Treatment of Detector Systematics via Likelihood-free Inference

NuXtract Workshop, Oct. 3rd, 2023

A paper by:

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Introduction: Monte-Carlo Forward-Folding

This nomenclature will be used all throughout the talk!

Produce MC

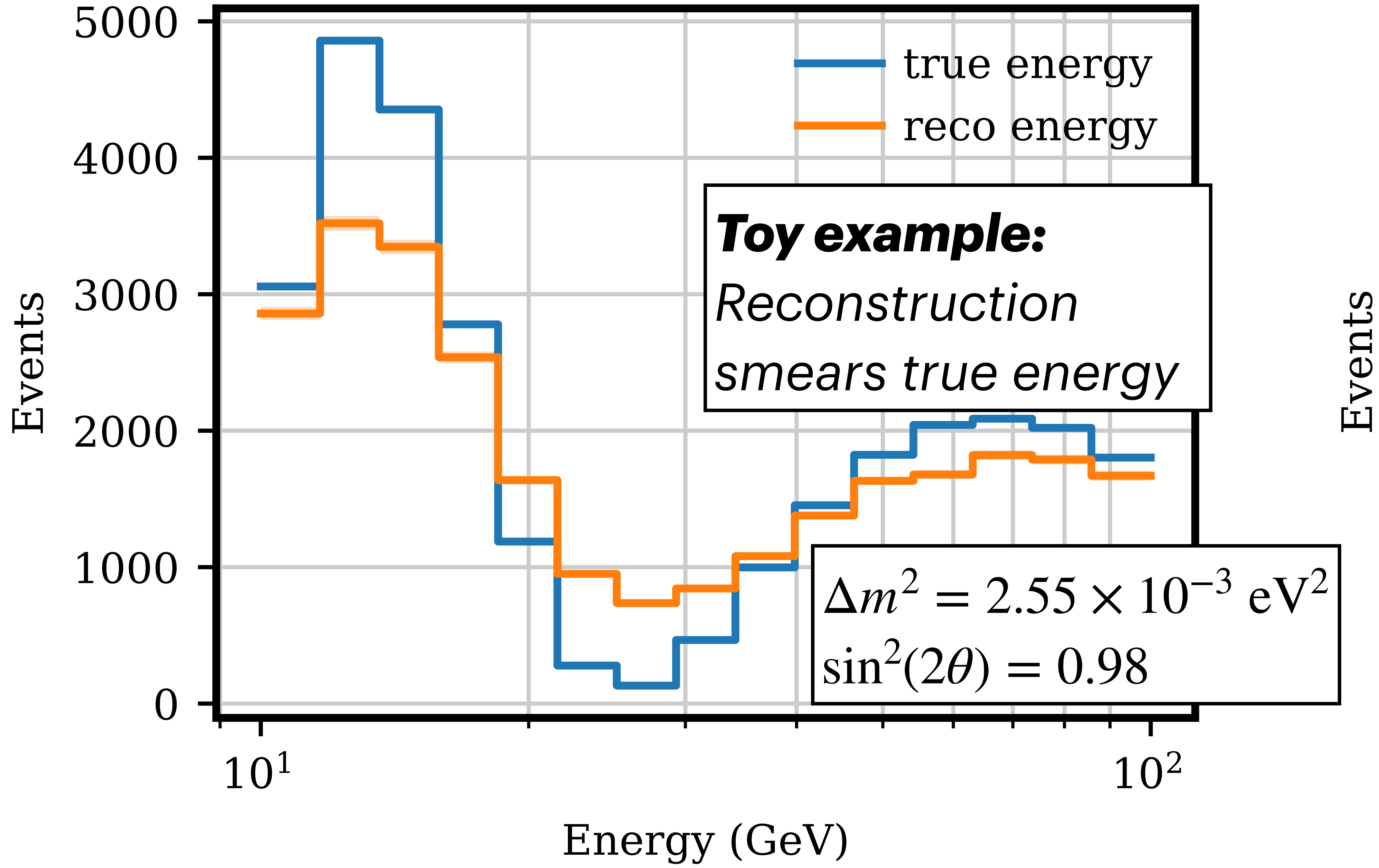
- $\mathbf{x}$ = true event properties (energy, direction, etc.)
- Simulated flux: $\Phi_{\mathrm{sim}}(\mathbf{x})$ (for example power law)

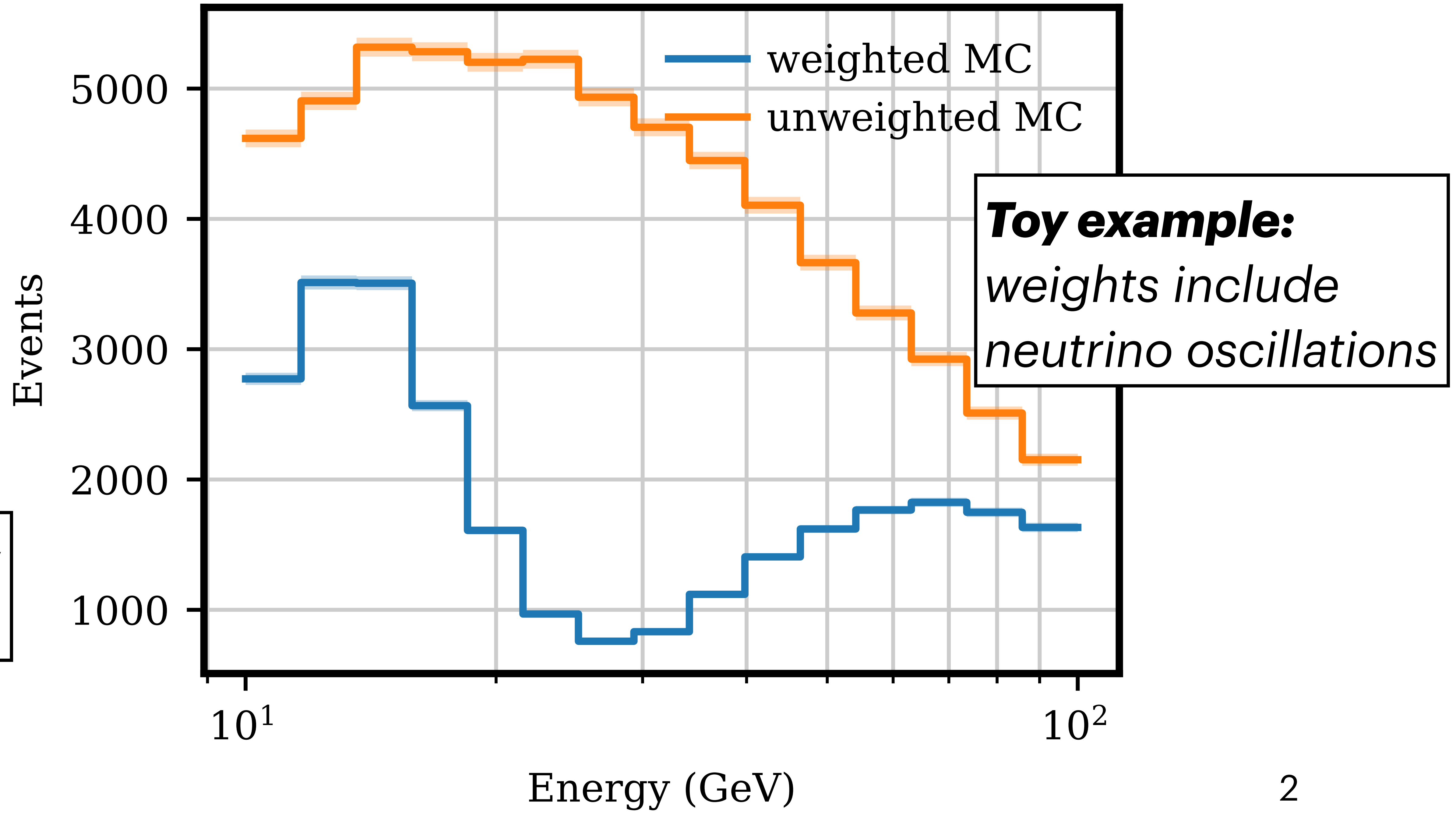
Detector Response

- $\mathbf{y}$ = reco. event properties
- α = detector properties
- $P(\mathrm{acc}\,|\,\mathbf{x}, \alpha)$ = acceptance
- $P(\mathbf{y}\,|\,\mathbf{x}, \alpha)$ = reconstruction

Weight Events

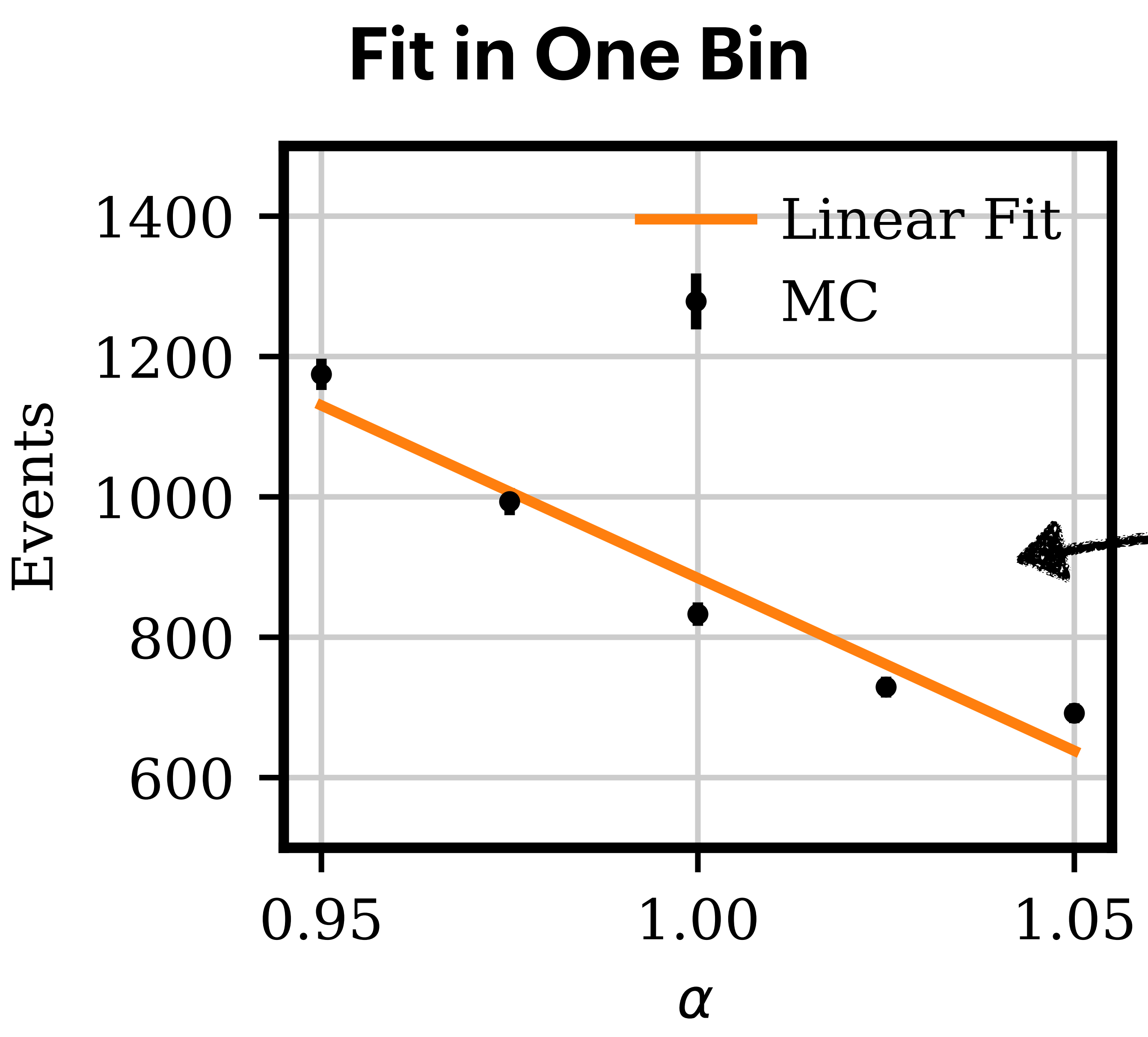
- $w = \Phi(\mathbf{x}\,|\,\theta)/\Phi_{\mathrm{sim}}(\mathbf{x})$
- θ = physics + nuisance parameters

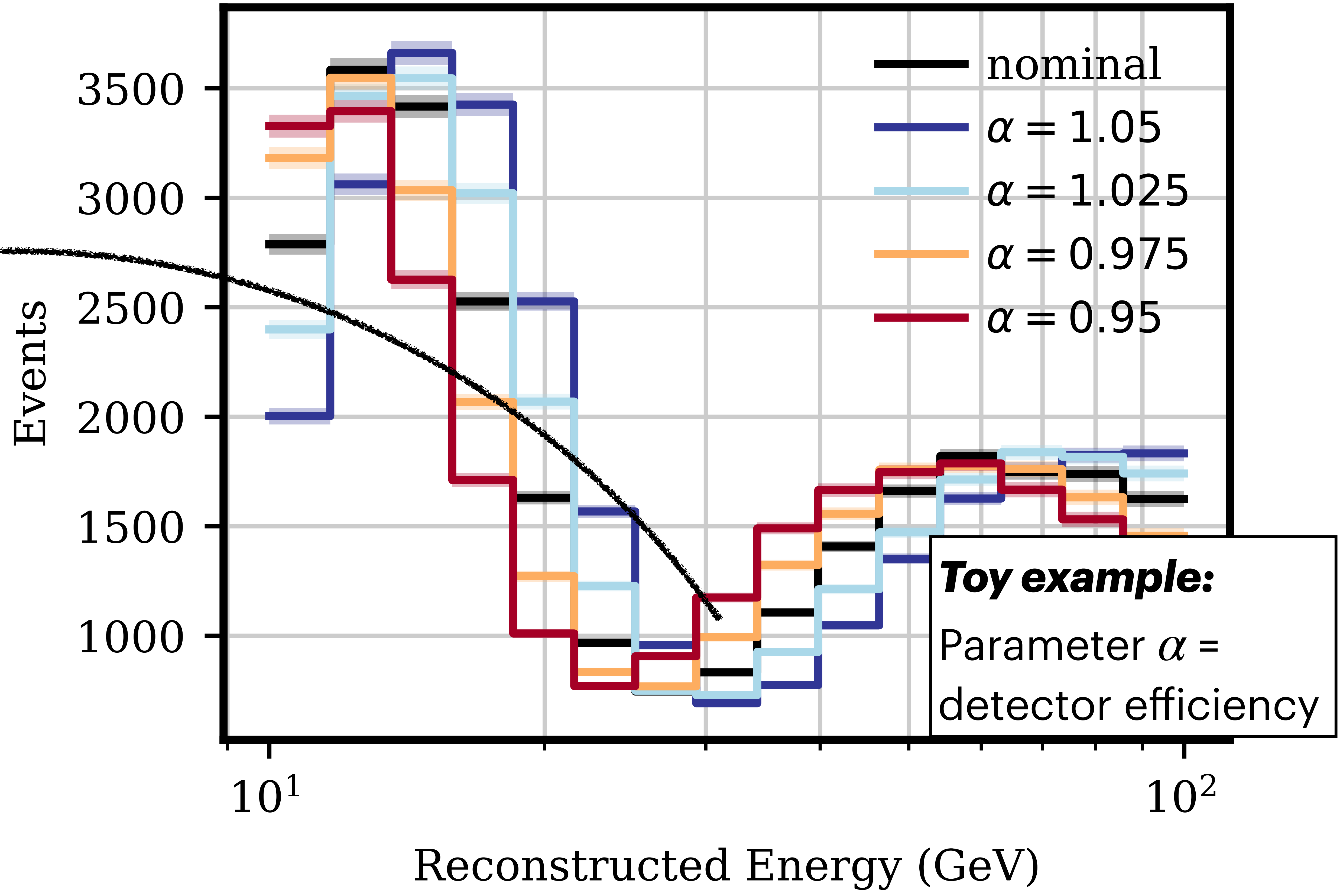




Modeling of Detector Effects

Bin-wise weighting method

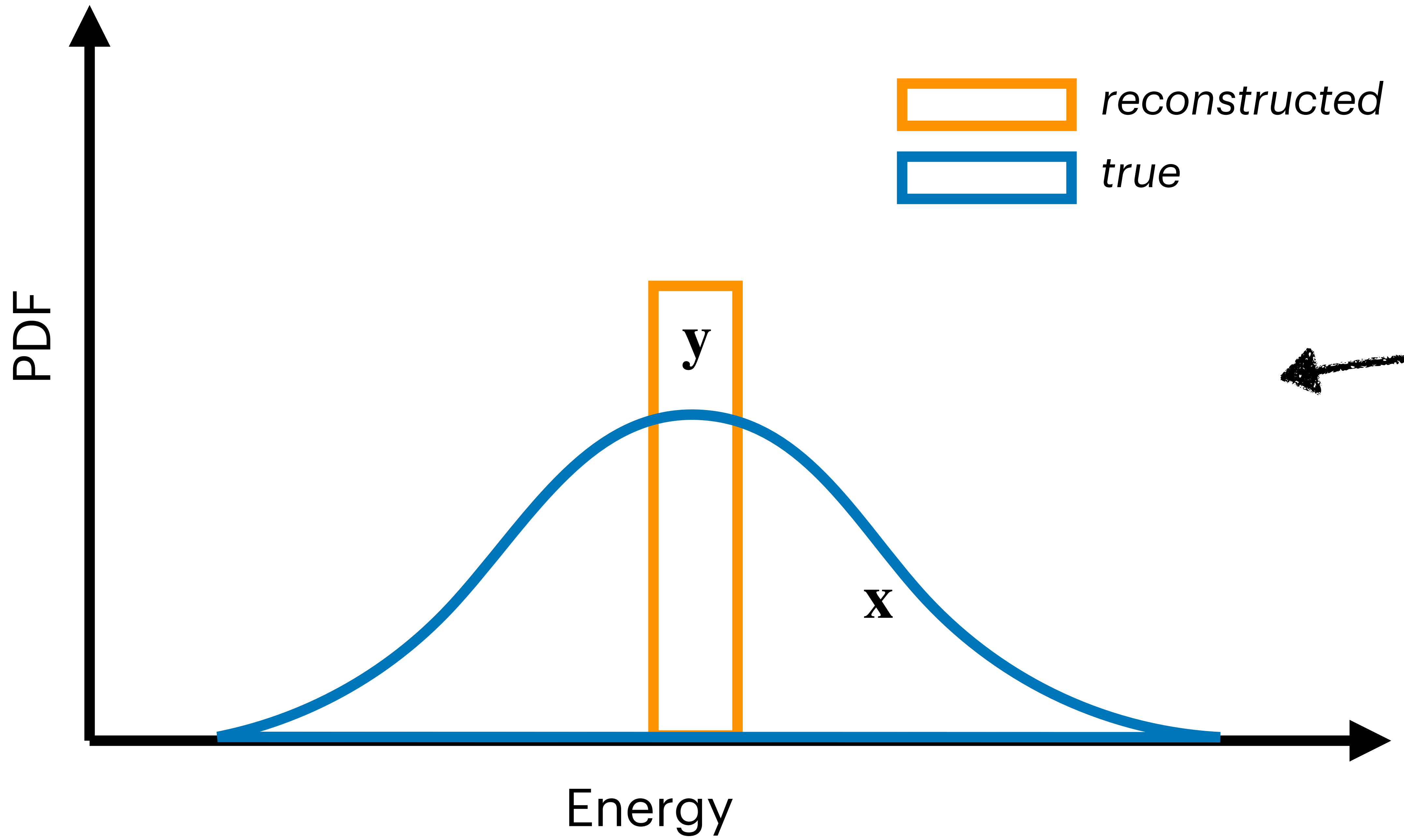


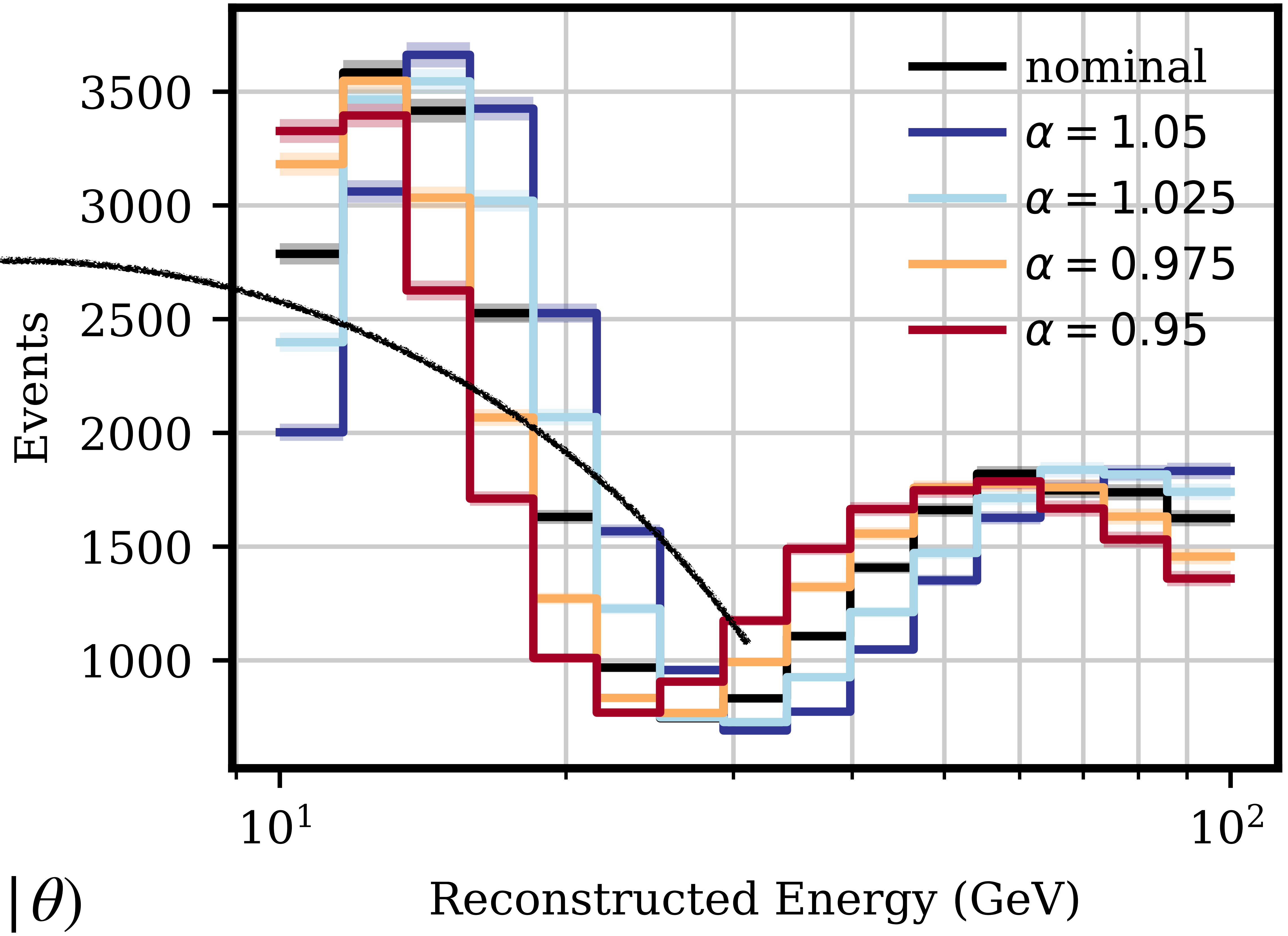


- **Simplest method:** Bin-wise gradients
- **Problem:** Depend on physics parameters θ

Bin-wise Weighting Methods

Implicit Marginalization



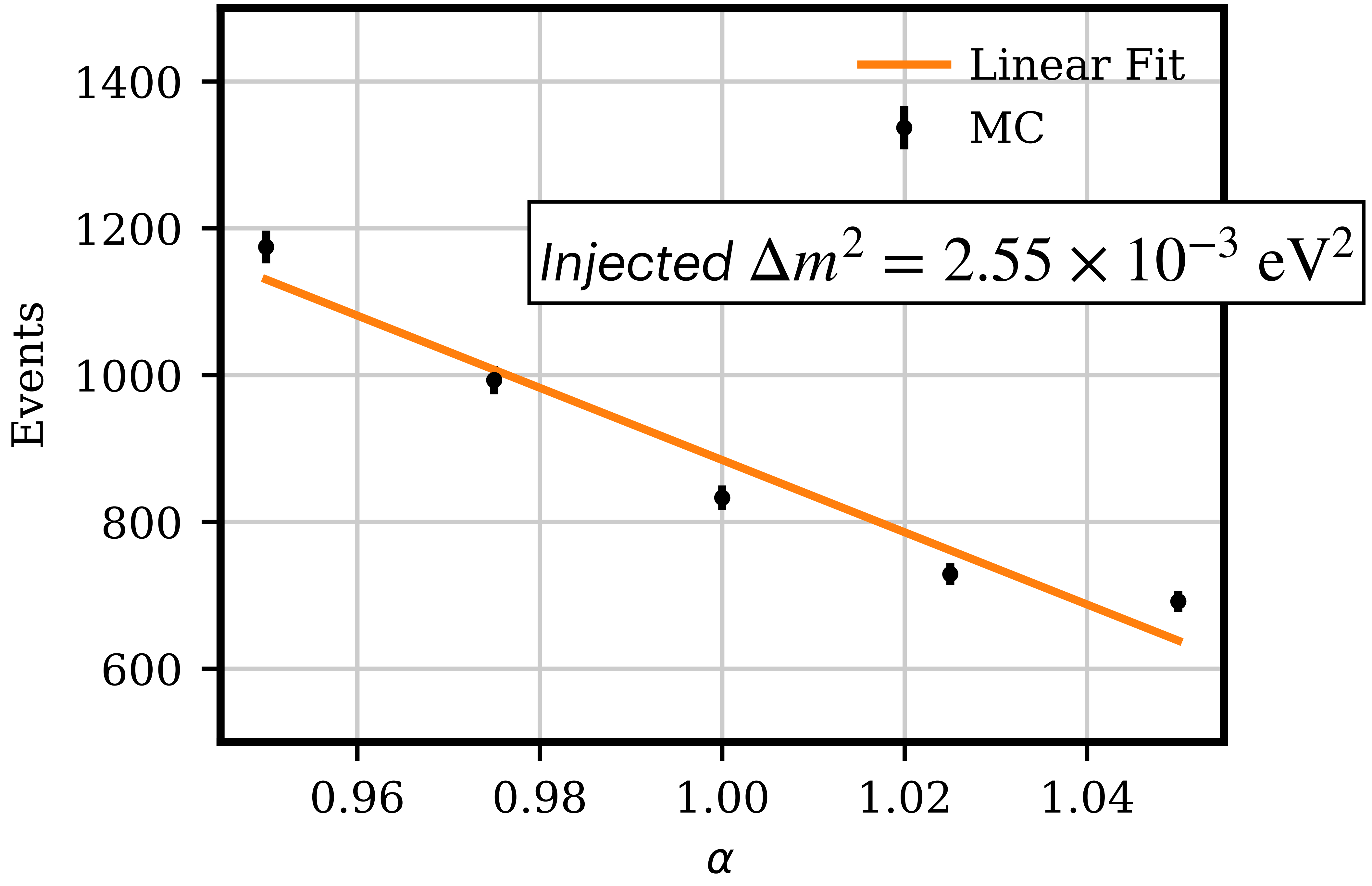


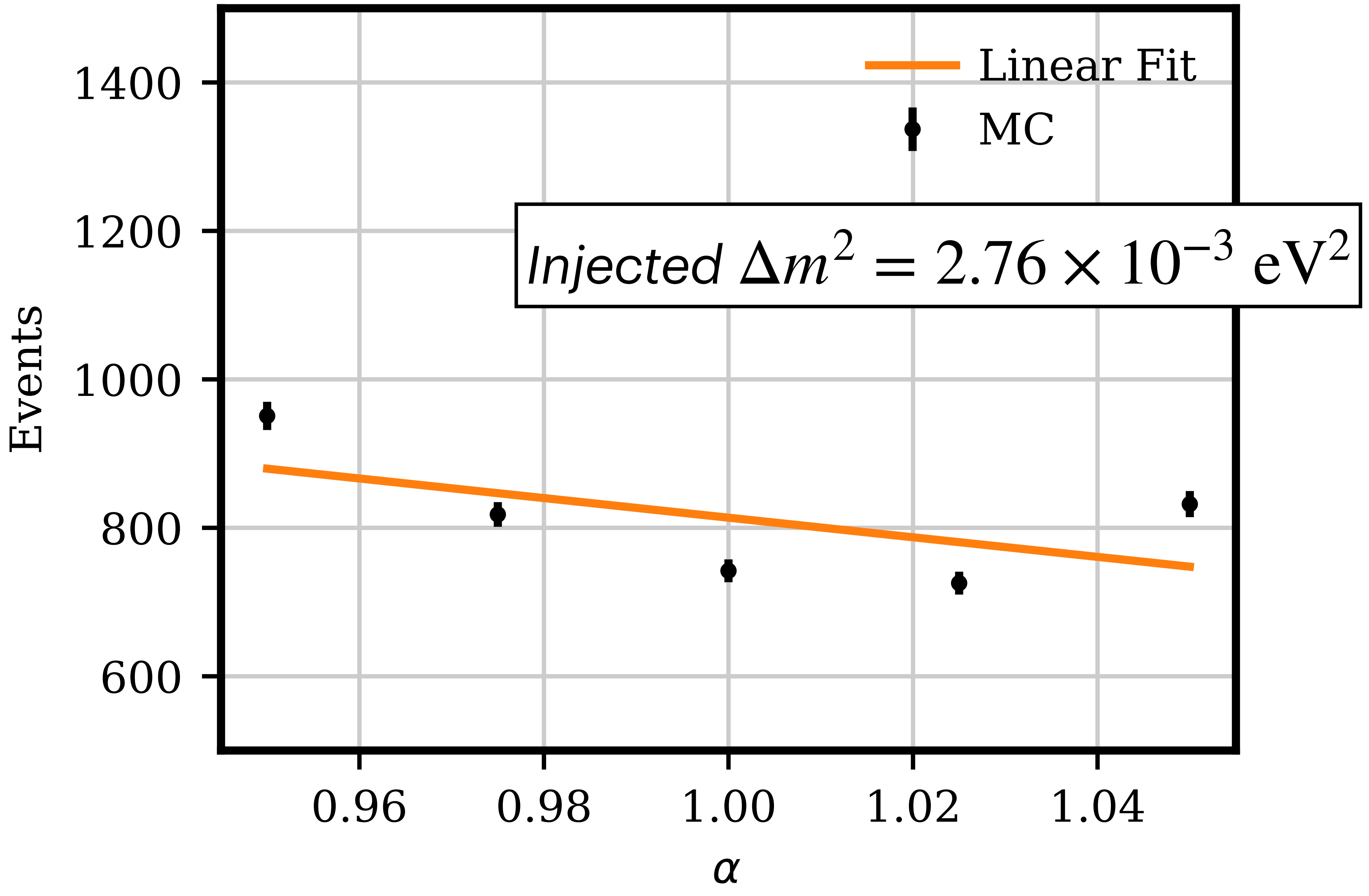
Expectation value in bin i:

$$\mu_i(\theta) = \int_{\boxed{\mathbf{y} \in \text{bin } i}} \mathrm{d}\mathbf{y} \int \mathrm{d}\mathbf{x} P(\mathbf{y} \,|\, \mathbf{x}, \alpha) P(\text{acc} \,|\, \mathbf{x}, \alpha) \frac{\Phi(\mathbf{x} \,|\, \theta)}{\Phi_{\text{sim}}(\mathbf{x})}$$

Bin-wise Weighting Methods

Gradients' dependence on Physics Parameters





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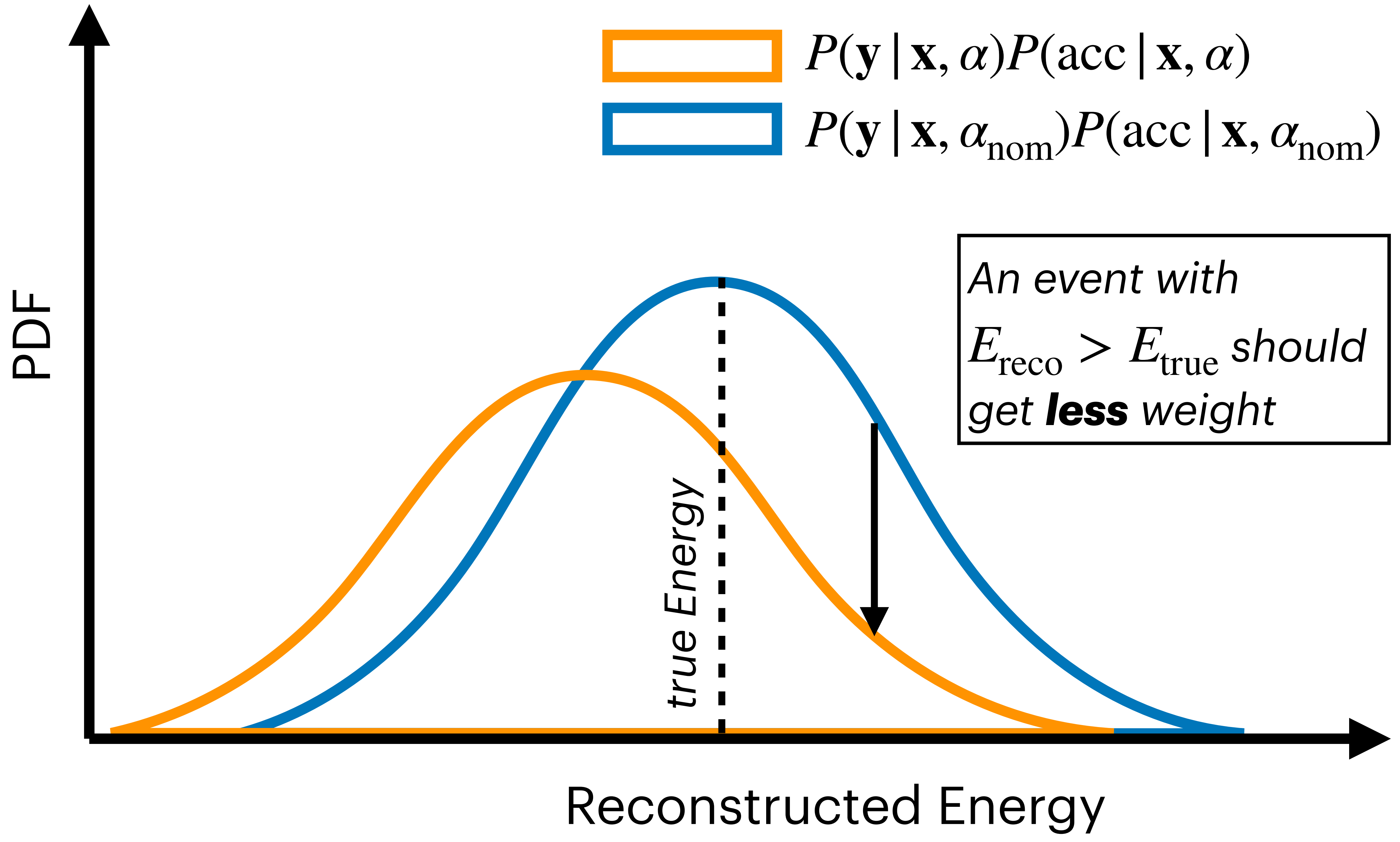
Gradient in one bin $\nabla_\alpha \mu_i$ requires integrating over true event properties

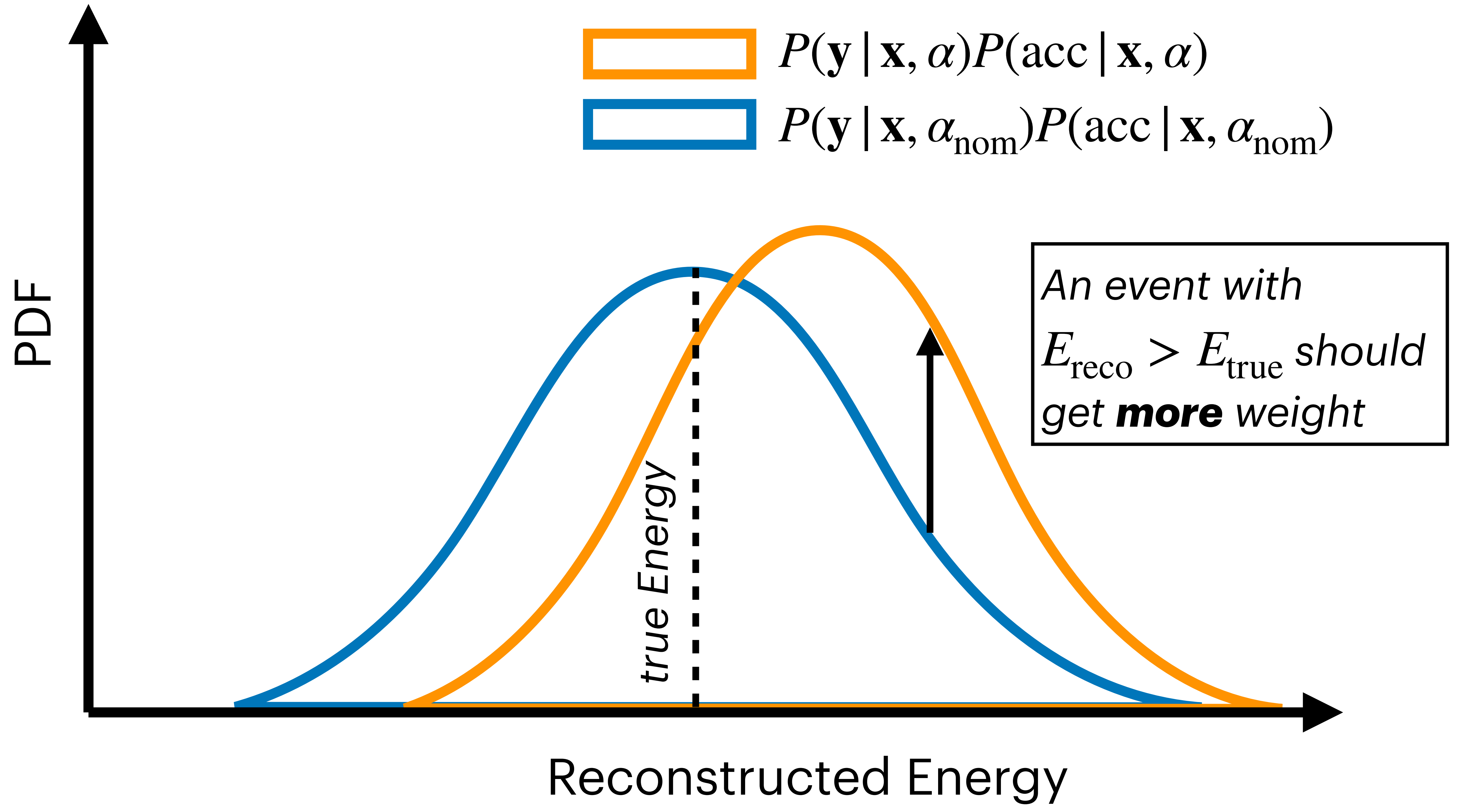
Decoupling Detector Effects

Event Weights Should be Independent from Initial Flux

Example: α = detector efficiency, $\alpha_{\text{nom}} = 1$



$\alpha < 1$: Reconstructed energy tends to be smaller than true energy



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Decoupling Detector Effects

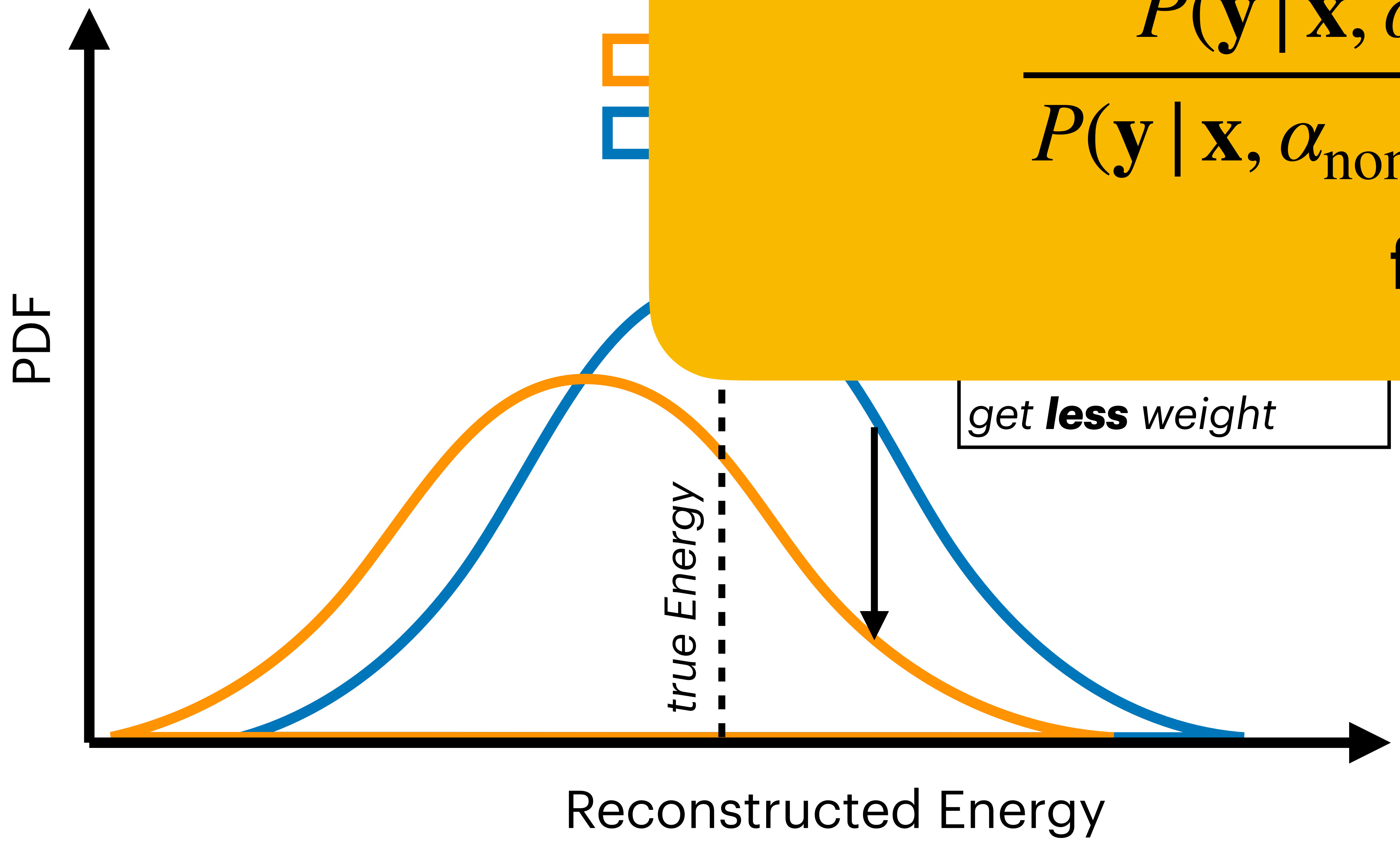
Event Weights Should be Independent from Initial Flux

Example: α = detector

But where do we get

$$\frac{P(\mathbf{y}\,|\,\mathbf{x},\alpha)P(\text{acc}\,|\,\mathbf{x},\alpha)}{P(\mathbf{y}\,|\,\mathbf{x},\alpha_{\text{nom}})P(\text{acc}\,|\,\mathbf{x},\alpha_{\text{nom}})}$$

from?



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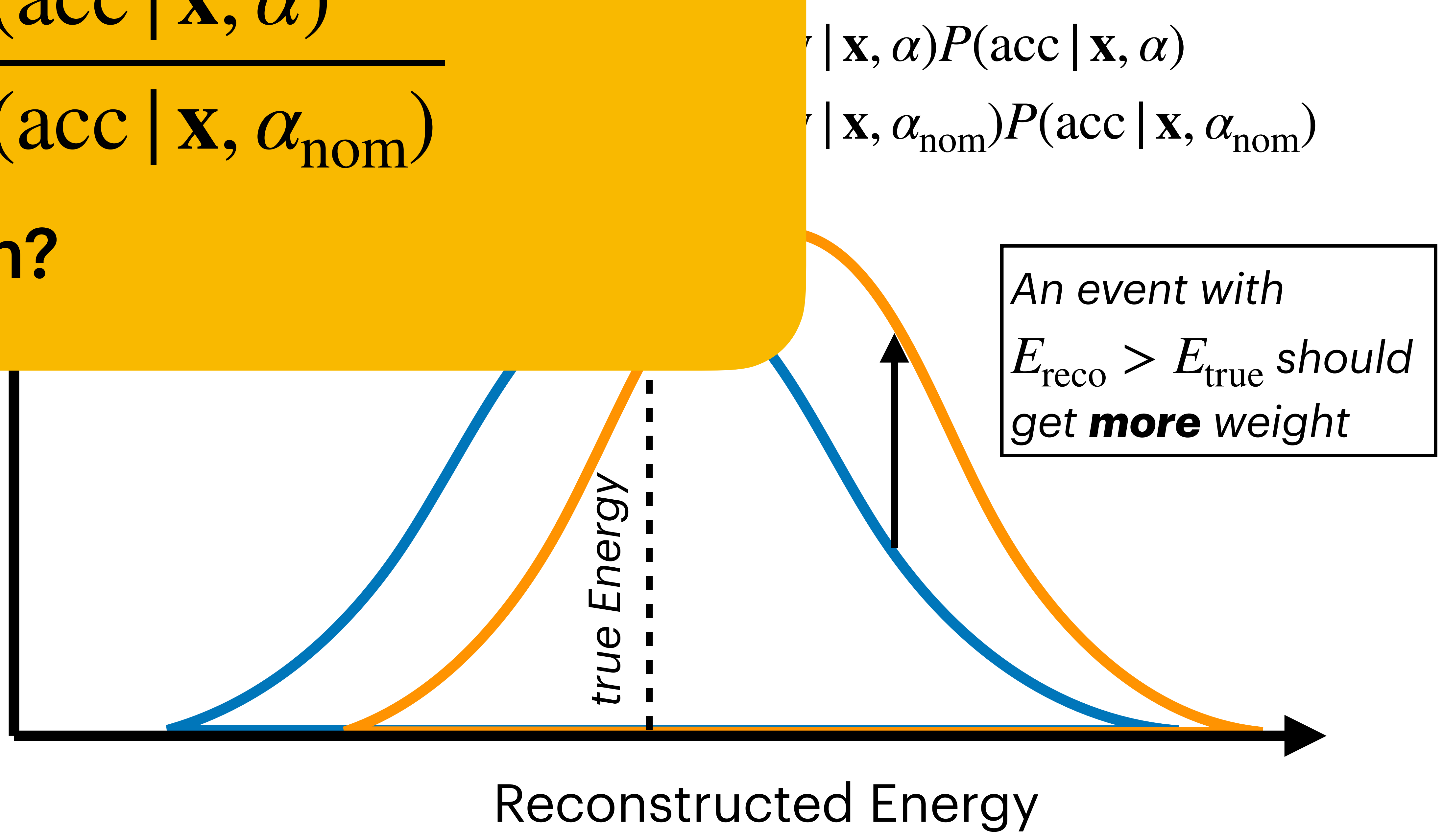

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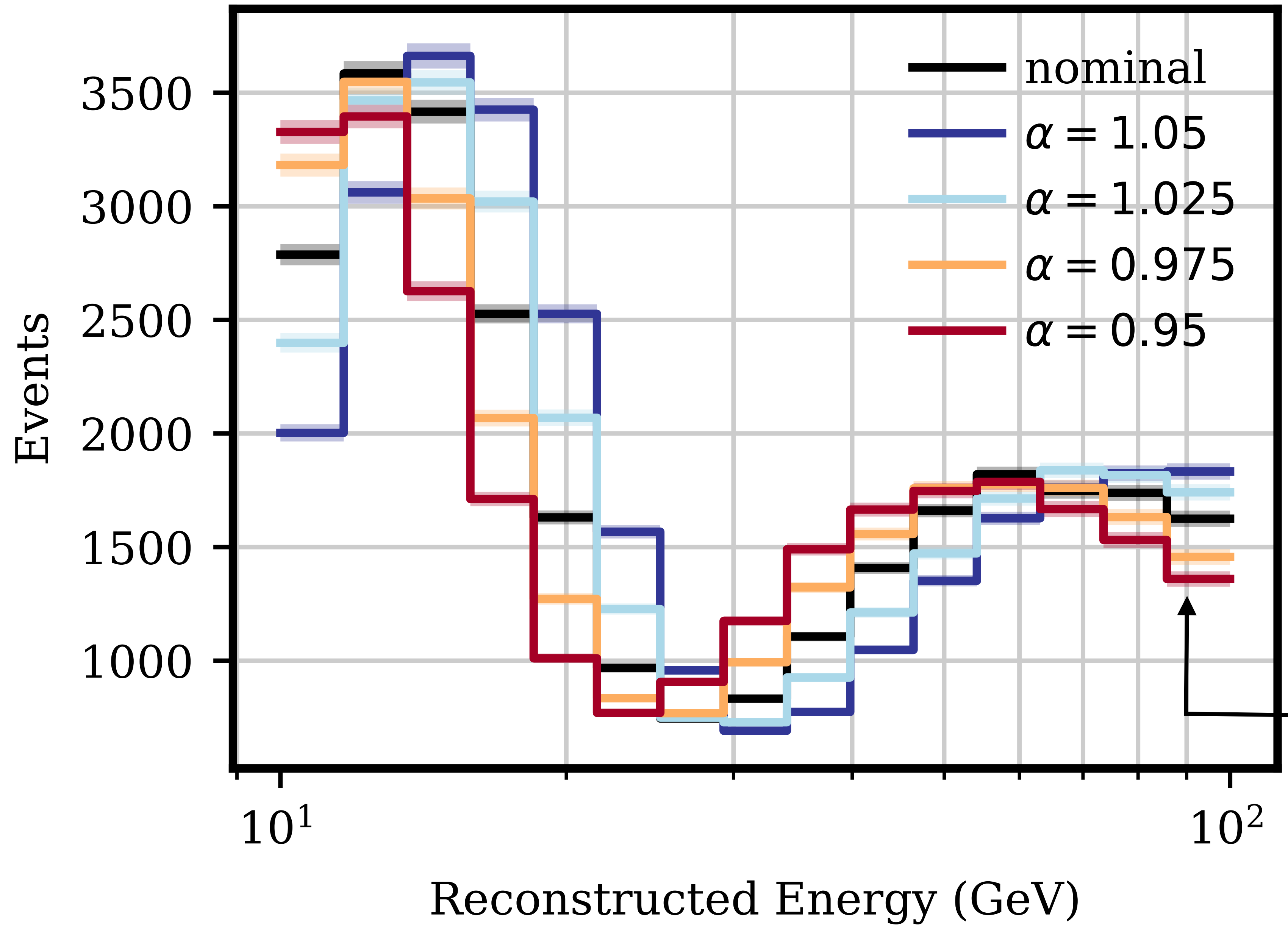
The Likelihood-free Inference Trick

Weighting from Nominal to Any Off-Nominal MC Set

Applying Bayes' Theorem:

index j = index of MC set

$$\frac{P(\mathbf{y}\,|\,\mathbf{x}, \alpha_k)P(\mathrm{acc}\,|\,\mathbf{x}, \alpha_k)}{P(\mathbf{y}\,|\,\mathbf{x}, \alpha_{\mathrm{nom}})P(\mathrm{acc}\,|\,\mathbf{x}, \alpha_{\mathrm{nom}})} = \frac{P(\alpha_k\,|\,\mathbf{x}, \mathbf{y})}{P(\alpha_{\mathrm{nom}}\,|\,\mathbf{x}, \mathbf{y})}$$



Treat each MC set as one discrete class

Just train a classifier to estimate posterior that an event with given $\mathbf{x}, \mathbf{y}$ belongs to set j!

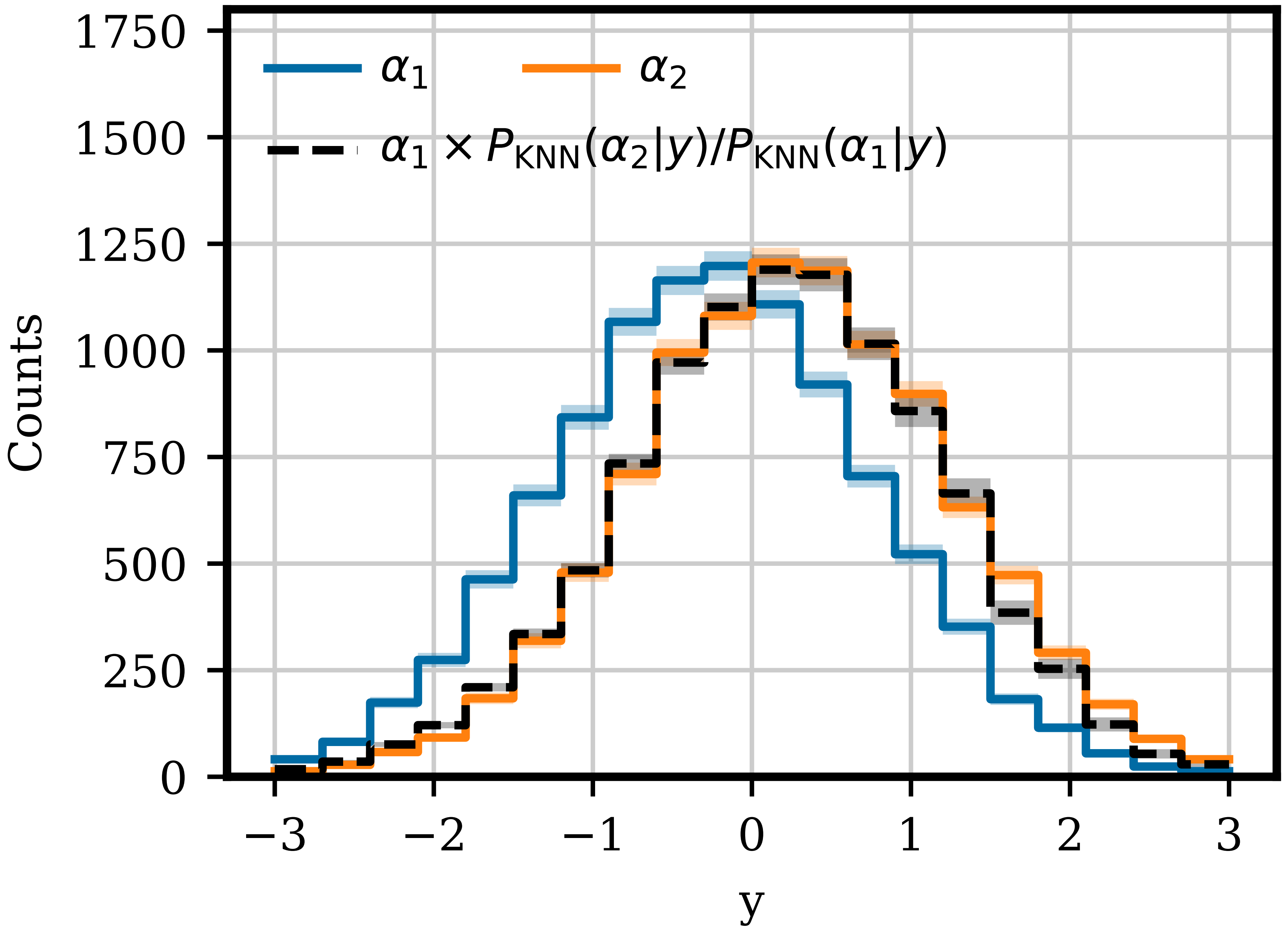
KNN Classifier Example

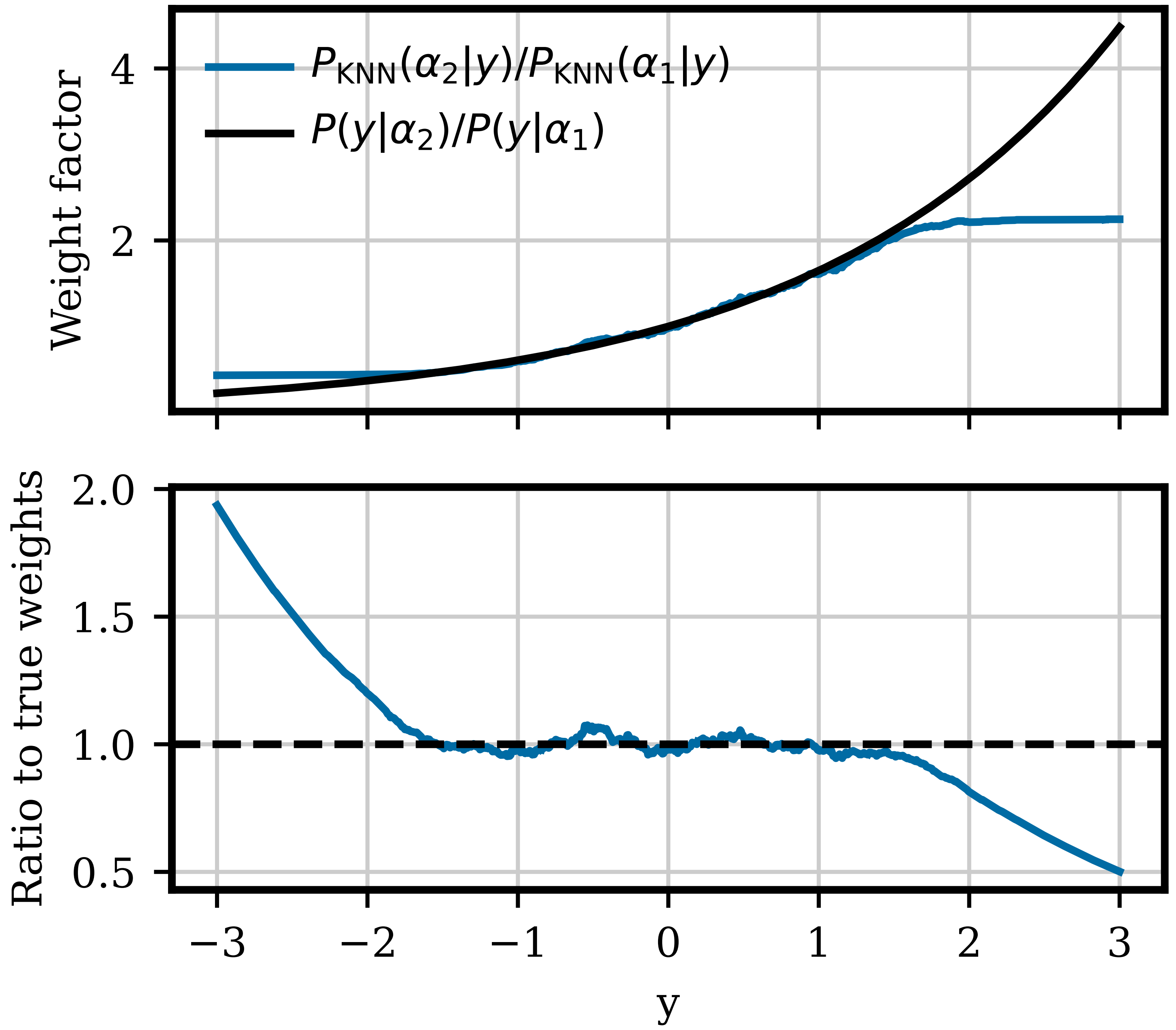
Simple and Robust Posterior Estimate

Sum over indices in neighborhood around $(\mathbf{x}, \mathbf{y})$ belonging to set k

KNN Classifier Equation:

$$P(\alpha = \alpha_k \,|\, \mathbf{x}, \mathbf{y}) = \frac{1}{N} \sum_{j \in \mathcal{N}_k(\mathbf{x},\mathbf{y})} 1$$





Making Event-Wise Gradients
Interpolating between Discrete MC Sets

- **Probability estimate** using softmax to normalize

$$\hat{P}(\alpha_k \,|\, \mathbf{x}_j, \mathbf{y}_j) = \text{softmax}\left(\mathbf{g}_j A\right) = \frac{\exp(\sum_n g_{jn} A_{nk})}{\sum_{k'} \exp(\sum_n g_{jn} A_{nk'})}$$

g_{jn} = gradient w.r.t. α_n for event j

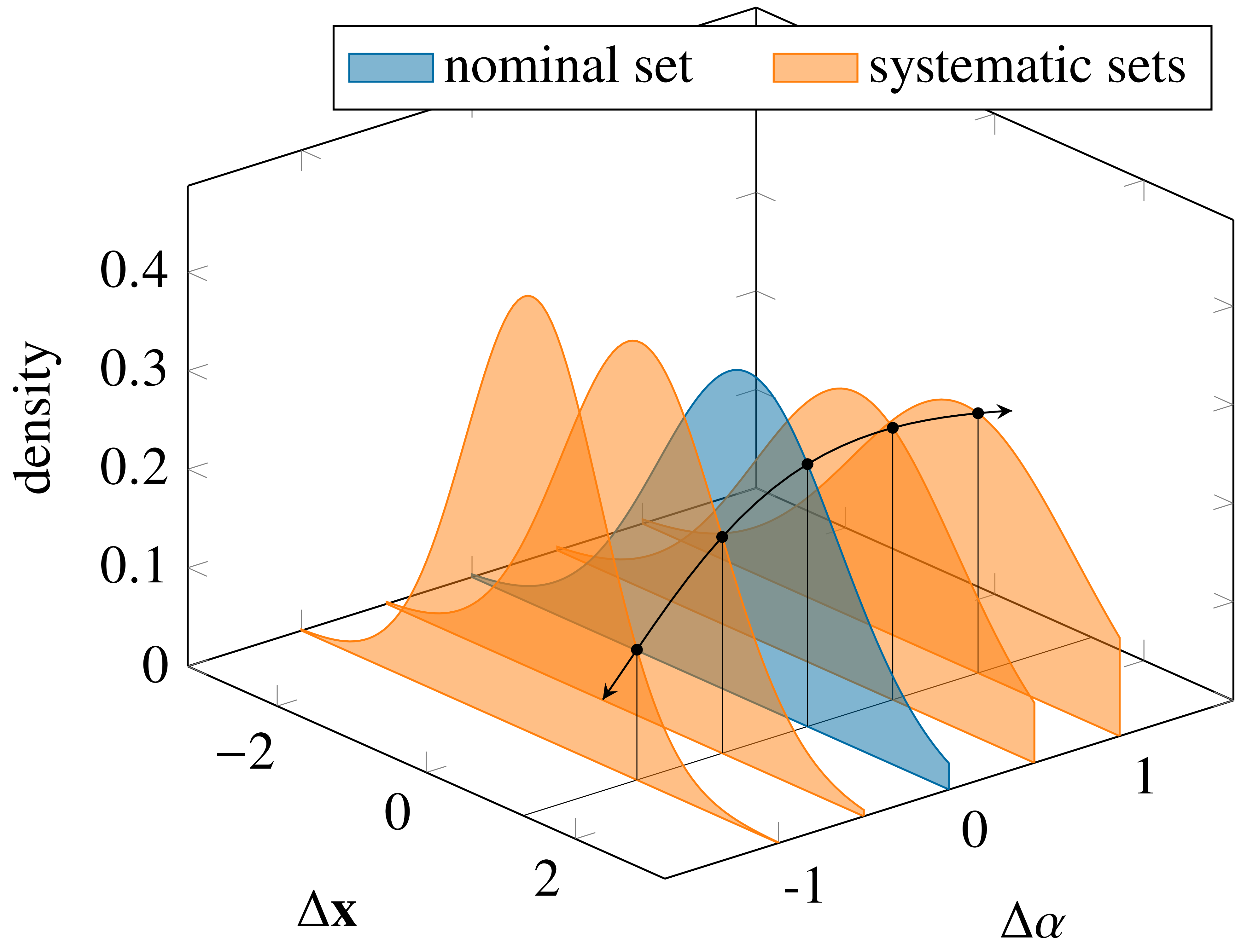
$$A_{nk} = \alpha_{n,k} - \alpha_{n,\,\text{nom}}$$

- **Loss function** to fit gradients g_{jn} is cross-entropy:

$$H_j = -\sum_k \log(\hat{P}(\alpha_k \,|\, \mathbf{x}_j, \mathbf{y}_j)) P_{\text{KNN}}(\alpha_k \,|\, \mathbf{x}_j, \mathbf{y}_j)$$

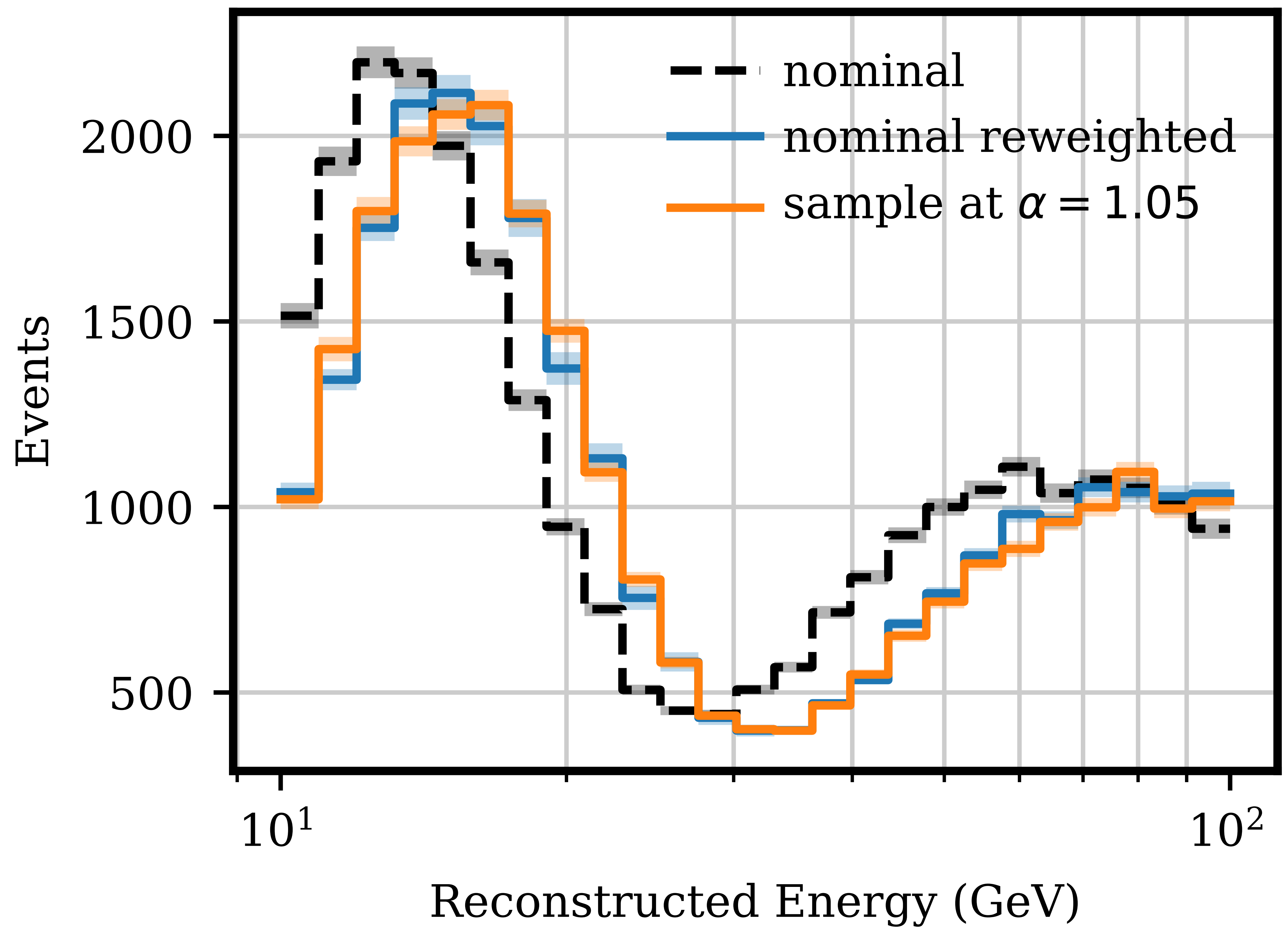
- **Interpolated weight** for every MC event during evaluation

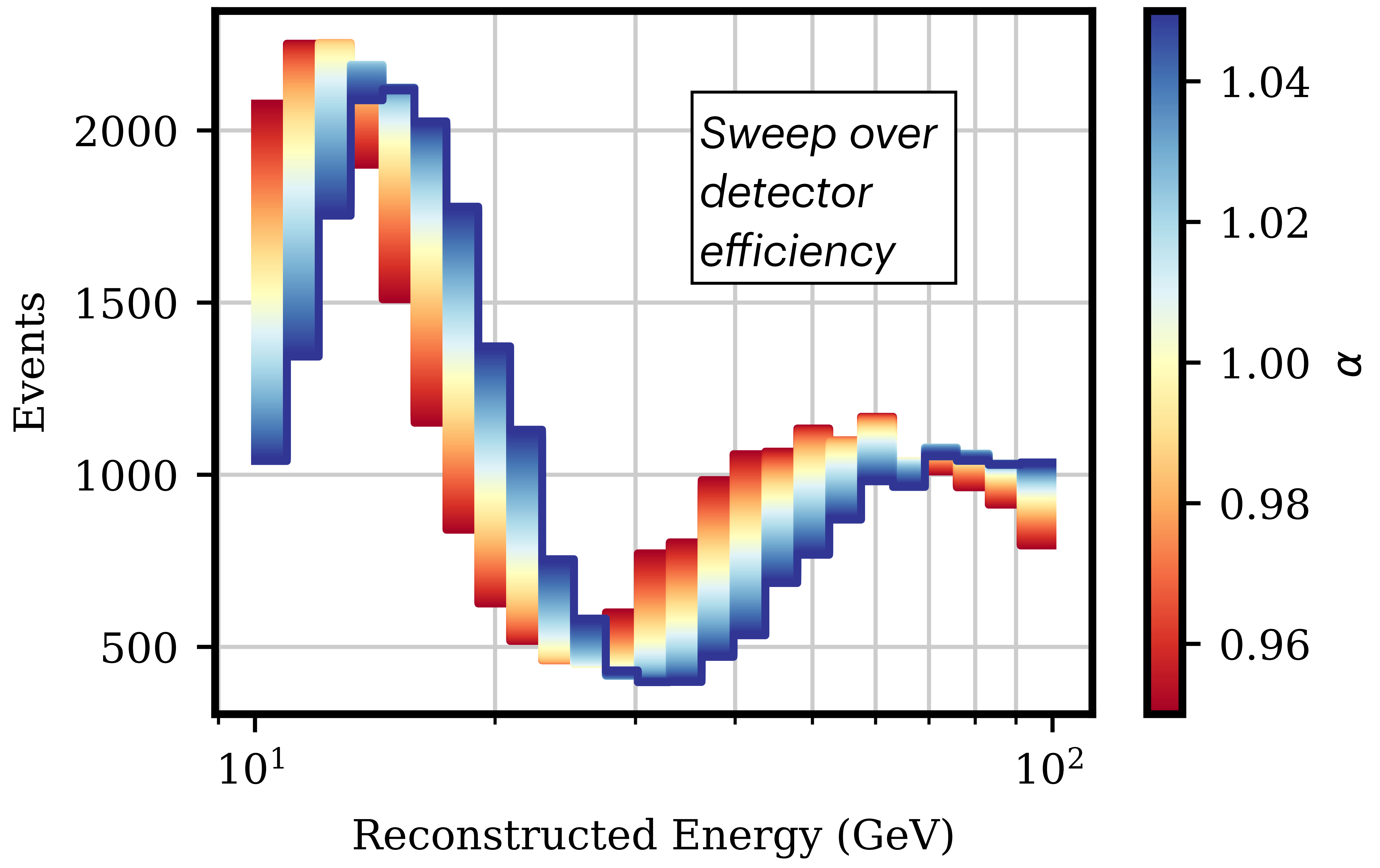
$$\hat{r}_j(\alpha) = \frac{\hat{P}(\alpha \,|\, \mathbf{x}_j, \mathbf{y}_j)}{\hat{P}(\alpha_{\text{nom}} \,|\, \mathbf{x}_j, \mathbf{y}_j)} = \exp\left(\sum_n g_{jn}(\alpha_n - \alpha_{n,\,\text{nom}})\right)$$



Toy MC Example

Reweighting between and in between MC sets

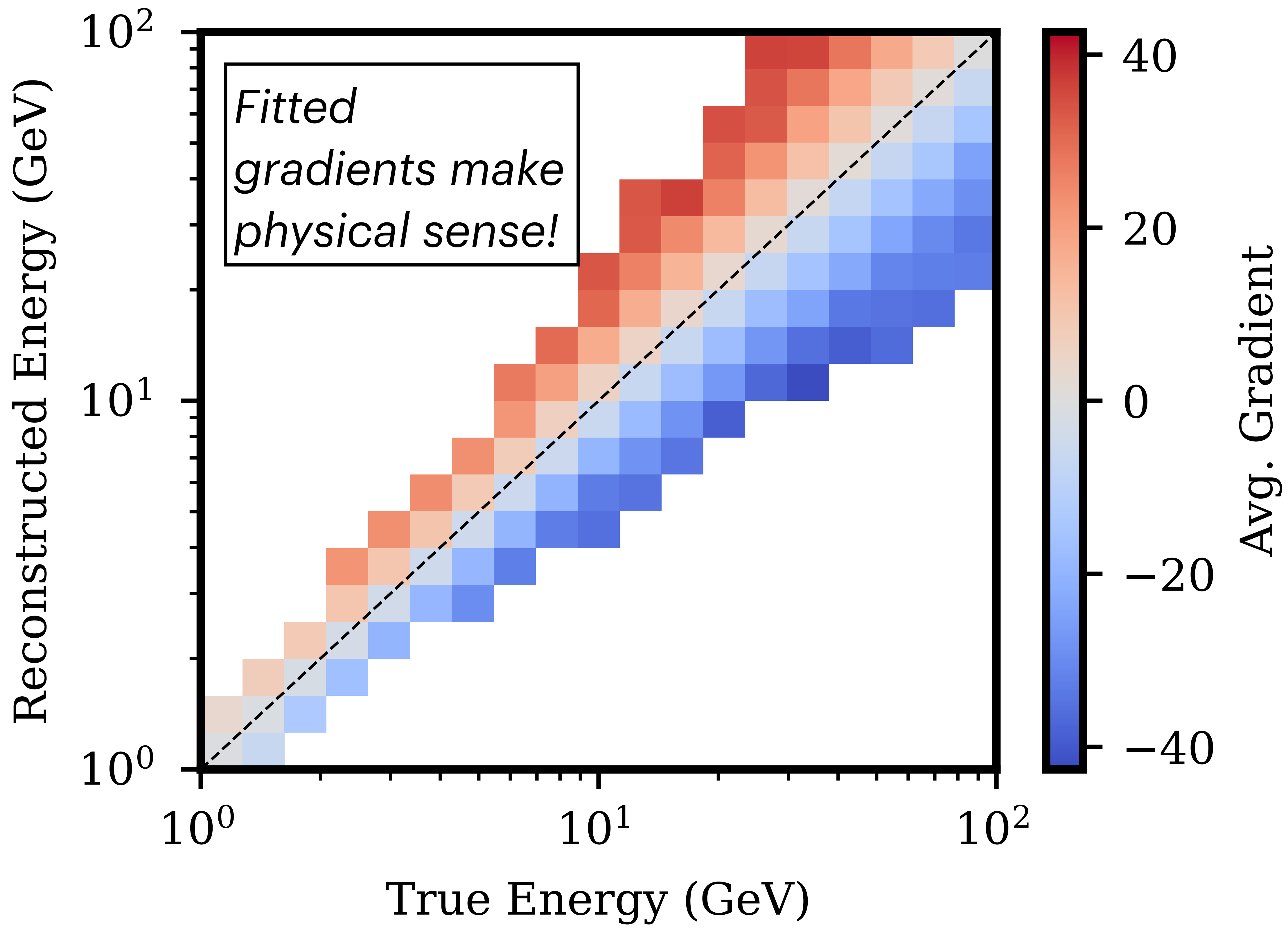


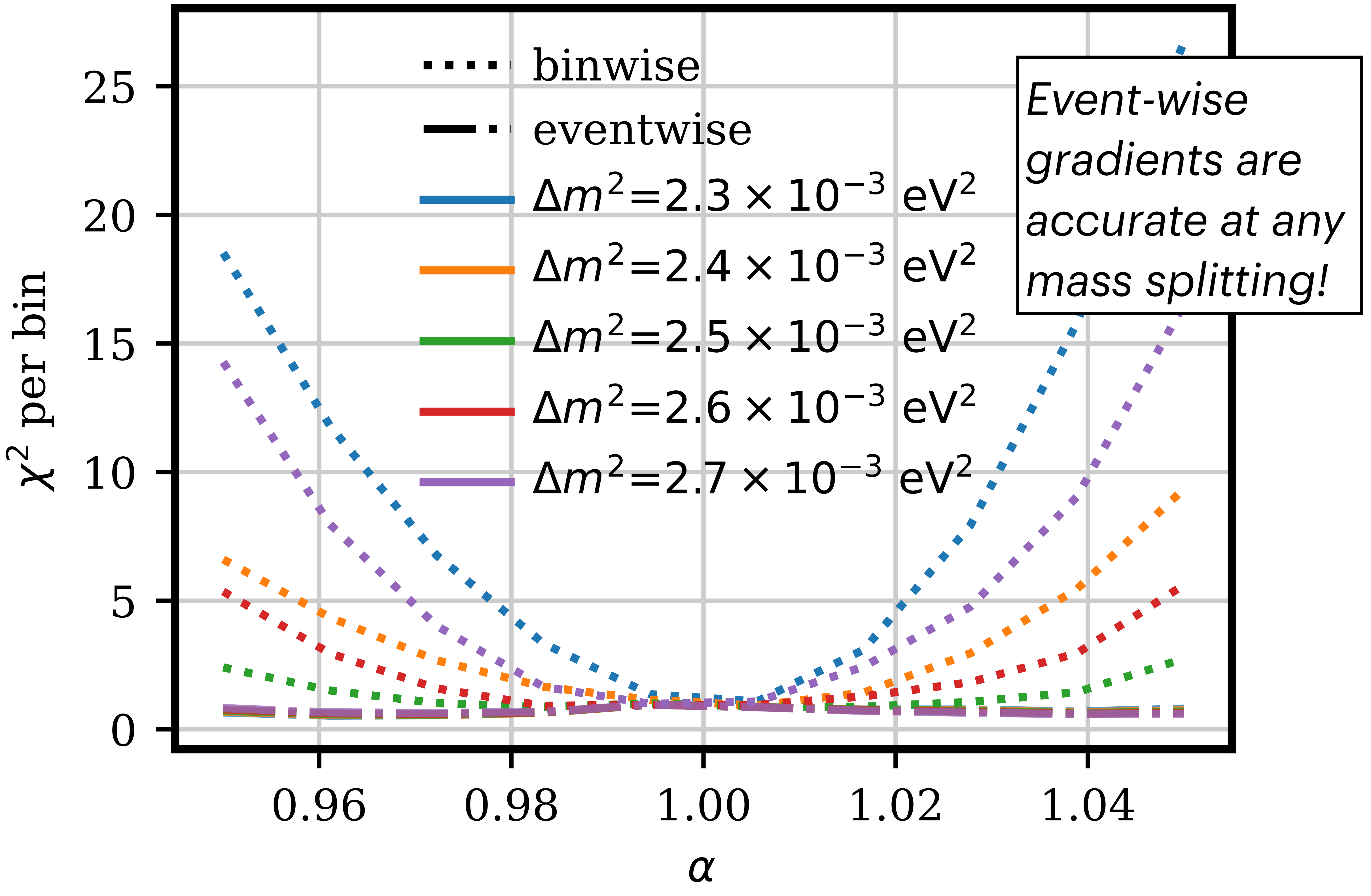


Note: The classifier was trained on the *unweighted* events!

Performance on Toy MC

Gradients make Sense and Produce Accurate Predictions





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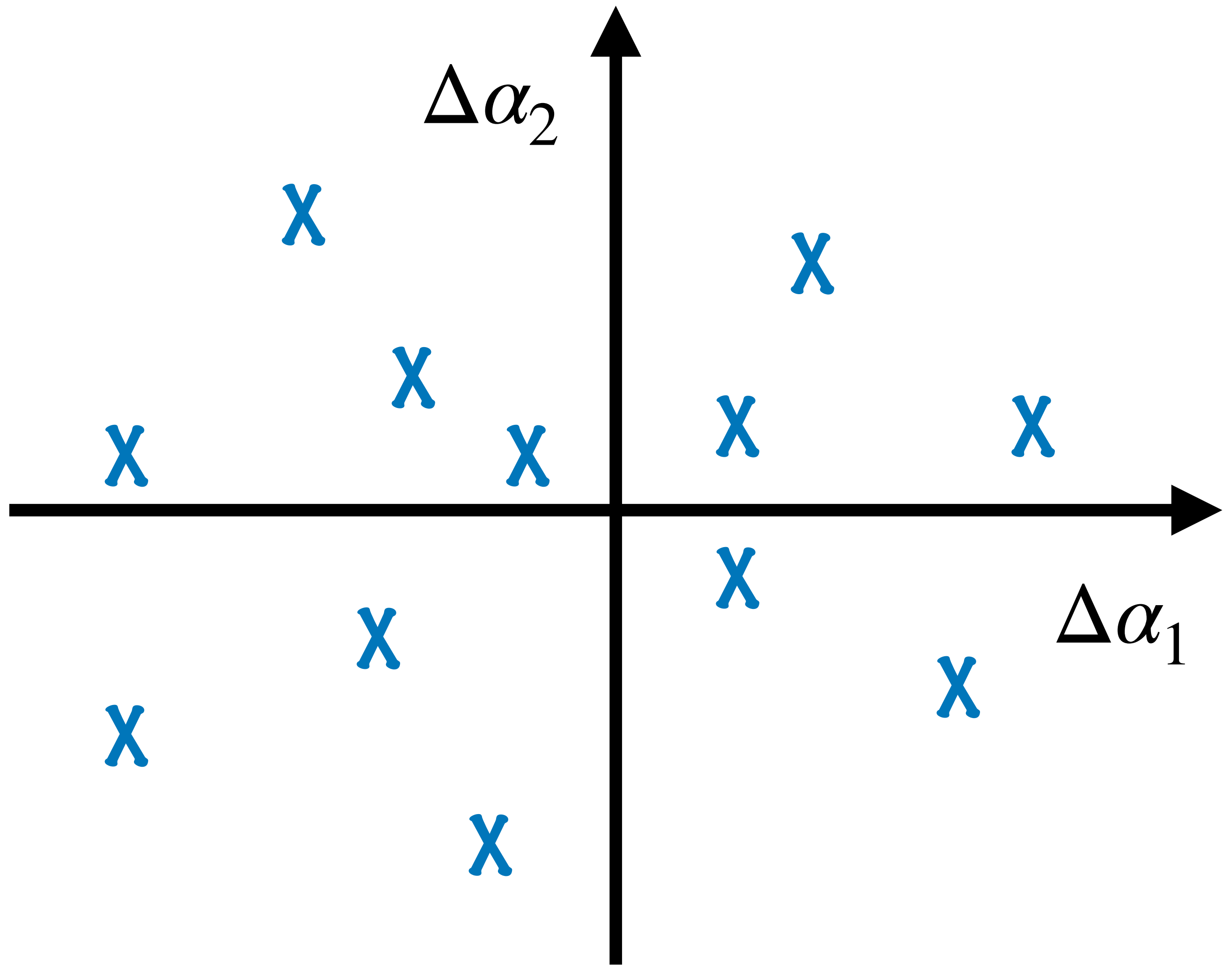

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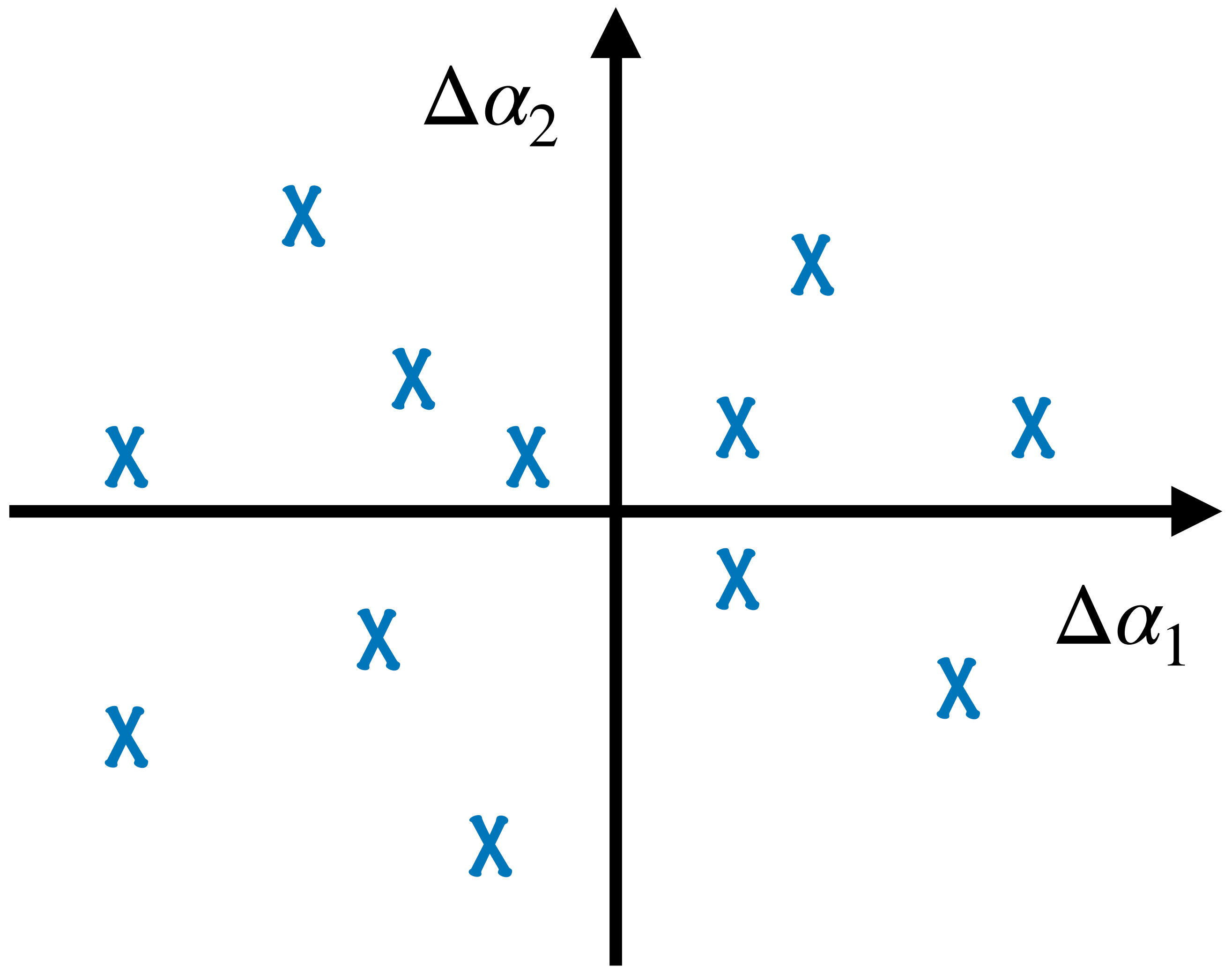

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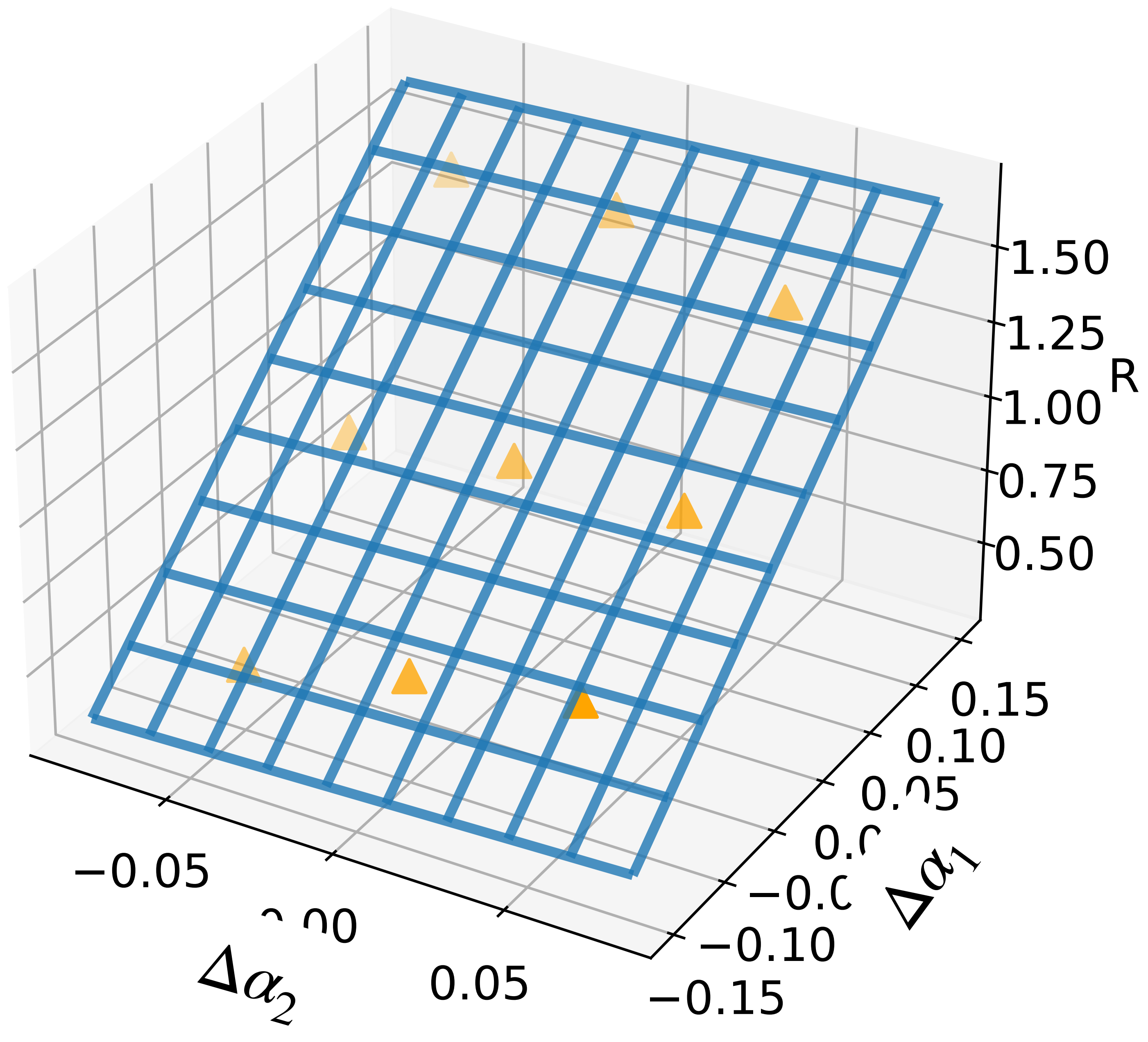

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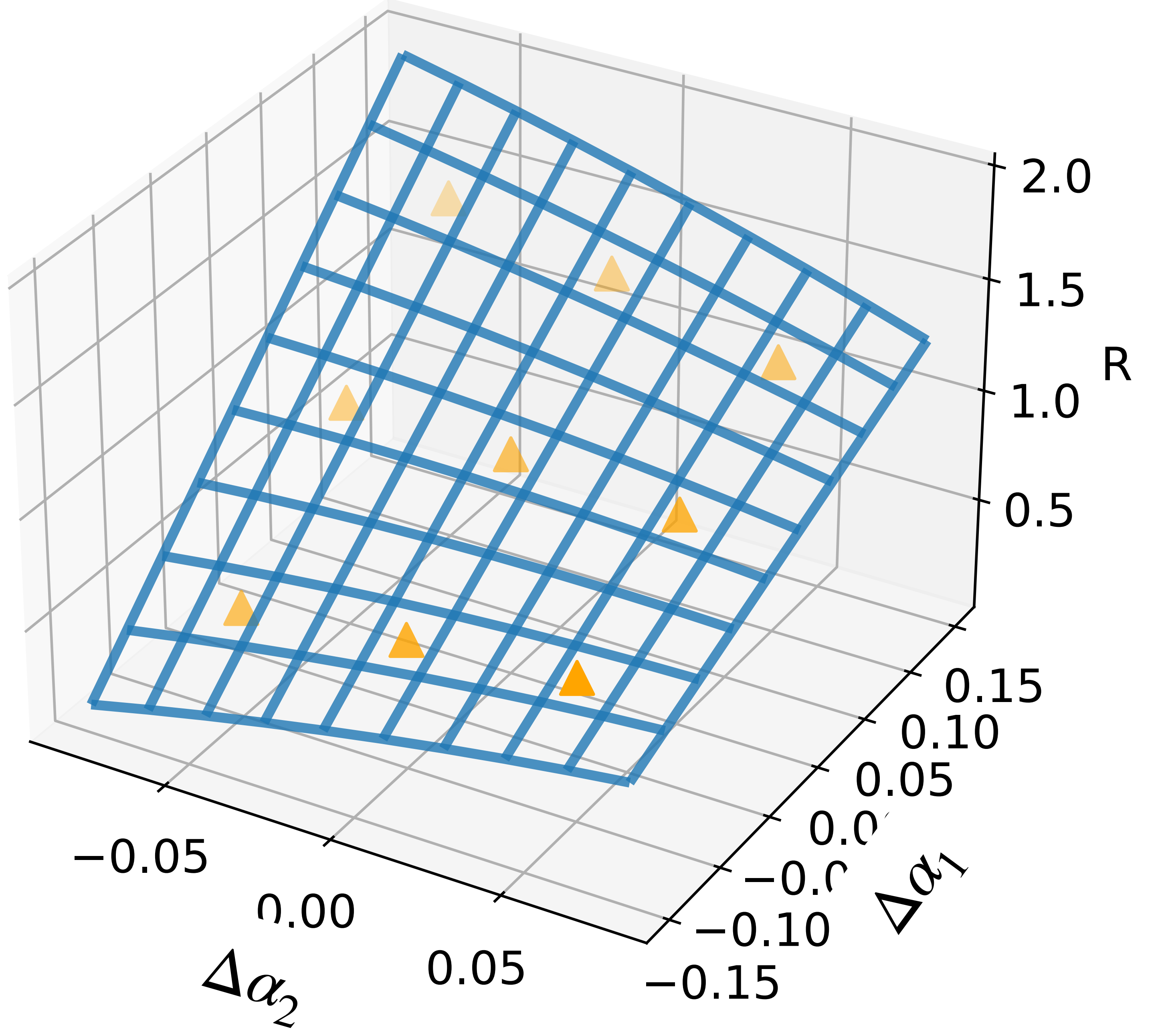

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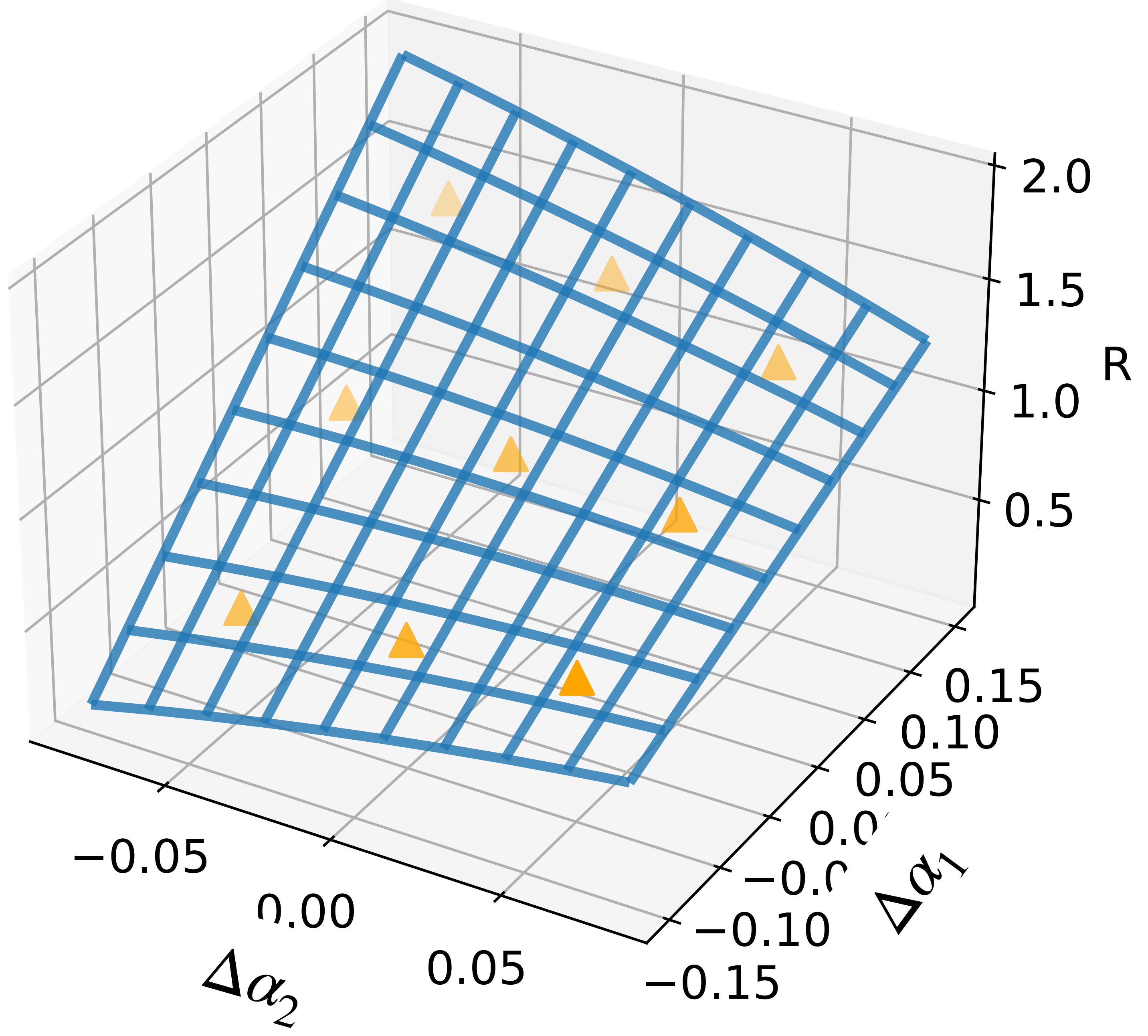

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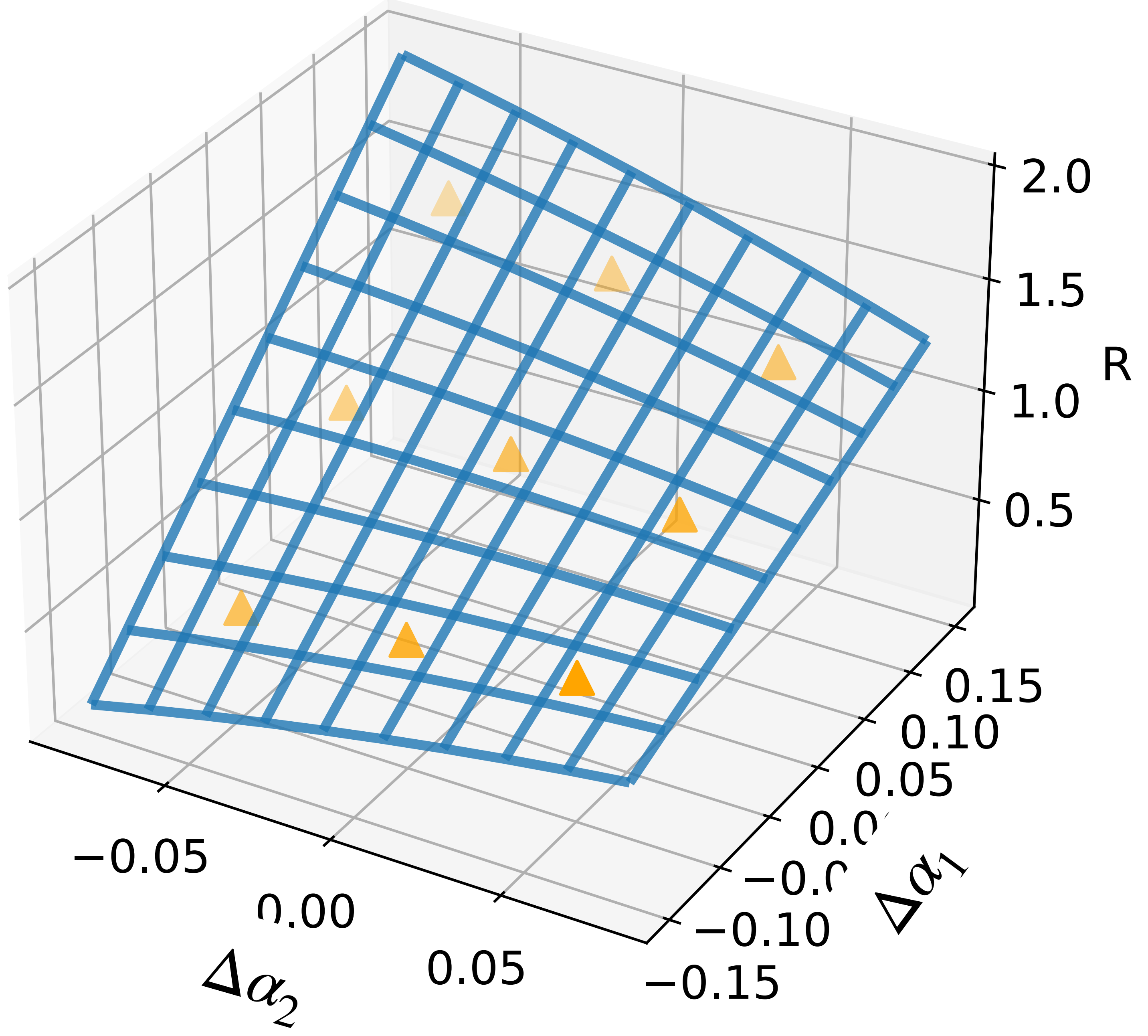

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Analyzers need only the last step!

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Thank You!

Backup

MC Event Weighting

How we get an expectation value in each bin

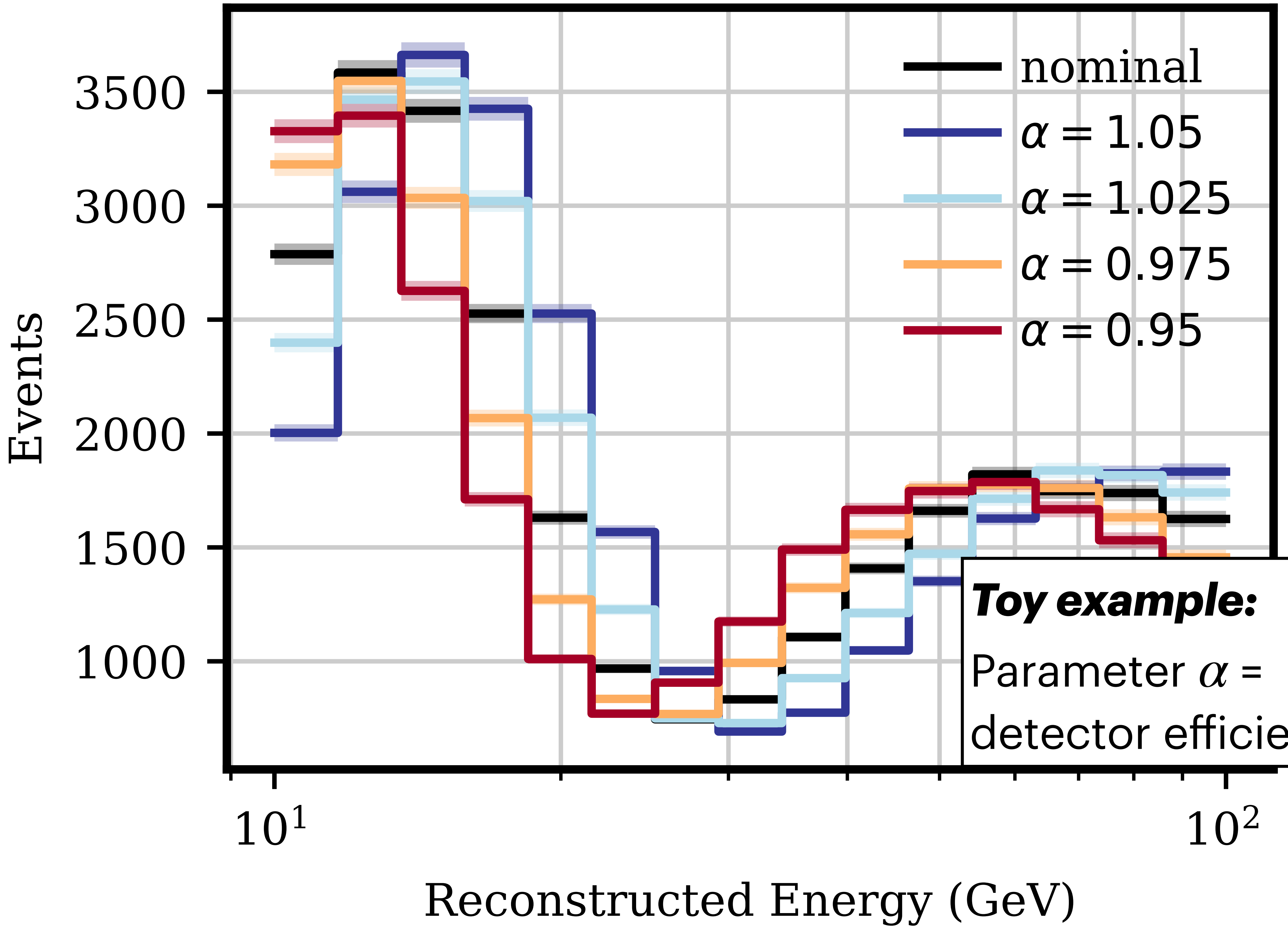
Full expression for expectation in each bin i:

$$\mu_i(\theta) = \int_{\mathbf{y}\in \text{bin } i} \mathrm{d}\mathbf{y} \int \mathrm{d}\mathbf{x} P(\mathbf{y}\,|\,\mathbf{x},\alpha) P(\text{acc}\,|\,\mathbf{x},\alpha) \frac{\Phi(\mathbf{x}\,|\,\theta)}{\Phi_{\text{sim}}(\mathbf{x})}$$

- **Flux, cross-sections, oscillations**:
  - Estimate bin count by weighting events:

$$\hat{\mu}_i(\theta) = \sum_j I(\mathbf{y}_j \in \text{bin } i) \frac{\Phi(\mathbf{x}_j\,|\,\theta)}{\Phi_{\text{sim}}(\mathbf{x}_j)}$$

- **Uncertainties of detector properties**:
  - How can we get $P(\text{acc}\,|\,\mathbf{x},\alpha)P(\mathbf{y}\,|\,\mathbf{x},\alpha)$?



Toy example:
Parameter α = detector efficiency

Goal of this Work

Decoupling Detector Response Weight from Physics Parameters

Basic intuition: Detector response should not depend on initial particle flux!

➡ Detector reacts to final state of each particle, doesn't know about flux or cross-sections

➡ Detector properties determine relationship between true and reconstructed variables

➡ If we knew $P(\mathbf{y} \mid \mathbf{x}, \alpha)P(\mathrm{acc} \mid \mathbf{x}, \alpha)$, we should be able to get the correct expectation value *independently* from θ

$$\hat{\mu}_i(\theta, \alpha) = \sum_j I(\mathbf{y}_j \in \mathrm{bin}\, i) \boxed{\frac{P(\mathbf{y}_j \mid \mathbf{x}_j, \alpha)P(\mathrm{acc} \mid \mathbf{x}_j, \alpha)}{P(\mathbf{y}_j \mid \mathbf{x}_j, \alpha_{\mathrm{nom}})P(\mathrm{acc} \mid \mathbf{x}_j, \alpha_{\mathrm{nom}})}} \frac{\Phi(\mathbf{x}_j \mid \theta)}{\Phi_{\mathrm{sim}}(\mathbf{x}_j)}$$

Event weight independent of θ

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- ✓ Automatically smooth over poor statistics in varied MC sets
  - ➡ Tune your classifier for the ideal balance of smoothness and over-fitting

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  - ➡ Tune your classifier for the ideal balance of smoothness and over-fitting
- ✓ No assumption of linearity of detector effects
- ✓ No assumption about how you space out your MC sets