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IRN Terascale, 26.10.2023

# Precision-Machine Learning for the Matrix Element Method

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

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

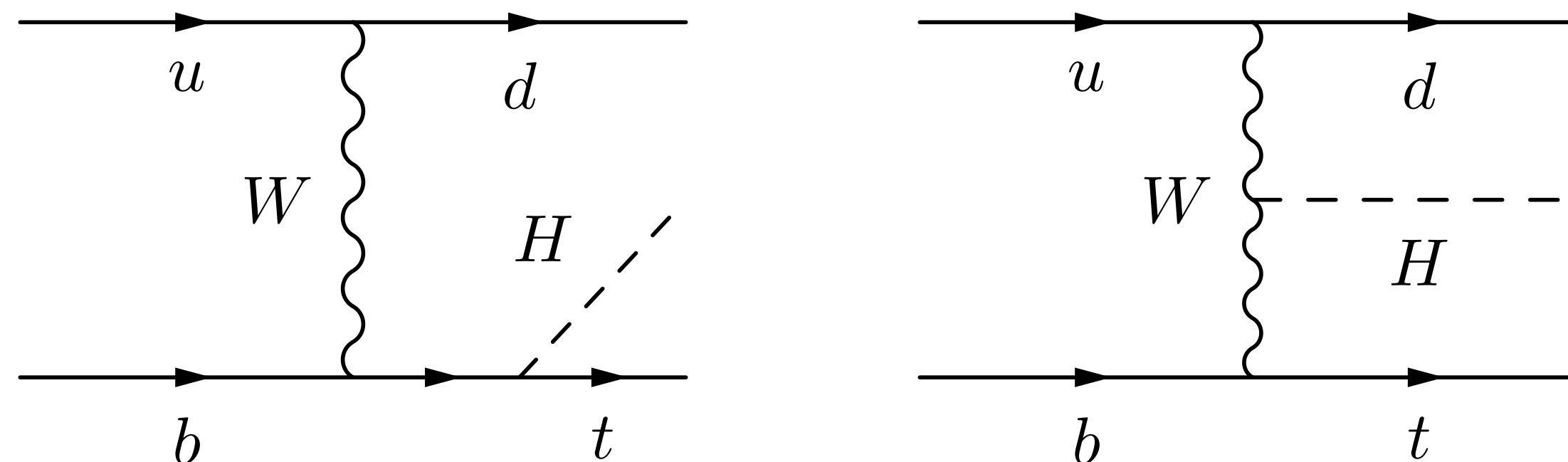
# The physics problem

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

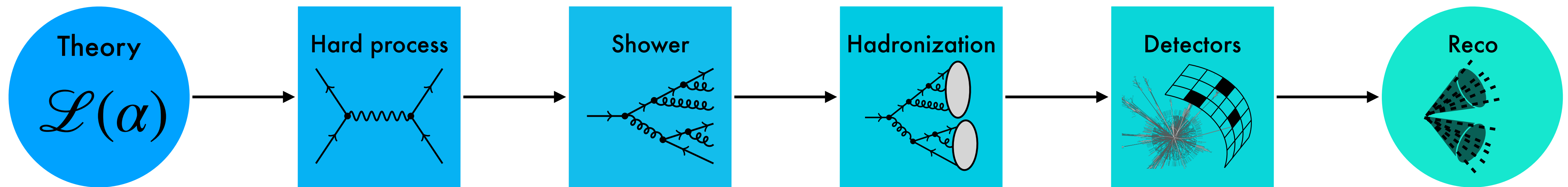
$$\mathcal{L}_{t\bar{t}H} = -\frac{y_t}{\sqrt{2}} \left[ \cos \alpha \bar{t}t + \frac{2}{3} i \sin \alpha \bar{t} \gamma_5 t \right] H$$

**The process:** Associated single-top and Higgs production

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

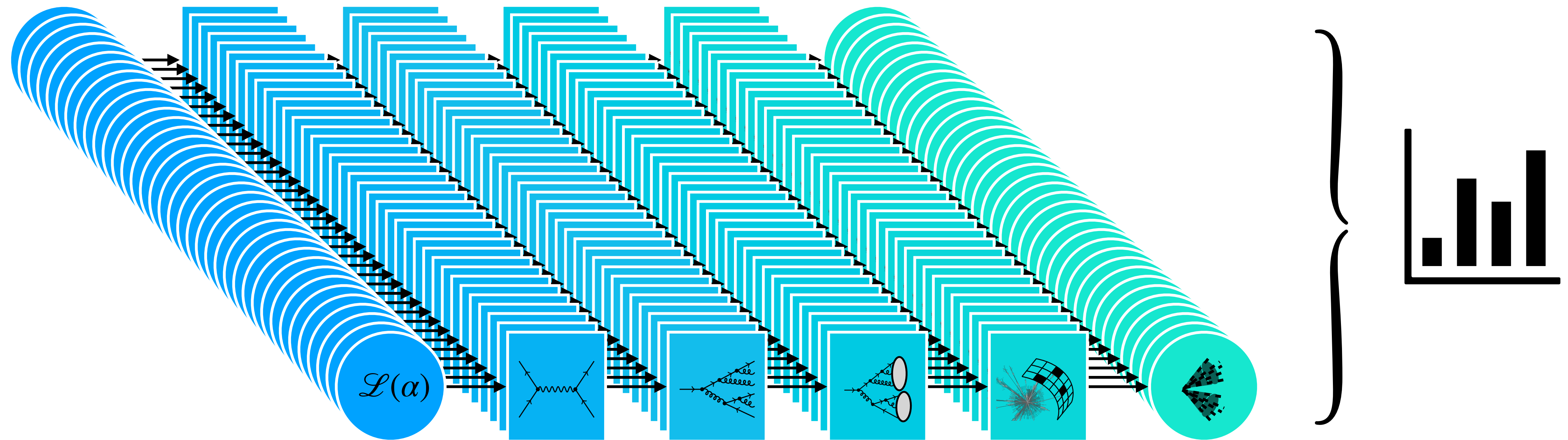


# From Theory to Experiment in LHC Physics



Each event undergoes reconstruction

# From Theory to Experiment in LHC Physics

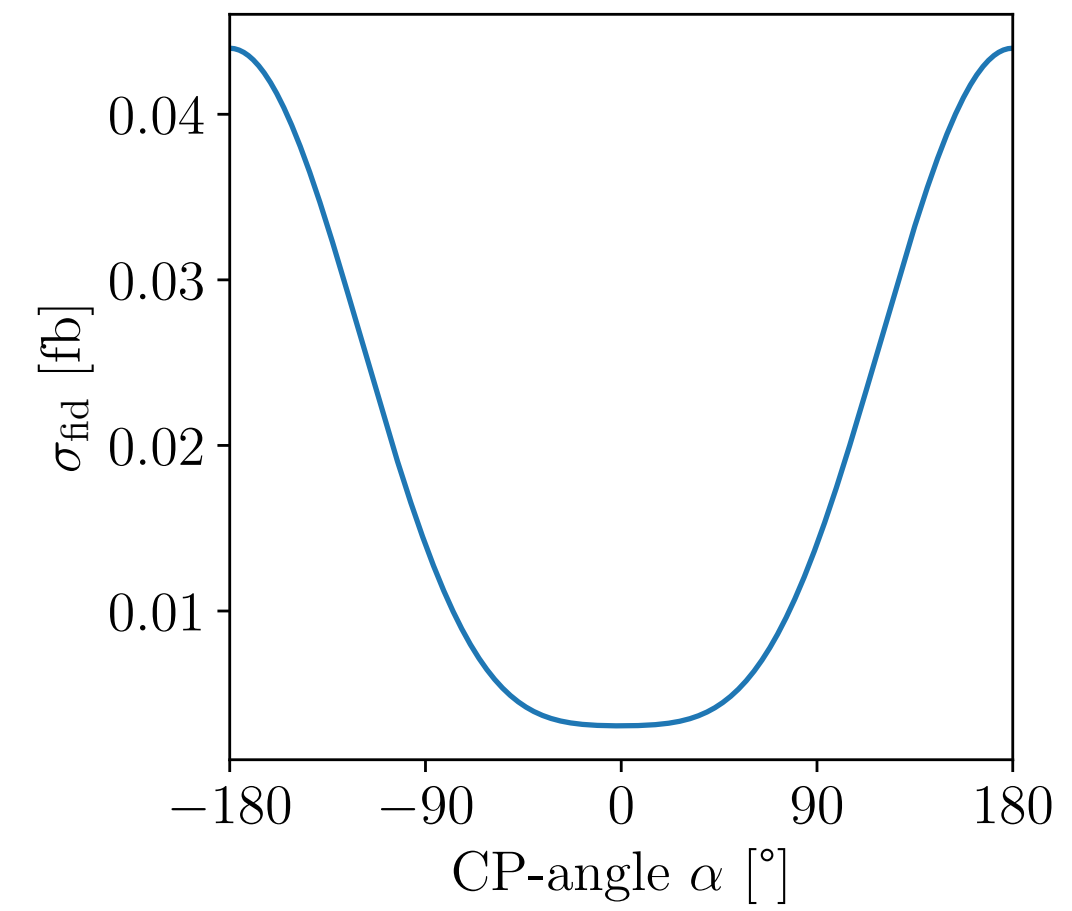


Event samples are combined into observable histogram

# Why is this a problem here?

Cross-section:

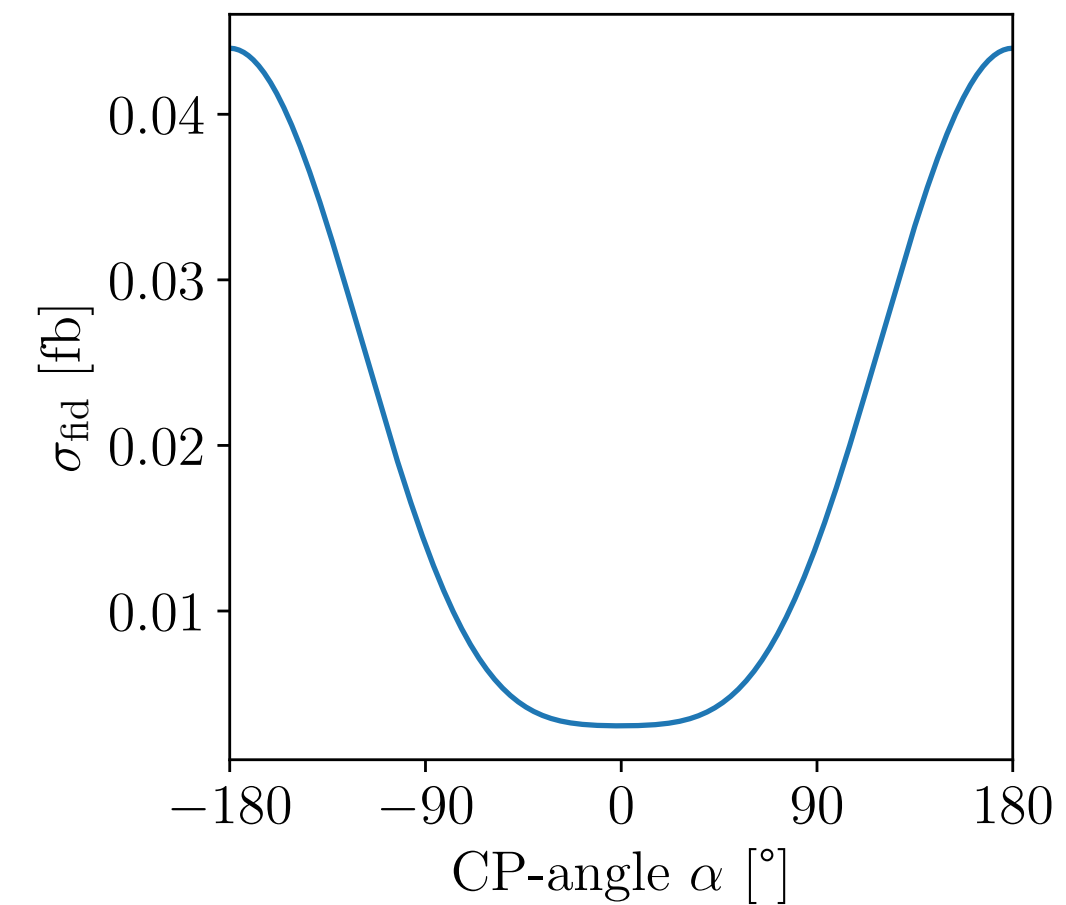
- very small
- insensitive to variations in  $\alpha$



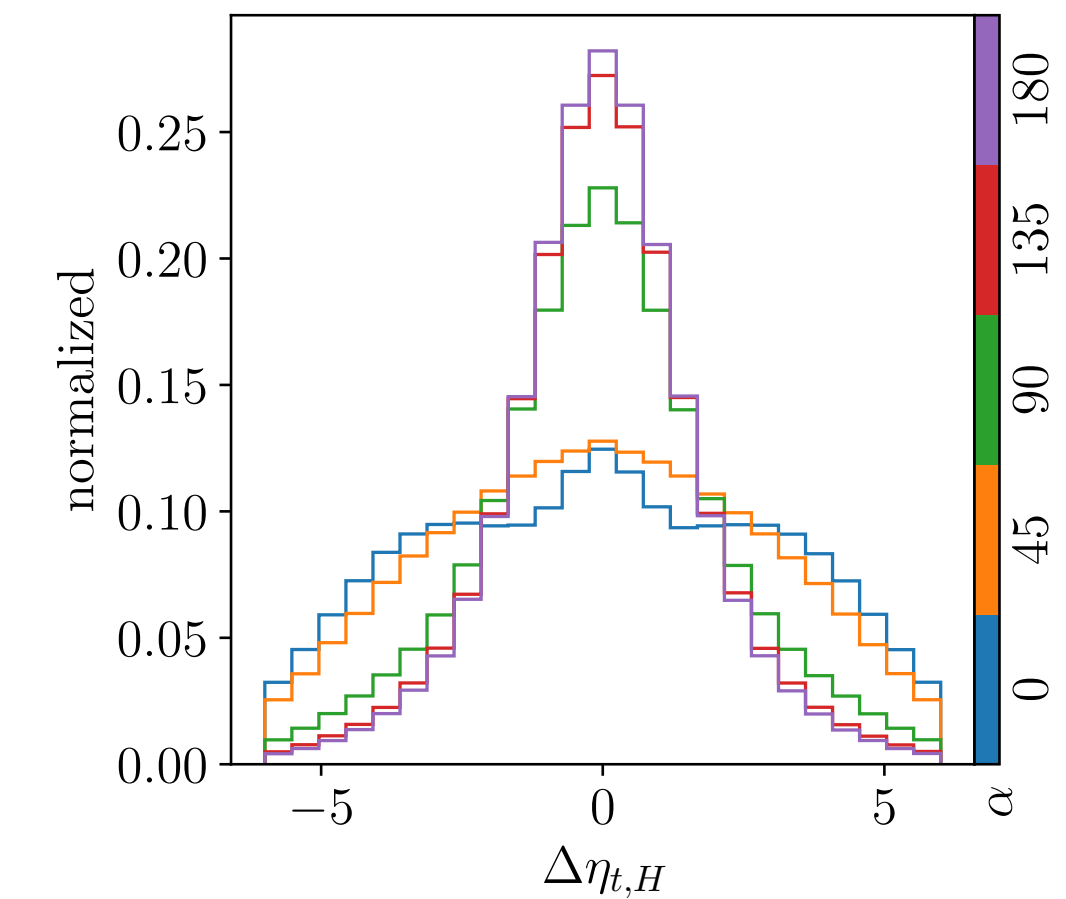
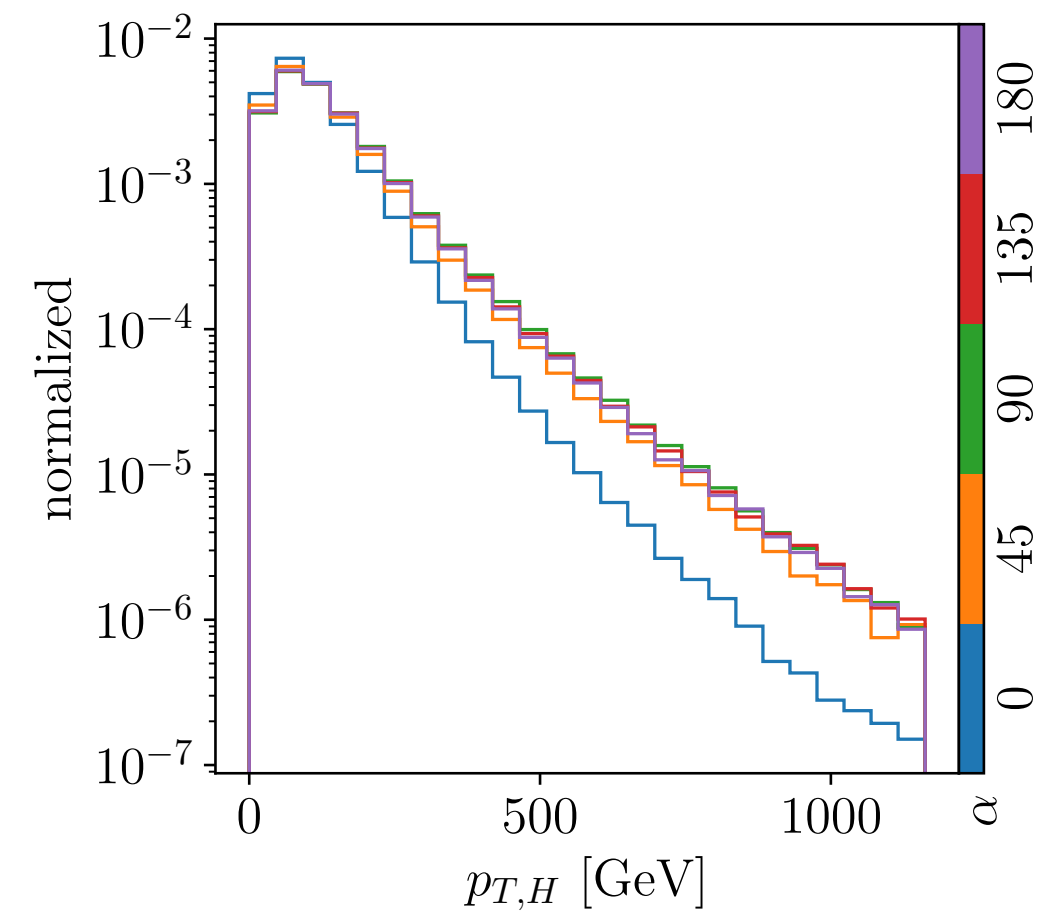
# Why is this a problem here?

Cross-section:

- very small
- insensitive to variations in  $\alpha$



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

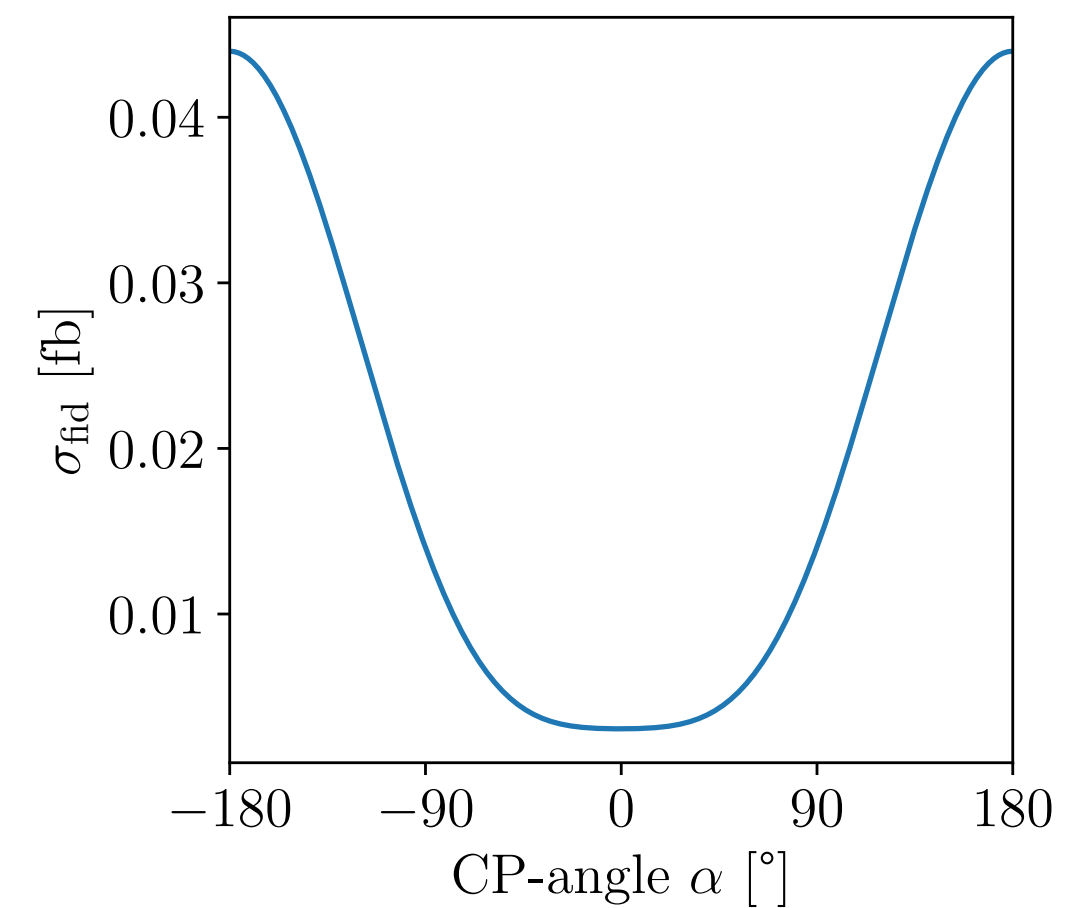


[Figures taken from Butter et al [arXiv:2210.00019](https://arxiv.org/abs/2210.00019)]

# Why is this a problem here?

Cross-section:

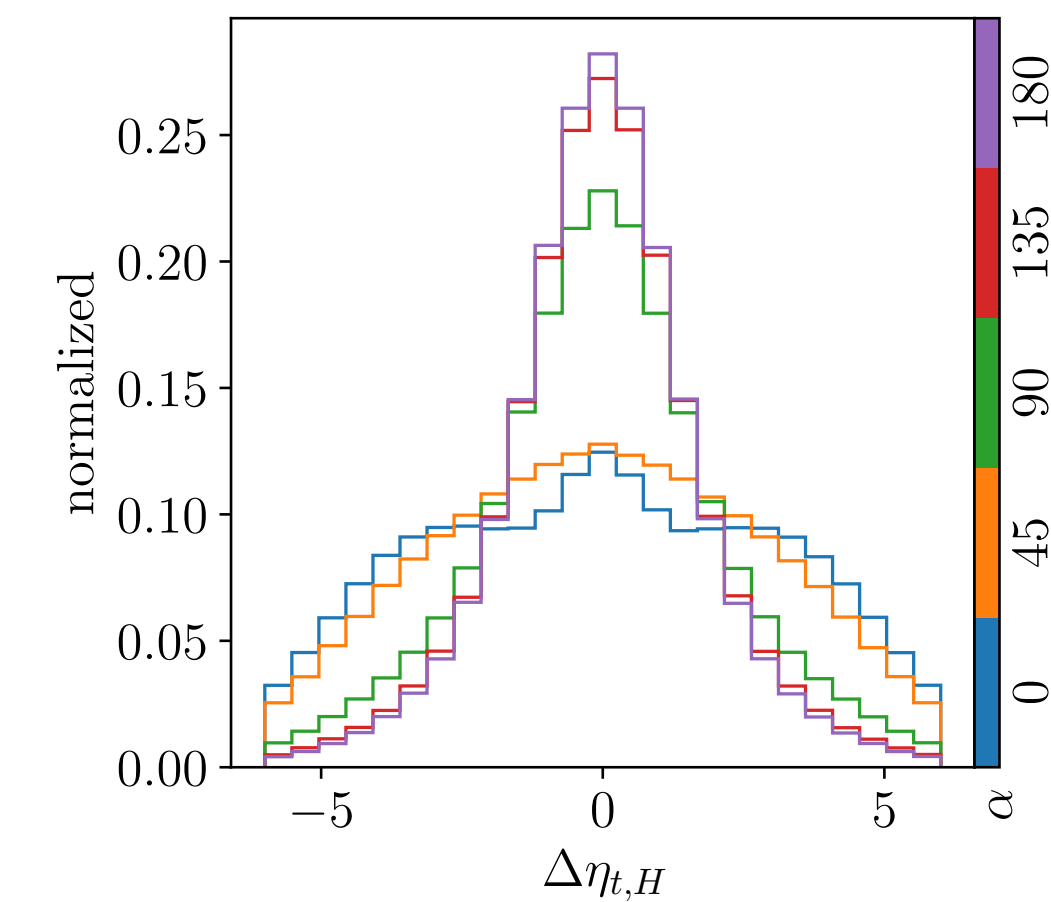
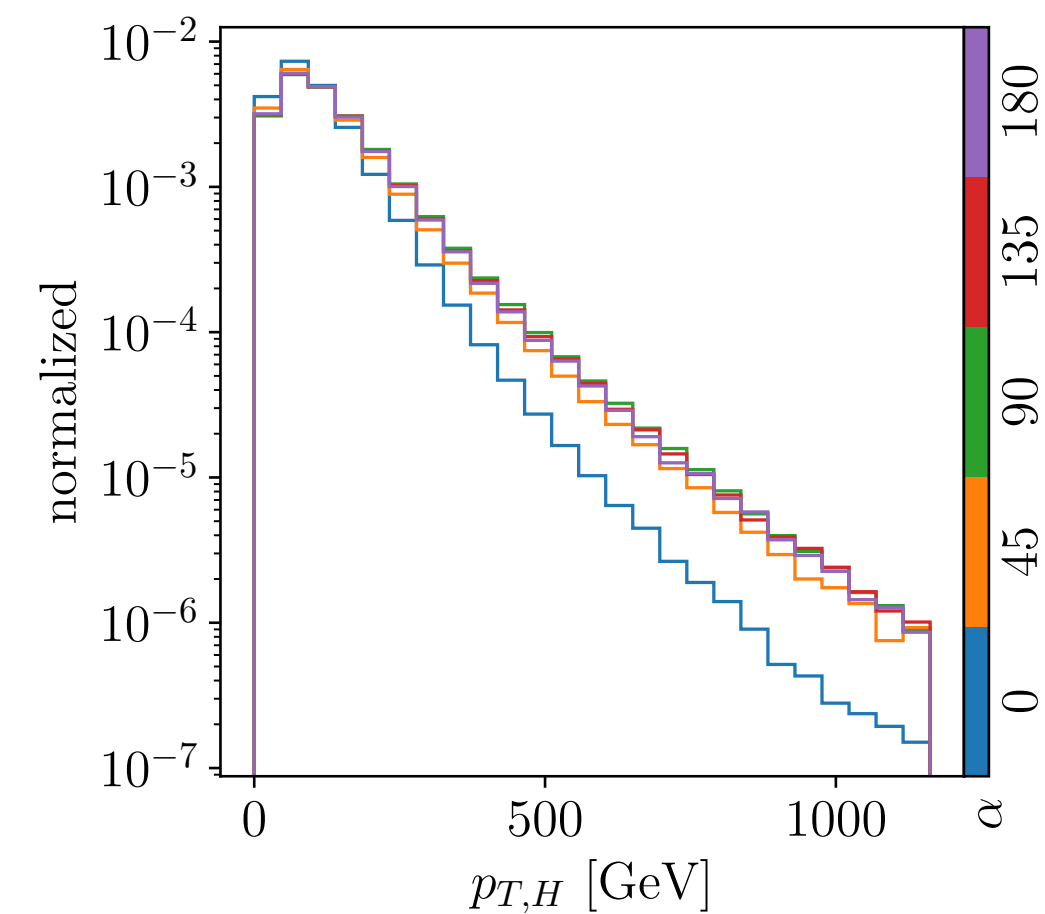
- very small
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Hard-scattering  $p(x_{\text{hard}} | \alpha)$  kinematics are sensitive

Need analysis method based on **kinematics**

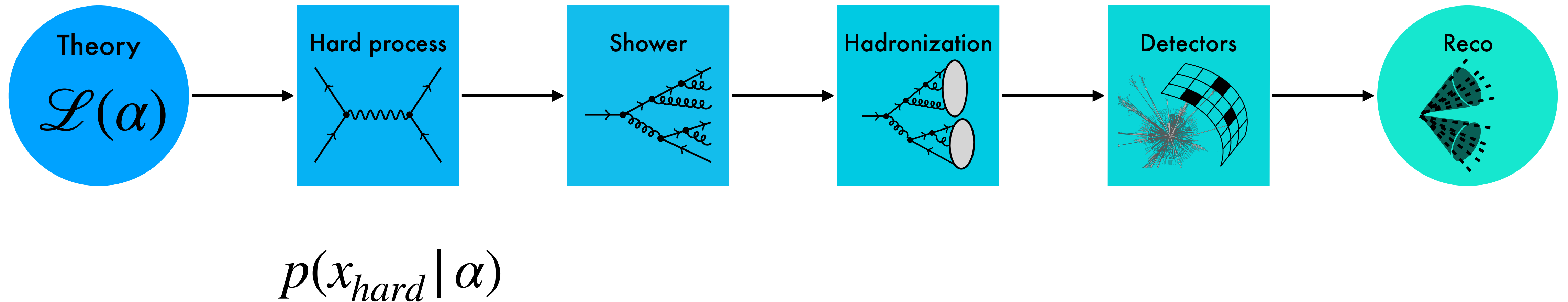
**Likelihood ratio** ideal test statistic according to Newman-Pearson lemma



[Figures taken from Butter et al [arXiv:2210.00019](https://arxiv.org/abs/2210.00019)]



# Going for the likelihood ratio

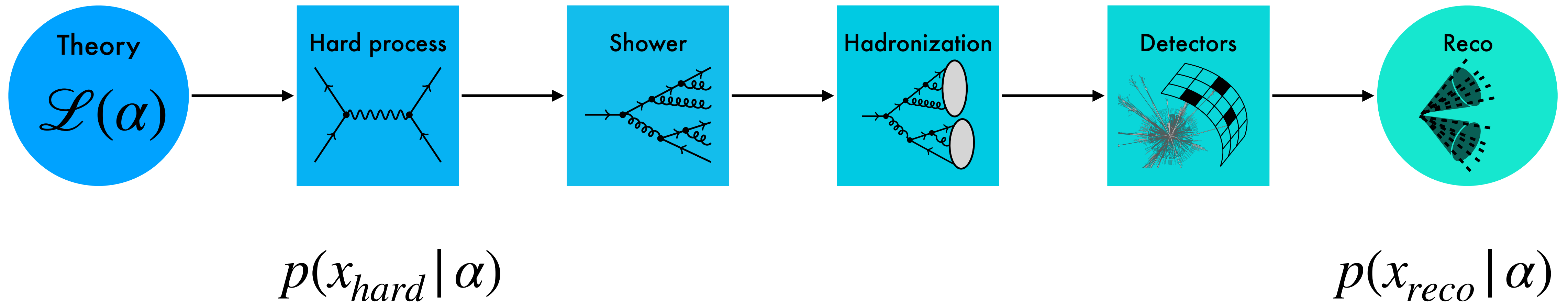


At hard-scattering level likelihood given by differential cross-section  $p(x_{hard} | \alpha) = \frac{1}{\sigma(\alpha)} \frac{d\sigma(\alpha)}{dx_{hard}}$

Unfortunately we do not measure at hard-scattering level

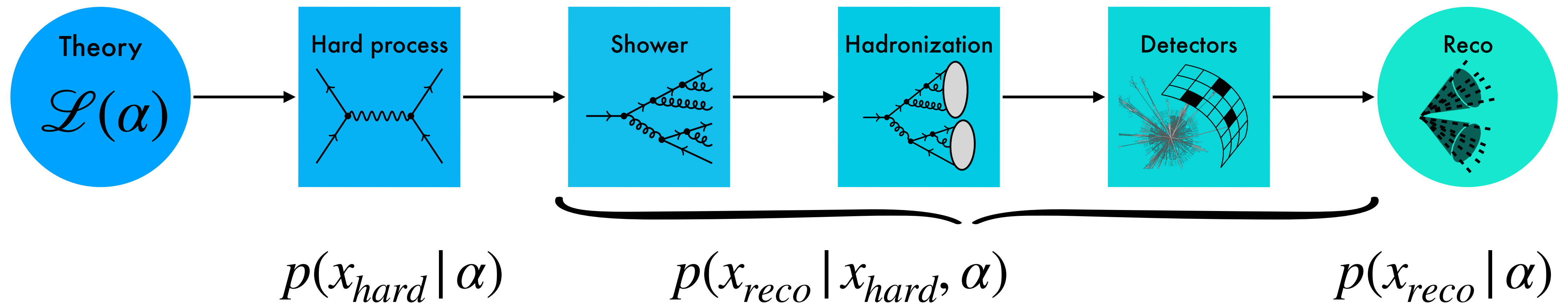


# Going for the likelihood ratio



**Need access to the likelihood at reconstruction level!**

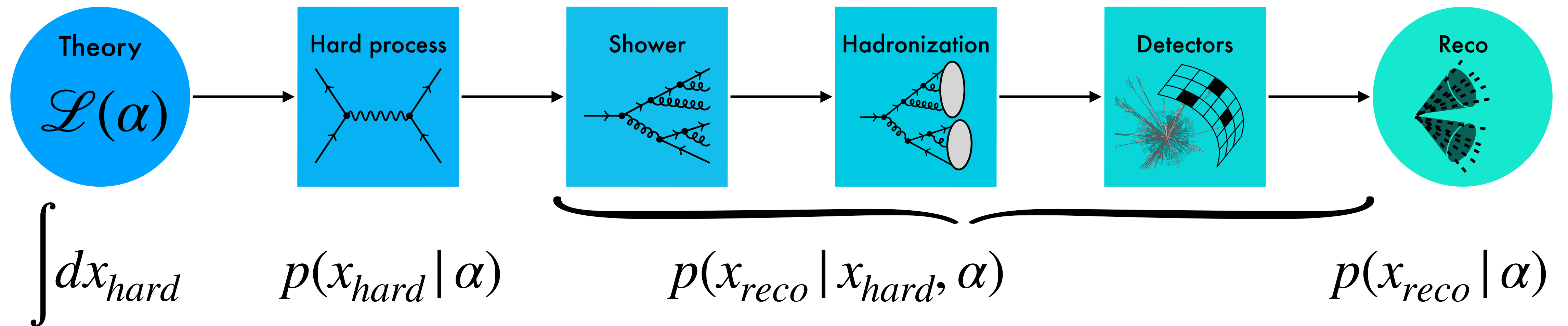
# Going for the likelihood ratio



Hard-scattering and reconstruction linked by forward transfer probability

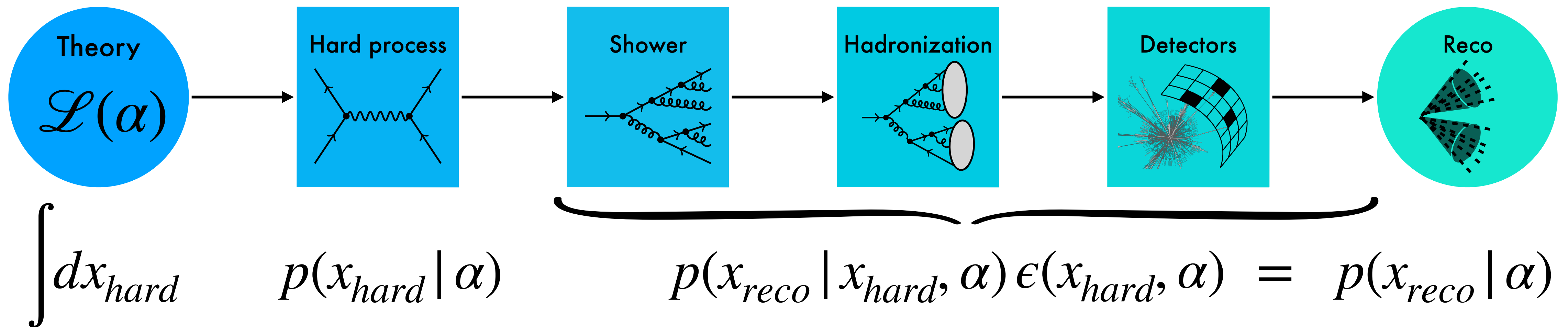
Forward transfer probability not known, encoded implicitly in forward simulation chain

# Going for the likelihood ratio



Integrate over all possible hard-scattering configurations

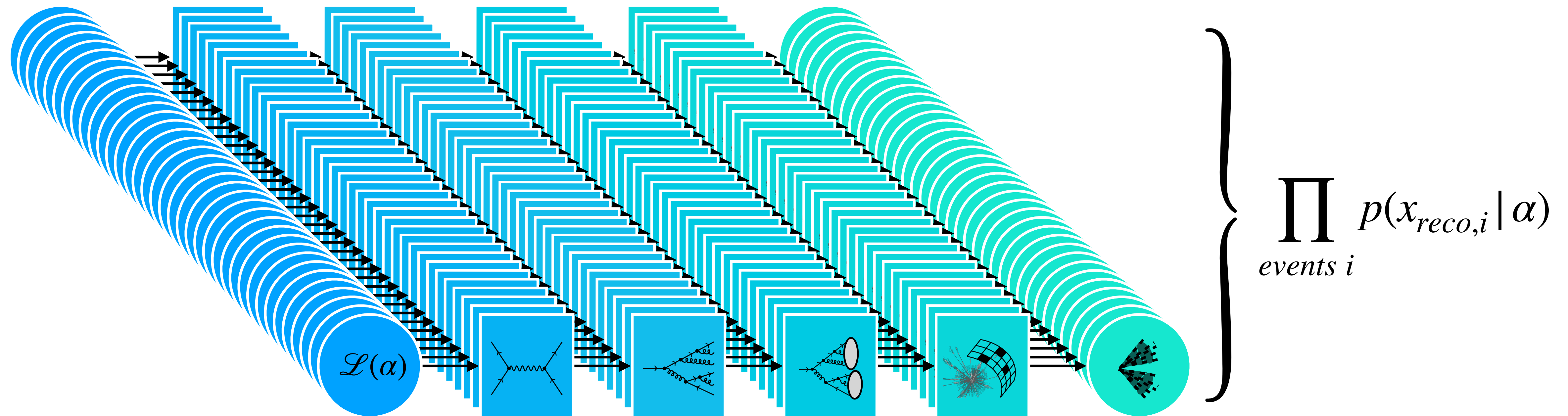
# Going for the likelihood ratio



Include an efficiency term to account for acceptance of events

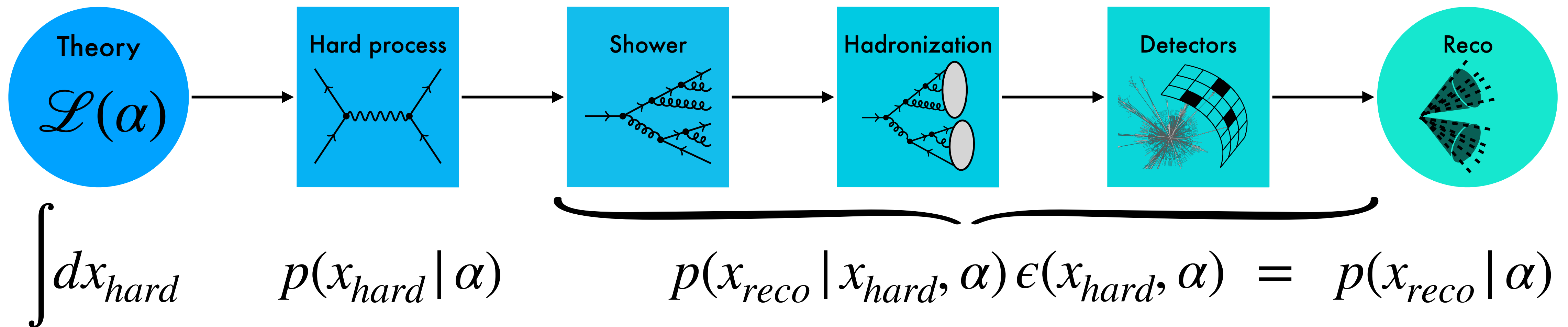
Encodes the probability that hard-scattering level configuration will pass reco level cuts

# Going for the likelihood ratio



Event likelihoods are combined into sample likelihoods

# The Matrix Element Method



+++ Unbinned and multivariate by design

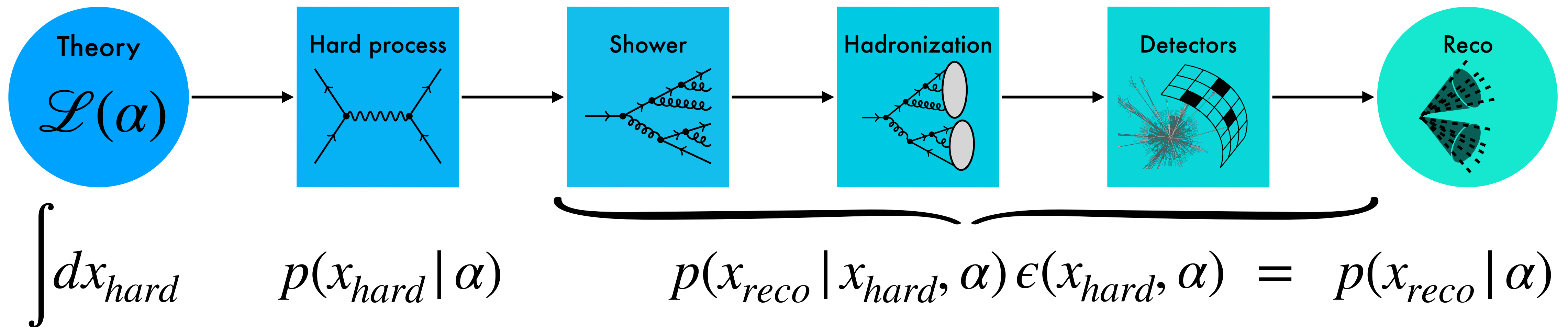
+++ Optimal use of information derived from Newman-Pearson lemma

— — 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 Newman-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

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

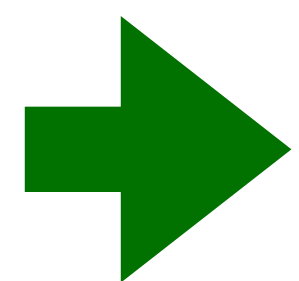
**Intractable**

# The Transfer Network

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

Transfer probability is analytically intractable

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



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

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

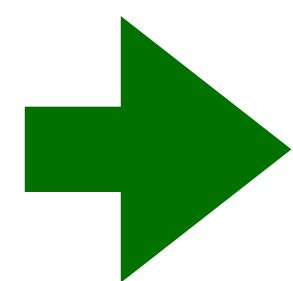
The term  $\epsilon(x_{hard})$  is highlighted with a red box and labeled "Unknown".

# The Acceptance Network

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

Efficiency at hard-scattering level is unknown

Transfer can be simulated to generate labeled data  $x_{hard} \rightarrow x_{reco}(x_{hard})$  }



Classifier Neural Network to encode the acceptance probability

# The Sampling Network

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



# The Sampling Network

$$\begin{aligned} p(x_{reco} | \alpha) &= \int dx_{hard} p(x_{hard} | \alpha) p(x_{reco} | x_{hard}) \epsilon(x_{hard}) \\ &= \left\langle \frac{1}{q(x_{hard})} p(x_{hard} | \alpha) p(x_{reco} | x_{hard}) \epsilon(x_{hard}) \right\rangle_{x_{hard} \sim q(x_{hard})} \end{aligned}$$

# The Sampling Network

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

# The Sampling Network

$$\begin{aligned} p(x_{reco} | \alpha) &= \int dx_{hard} p(x_{hard} | \alpha) p(x_{reco} | x_{hard}) \epsilon(x_{hard}) \\ &= \left\langle \frac{1}{q(x_{hard})} p(x_{hard} | \alpha) p(x_{reco} | x_{hard}) \epsilon(x_{hard}) \right\rangle_{x_{hard} \sim q(x_{hard})} \end{aligned}$$

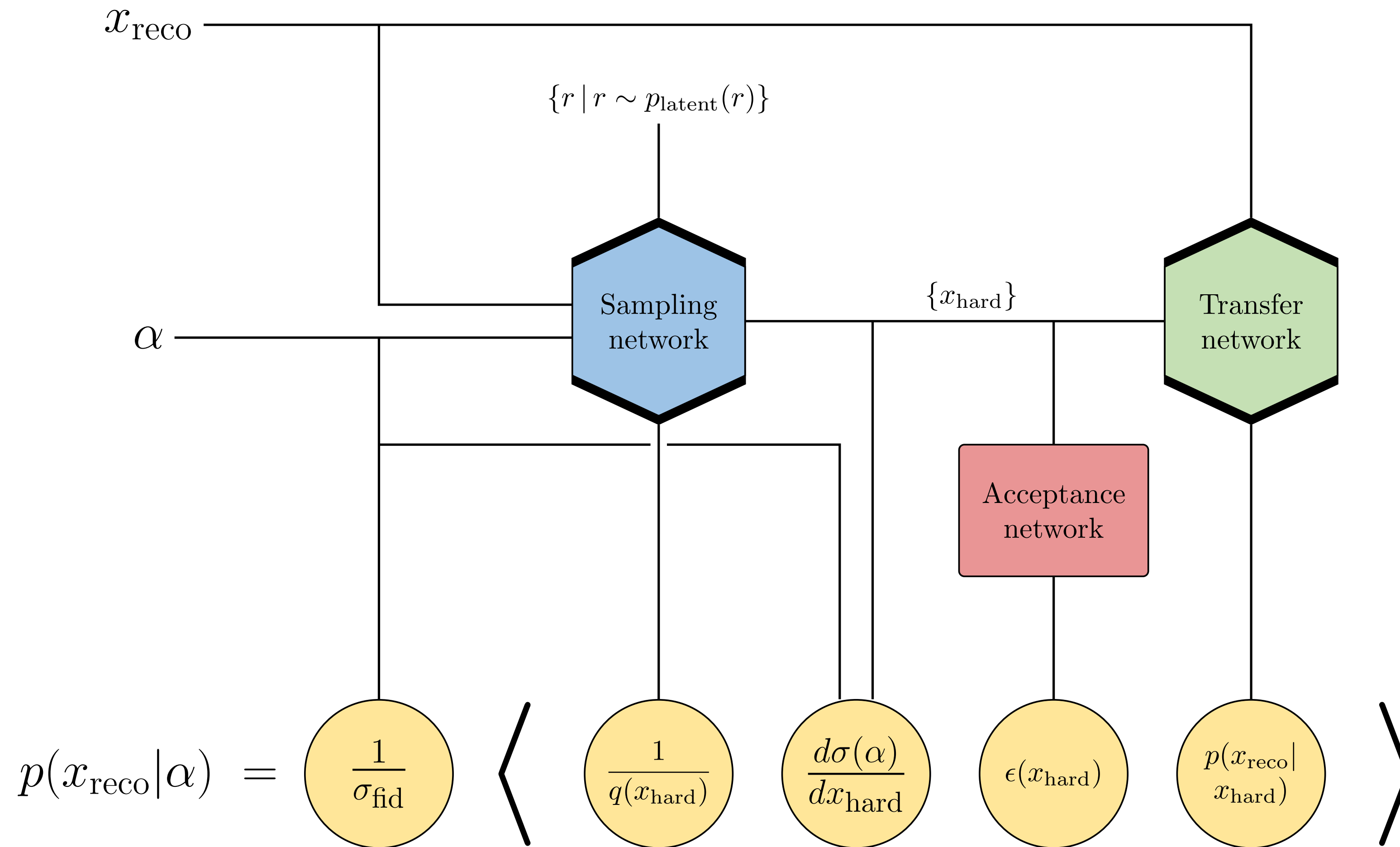
Integral becomes trivial if :  $q(x_{hard}) \propto p(x_{hard} | x_{reco}, \alpha) \epsilon(x_{hard})$



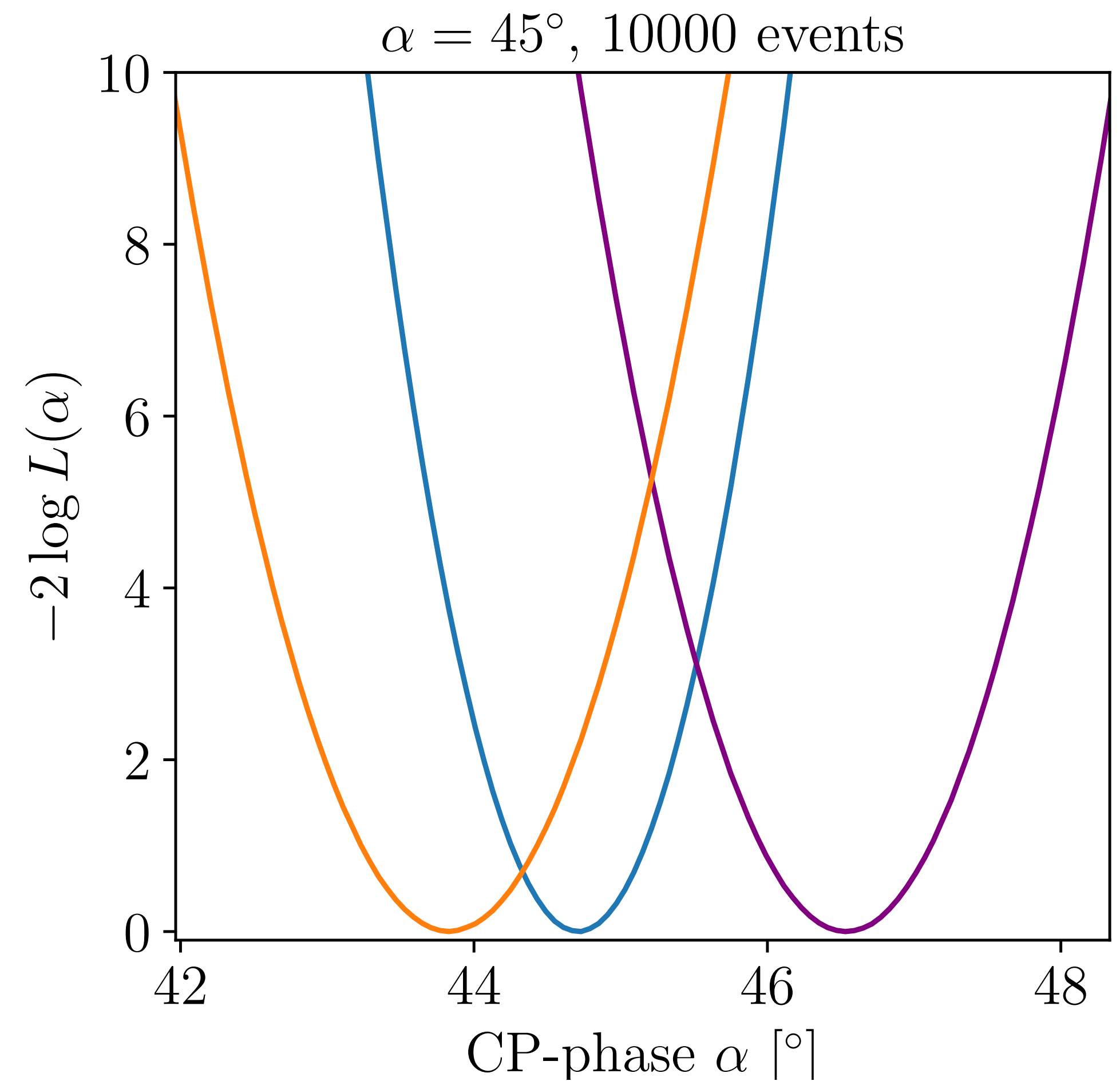
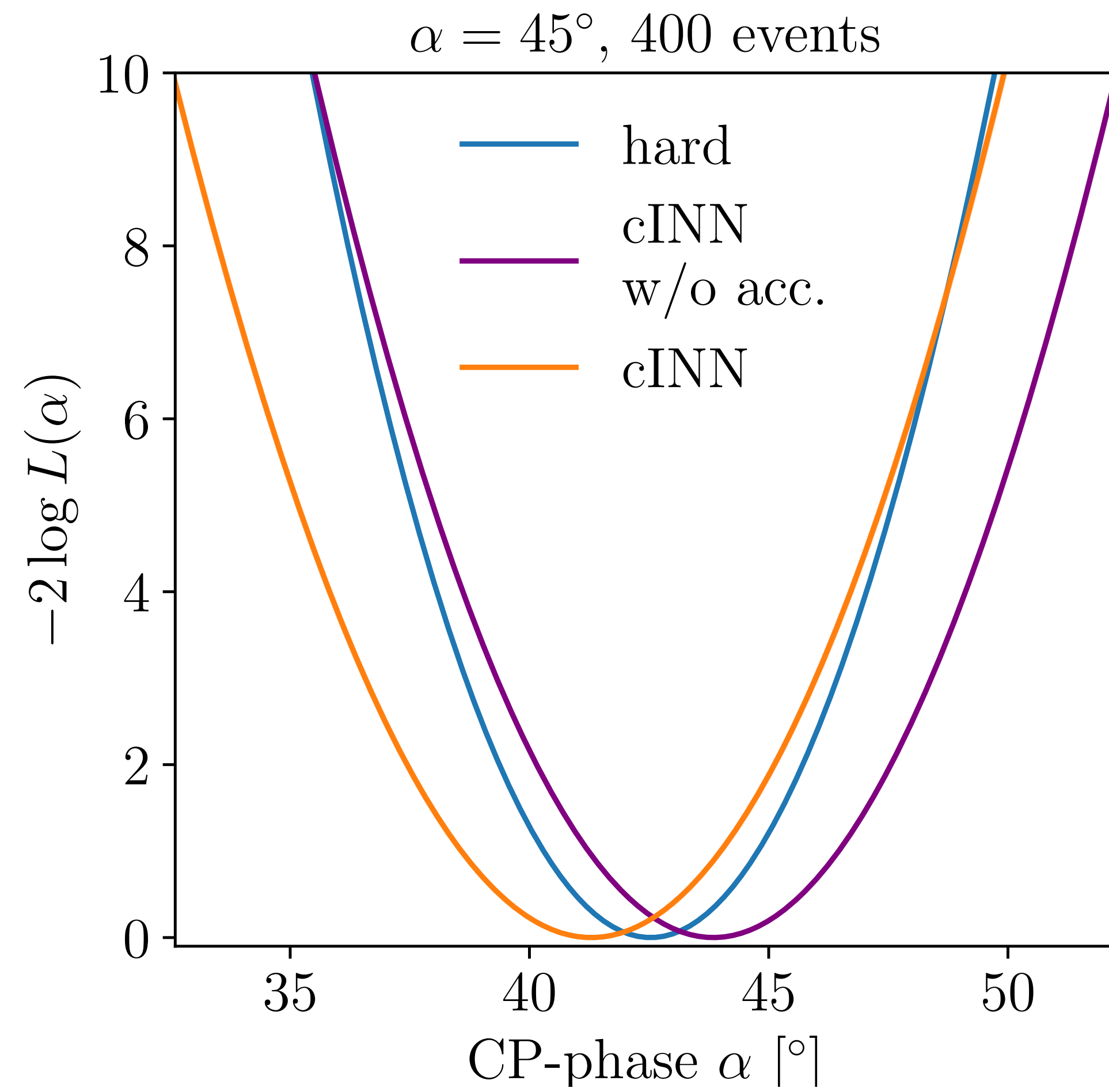
Generative Neural Network to encode sampling distribution

$$r \sim p_{latent}(r) \longleftrightarrow x_{hard}(r) \sim q_{\phi}(x_{hard})$$

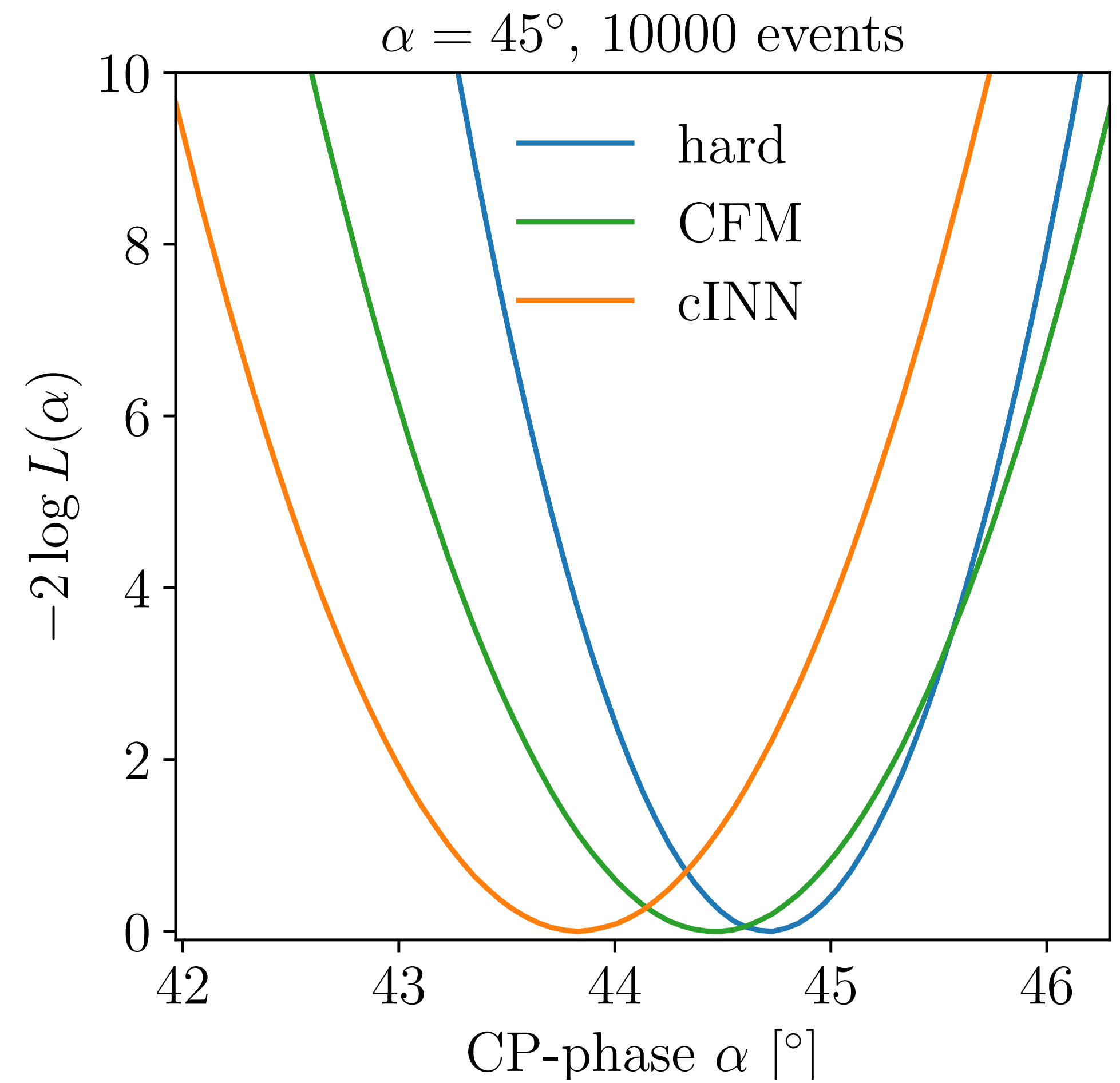
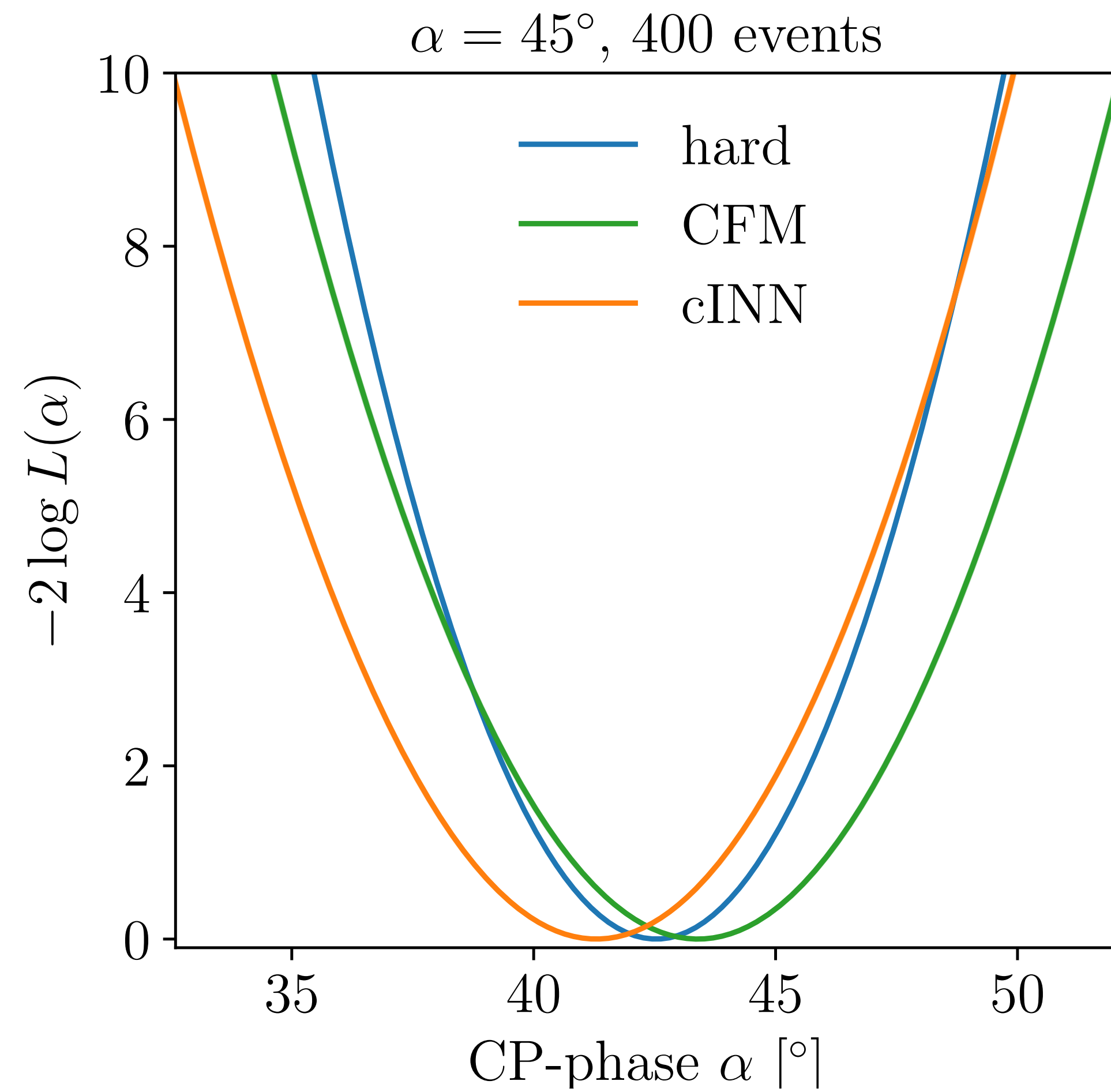
# Machine-learned MEM



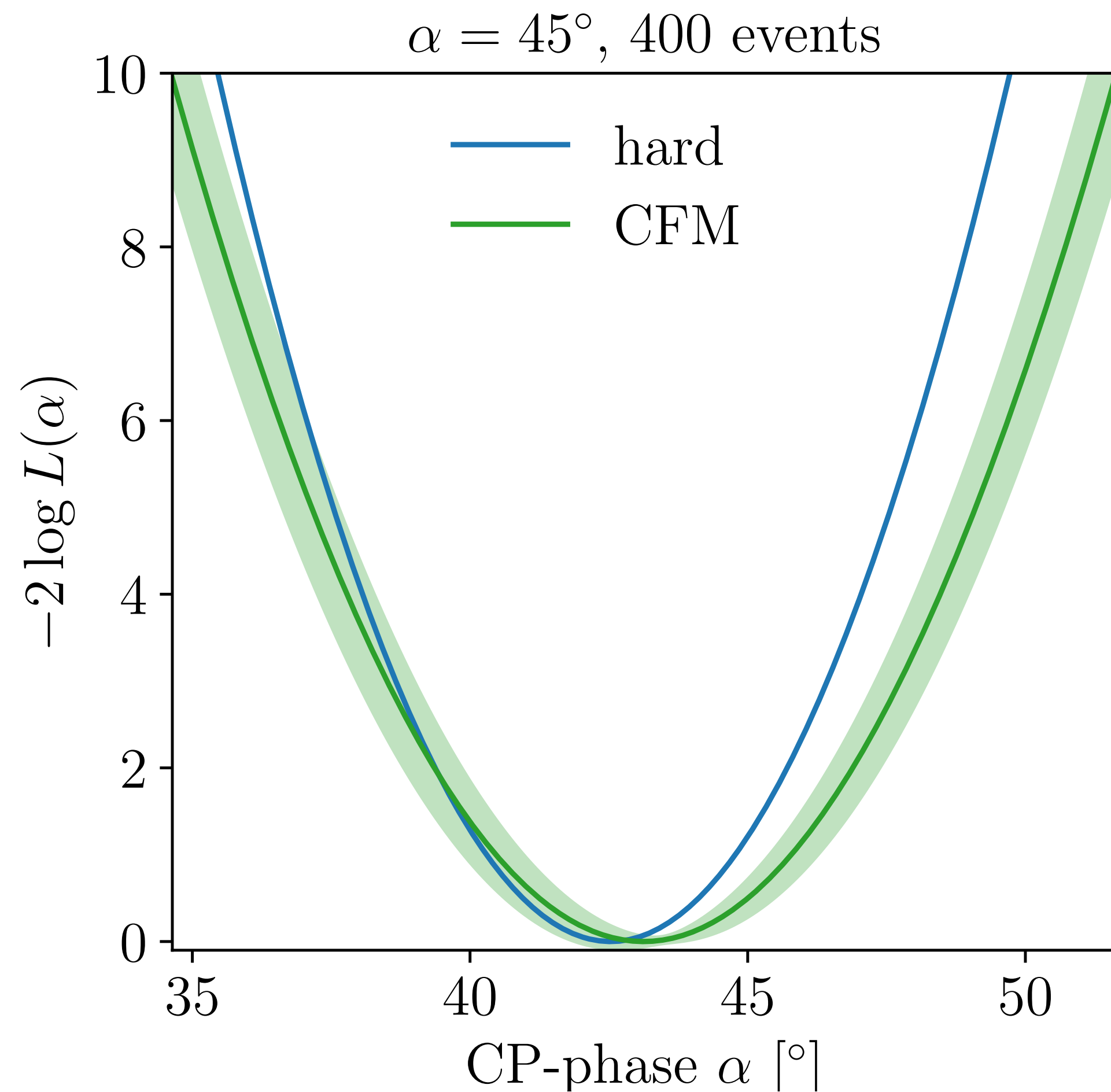
# Baseline Results



# Transfer-Diffusion Results



# Estimating Uncertainty



Estimate uncertainty using replicas:

**Integration uncertainty:**

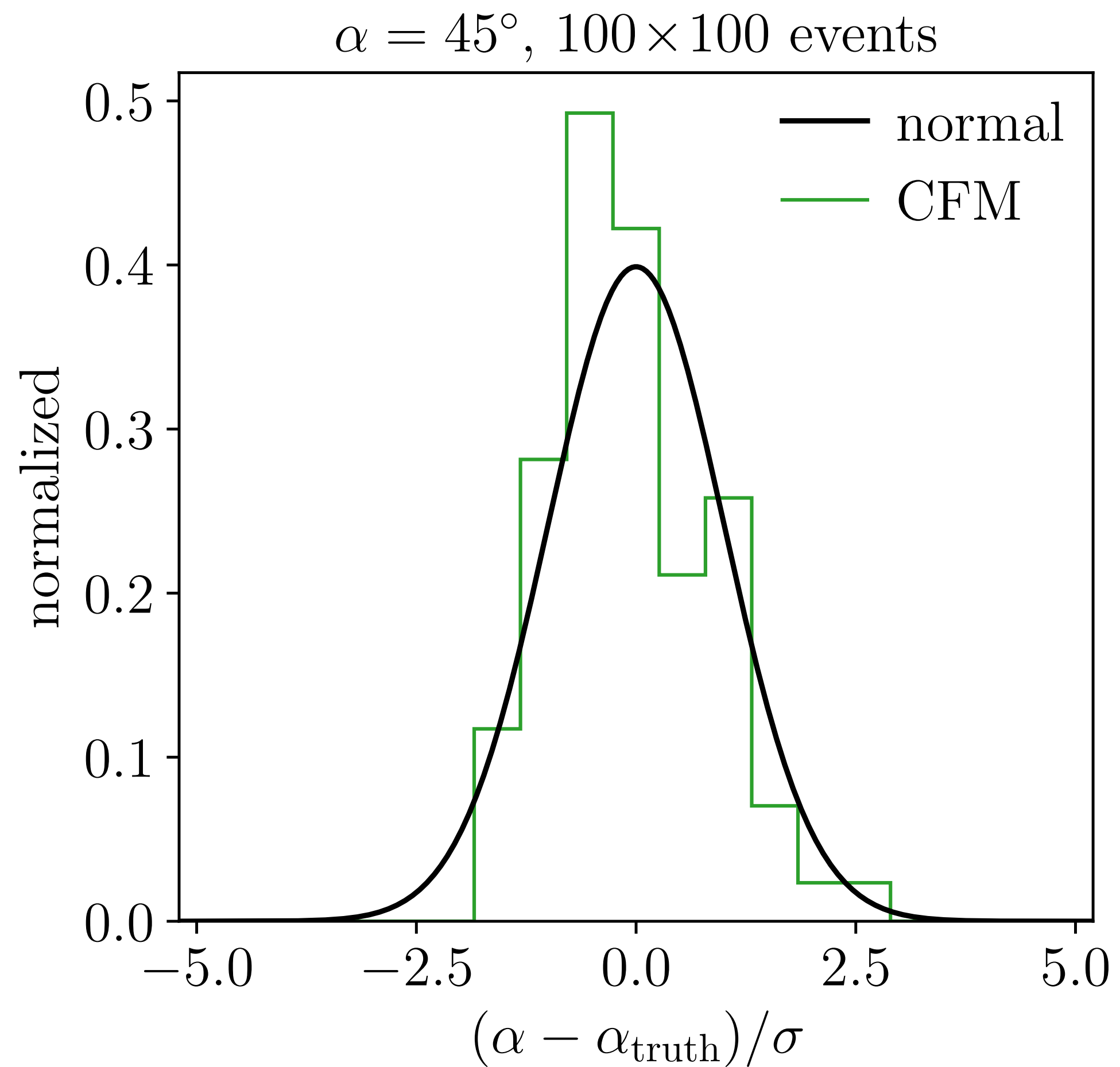
Resample the MC points using bootstrapping

**Network uncertainty:**

Use Bayesian NN and resample for each replica



# Estimating Calibration



Divide the 10k events into 100 samples of 100 events

Look at this distribution of the minima around the true  $\alpha$

# Summary and Outlook

Modern machine learning makes the MEM tractable and scaleable

We present a state-of-the-art three network setup consisting of

- 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  $q(x_{hard})$

Bootstrapping and Bayesian NNs allow us to capture the uncertainties

Extend our formalism to NLO, both on the physics and the ML side

Test our setup on an actual analysis and/or more challenging processes