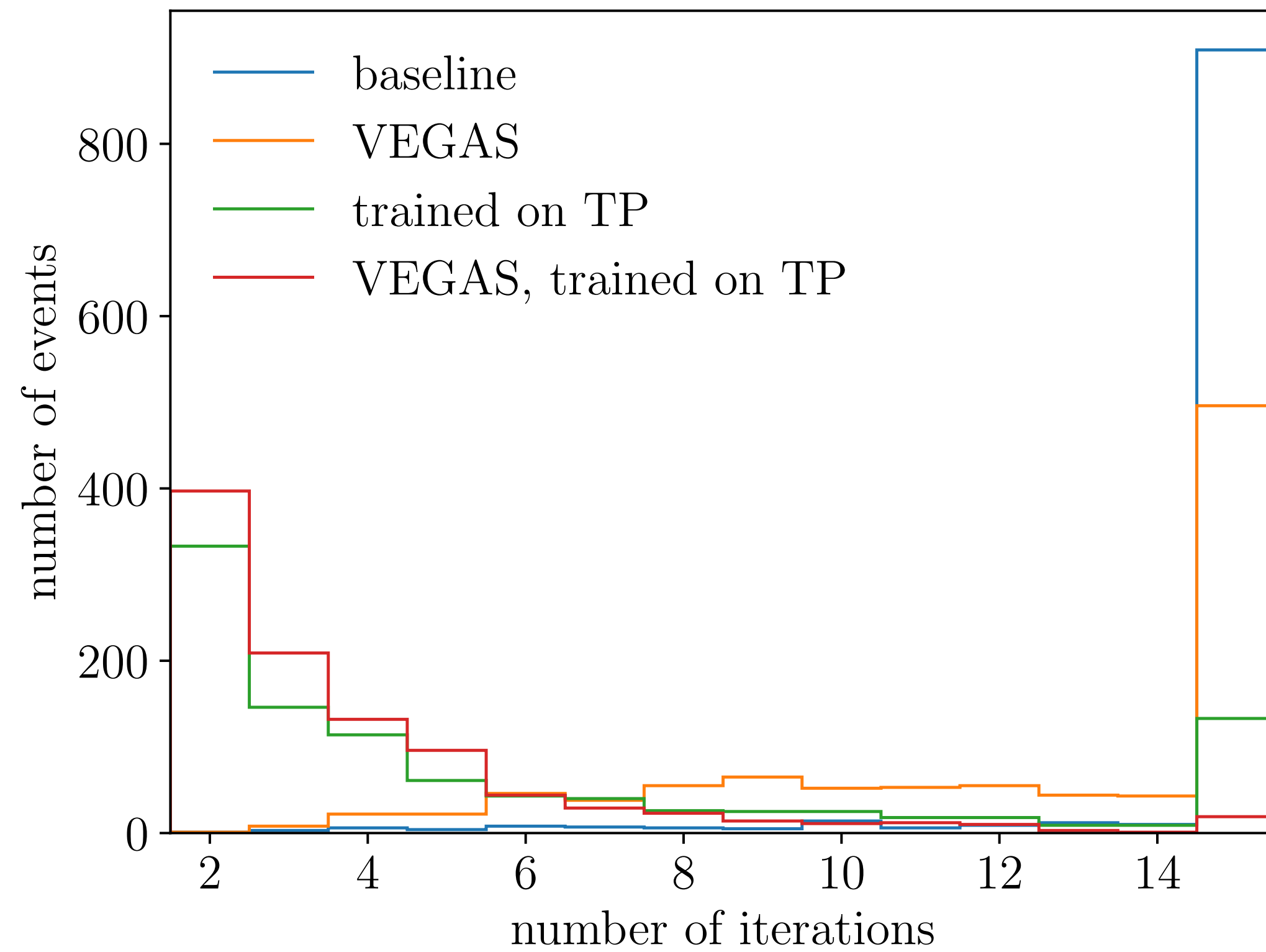
2

In practice $q_{\theta}(x_{hard}) \neq q_{ideal}(x_{hard})$

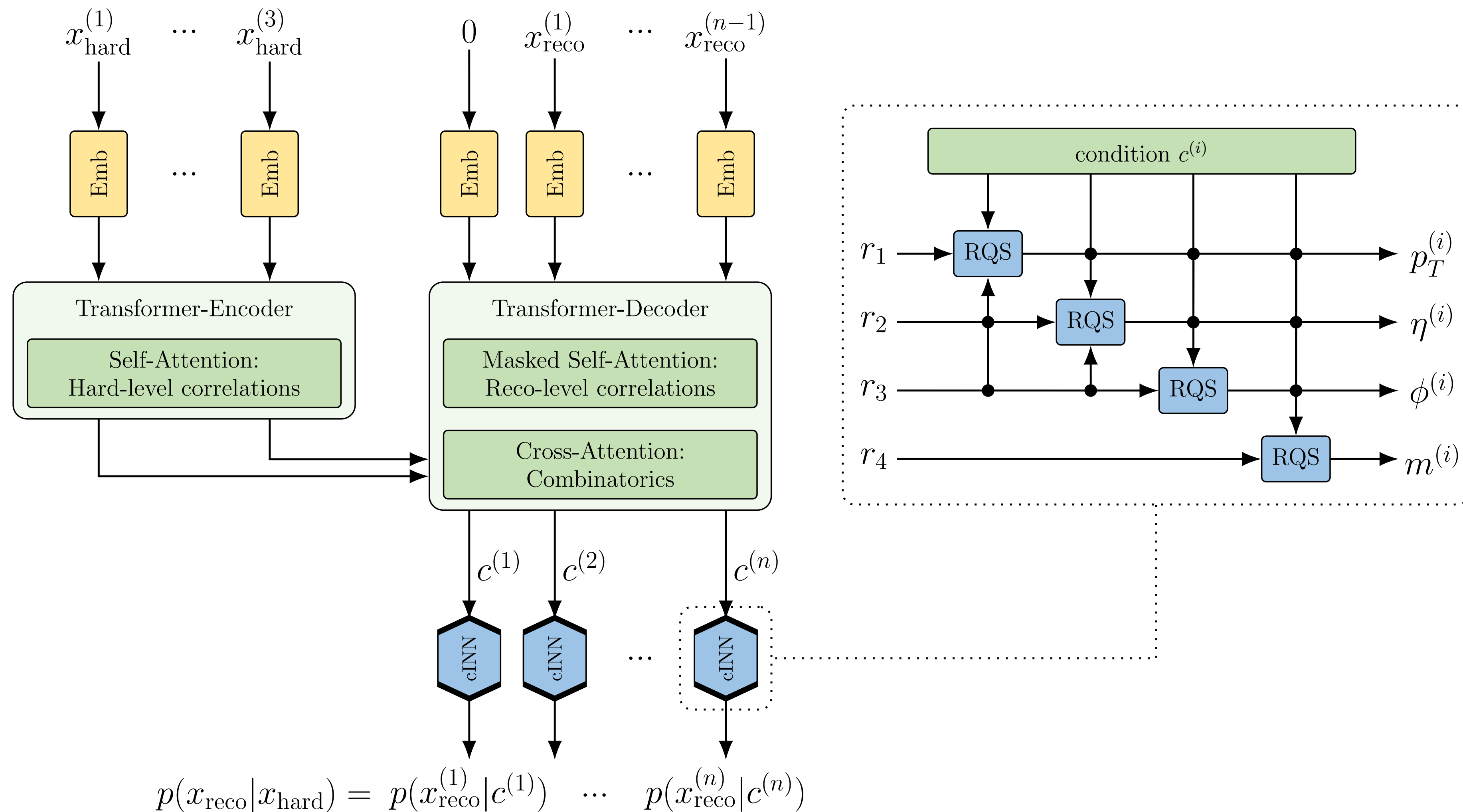


Further refine the cINN latent space with a VEGAS grid

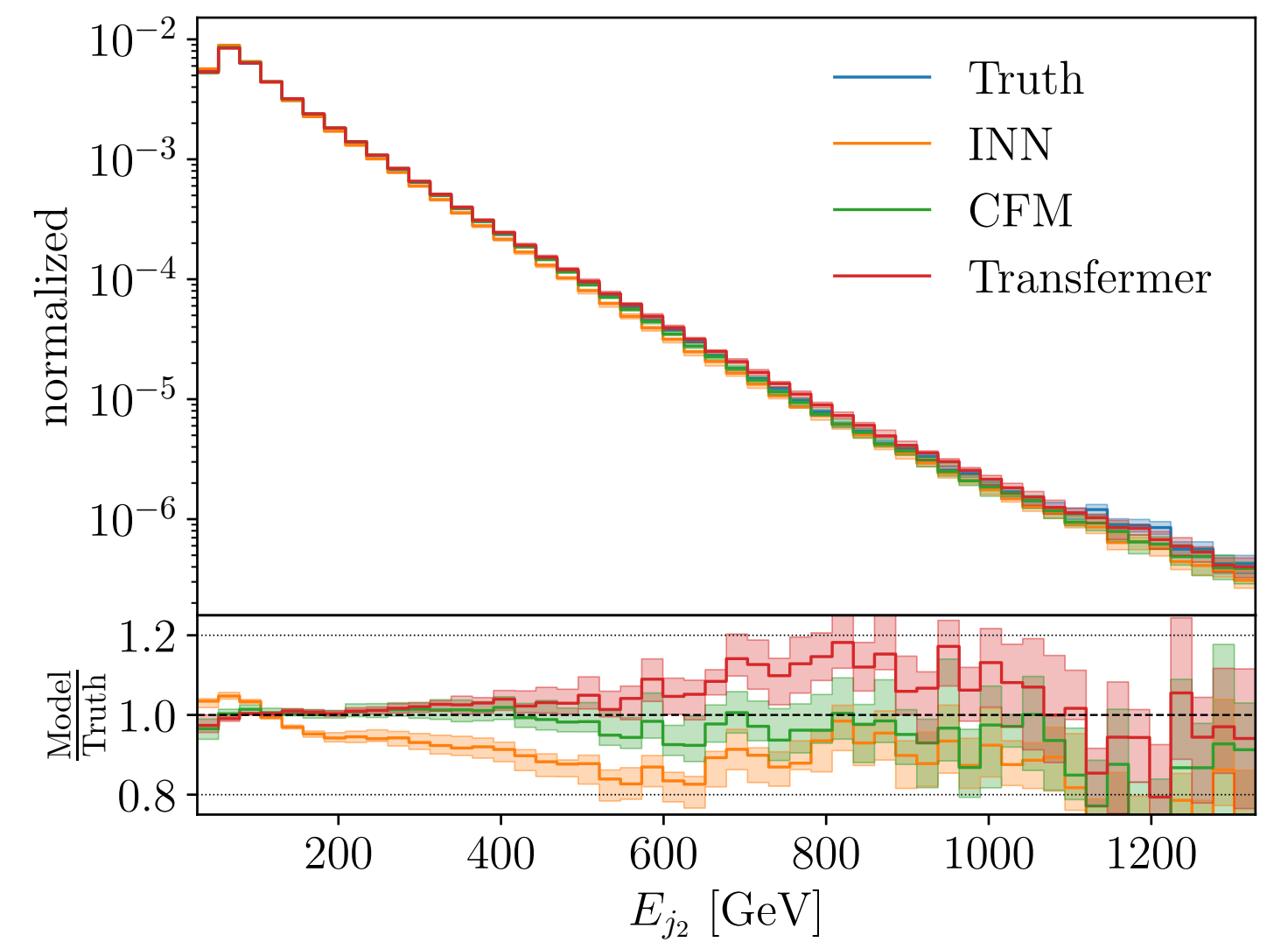
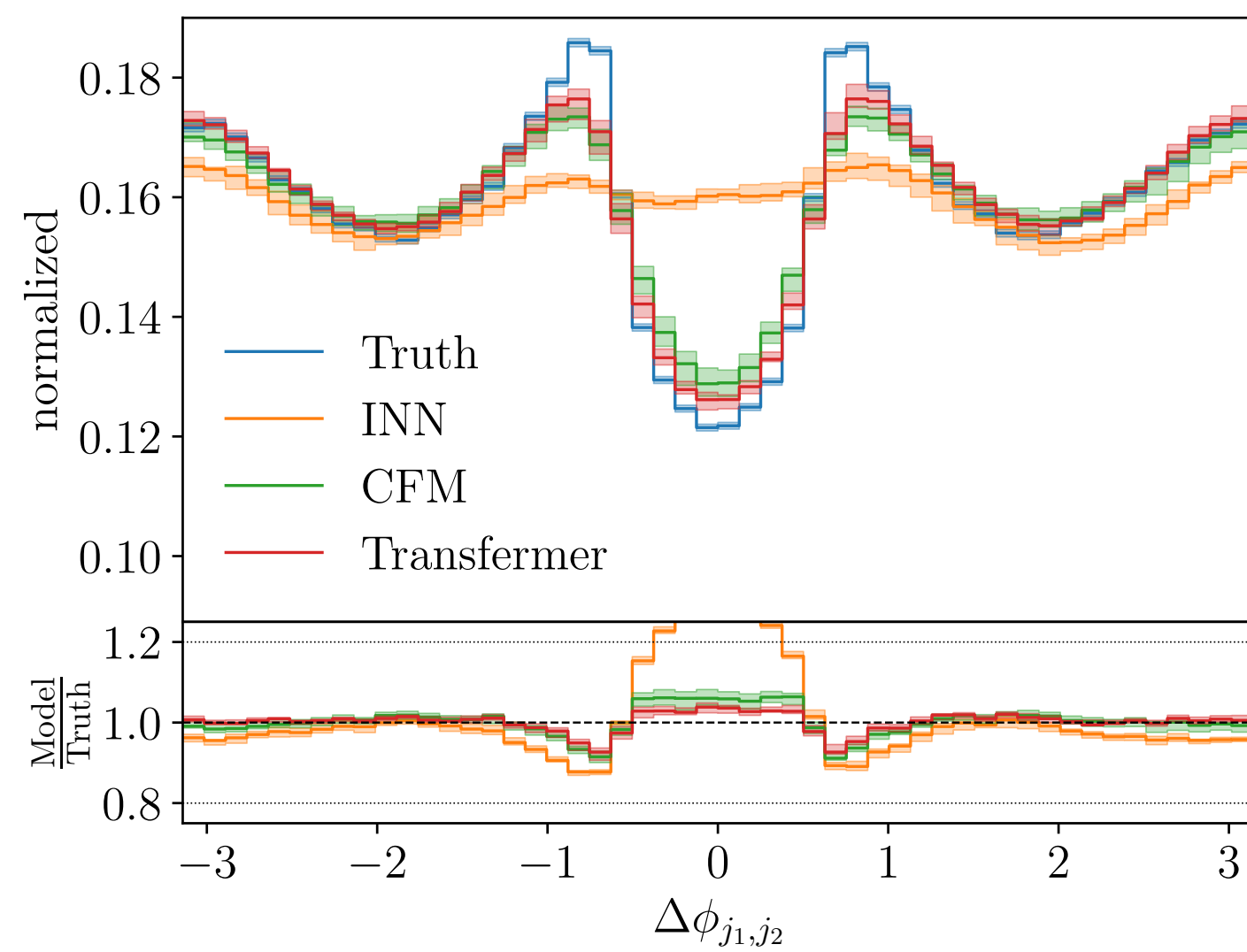
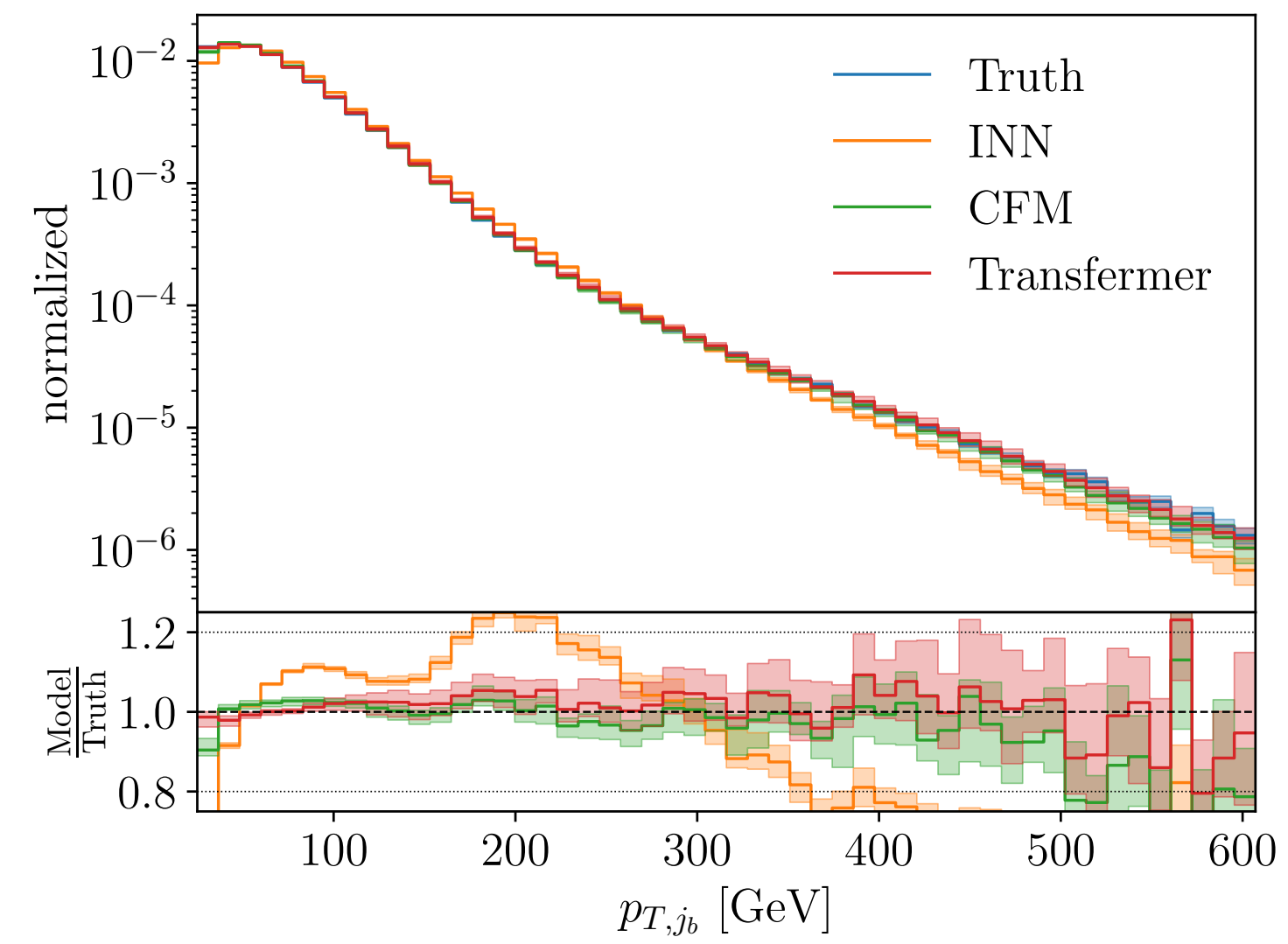
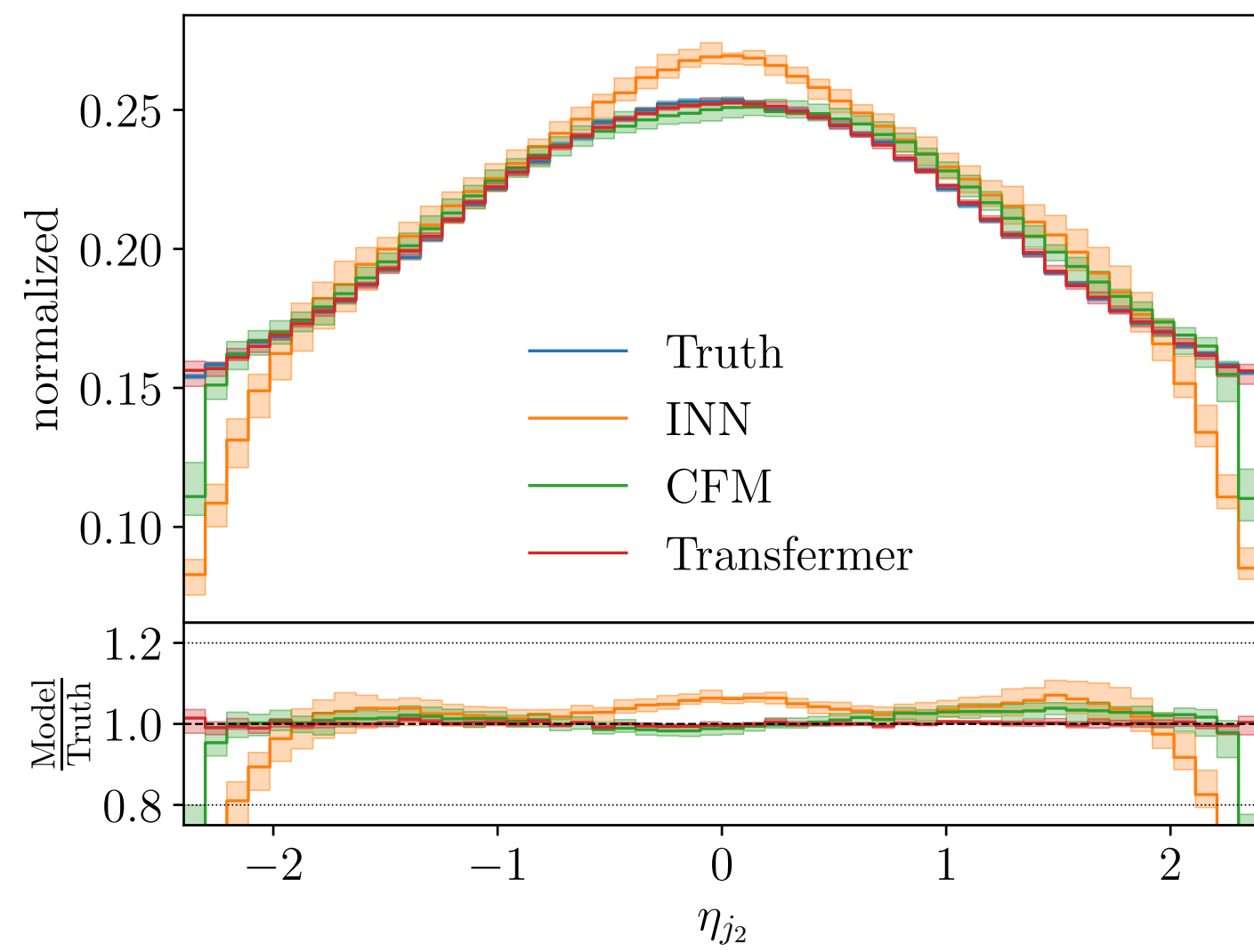
Improving integration convergence



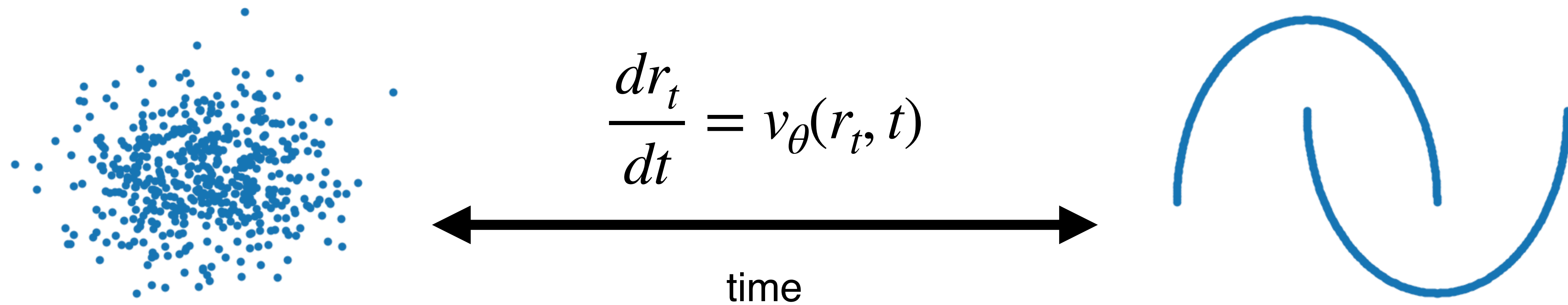
The Transformer (Transfer-Transformer)



Transfer-Network observables



Conditional Flow Matching



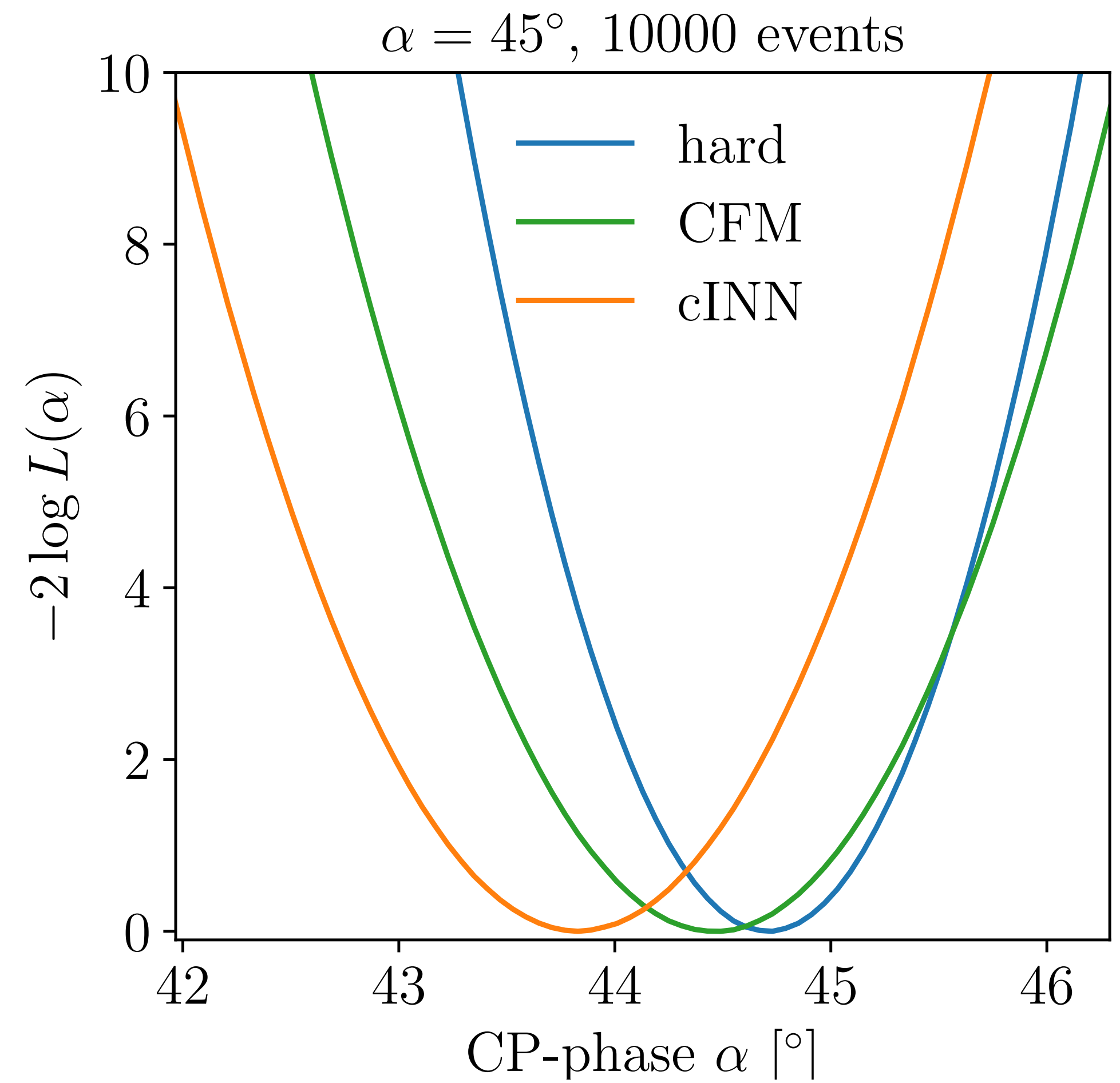
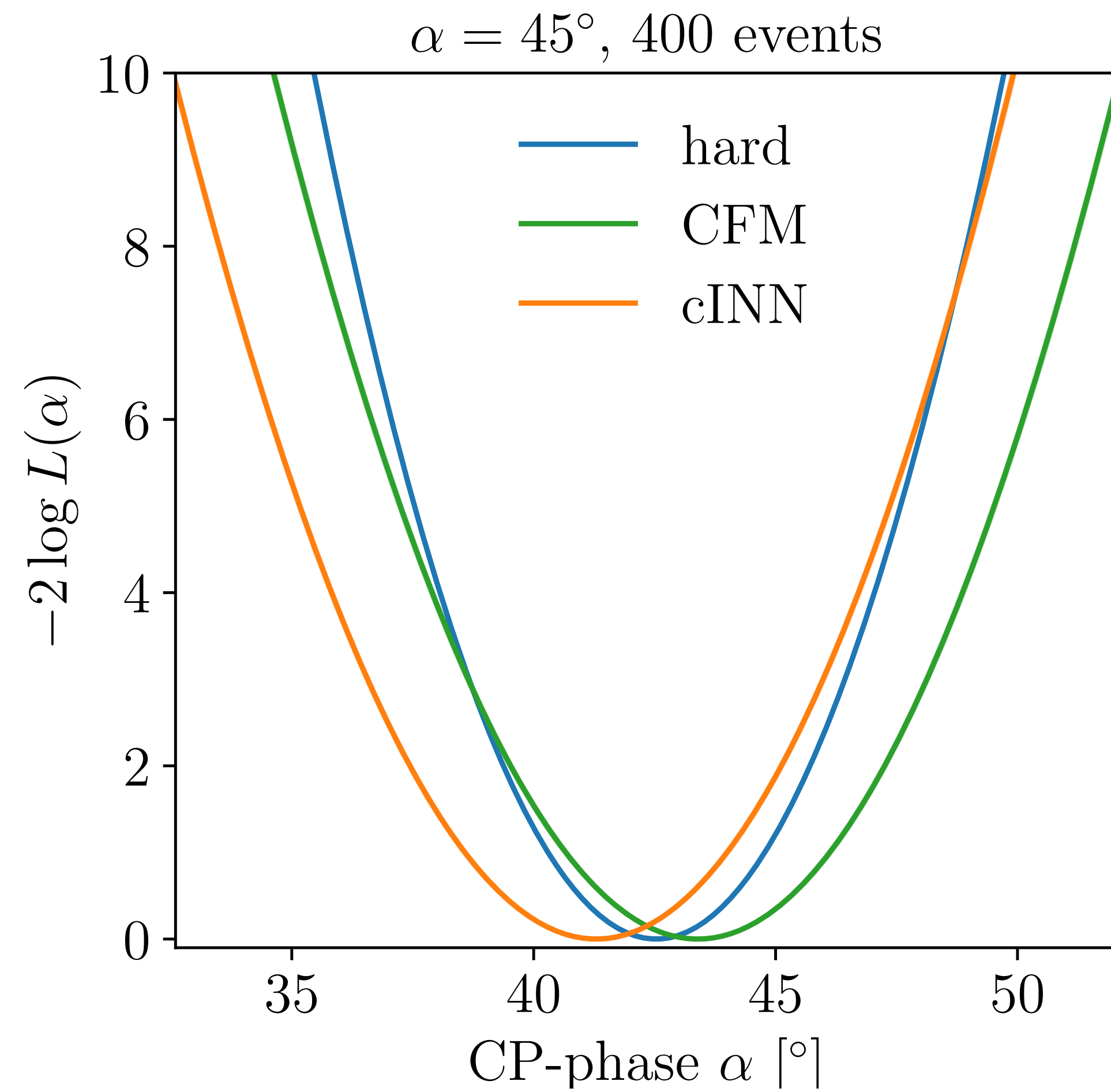
$$r_1 \sim P_{latent}(r)$$

$$r_0 \sim P_{target}$$

ODE defines invertible mapping: $r_1 = G_\theta^{-1}(r) = r_1 + \int_1^0 v_\theta(r_t, t) dt$

$$p_\theta(x) = p_{latent}(G_\theta(x)) \underbrace{\left| \det J_{G_\theta} \right|}_{\exp\left(\int_0^1 \nabla_r v_\theta(r_t, t) dt\right)}$$

Transfer-Diffusion Results



Transfermer Results

