# An implementation of Neural Simulation-Based Inference for Parameter Estimation in ATLAS

ML4Jets2024
07 November 2024

Arnaud Maury, on behalf of the ATLAS Collaboration

*Run 2 analysis of the off-shell Higgs boson decaying into four leptons*

1 analysis, 2 papers:

- A Physics measurement paper:
  https://atlas.web.cern.ch/Atlas/GROUPS/PHYSICS/CONFNOTES/ATLAS-CONF-2024-016/

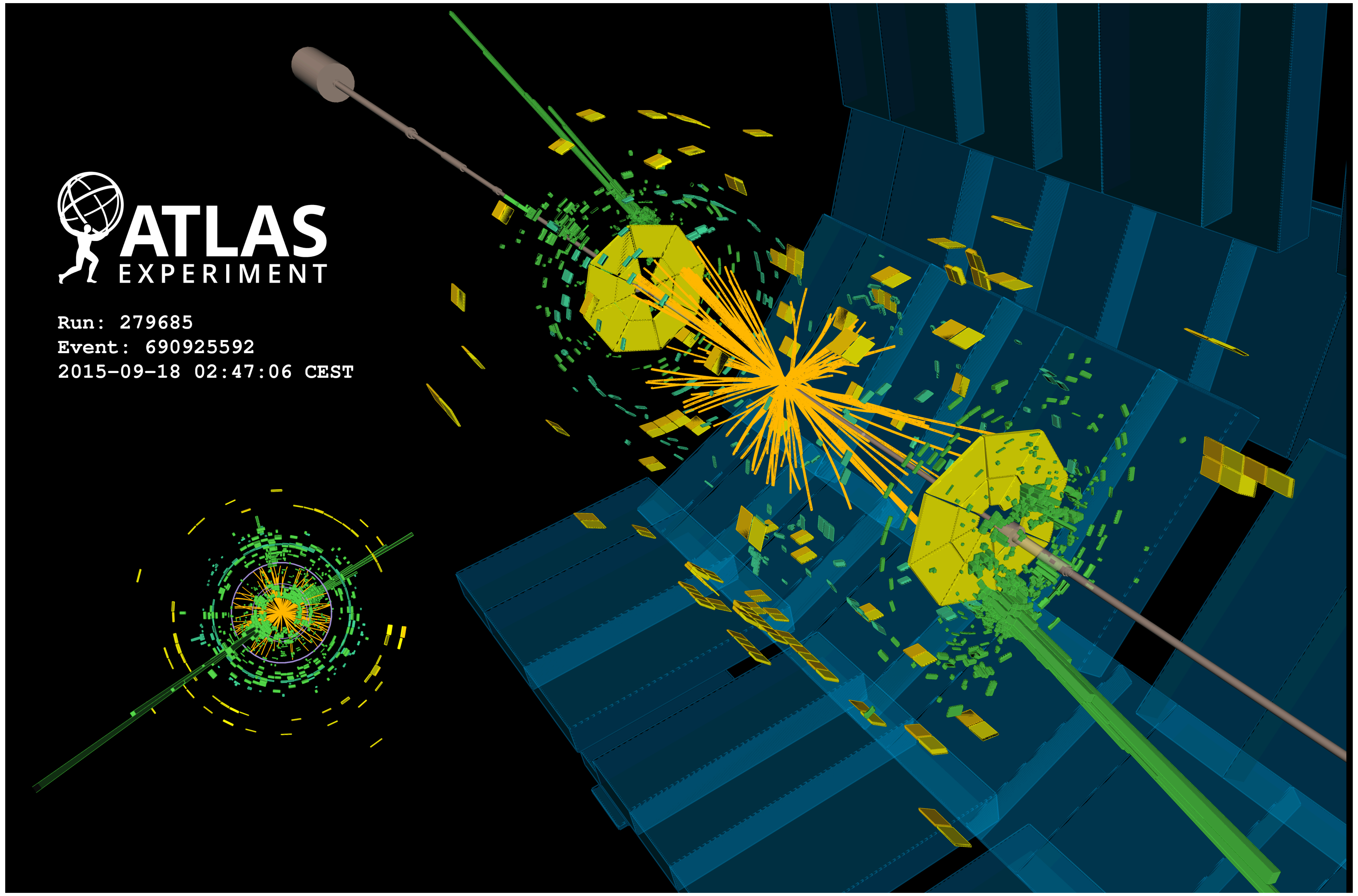
- An ML-focused methodology paper (this talk):
  https://atlas.web.cern.ch/Atlas/GROUPS/PHYSICS/CONFNOTES/ATLAS-CONF-2024-015/

# The motivation for Neural Simulation-Based Inference (NSBI)

# Typical LHC Workflow

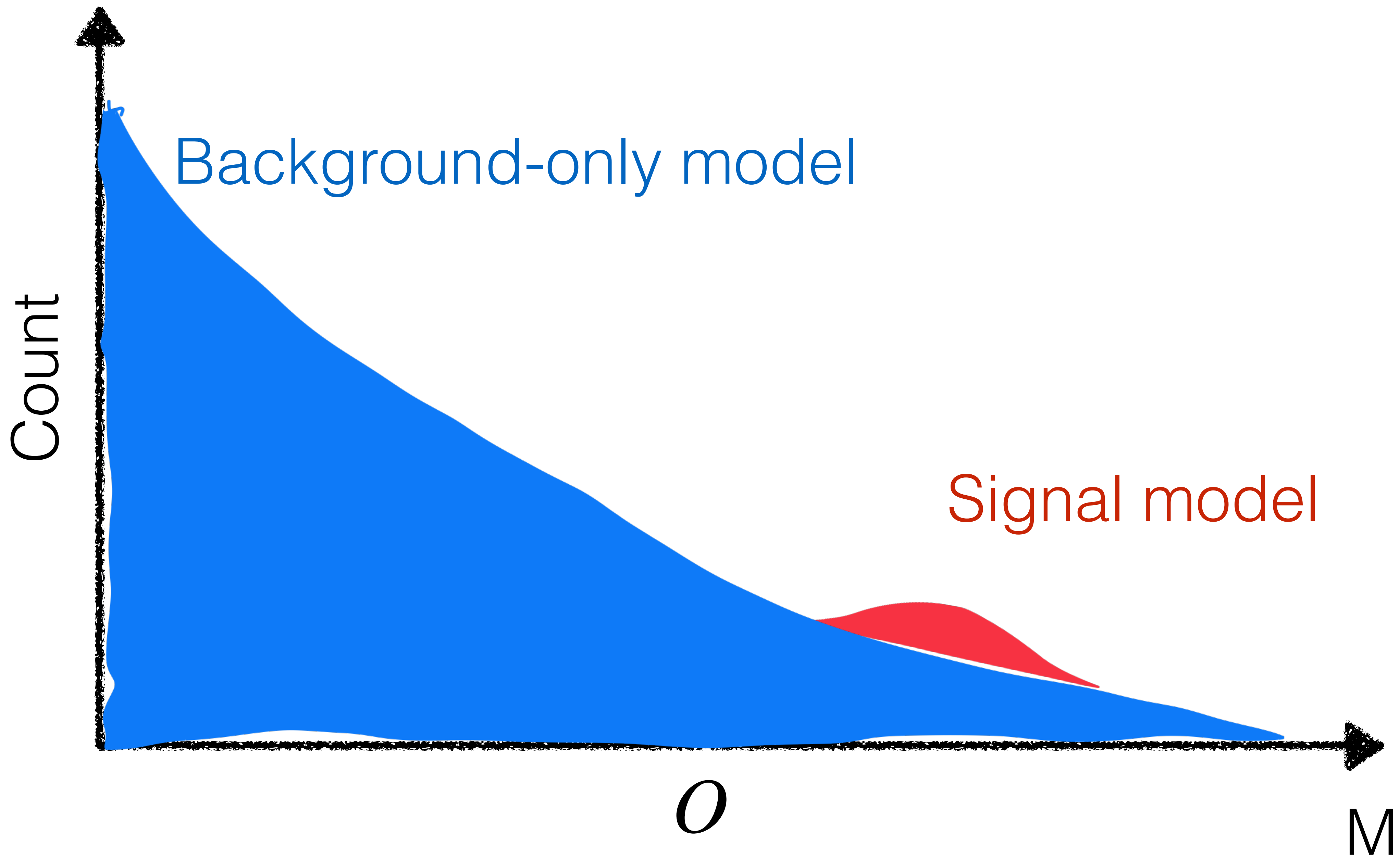
- Detector has O(100 million) sensors
- Can’t build 100M dimensional histogram

- Reconstruction pipeline, event selection
- Design sensitive one-dimensional observable

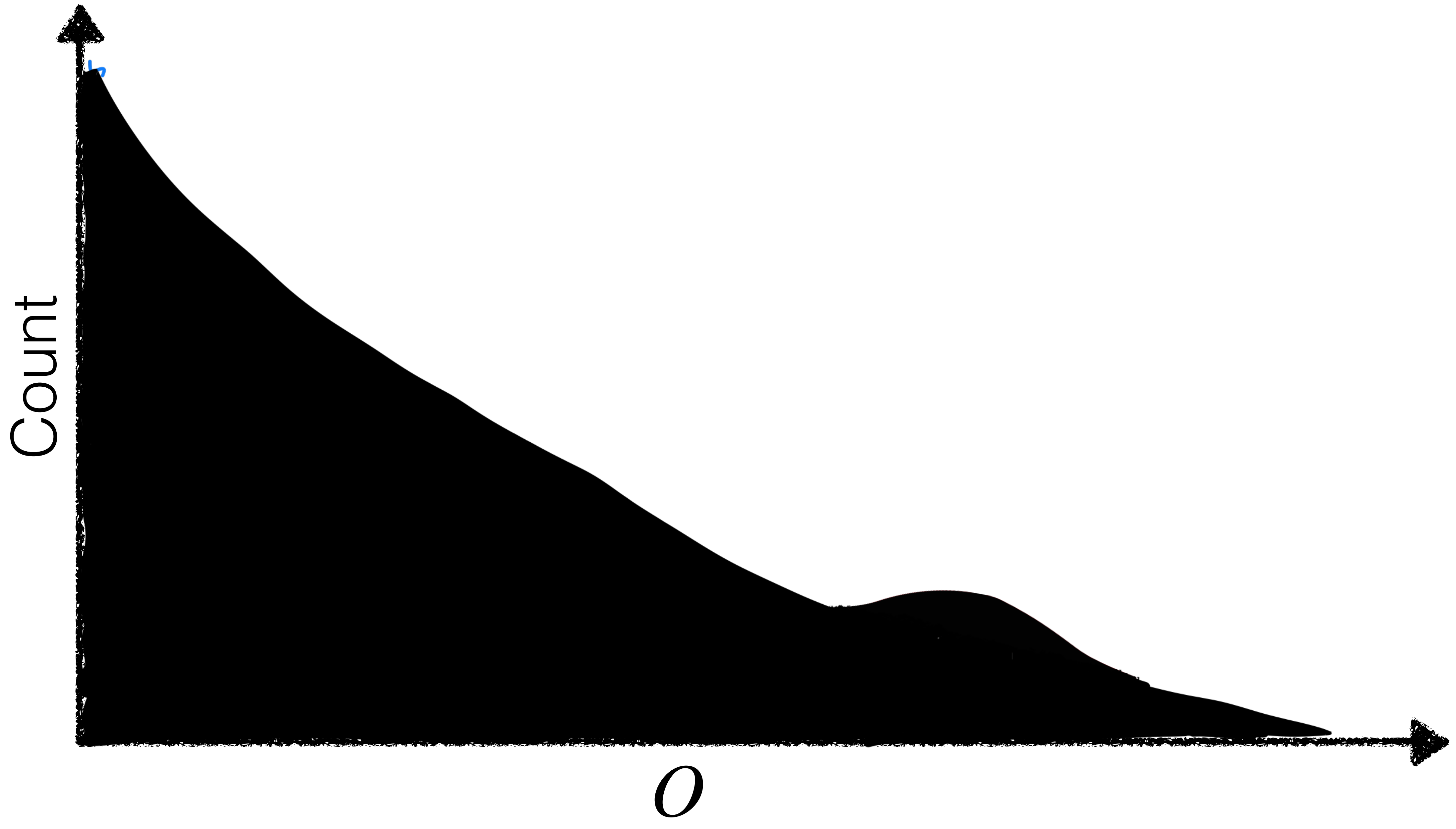


# Density Estimation: What we're used to doing..

Theory Predictions




Data




Measure signal strength $\mu$

With histograms we can ask "Given the data, what is the likelihood of $\mu = 1$ hypothesis vs $\mu = 2$ hypothesis?"

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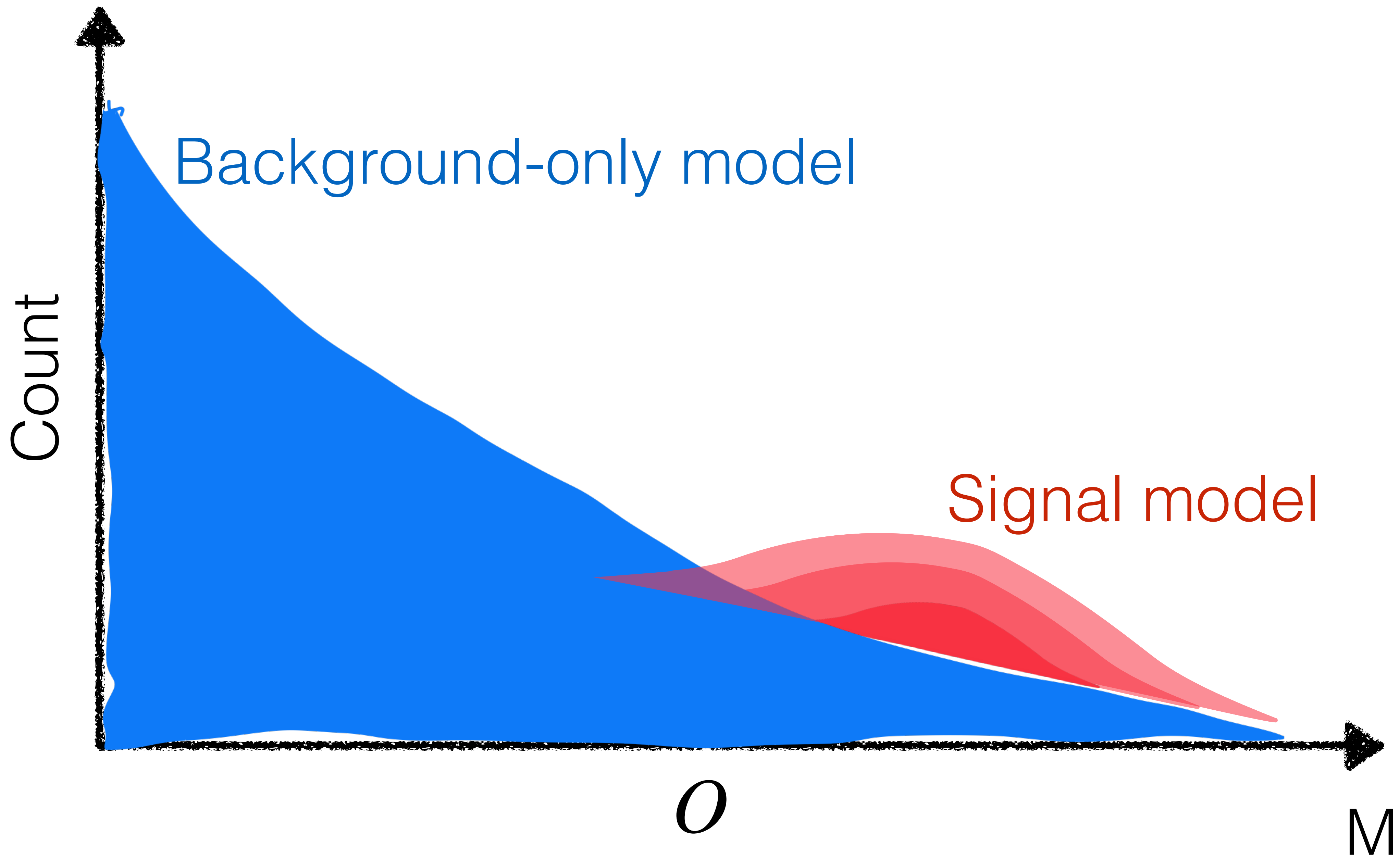


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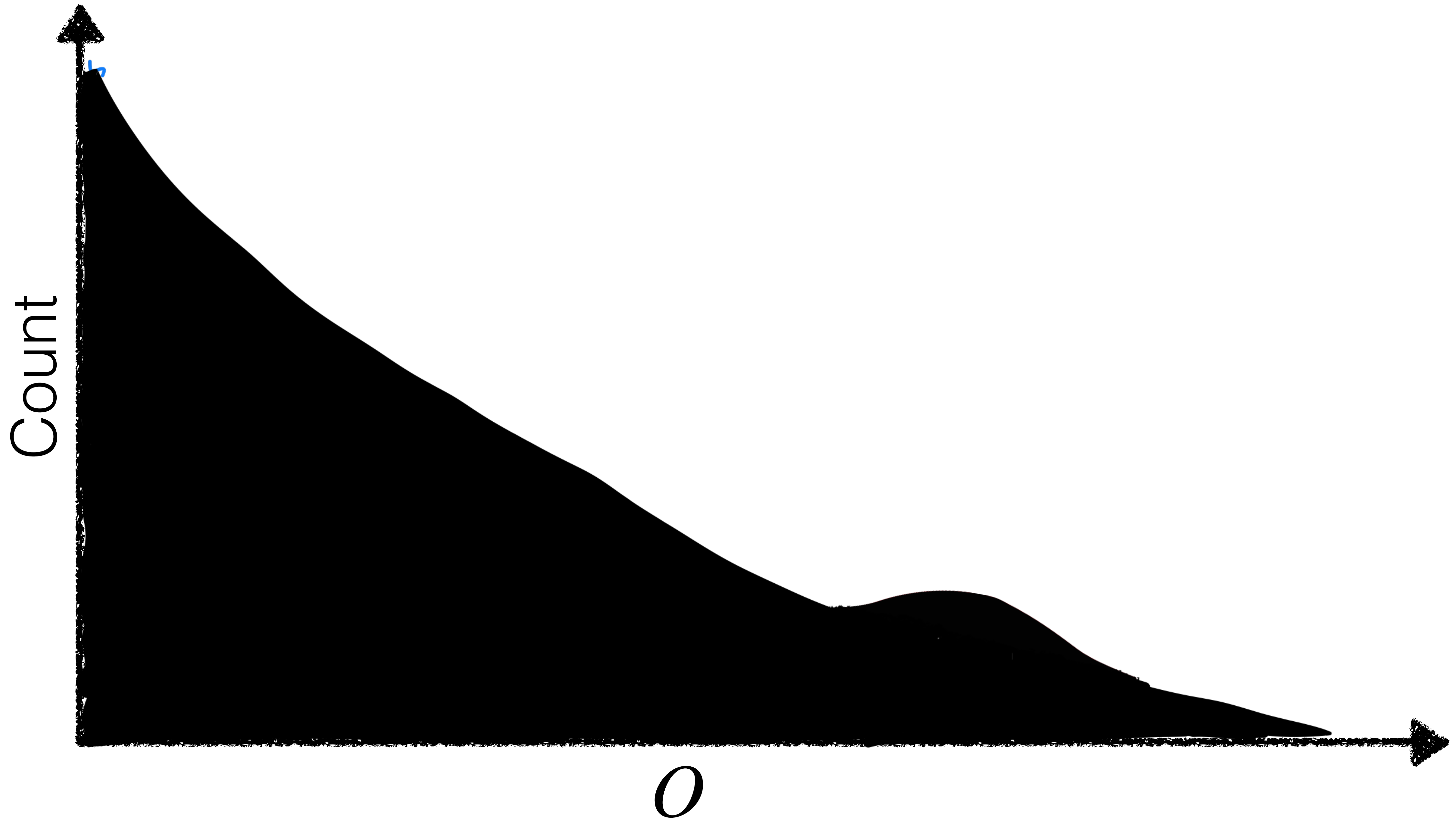


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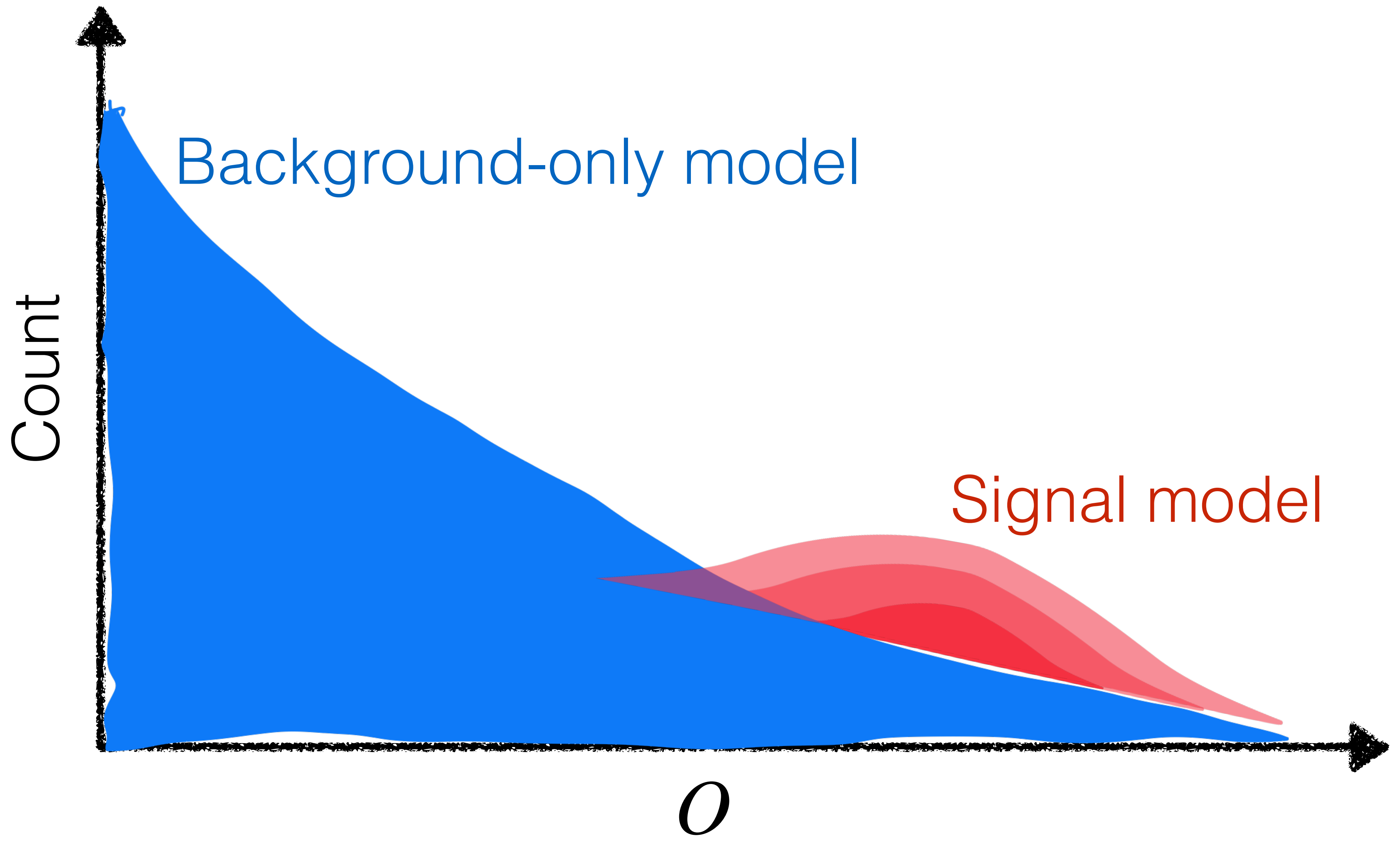
# New challenge: Non-linear changes in kinematics (w.r.t. parameter of interest)

Campbell et al: arXiv:1311.3589

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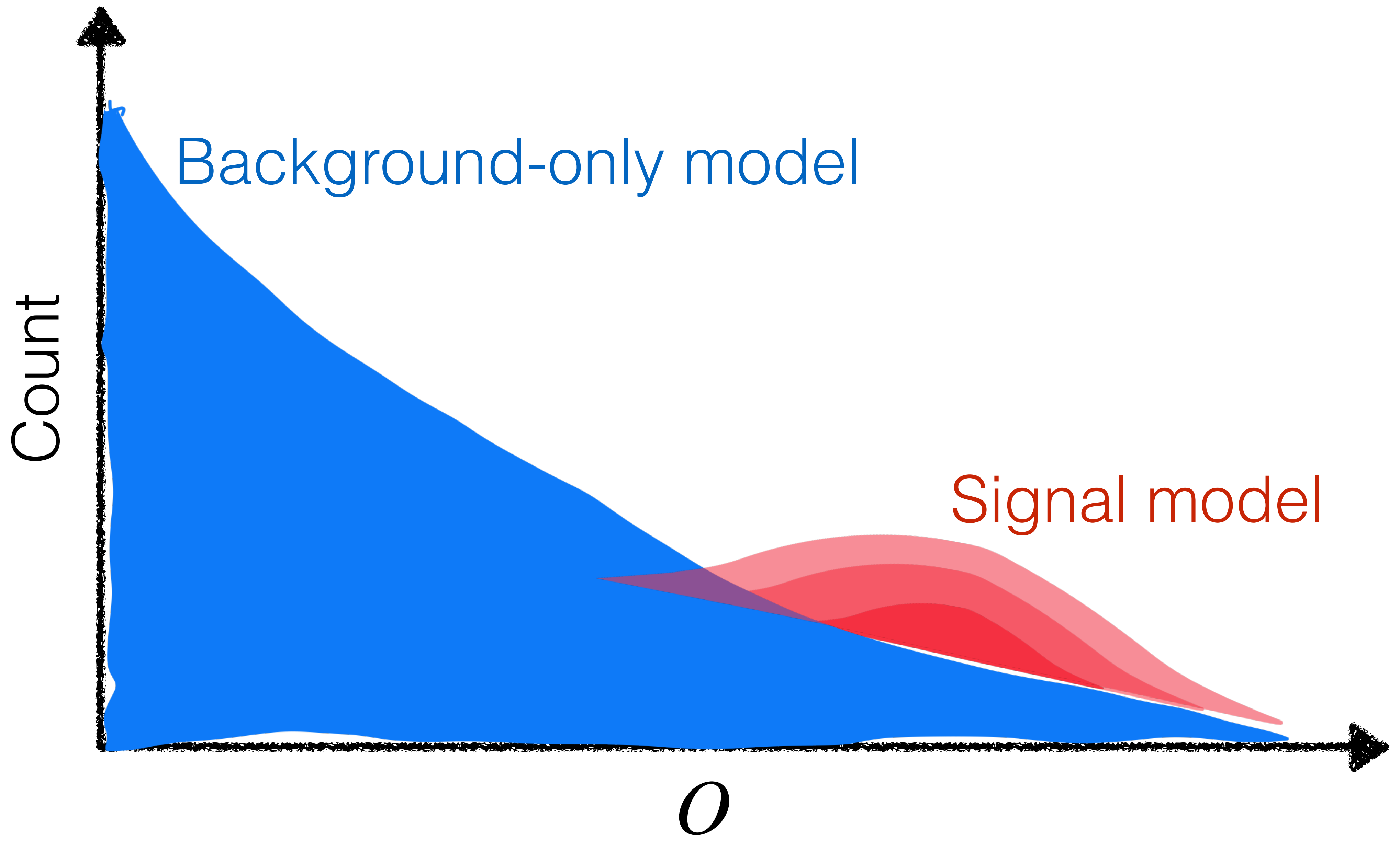


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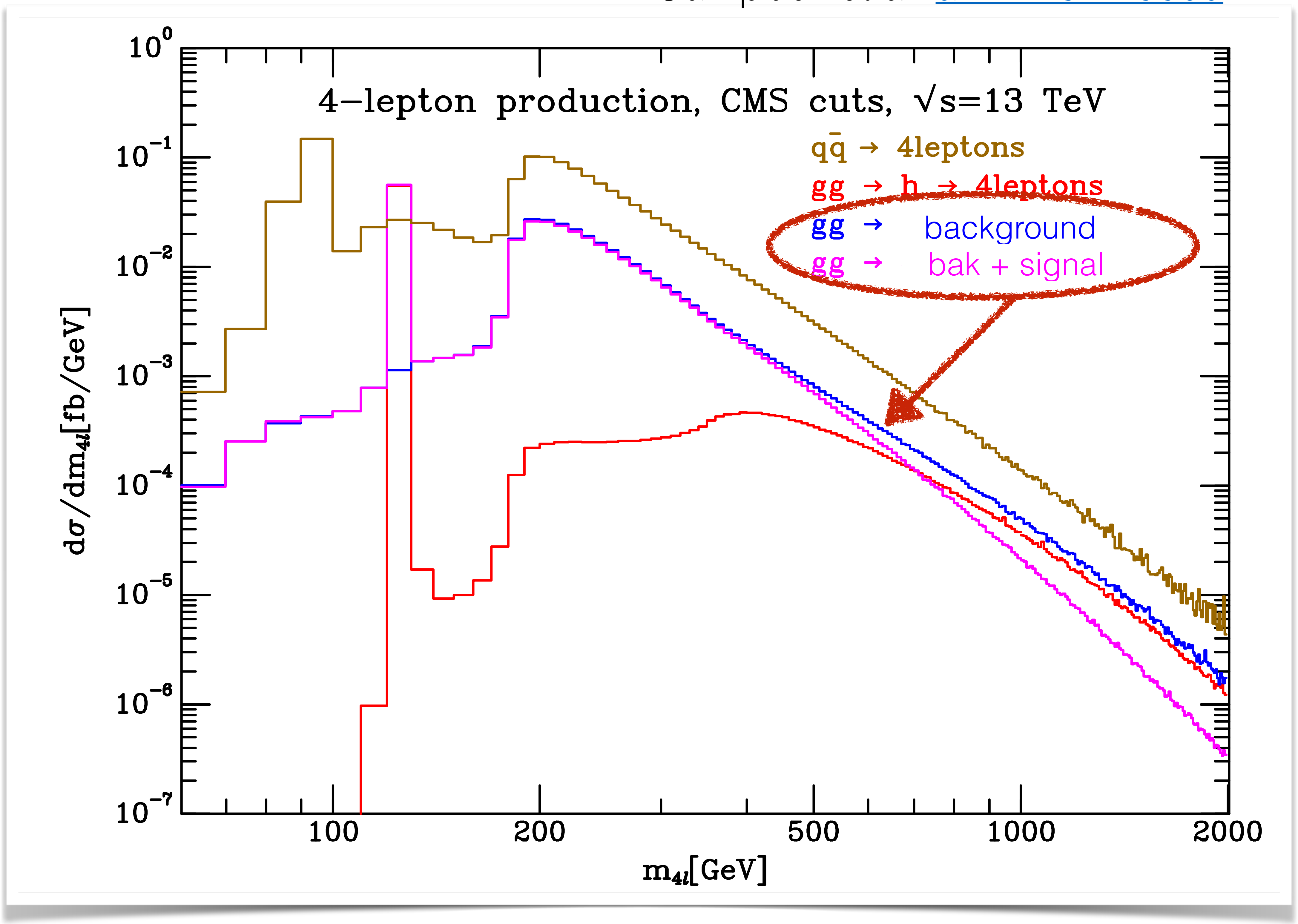


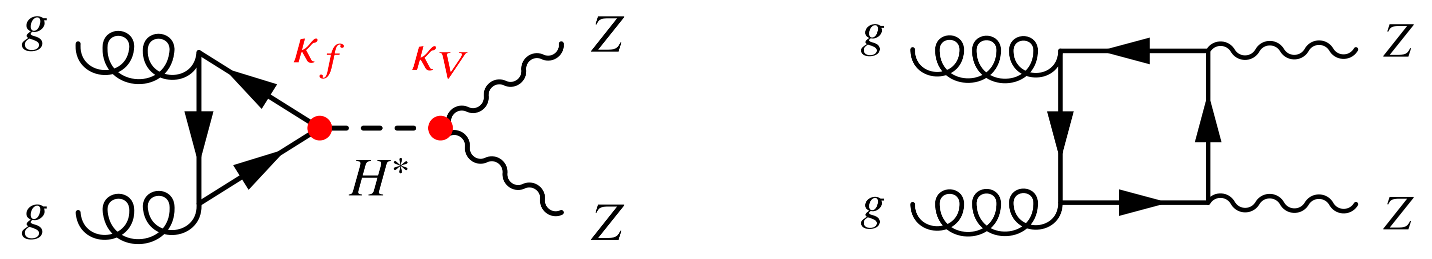


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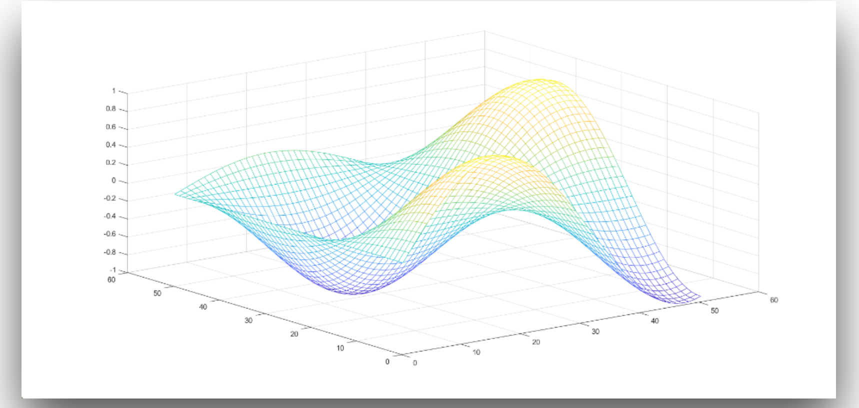
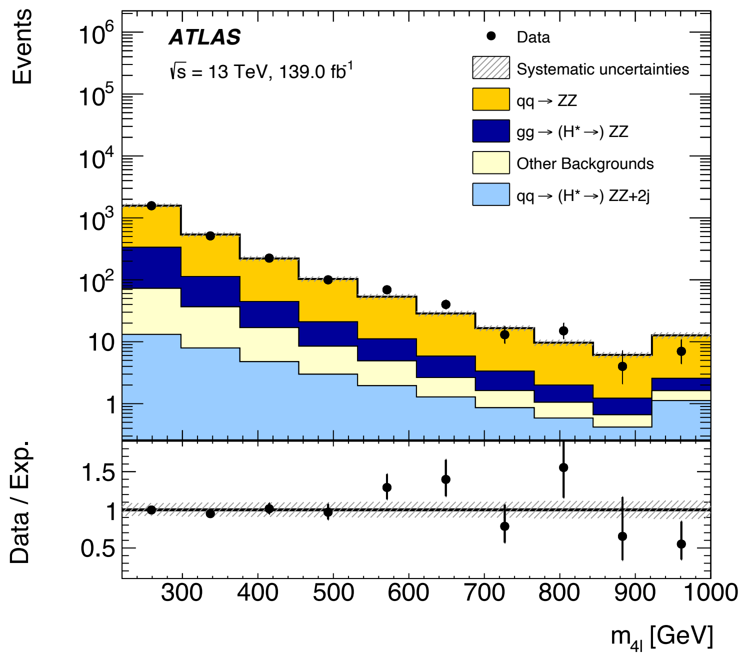
# "Neural Simulation-Based Inference"

## Traditional framework:



High-dim data

Summarisation to histogram →

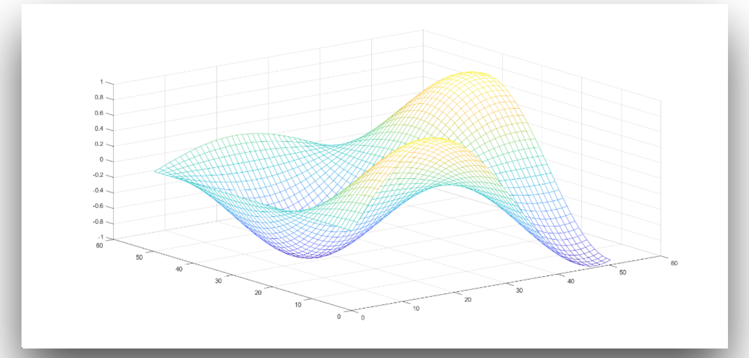



Summary Histogram → **Statistical Fit** → Likelihood $\mathscr{L}(\mu_1 | \mathscr{D})$

$\mu_1$ → **Statistical Fit**

$\mu$ is now arbitrary parameter of interest(s)

## The neural inference framework:



High-dim data

Obs Data → **Neural Networks** → Likelihood Ratio $\left(\frac{\mathscr{L}(\mu_1 | \mathscr{D})}{\mathscr{L}(ref | \mathscr{D})}\right)$

$\mu_1$ → **Neural Networks**

# "Neural Simulation-Based Inference"

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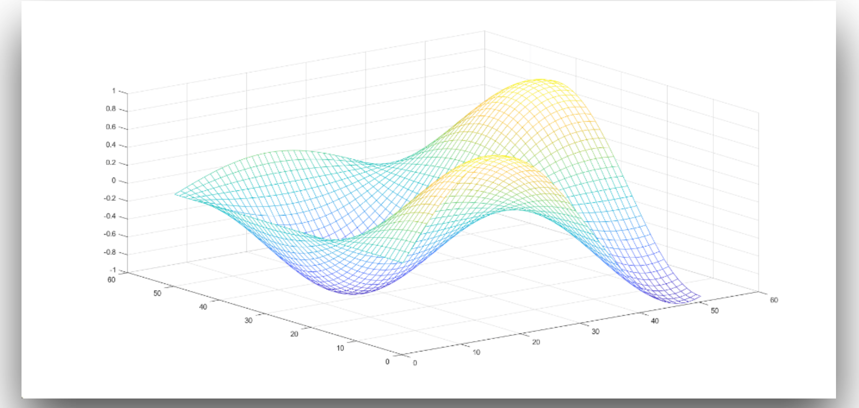

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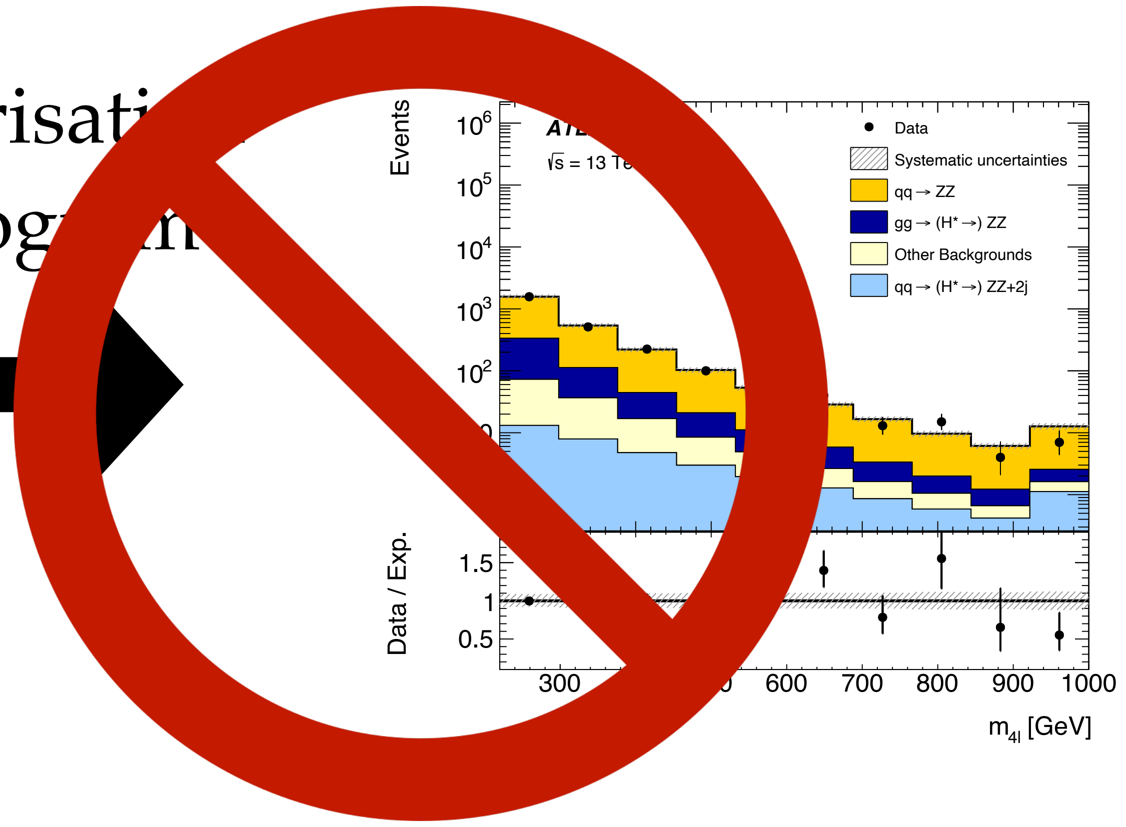


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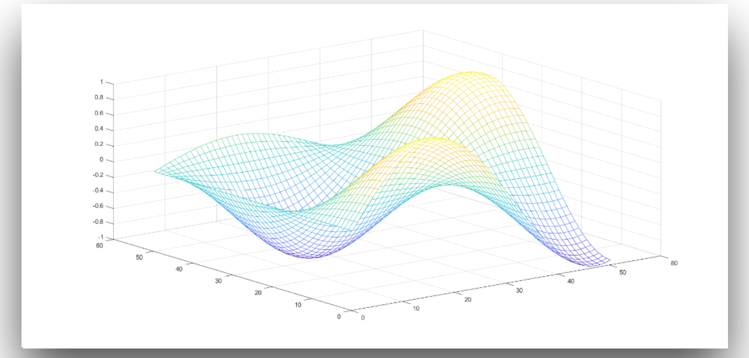

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Open problems to extend to full ATLAS analysis:

- Robustness: Design and validation
- Systematic Uncertainties: Incorporate them into likelihood (ratio) model
- Neyman Construction: Sampling pseudo-experiments in a per-event analysis

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General Formula

$$p(x_i|\mu) = \frac{1}{\nu(\mu)} \sum_{j}^{C} f_j(\mu) \cdot \nu_j \ p_j(x_i)$$

$j$ runs over different physics process
(Eg. $gg \rightarrow H^* \rightarrow 4l$, $gg \rightarrow ZZ \rightarrow 4l$)

Example use case

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Estimated using an ensemble of networks

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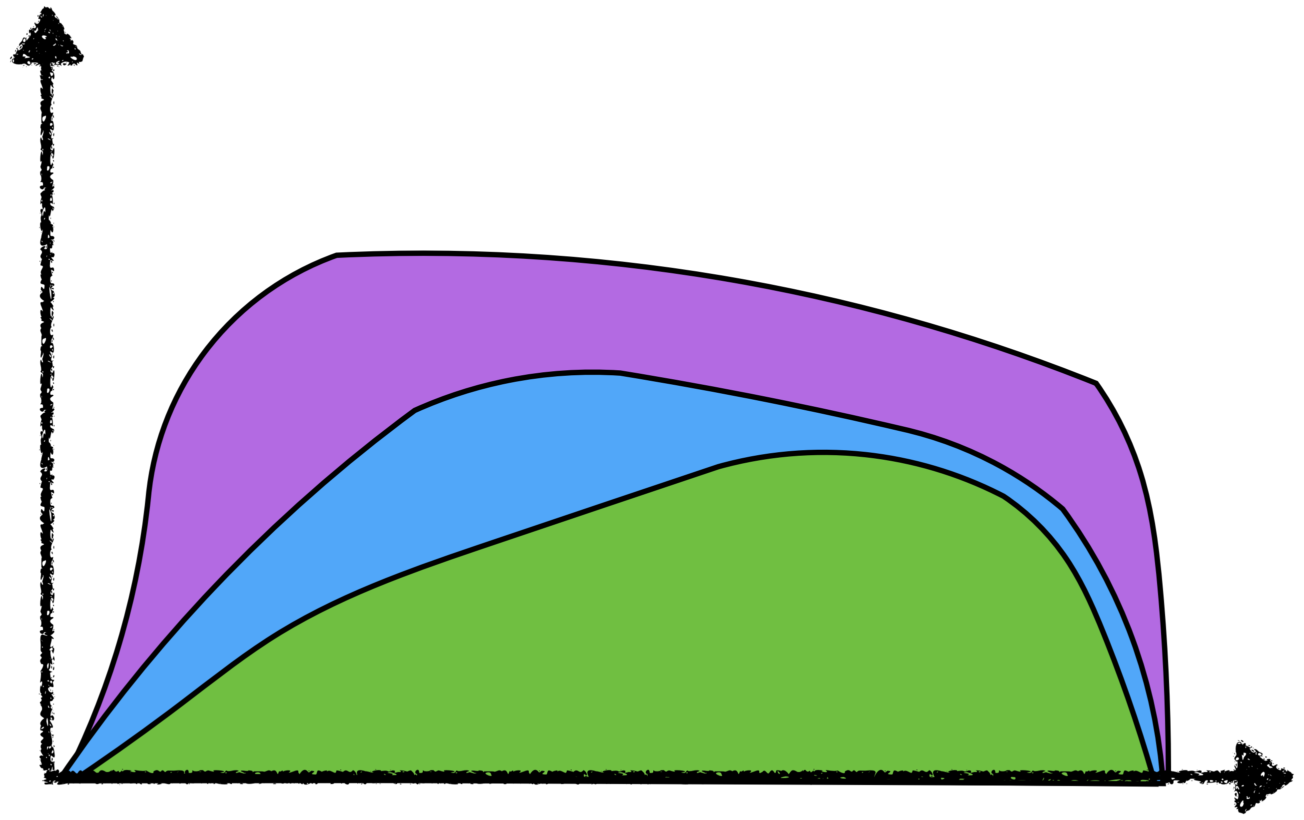
$H_{ref}$ : Reference hypothesis

$H_\mu$

Hypothesis



VS

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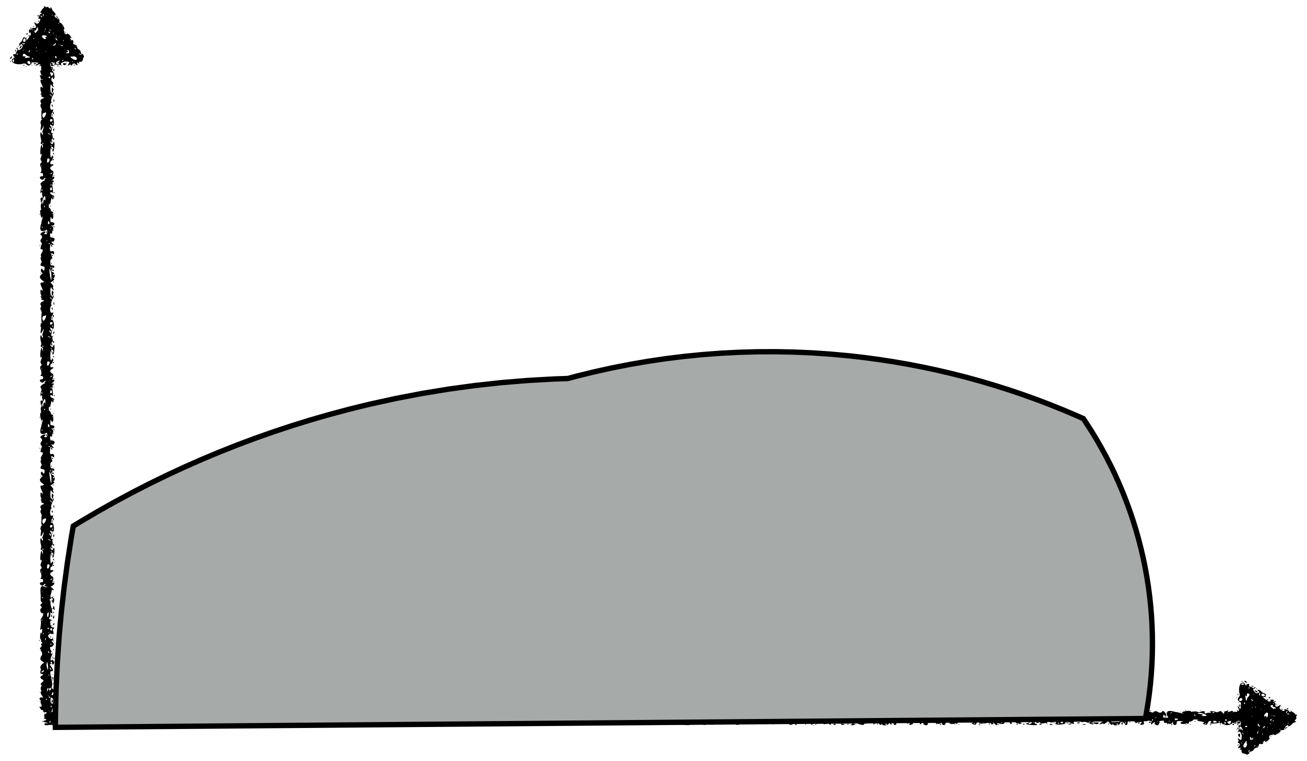

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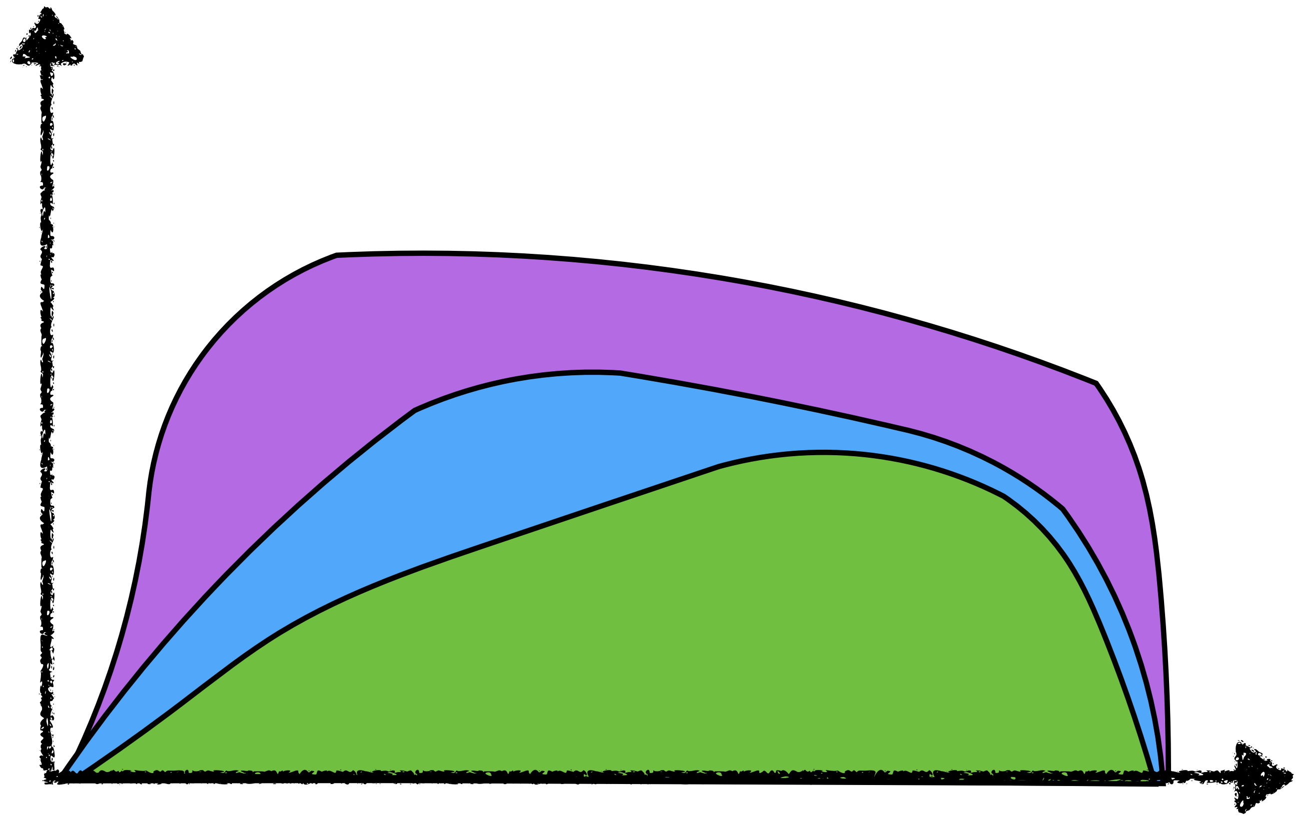

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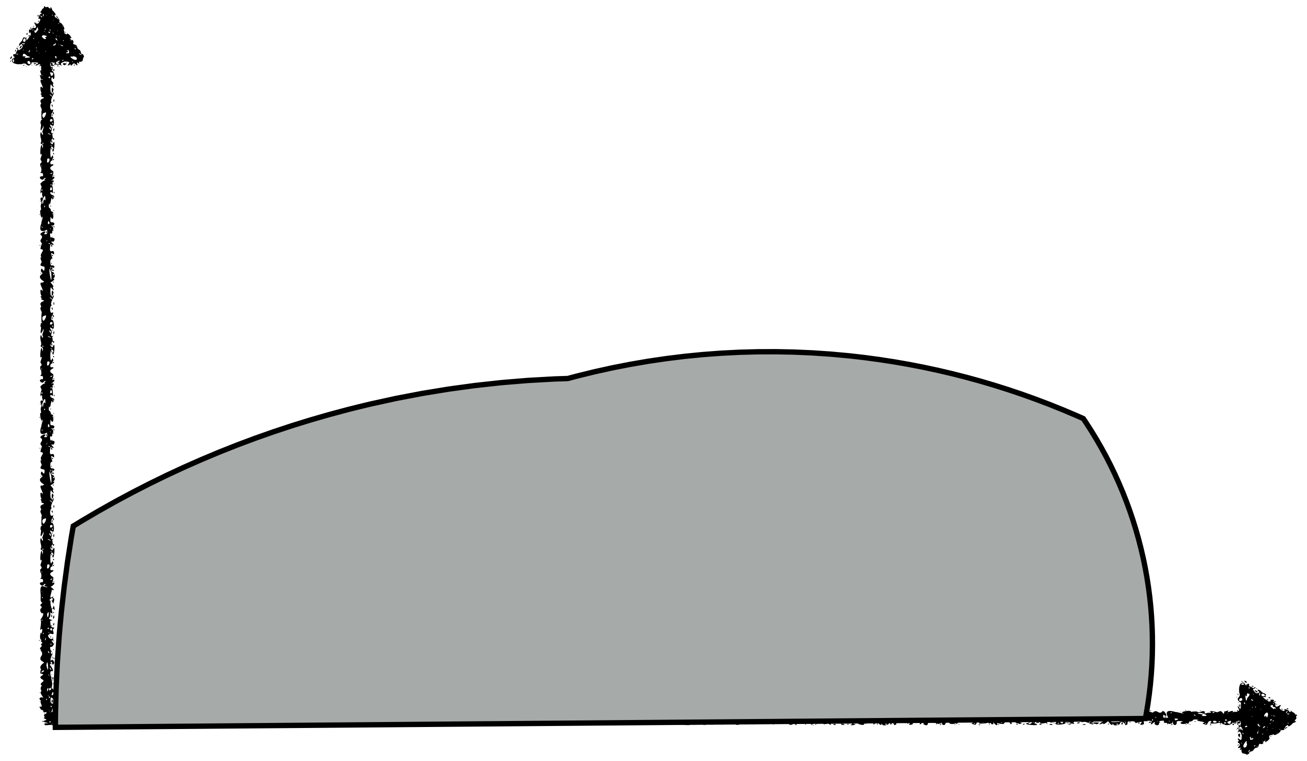

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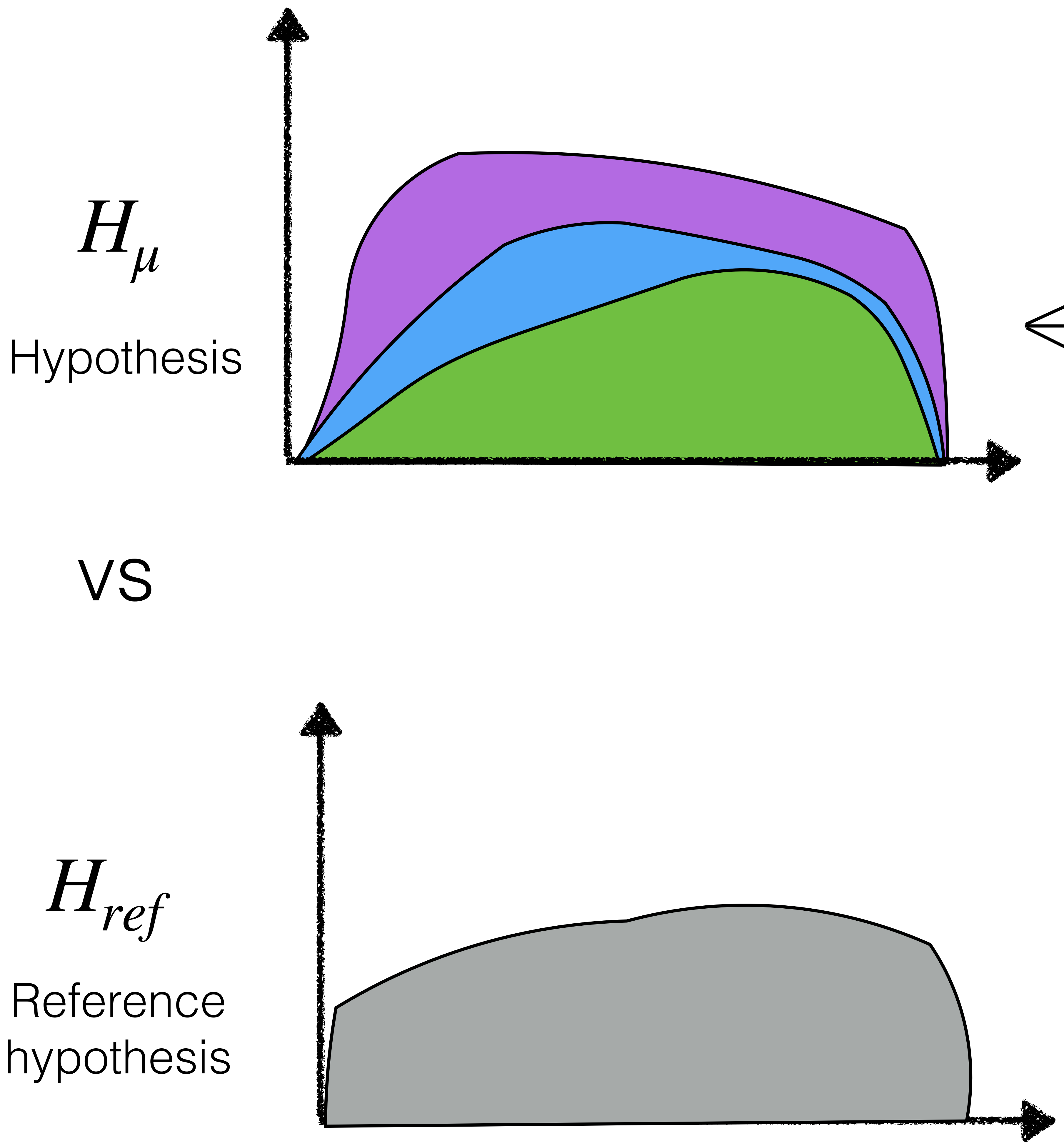


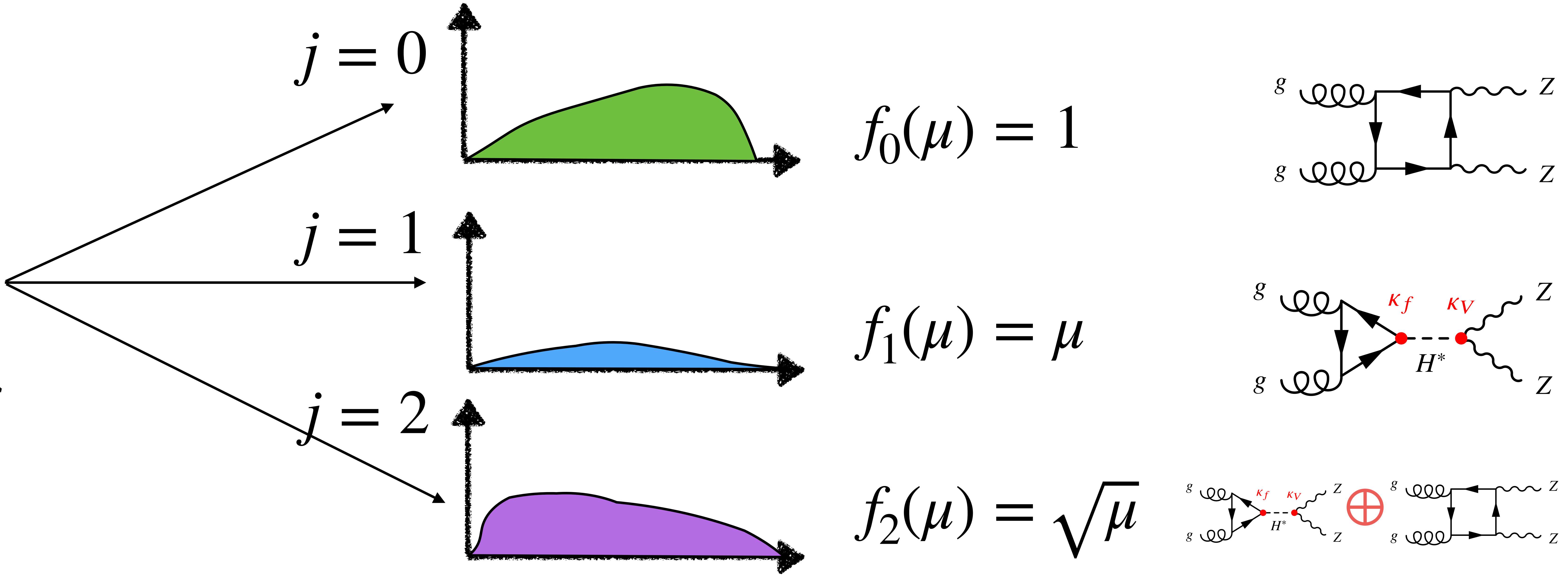


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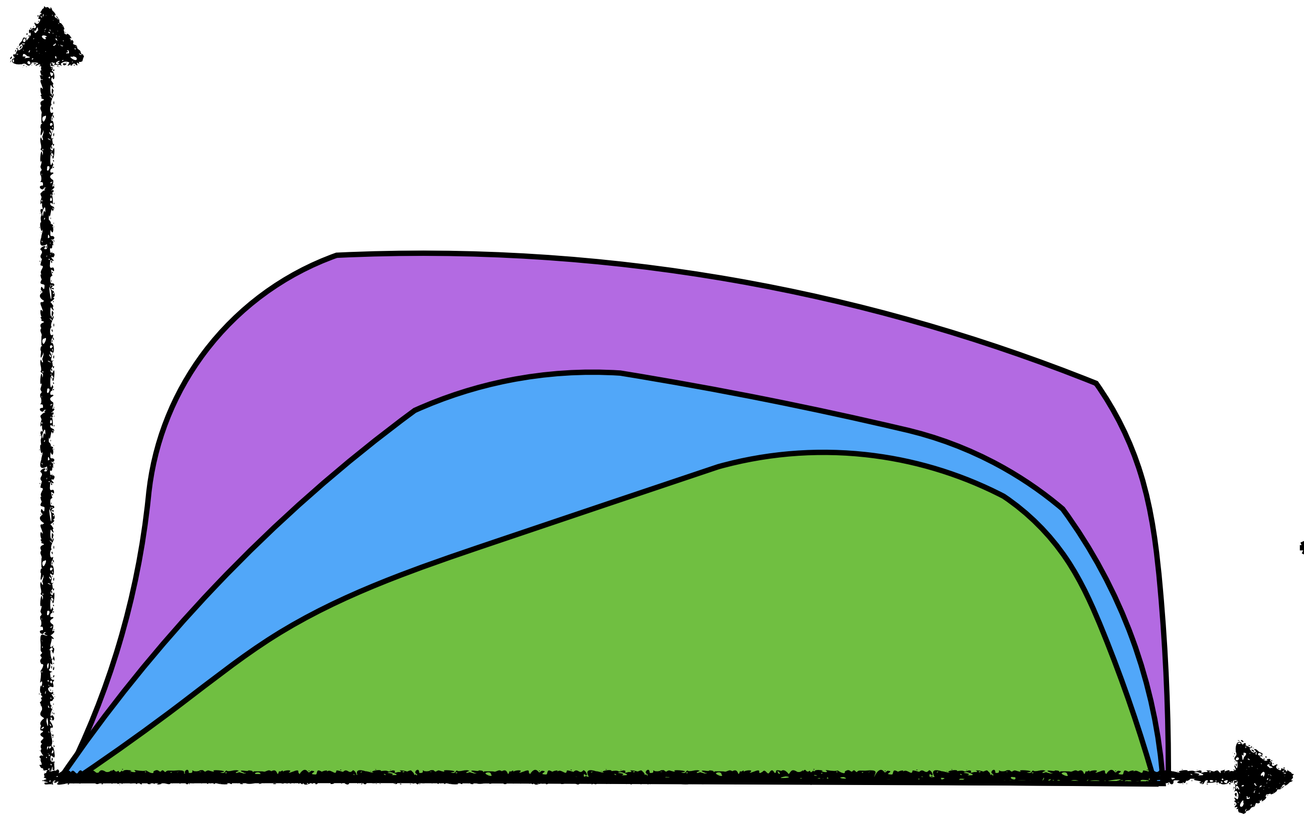

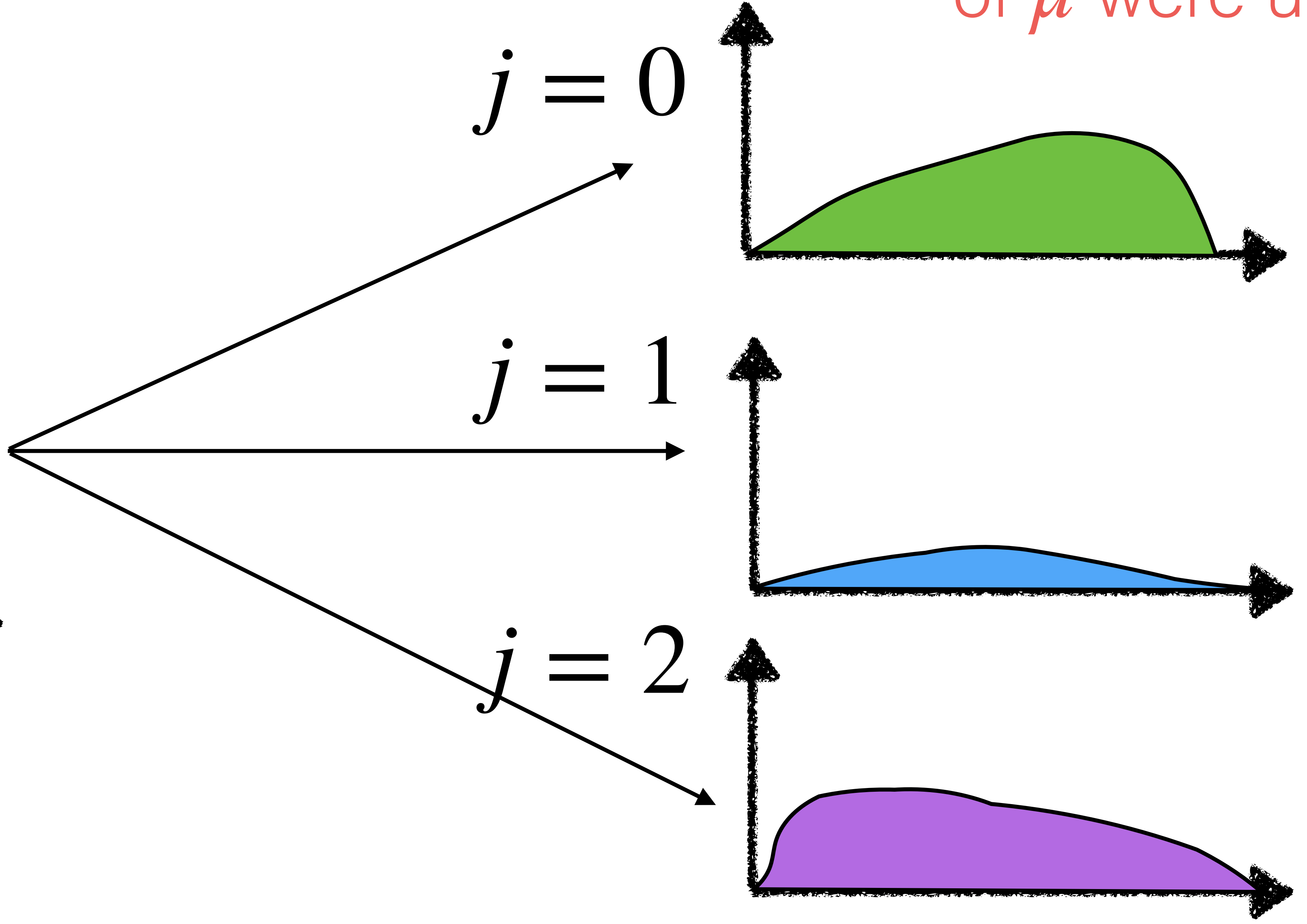


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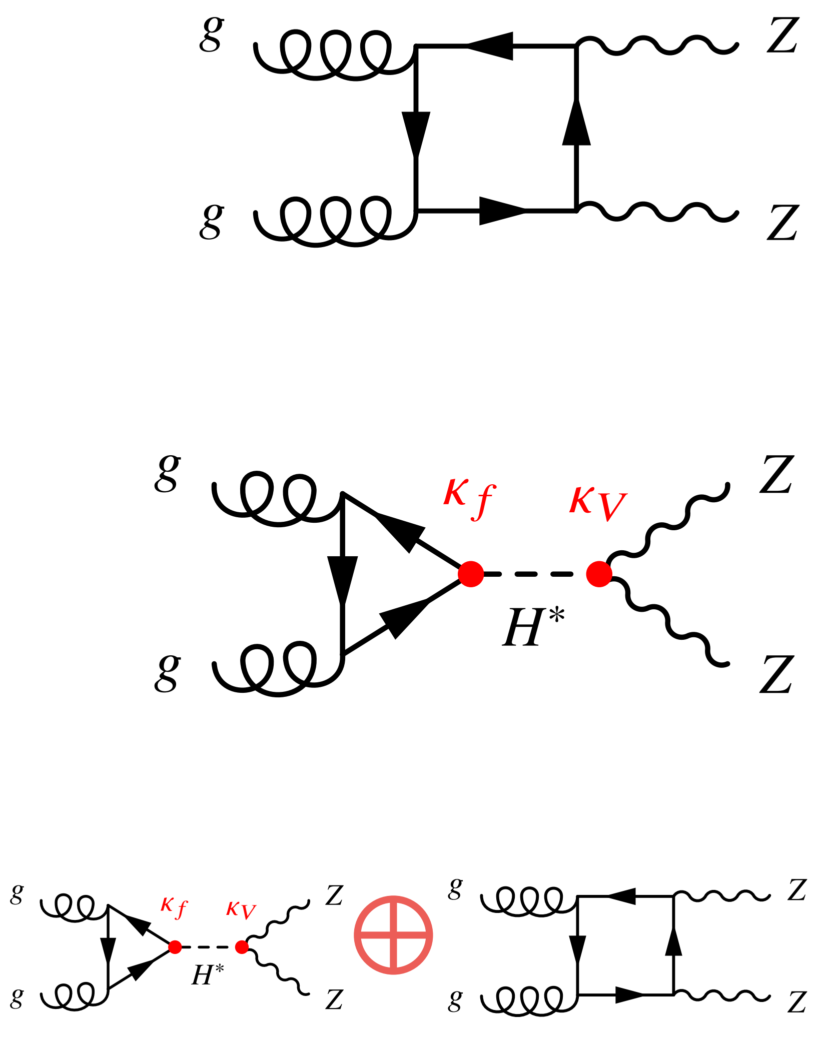


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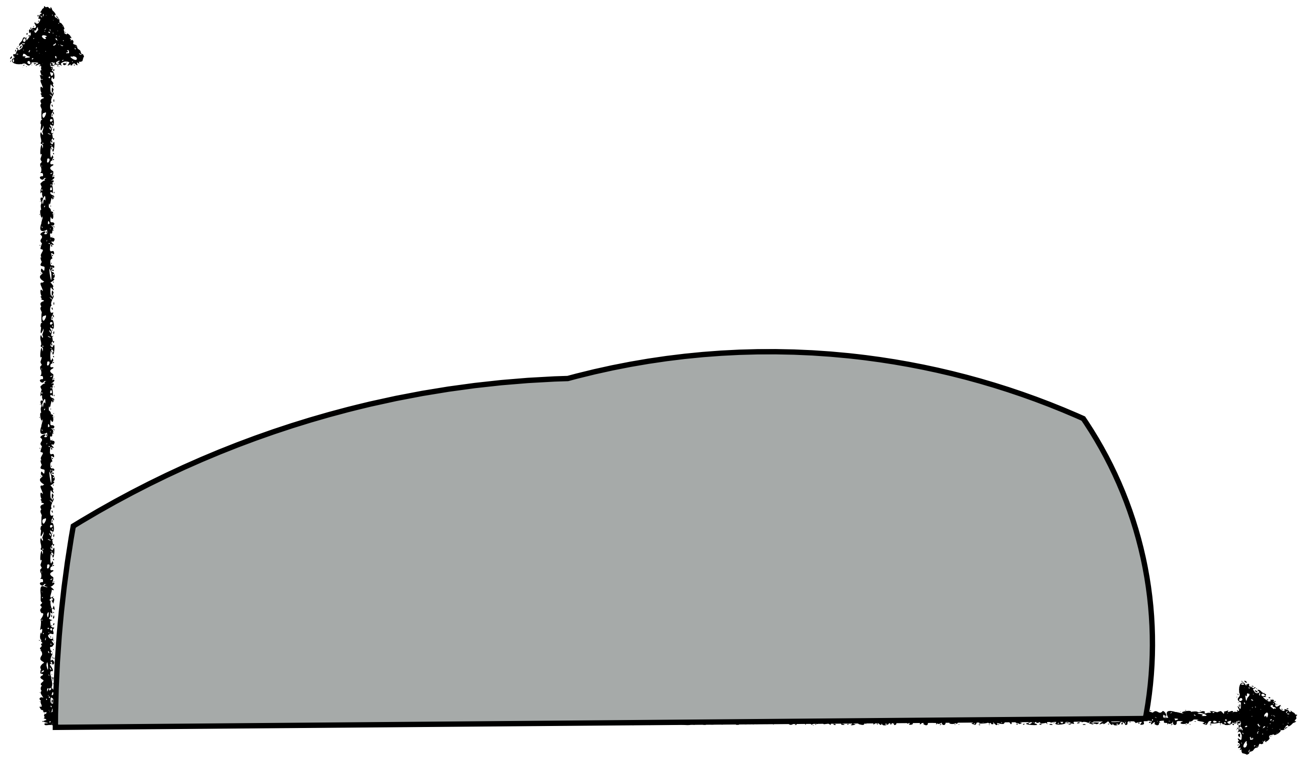

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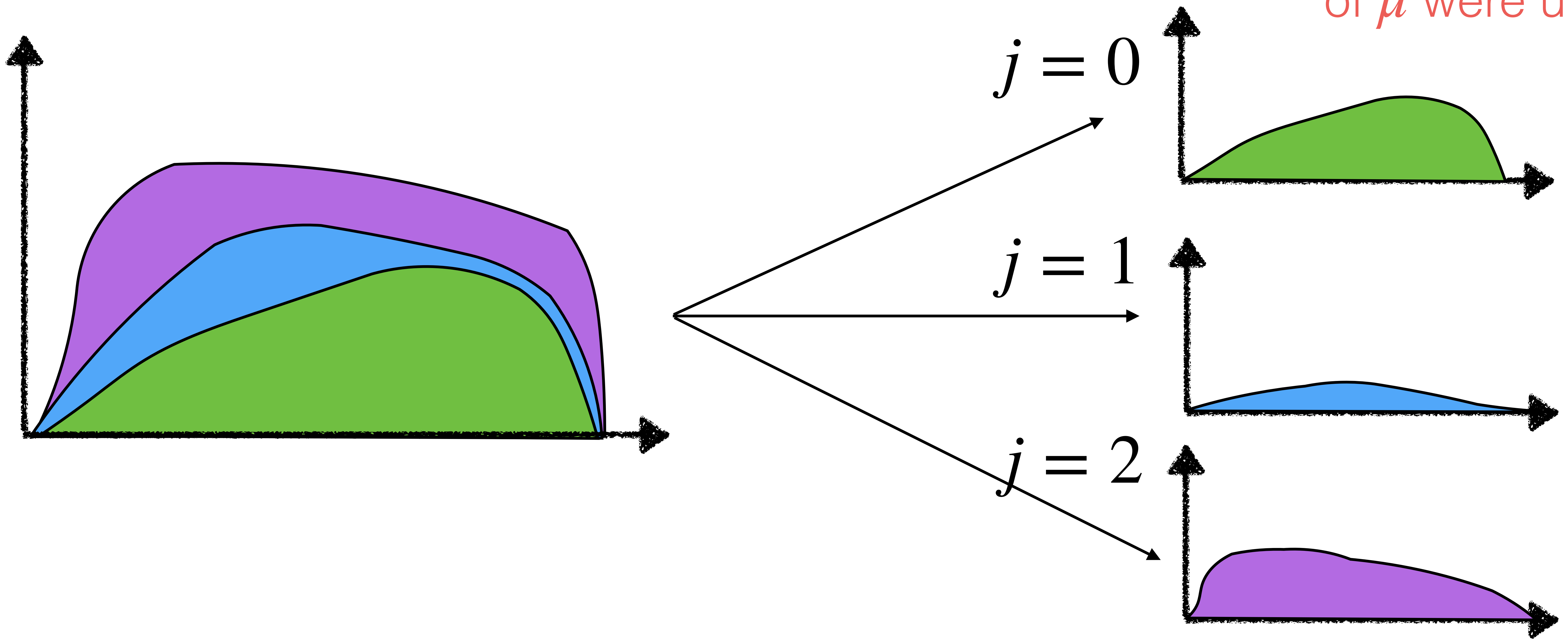


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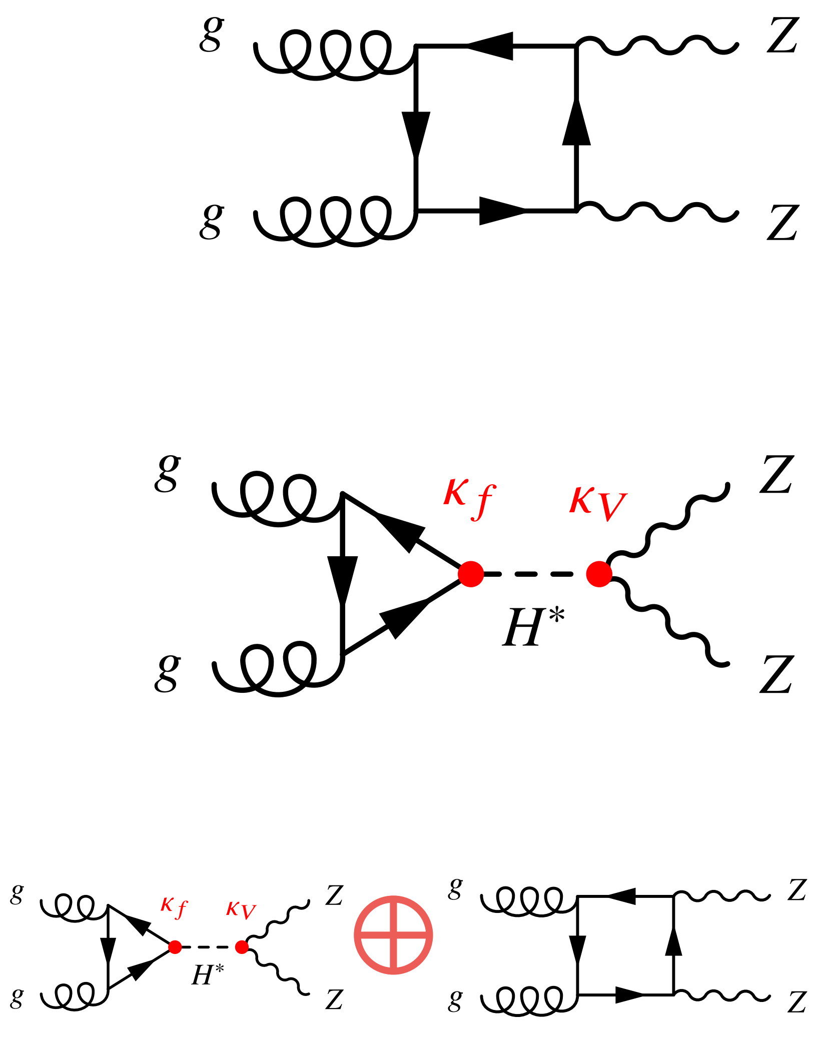


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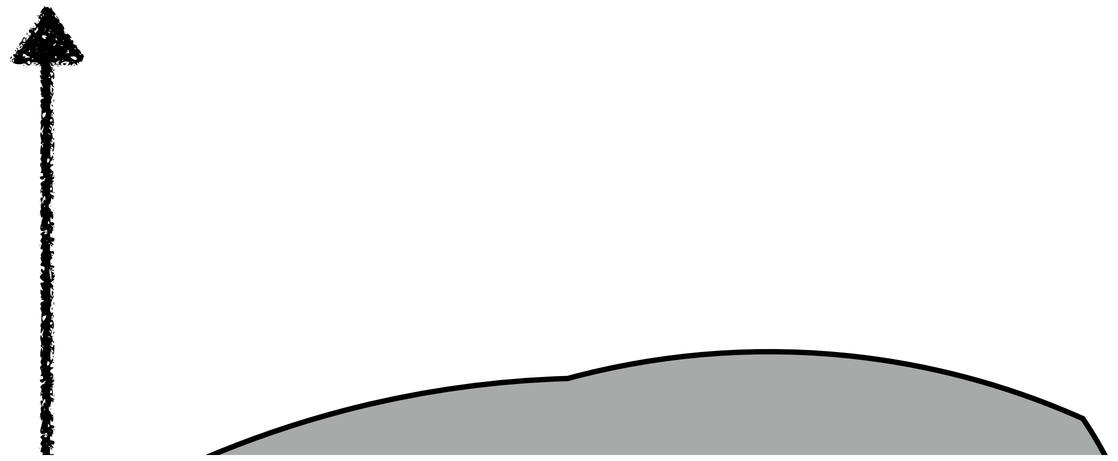

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F
h

**Analytically parameterised in $\mu$**, allows to get LR for any hypothesis $\mu$ without training parameterised networks !

A separate classifier per physics process j
(Eg. $gg \to H^* \to 4l$, $gg \to ZZ \to 4l$)

# Reference Sample

A combination of signal samples, to ensure there's non-vanishing support in pre-selected region

$$p_{\text{ref}}(x_i) = \frac{1}{\sum_k \nu_k} \sum_{k}^{C_{\text{signals}}} \nu_k \cdot p_k(x_i)$$

⇒ In our dataset, $p_{ref}(\cdot) = p_S(\cdot)$

Choice of $p_{ref}(\cdot)$ can be made purely on numerical stability of training,
as it drops out from the likelihood ratio

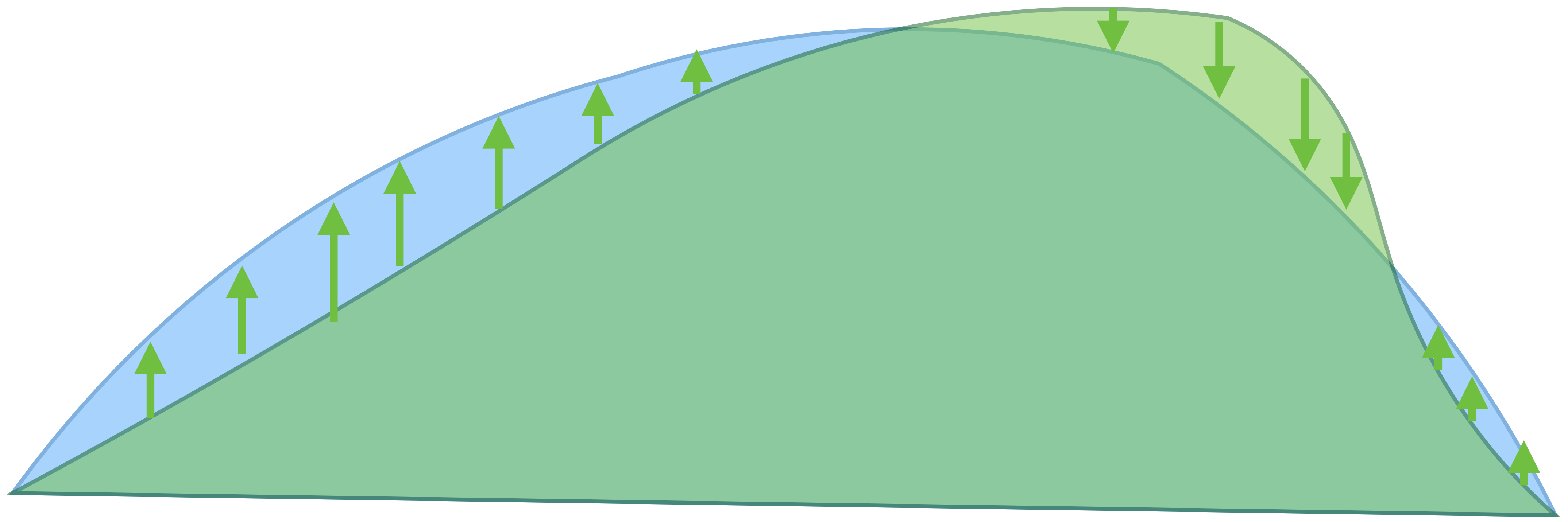
$$t_\mu = -2\ln\left(\frac{L_{\text{full}}(\mu, \hat{\hat{\alpha}})/\cancel{L_{\text{ref}}}}{L_{\text{full}}(\hat{\mu}, \hat{\alpha})/\cancel{L_{\text{ref}}}}\right)$$

# Validate quality of LR estimation with re-weighting task

Reweighting: Calculate weights $w_i$ for events $x_i$ in green sample to match blue sample

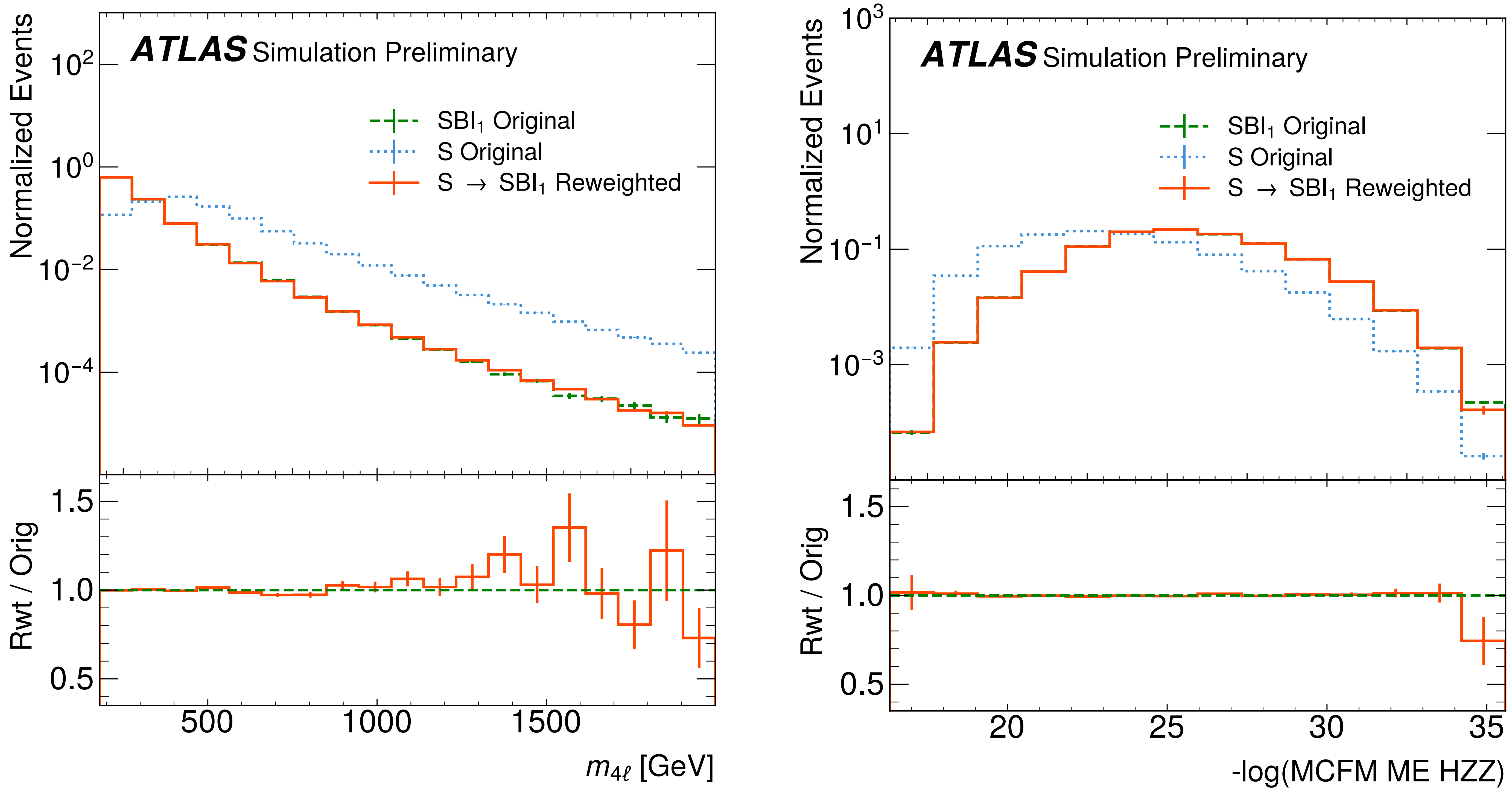
$$w_i = r_j(x_i) = \frac{p_j(x_i)}{p_{ref}(x_i)}$$

Already estimated using an ensemble of networks



# Re-weight closures

Source
Target
RW




$m_{4l}$

Matrix-Element-based Observable (ggF from MCFM)

**High-Dim Classifier Test:**
Train independent classifier on RW vs Target, AUC=0.5 ⇒ LRs well estimated

See additional closure tests

Open problems to extend to full ATLAS analysis:

- ✓ Robustness: Design and validation
- ‣ Systematic Uncertainties: Incorporate them into likelihood (ratio) model
- • Neyman Construction: Sampling pseudo-experiments in a per-event analysis

# Systematic uncertainties

## Experimental uncertainties:

Eg. Inaccuracies in the calibration of our detector

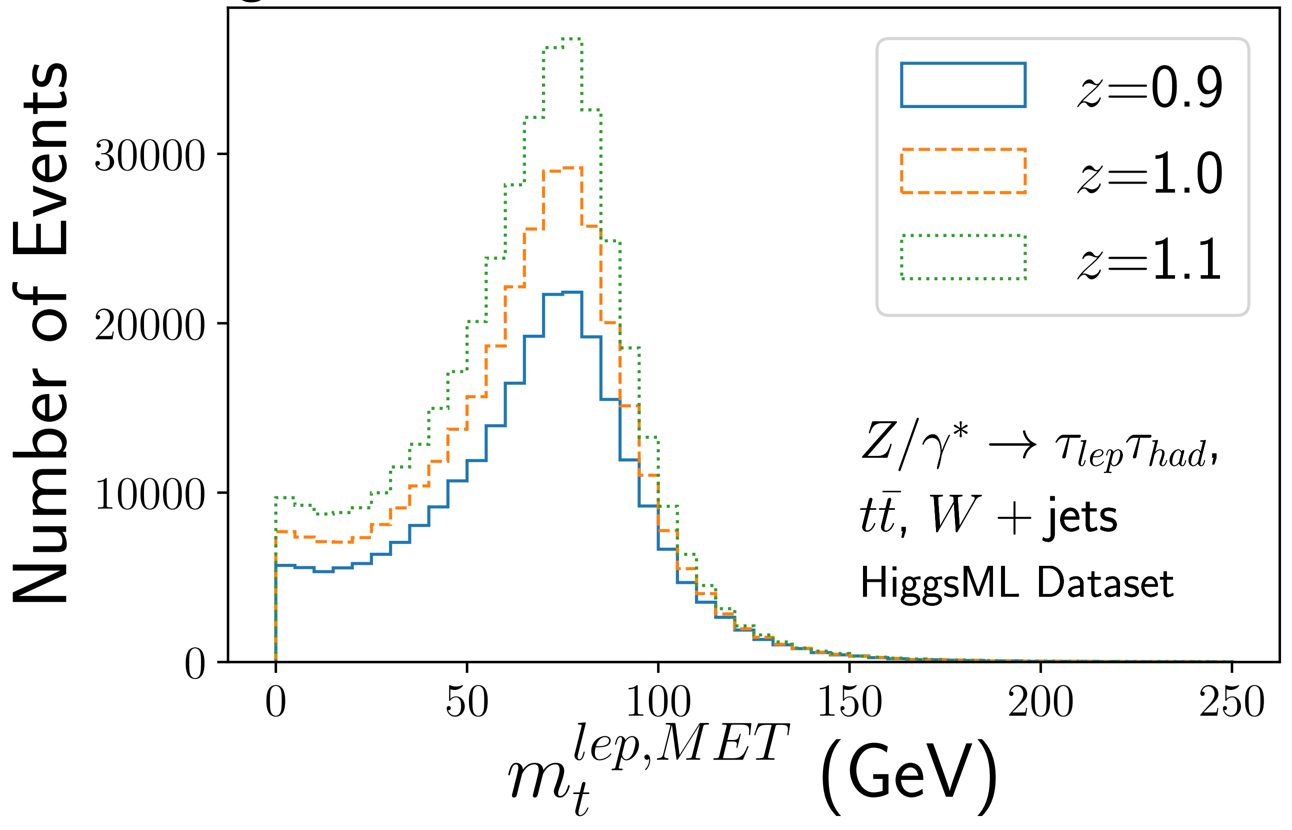



Image: arXiv:2105.08742

## Theory uncertainties:

Eg. Inability to compute QFT to infinite order

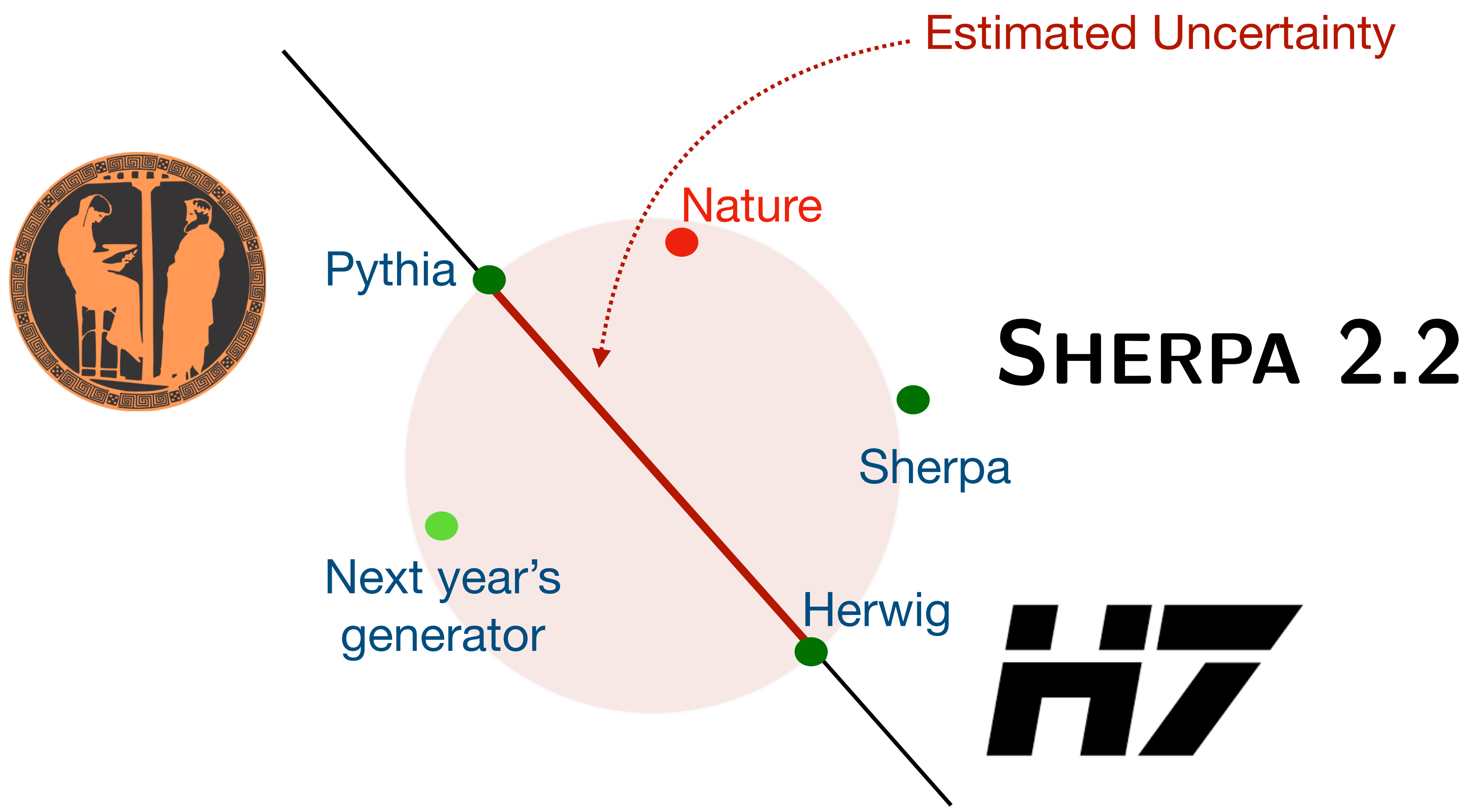



Image: arXiv:2109.08159

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Theory uncertainties:
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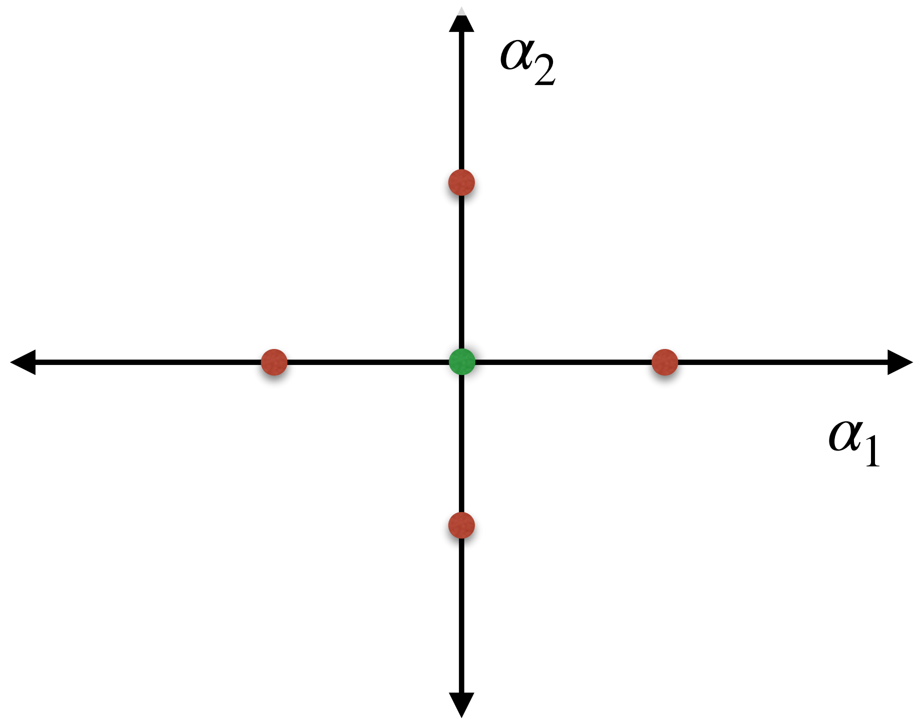
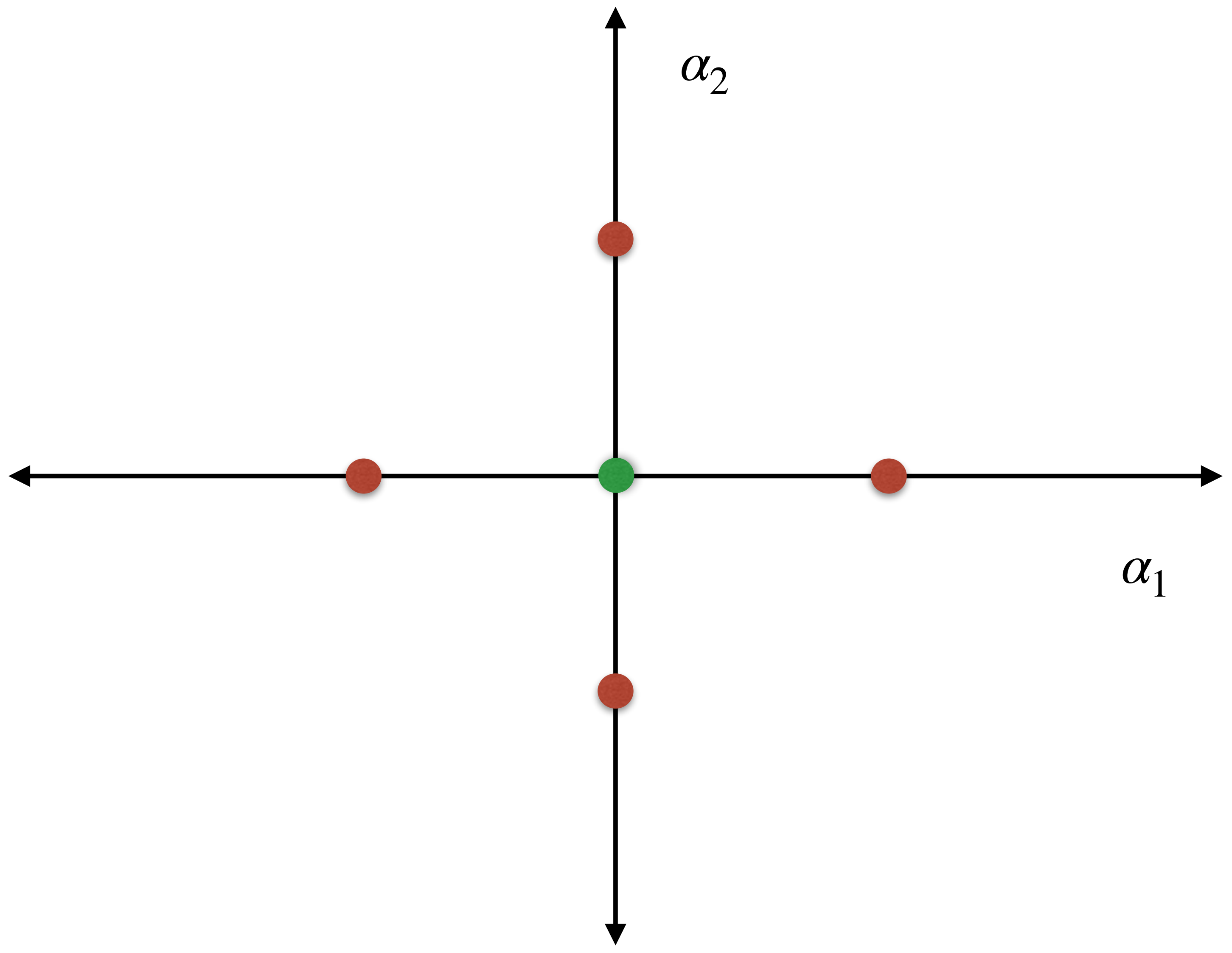
- We only have simulations at 3 variations of each nuisance parameter $\alpha_k$



# Known interpolation strategies

See formula used

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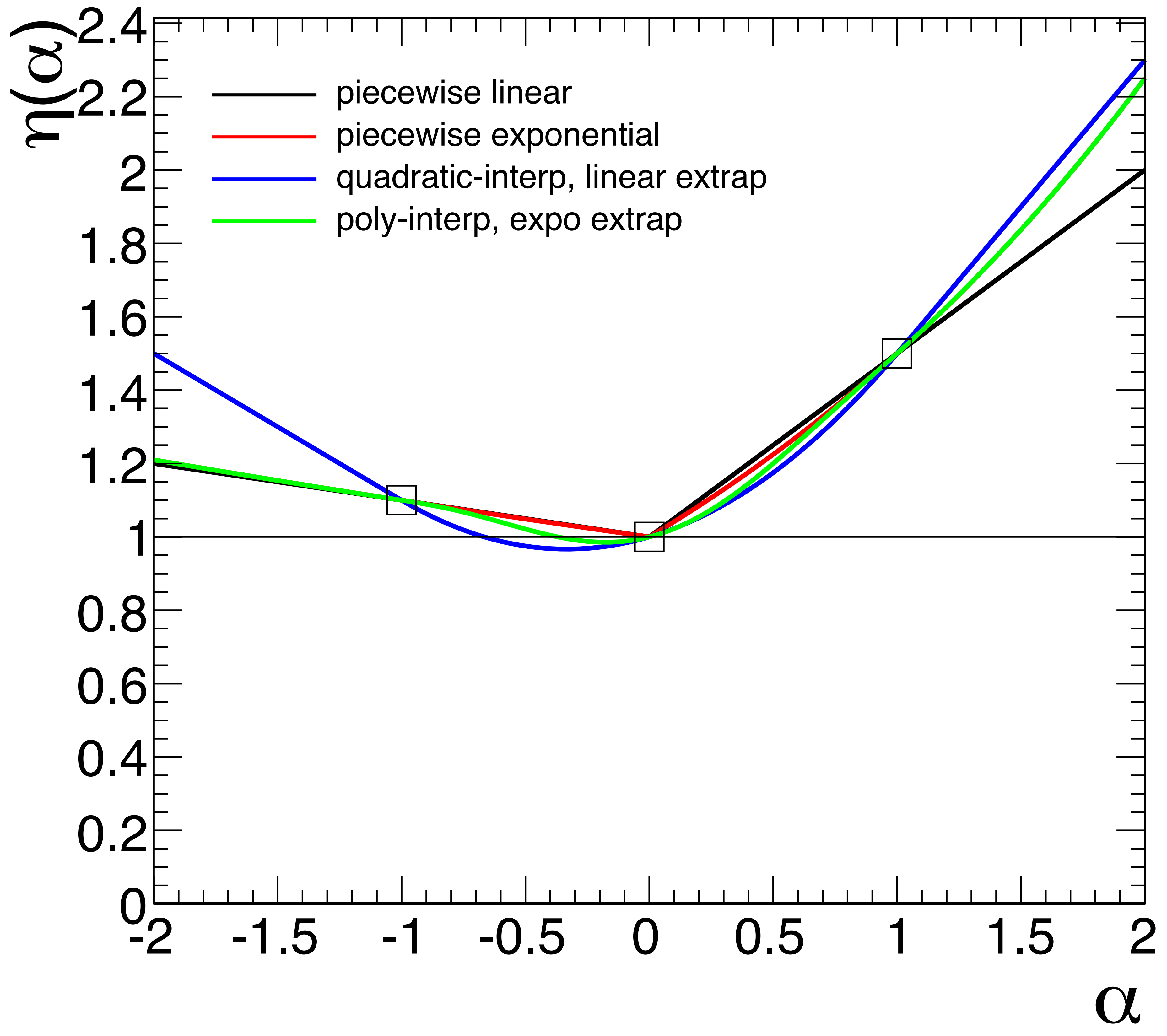
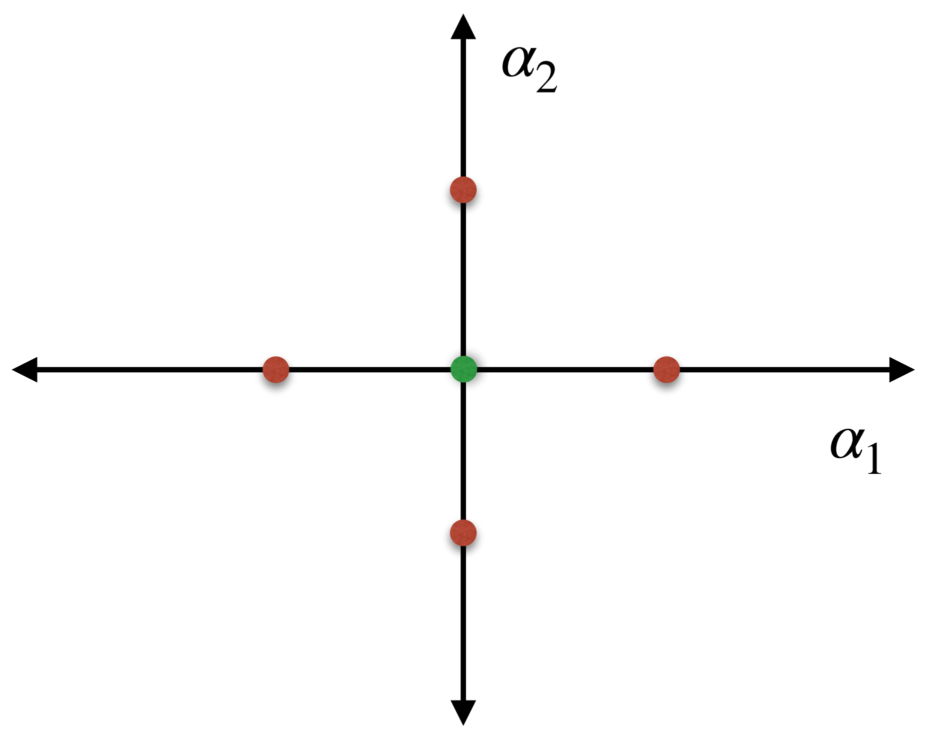



⇒ Combine these traditional interpolation with neural network estimation of per-event likelihood ratios

# Probability density ratio including nuisance parameters ($\alpha$)

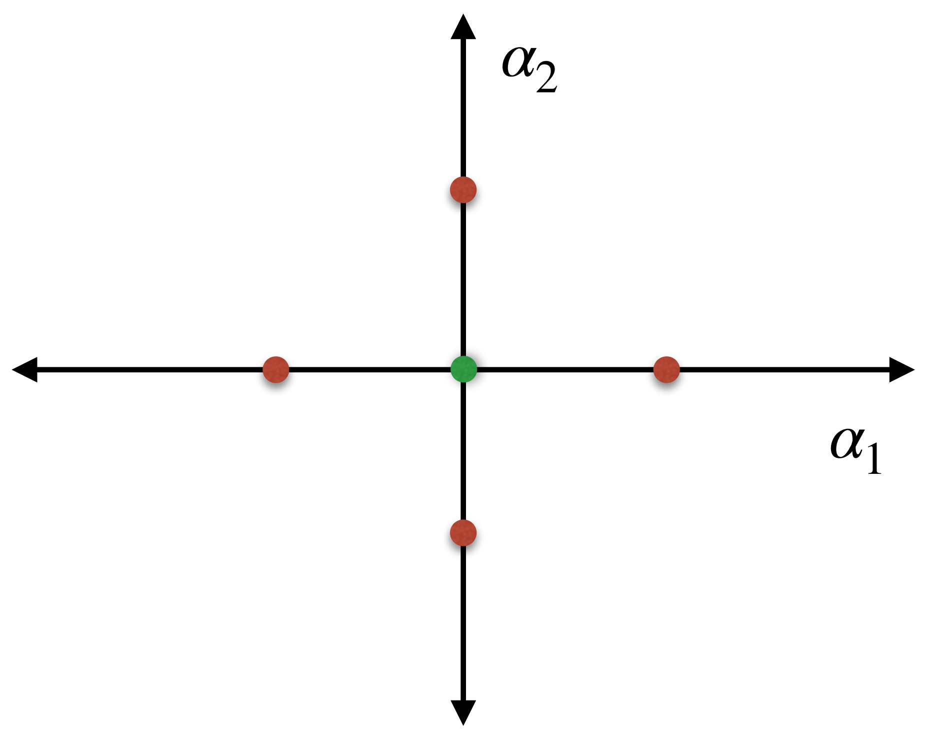
$$\frac{p(x_i \mid \mu, \alpha)}{p_{ref}(x_i)} =$$




See details of vertical interpolation for $G_j(\alpha_k)$, $g_j(x_i, \alpha_k)$

# Probability density ratio including nuisance parameters ($\alpha$)

$$\frac{p(x_i | \mu, \alpha)}{p_{ref}(x_i)} = \frac{1}{\nu(\mu, \alpha)} \sum_j^C f_j(\mu) \cdot \nu_j \cdot \frac{p_j(x_i)}{p_{ref}(x_i)} \cdot \prod_k^{N_{syst}} G_j(\alpha_k) \cdot g_j(x_i, \alpha_k)$$




$$g_j(x_i, \alpha_k) = \frac{p_j(x_i, \alpha_k)}{p_j(x_i)}$$

See details of vertical interpolation for $G_j(\alpha_k)$, $g_j(x_i, \alpha_k)$

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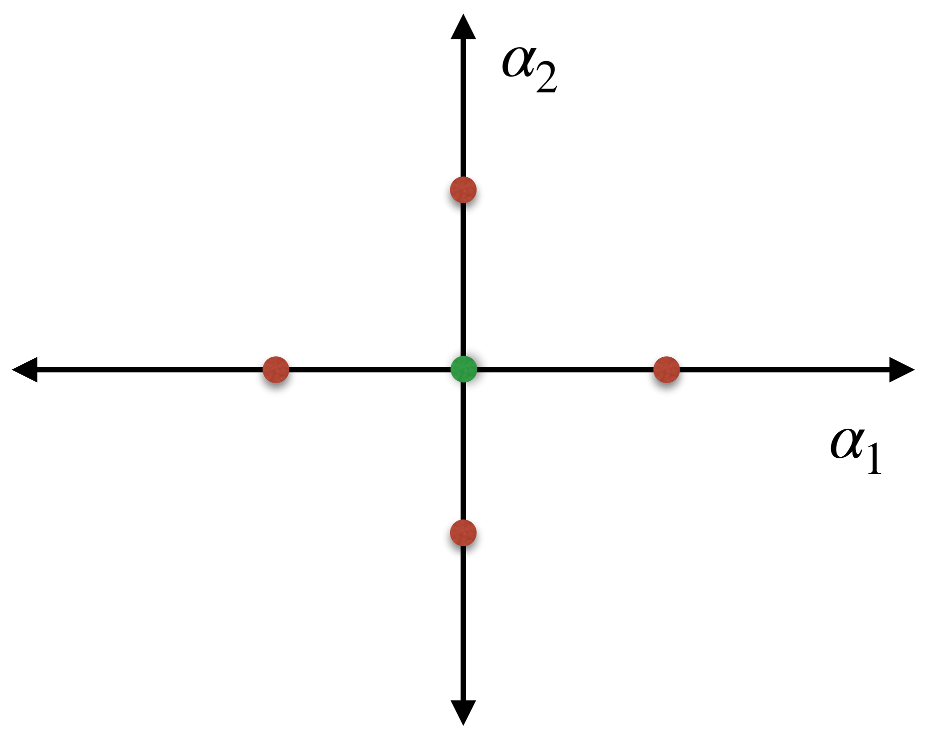
We have this already

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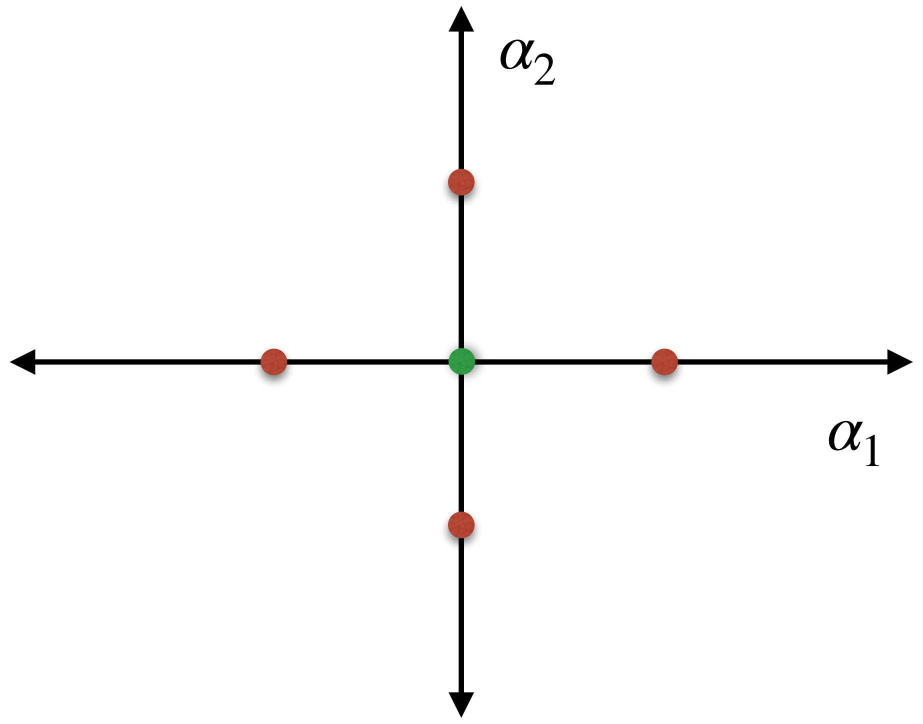
We have this already

Estimate from simulations and existing interpolation methods

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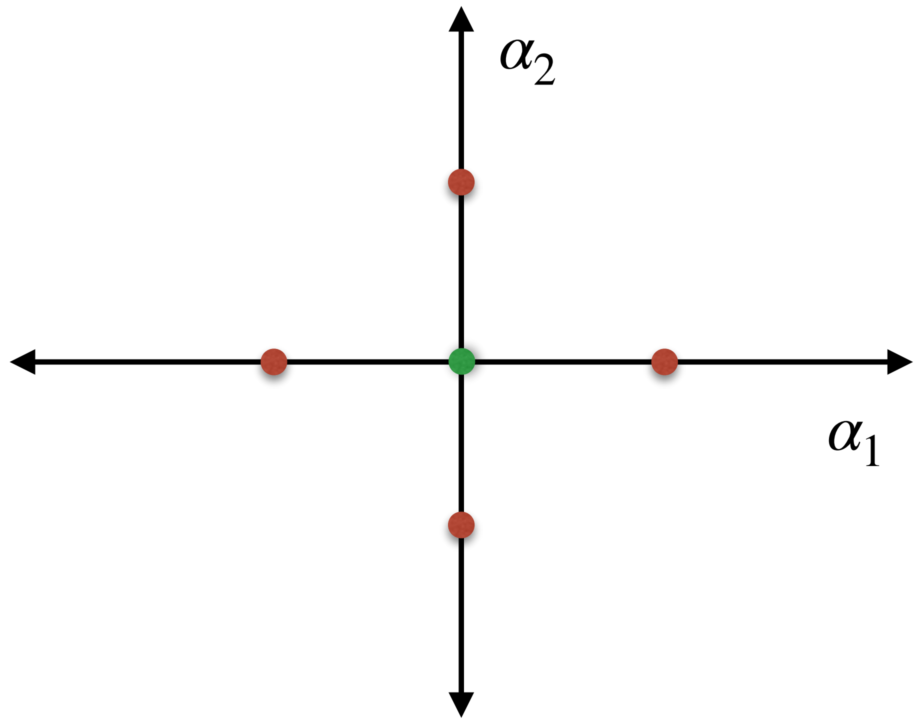
We have this already

Estimated using another ensemble of networks and interpolation methods

Estimate from simulations and existing interpolation methods

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See details of vertical interpolation for $G_j(\alpha_k)$, $g_j(x_i,\alpha_k)$

# Final test statistic

$$\frac{L_{\text{full}}(\mu, \alpha | \mathcal{D})}{L_{\text{ref}}(\mathcal{D})} = \text{Pois}(N_{\text{data}} | \nu(\mu, \alpha)) \prod_{i}^{N_{\text{data}}} \frac{p(x_i | \mu, \alpha)}{p_{\text{ref}}(x_i)} \prod_{k} \text{Gaus}(a_k | \alpha_k, \delta_k)$$

# Final test statistic

From previous slide

$$\frac{L_{\text{full}}(\mu, \alpha|\mathcal{D})}{L_{\text{ref}}(\mathcal{D})} = \text{Pois}(N_{\text{data}}|\nu(\mu, \alpha)) \prod_{i}^{N_{\text{data}}} \frac{p(x_i|\mu, \alpha)}{p_{\text{ref}}(x_i)} \prod_{k} \text{Gaus}(a_k|\alpha_k, \delta_k)$$

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From previous slide

Prod over events

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Rate term

Prod over events

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From previous slide

Rate term

Prod over events

Constrain term

# Final test statistic

From previous slide

$$\frac{L_{\text{full}}(\mu,\alpha|\mathcal{D})}{L_{\text{ref}}(\mathcal{D})} = \text{Pois}(N_{\text{data}}|\nu(\mu,\alpha)) \prod_{i}^{N_{\text{data}}} \frac{p(x_i|\mu,\alpha)}{p_{\text{ref}}(x_i)} \prod_{k} \text{Gaus}(a_k|\alpha_k,\delta_k)$$

Rate term

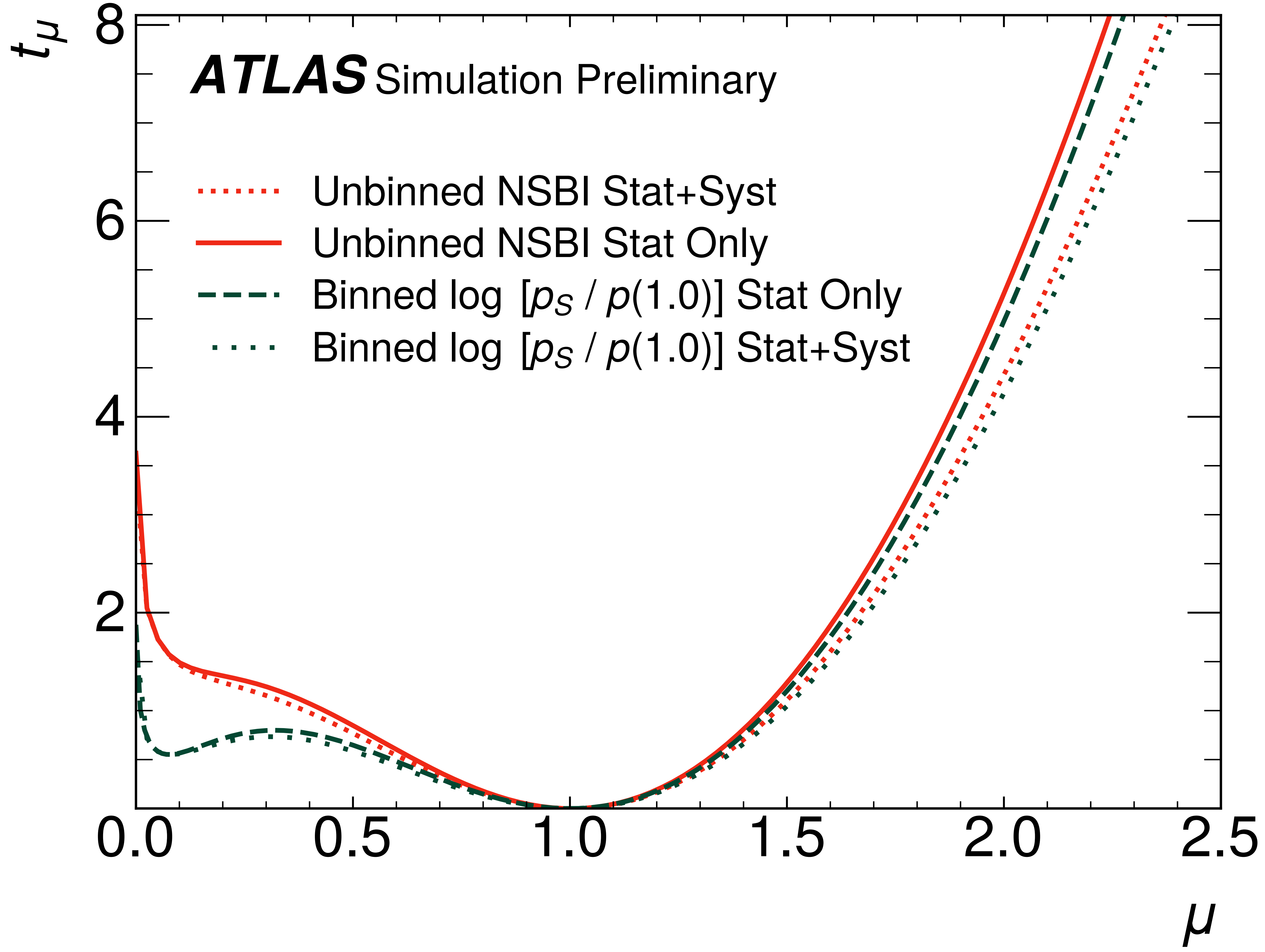
Prod over events

Constrain term

Profiling: $$t_\mu = -2\ln\left(\frac{L_{\text{full}}(\mu,\hat{\hat{\alpha}})/\cancel{L_{\text{ref}}}}{L_{\text{full}}(\hat{\mu},\hat{\alpha})/\cancel{L_{\text{ref}}}}\right)$$

This is why we define $p_{ref}$ to be independent of $\mu$

# Negative Likelihood Ratio result



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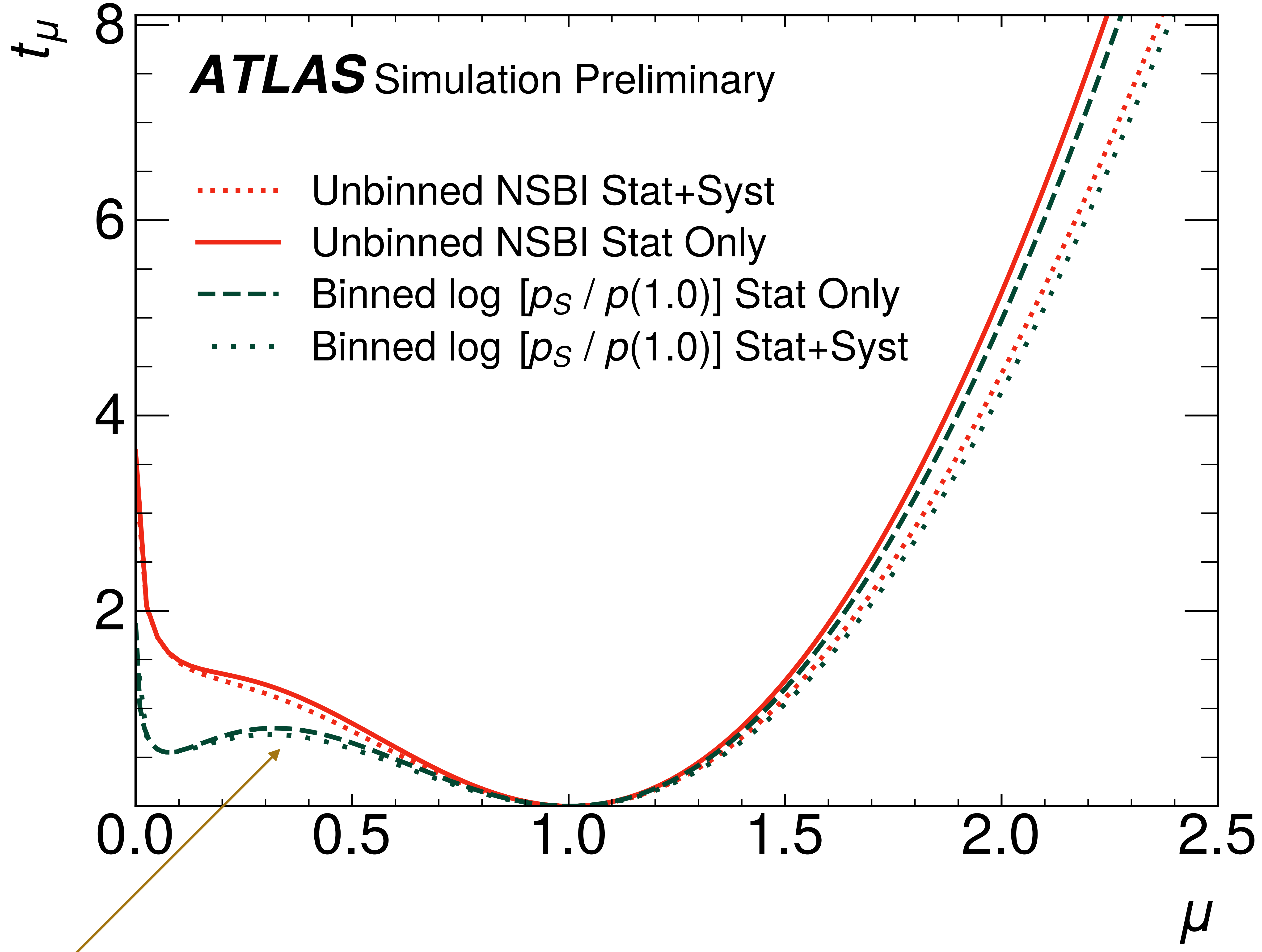


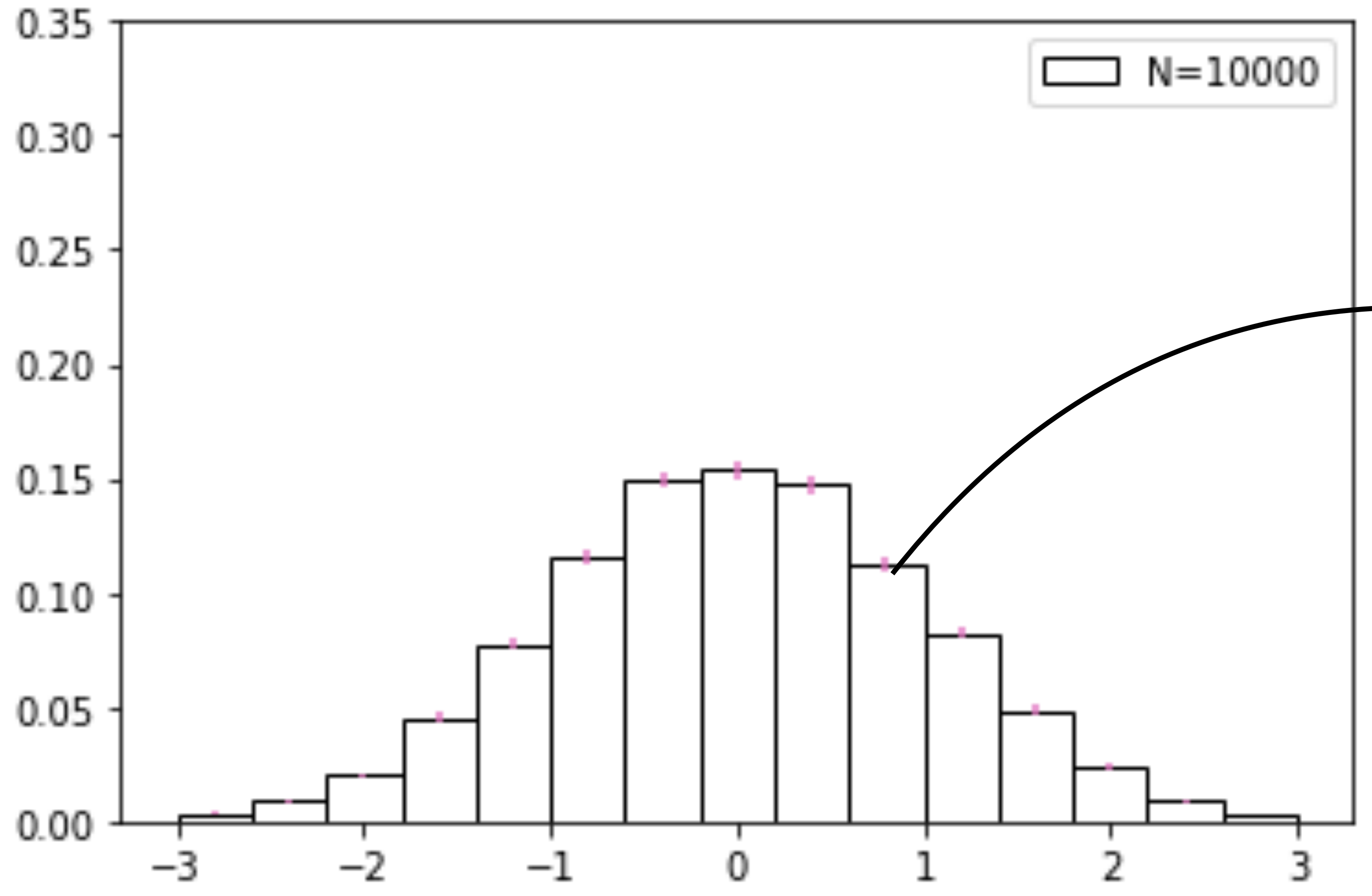

Non-parabolic shape due to non-linear effects from quantum interference

Open problems to extend to full ATLAS analysis:

- ✓ Robustness: Design and validation
- ✓ Systematic Uncertainties: Incorporate them into likelihood (ratio) model
- ‣ Neyman Construction: Sampling pseudo-experiments in a per-event analysis

# Sampling (per-event) pseudo-experiments using bootstrapping

Traditionally:

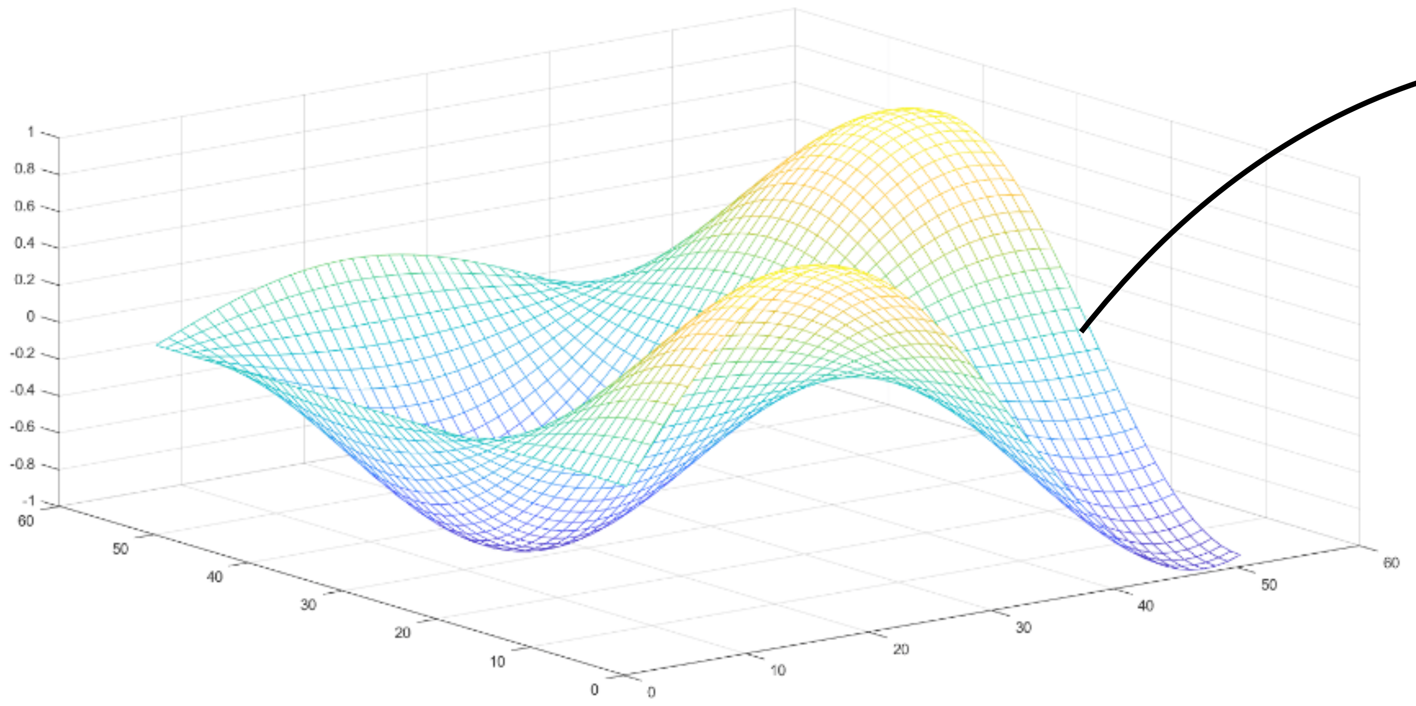



Poisson per bin

Asimov Histogram

$$N_i^{toy} = Poisson(N_i^{Asimov})$$

NSBI:



Poisson per event

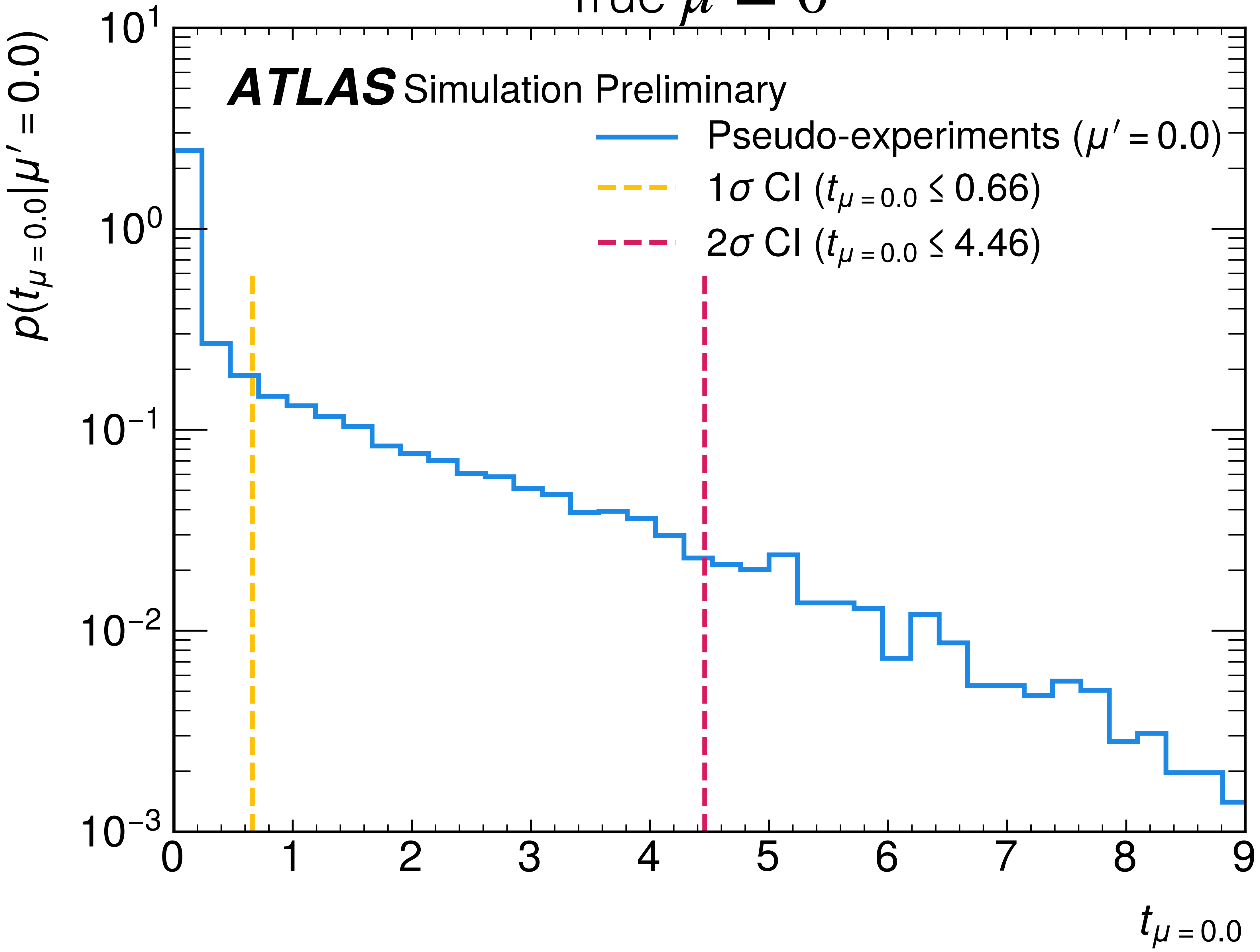
$$w_i^{toy} = Poisson(w_i^{Asimov})$$

('Unweighted' events, i.e. integer weights)

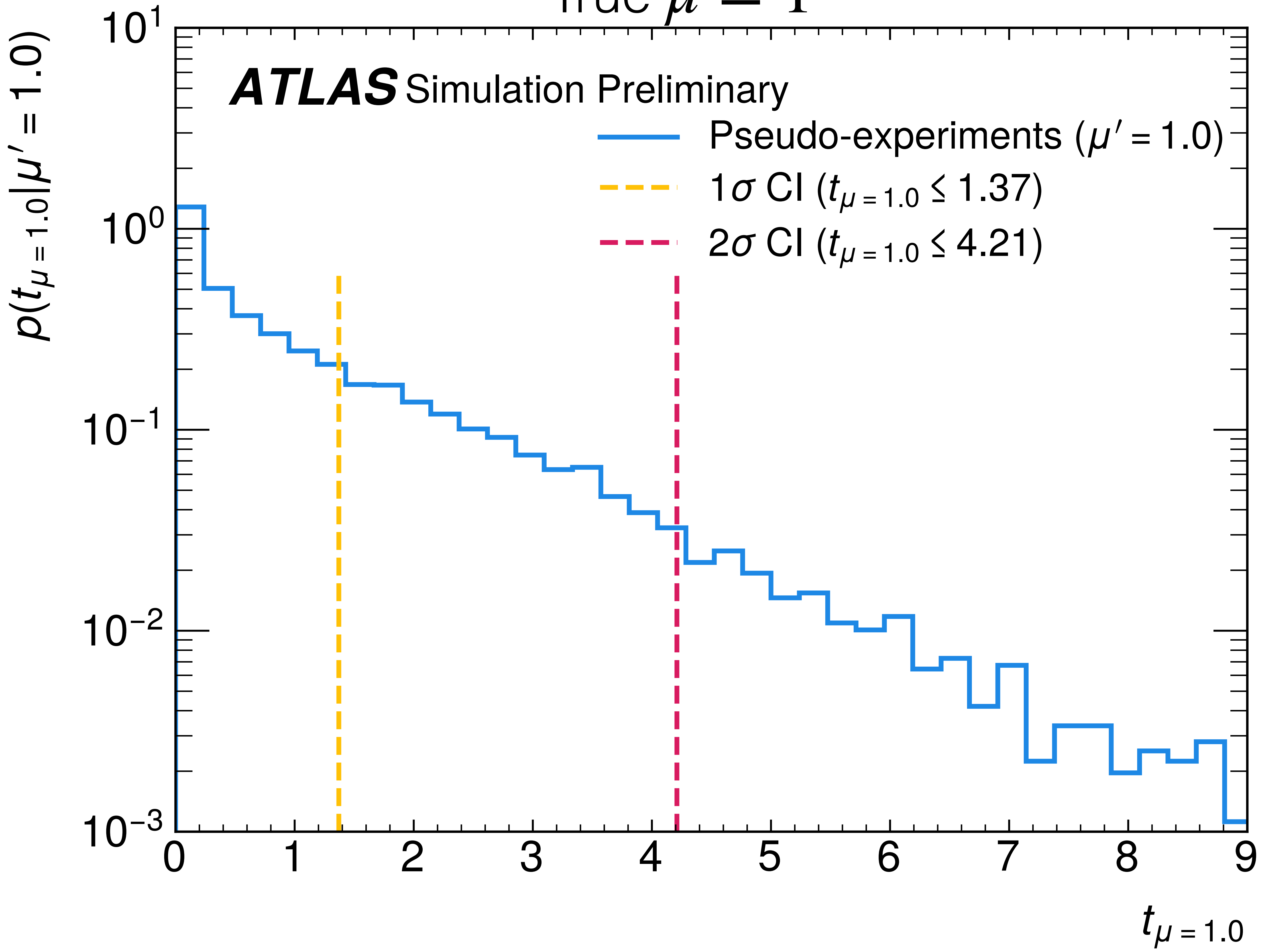
# Neyman Construction

- For each hypothesis:
  - Generate pseudo-experiments using bootstrapping
  - Compute the test statistic at the value of the considered hypothesis
  - Integrate up to 68.27% (95.45%) to determine $1\sigma$ ($2\sigma$) CI as a function of the parameter of interest

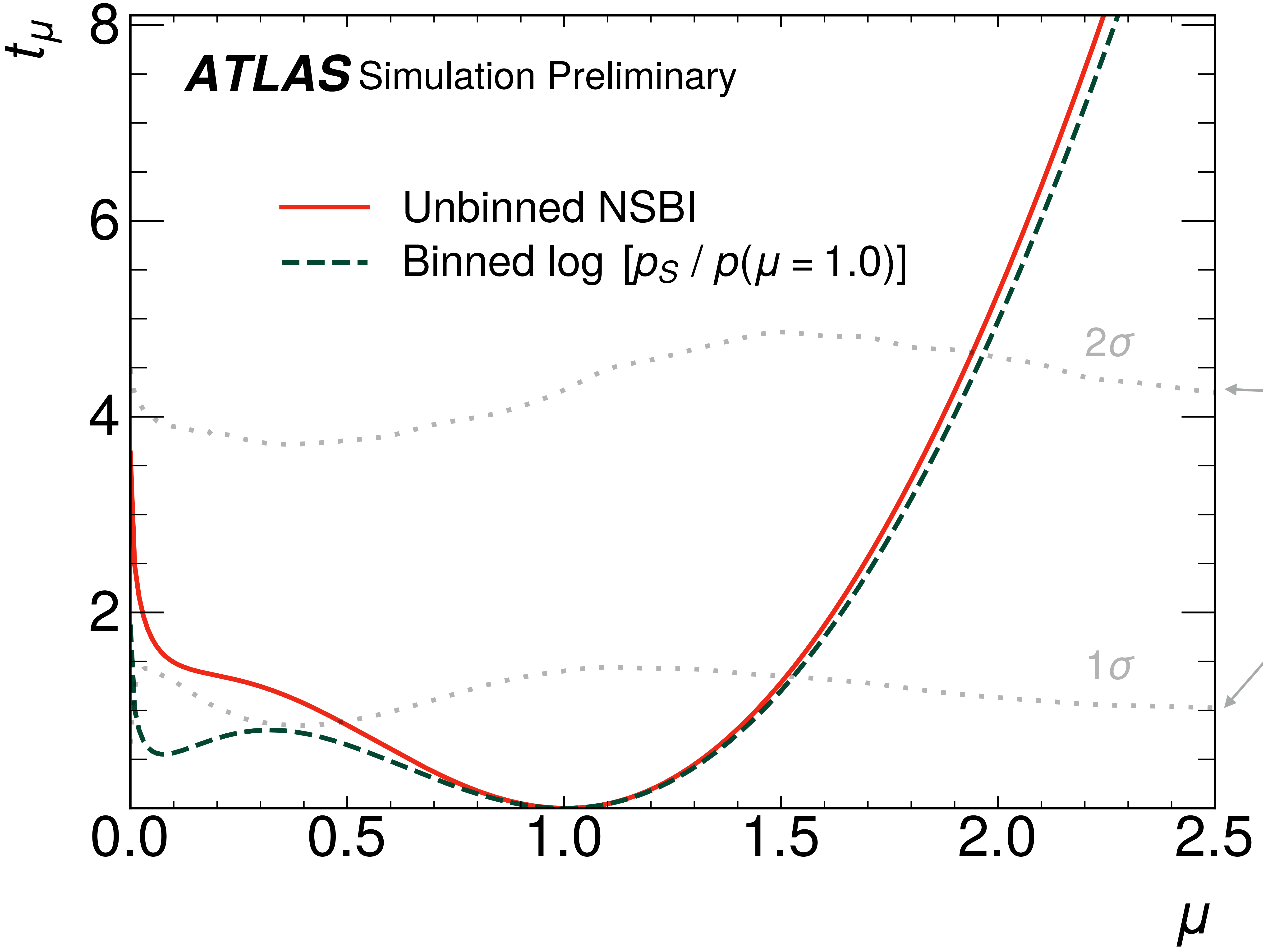
True $\mu = 0$




True $\mu = 1$



# Confidence belts




Similar to structure seen in histogram analysis

Why does NSBI work better than traditional analyses?

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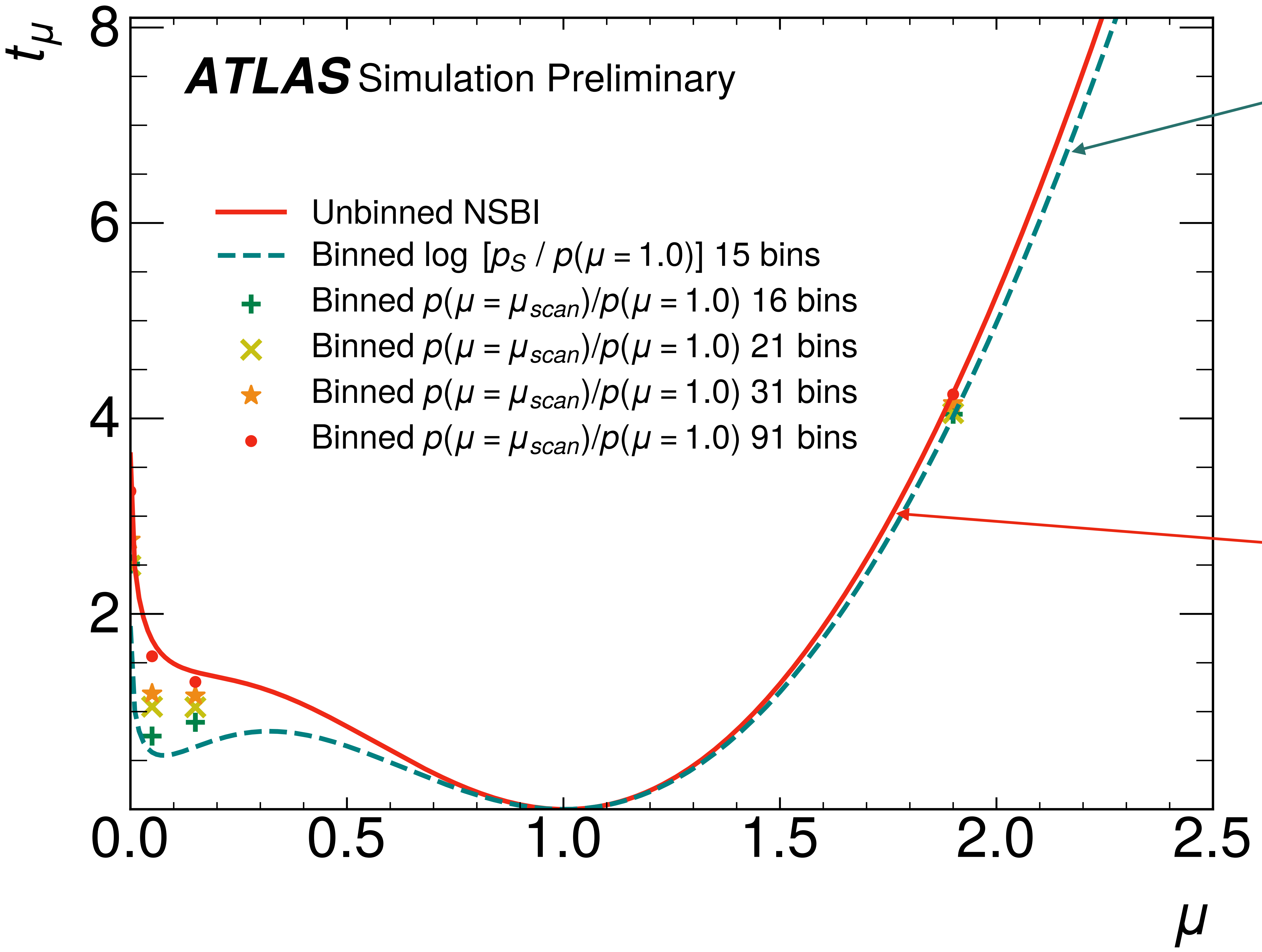
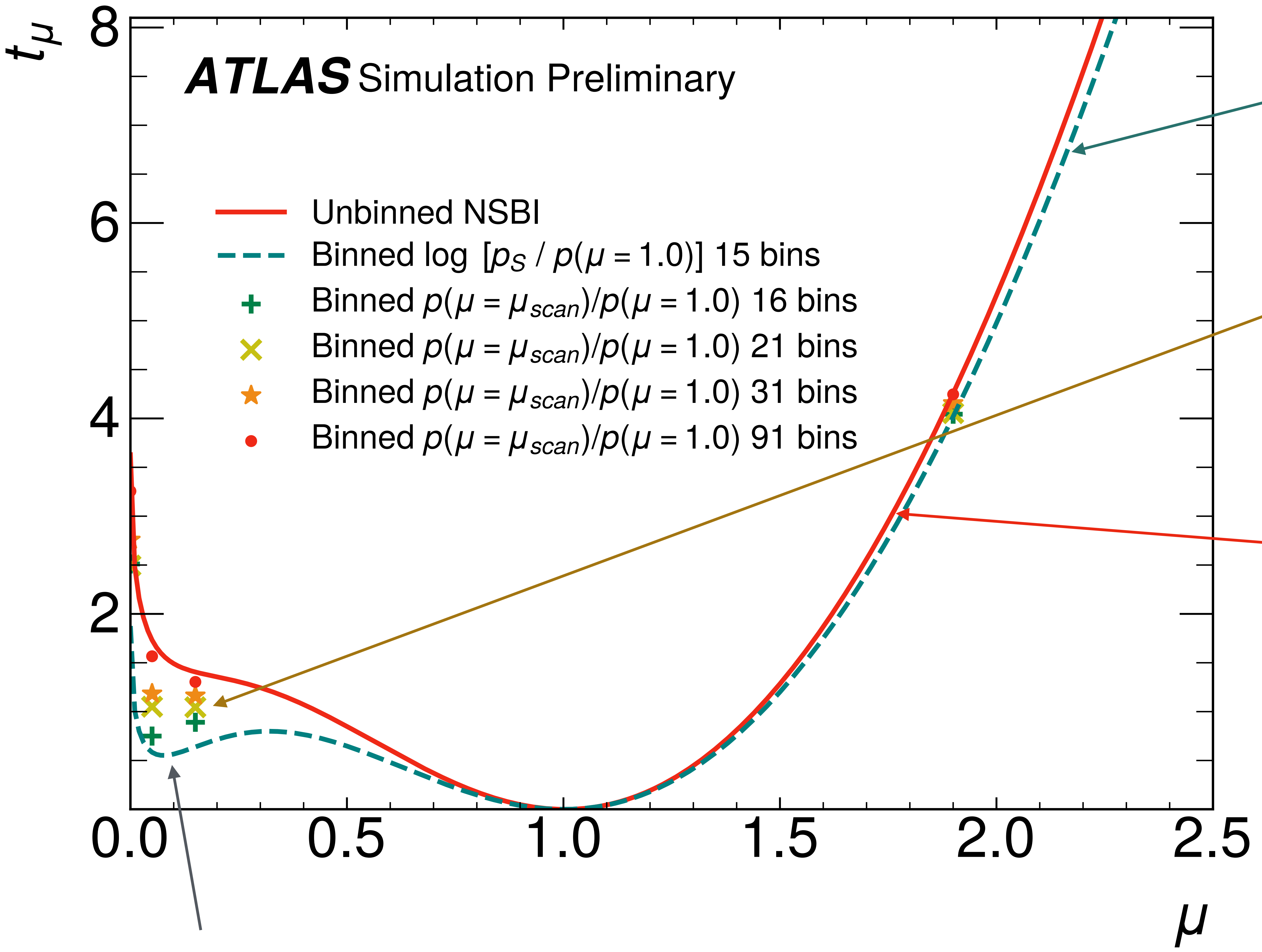



$O_{\text{fixed}} = \log \frac{p_S(x_i)}{p_{SBI}(x_i)}$: Similar to histogram analysis

NSBI: Parameterised, unbinned

# Why does it work better than traditional analyses?

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$O_\mu = \frac{p(x_i|\mu)}{p(x_i|\mu = 1)}$: Parameterised observable, histogram fit

NSBI: Parameterised, unbinned

Significant improvement in quantum interference impacted region

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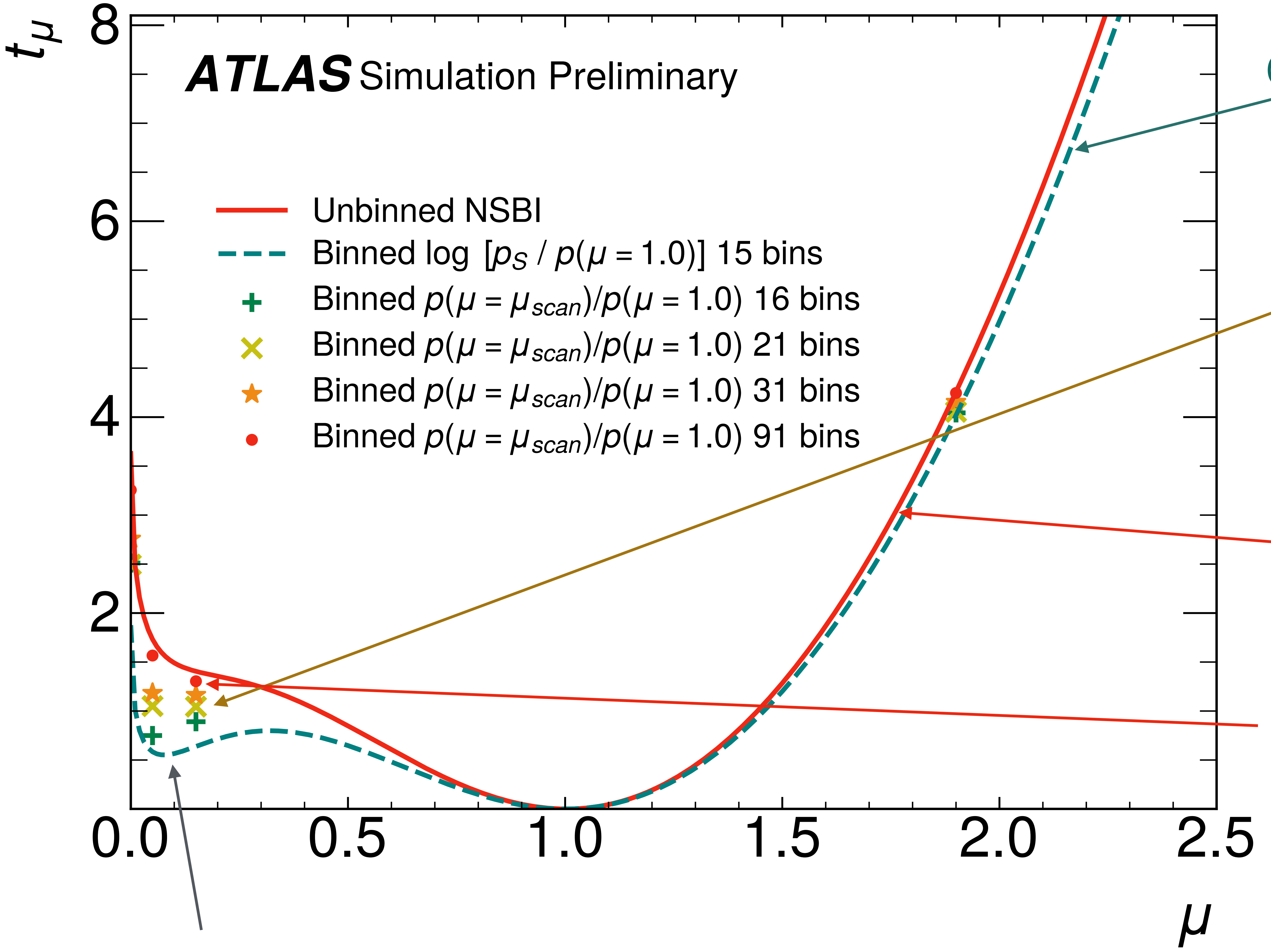


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$O_\mu = \frac{p(x_i \mid \mu)}{p(x_i \mid \mu = 1)}$: Parameterised observable, histogram fit

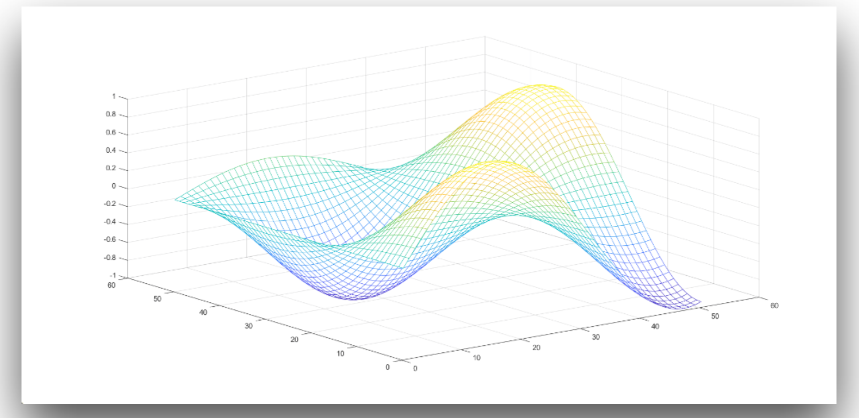
NSBI: Parameterised, unbinned

$O_\mu$ approaches NSBI as nBins $\to \infty$

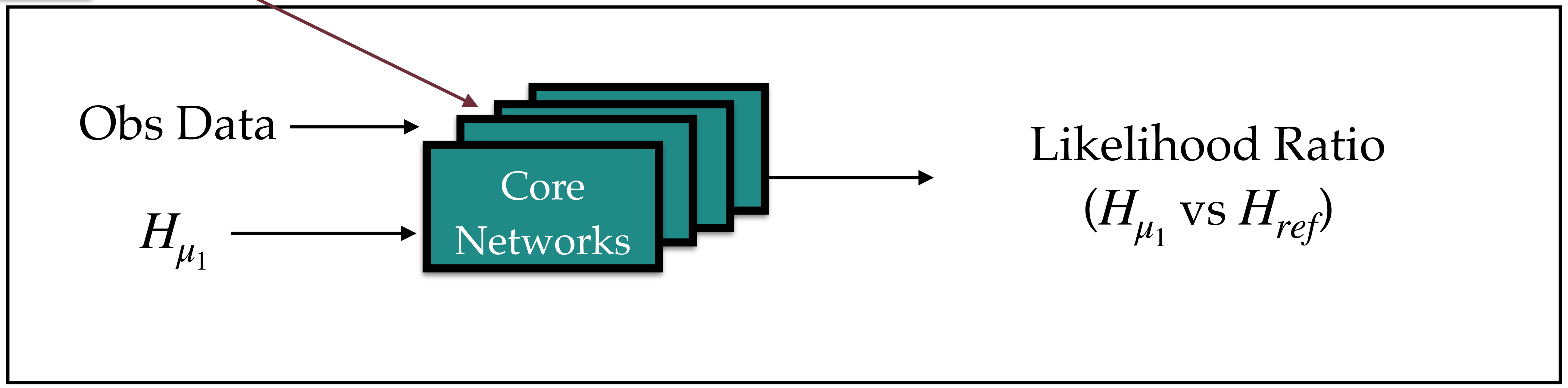
Significant improvement in quantum interference impacted region

# Big picture of the implementation of NSBI for Parameter Estimation in ATLAS

Ensemble; Statistical uncertainty on density ratios



$O(16)$ observables



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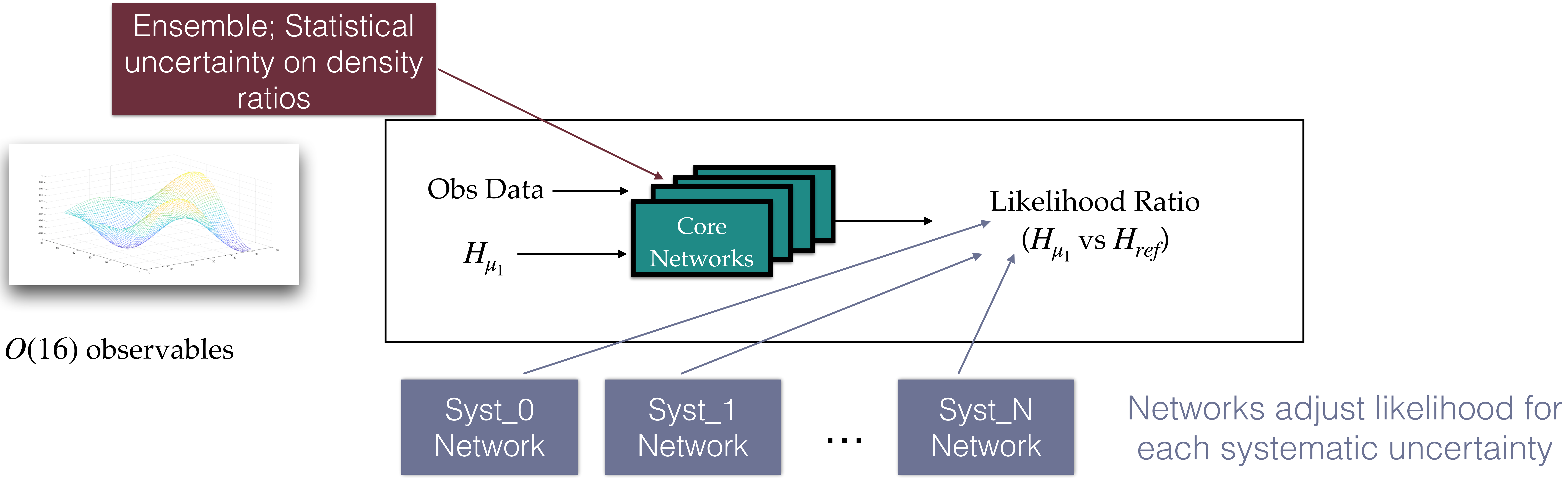
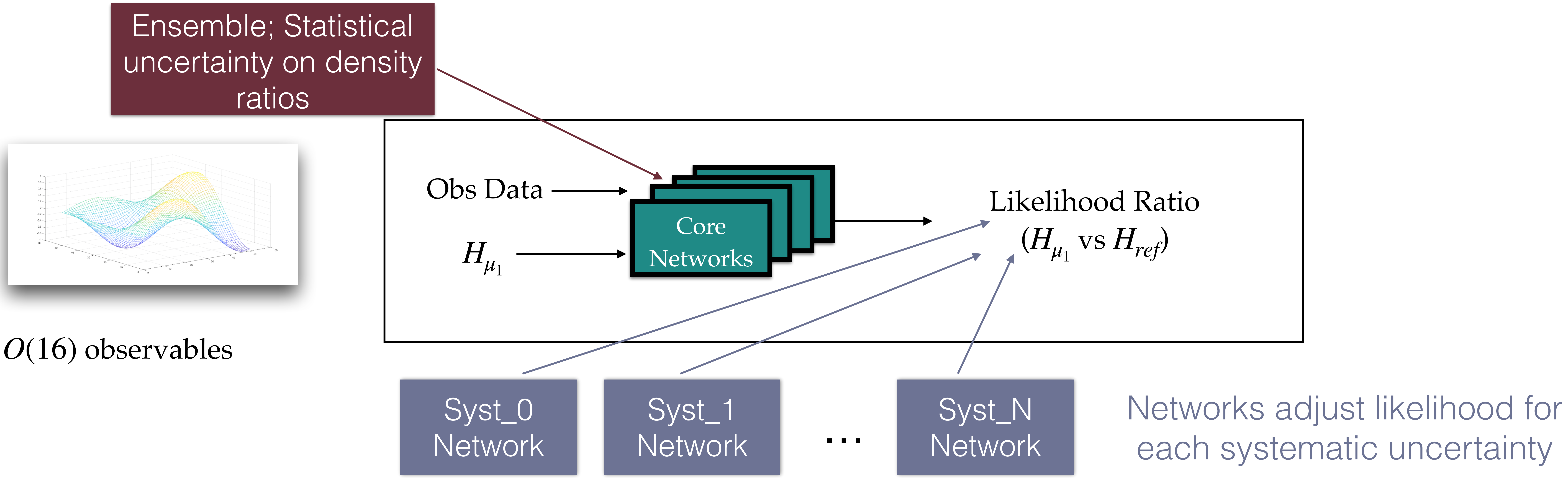


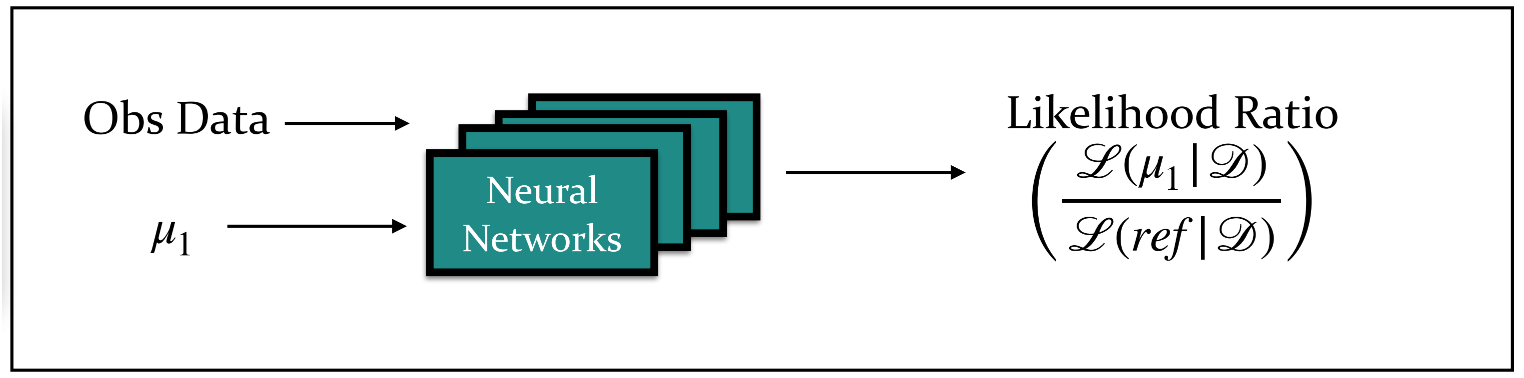
# Big picture of the implementation of NSBI for Parameter Estimation in ATLAS

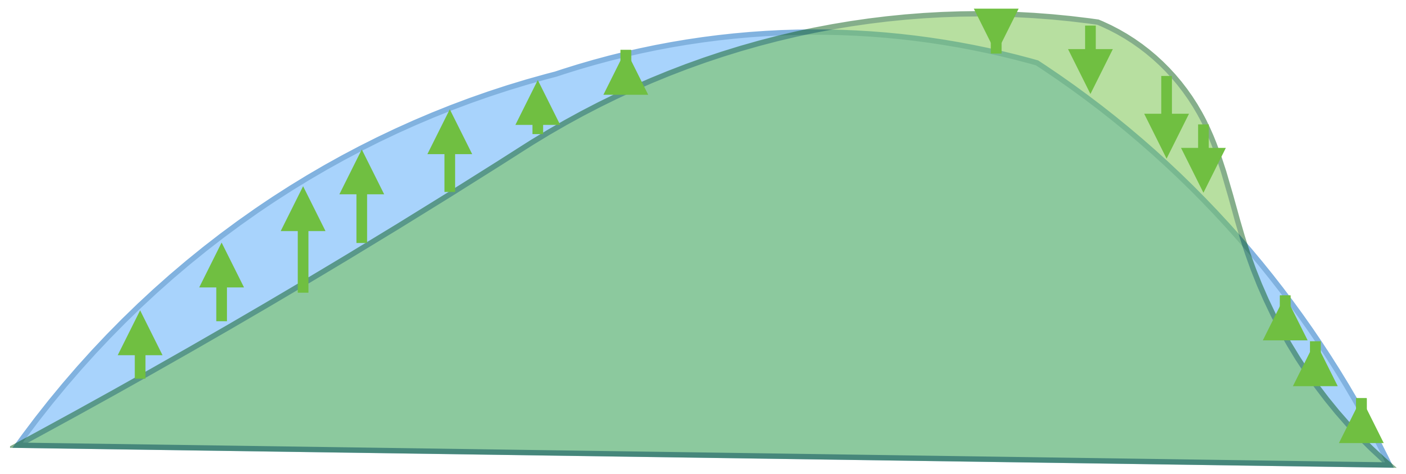



- ✦ Train $O(10^3)$ networks on TensorFlow
- ✦ **Computing resources provided by Google, SMU,** other HPC clusters
- ✦ Fits with JAX

# Conclusion

- Developed a complete statistical framework for high-dimensional statistical inference
  - Builds upon traditional methodology in ATLAS
  - Developed diagnostic tools for validation
- Such methods are crucial for analyses where kinematic distributions change non-linearly with the parameter of interest, eg. EFT studies
- Weaknesses: Same as traditional analyses, requires well trained networks



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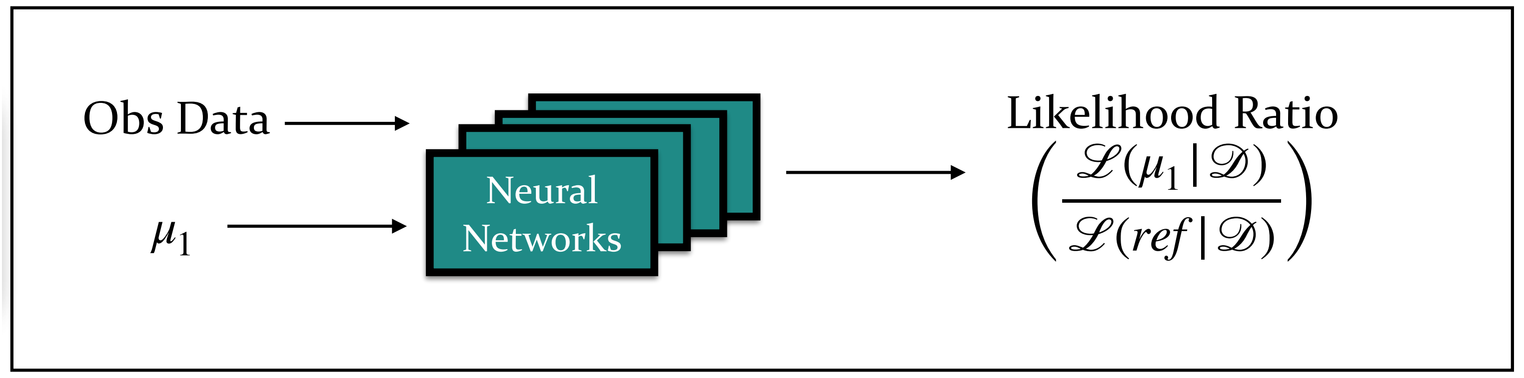


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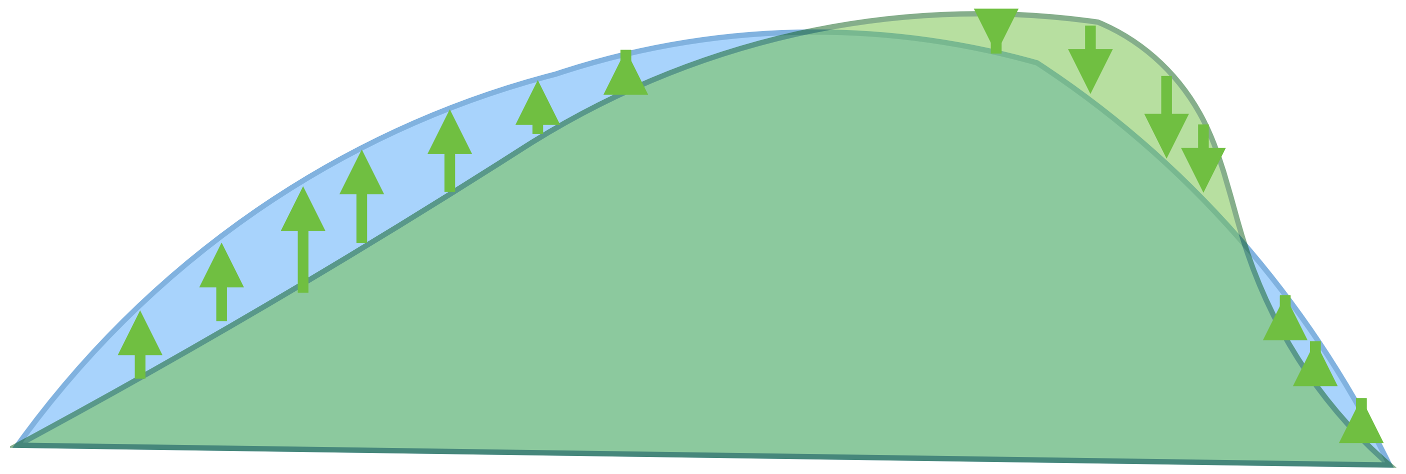

Thanks!

# Backup

# Building a 'Search-Oriented Mixture Model'

$$p(x_i|\mu) = \frac{1}{\nu(\mu)} \sum_{j}^{C} f_j(\mu) \cdot \nu_j \, p_j(x_i)$$

$x_i$ is one individual event

$j$ runs over different physics process (Eg. $gg \rightarrow H^* \rightarrow 4l$, $gg \rightarrow ZZ \rightarrow 4l$)

Event rates

Comes from theory model chosen to interpret data

$$p_{\mathrm{ref}}(x_i) = \frac{1}{\sum_k \nu_k} \sum_{k}^{C_{\mathrm{signals}}} \nu_k \cdot p_k(x_i)$$

Define a 'reference' density with support over entire region of analysis
Does not have to be physical !

# Choice of observable

# Choice of observable

$$\mathcal{L}(\mu\,|\,\mathcal{D}) = p(\mathcal{D}\,|\,\mu)$$

Neyman–Pearson lemma: Likelihood ratio is the most powerful test statistic

We want to compare likelihoods: $$\frac{p(\mathcal{D}\,|\,\mu)}{p(\mathcal{D}\,|\,\mu_0)}$$

# Choice of observable

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$$\mathcal{L}(\mu \mid \mathcal{D}) = p(\mathcal{D} \mid \mu)$$

Neyman–Pearson lemma: Likelihood ratio is the most powerful test statistic

We want to compare likelihoods: $$\frac{p(\mathcal{D} \mid \mu)}{p(\mathcal{D} \mid \mu_0)}$$

A neural network classifier trained on S vs B, estimates the decision function*: $$s(x_i) = \frac{p(x_i \mid S)}{p(x_i \mid S) + p(x_i \mid B)}$$

* Equal class weights

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Which contains all the information required for the likelihood ratio:

$$\frac{p(x_i \,|\, \mu)}{p(x_i \,|\, \mu = 0)} = \frac{\mu \cdot \sigma_S \cdot p(x_i \,|\, S) + \sigma_B \cdot p(x_i \,|\, B)}{\sigma_B \cdot p(x_i \,|\, B)} = \mu \cdot \frac{\sigma_S}{\sigma_B} \cdot \frac{s(x_i)}{1 - s(x_i)} + 1.$$

Same observable $s$ is optimal to test all $\mu$ hypotheses!

No need to develop separate analysis per hypothesis $\mu$

* Equal class weights

# What breaks down?

$$P(X) = |M_s(X) + M_b(X)|^2 = \underbrace{|M_s(X)|^2}_{P_s(X)} + \underbrace{|M_b(X)|^2}_{P_b(X)} + 2\,\underbrace{\mathrm{Re}(\overline{M_s(X)} M_b(X))}_{P_i(X)}$$

$$N_{exp} = \mu \cdot S + B + \sqrt{\mu} \cdot I$$

A neural network classifier trained on S vs B, estimates the decision function: $s(x_i) = \frac{p(x_i|S)}{p(x_i|S) + p(x_i|B)}$

Which contains all the information required for the likelihood ratio:

$$\frac{p(x_i|\mu)}{p(x_i|\mu=0)} = \frac{\mu \cdot \sigma_S \cdot p(x_i|S) + \sigma_B \cdot p(x_i|B)}{\sigma_B \cdot p(x_i|B)} = \mu \cdot \frac{\sigma_S}{\sigma_B} \cdot \frac{s(x_i)}{1 - s(x_i)} + 1.$$

Same observable $s$ is optimal to test all $\mu$ hypotheses!
No need to develop separate analysis per hypothesis $\mu$

8

No longer in this convenient spacial case: The same observable **no longer optimal due to non-linear effects** coming from quantum interference

Also **does not generalise to an arbitrary theory parameter** $\theta$, (eg. Effective Field Theory parameters)

Can we modify the LHC analysis methodology to **design near-optimal analyse for the general case?**

Cranmer et al

# Estimating high-dimensional density ratios

$$\mathscr{L}(\mu \mid \mathscr{D}) = p(\mathscr{D} \mid \mu)$$

Neyman–Pearson lemma: Likelihood ratio is the most powerful test statistic

We want to compare likelihoods: $$\frac{p(\mathscr{D} \mid \mu)}{p(\mathscr{D} \mid ref)}$$

A neural network classifier trained on simulated samples from $\theta_1$ vs simulated samples from $ref$, estimates the decision function:

$$s(x_i) = \frac{p(x_i \mid \mu_1)}{p(x_i \mid \mu_1) + p(x_i \mid ref)}$$

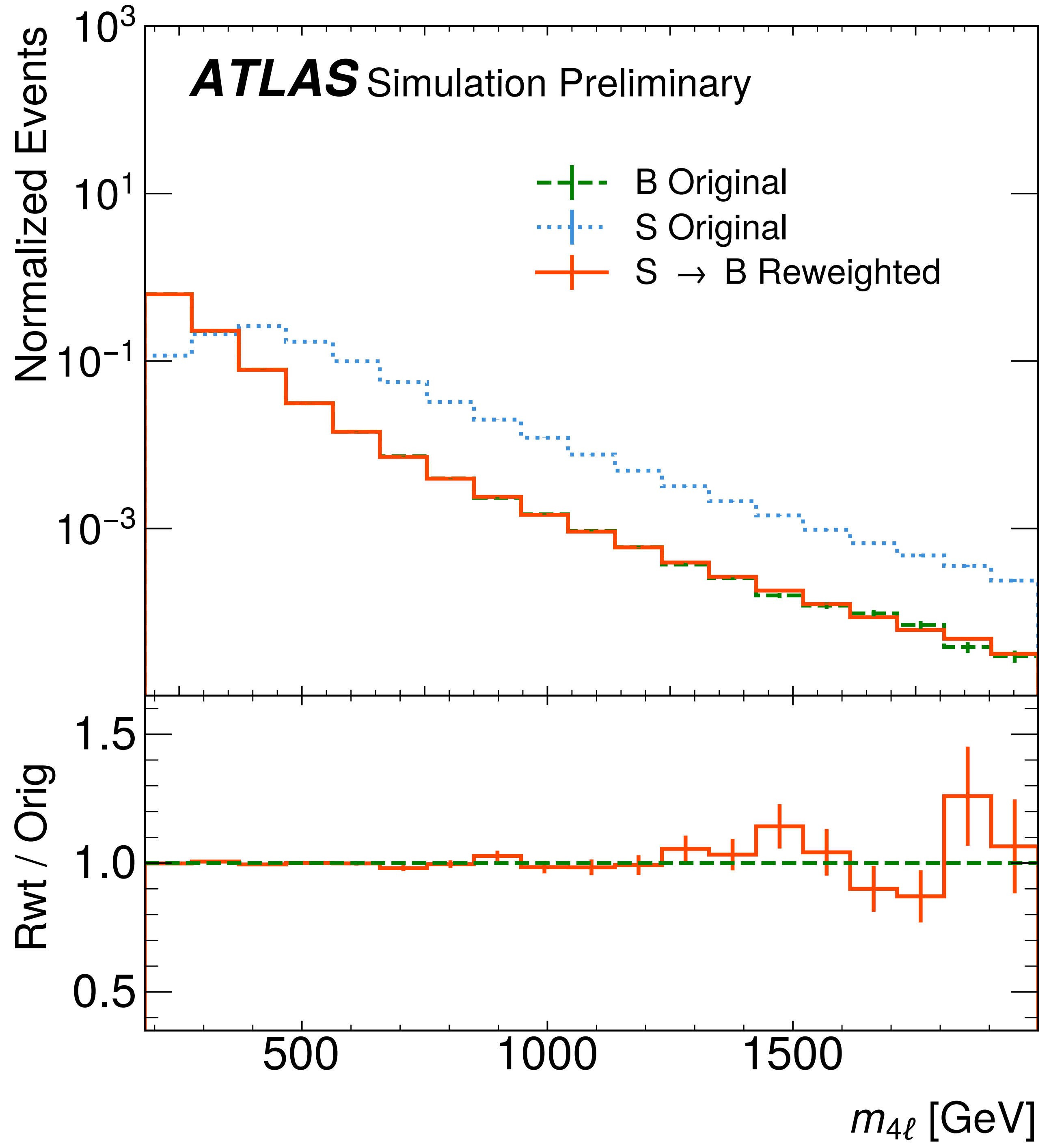
Which contains all the information required for the likelihood ratio:

$$\frac{p(x_i \mid \mu_1)}{p(x_i \mid ref)} = \frac{s(x_i)}{1 - s(x_i)}$$

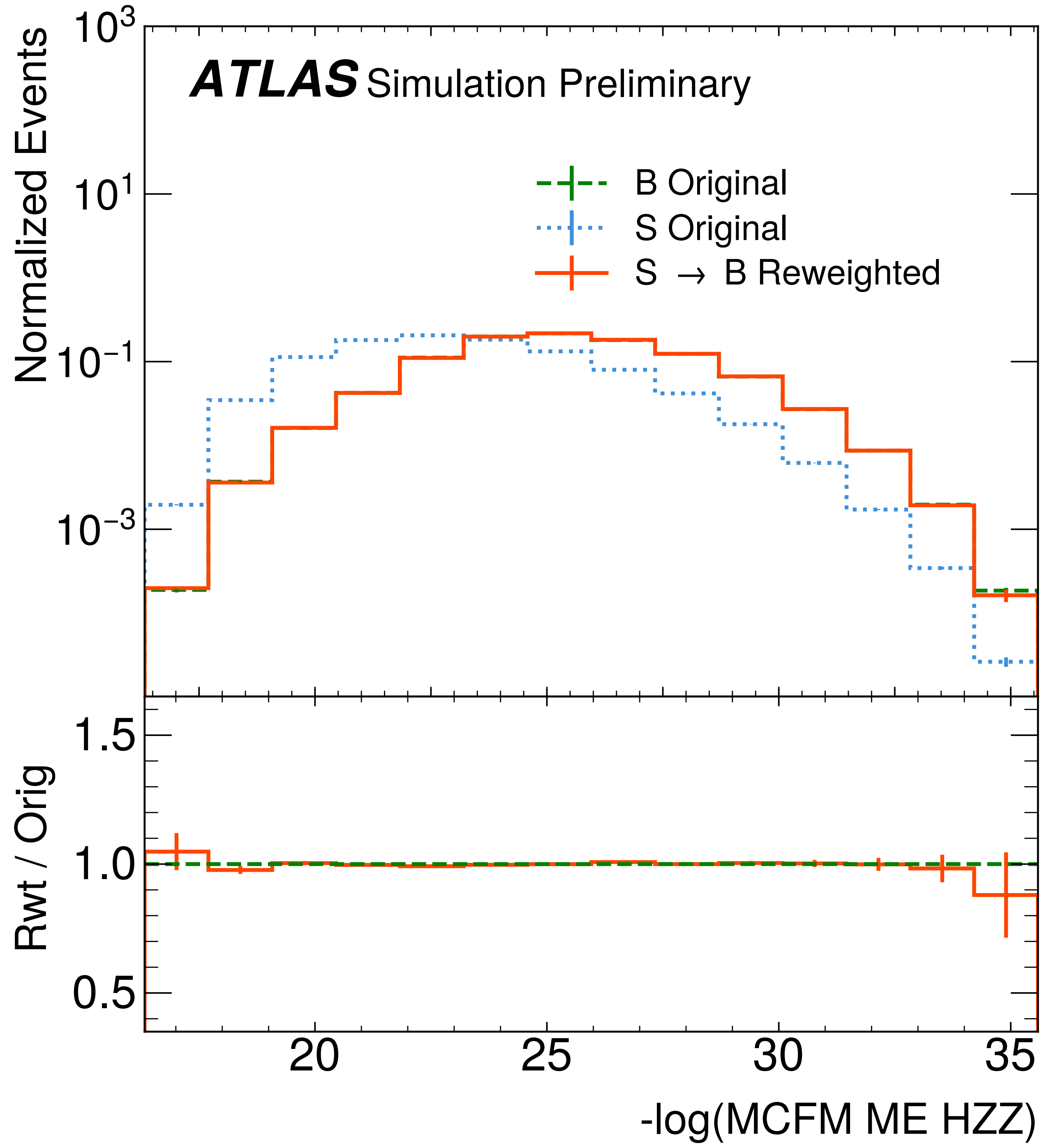
- Optimal statistic to test each value of $\mu$
- We get the LR *per event* (unbinned)

# Re-weight closures for B

Source
Target
RW




$m_{4l}$



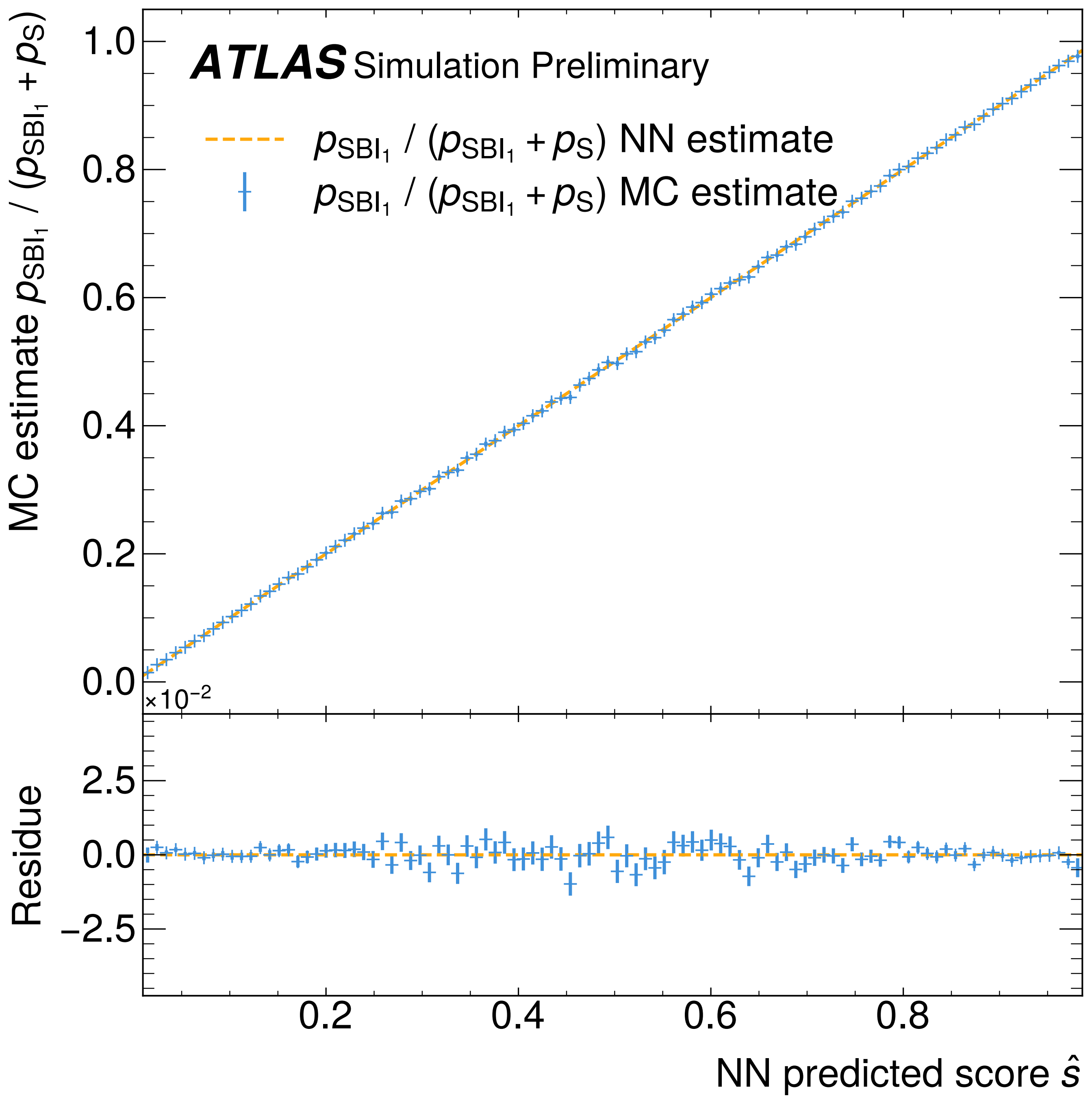

Matrix-Element-based Observable
(ggF from MCFM)

# Calibration Curves

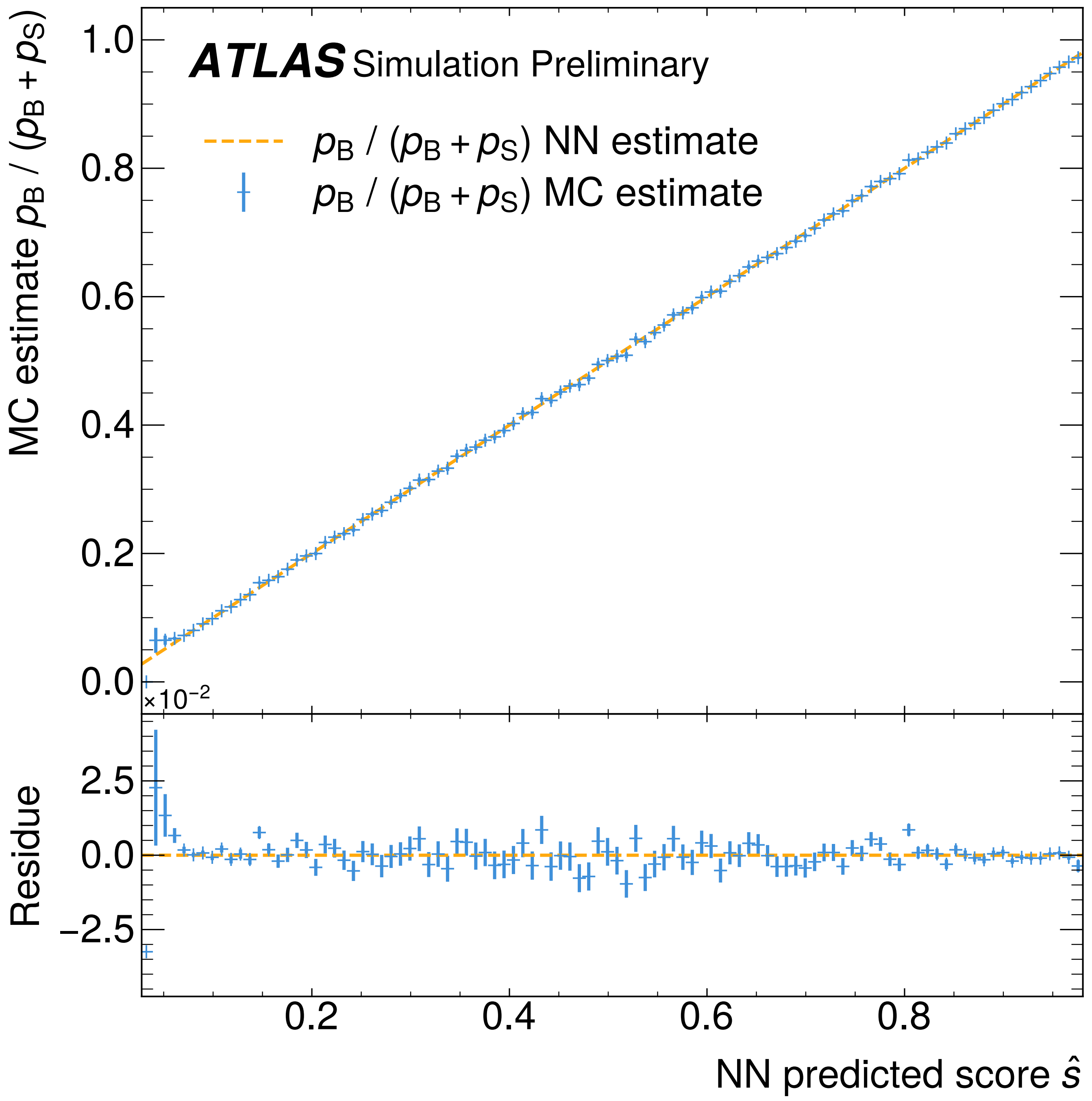
$$\frac{P_{SBI}}{P_{SBI} + P_{ref}}$$

$$\frac{P_B}{P_B + P_{ref}}$$

Binned estimate




Ensemble prediction

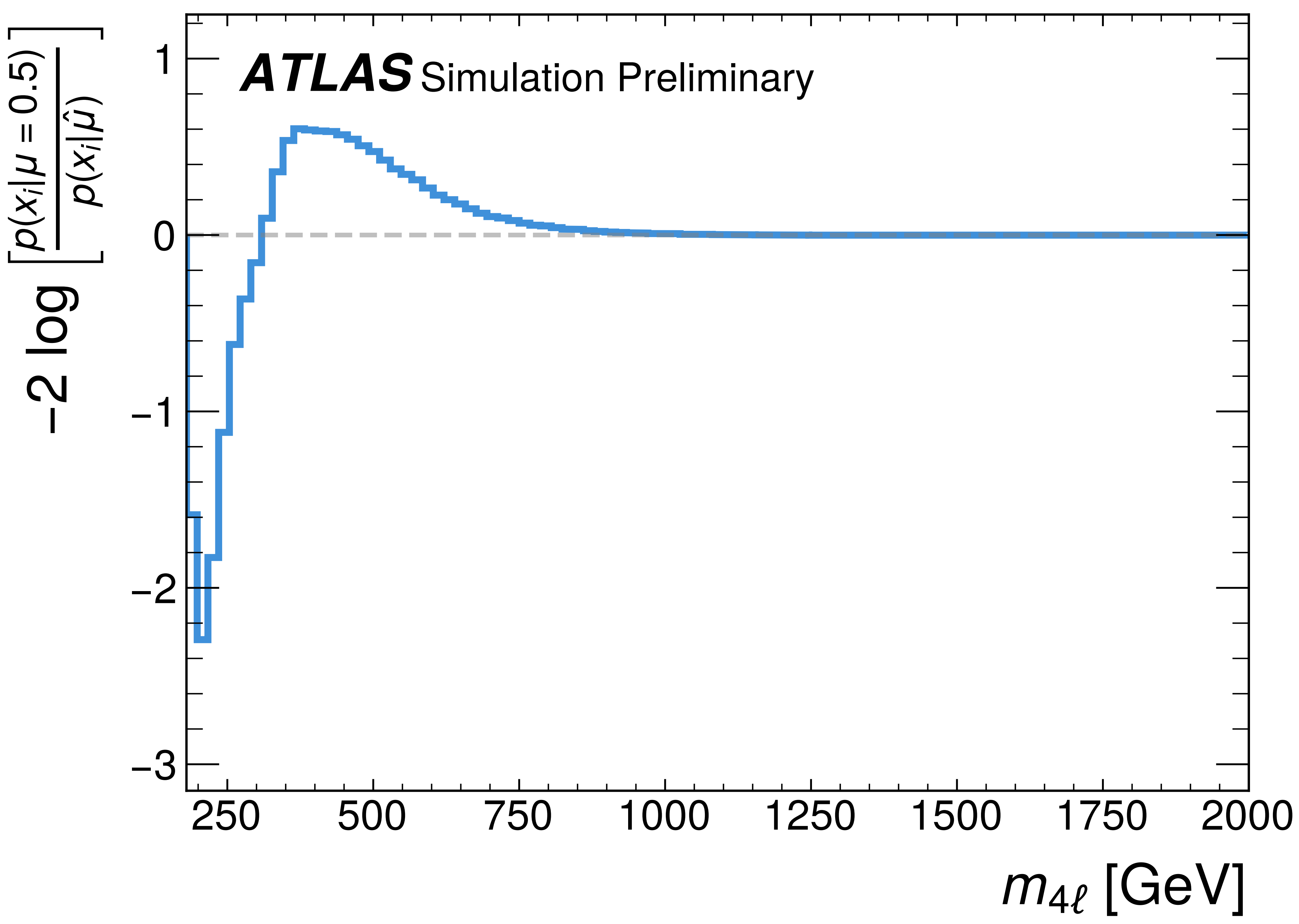


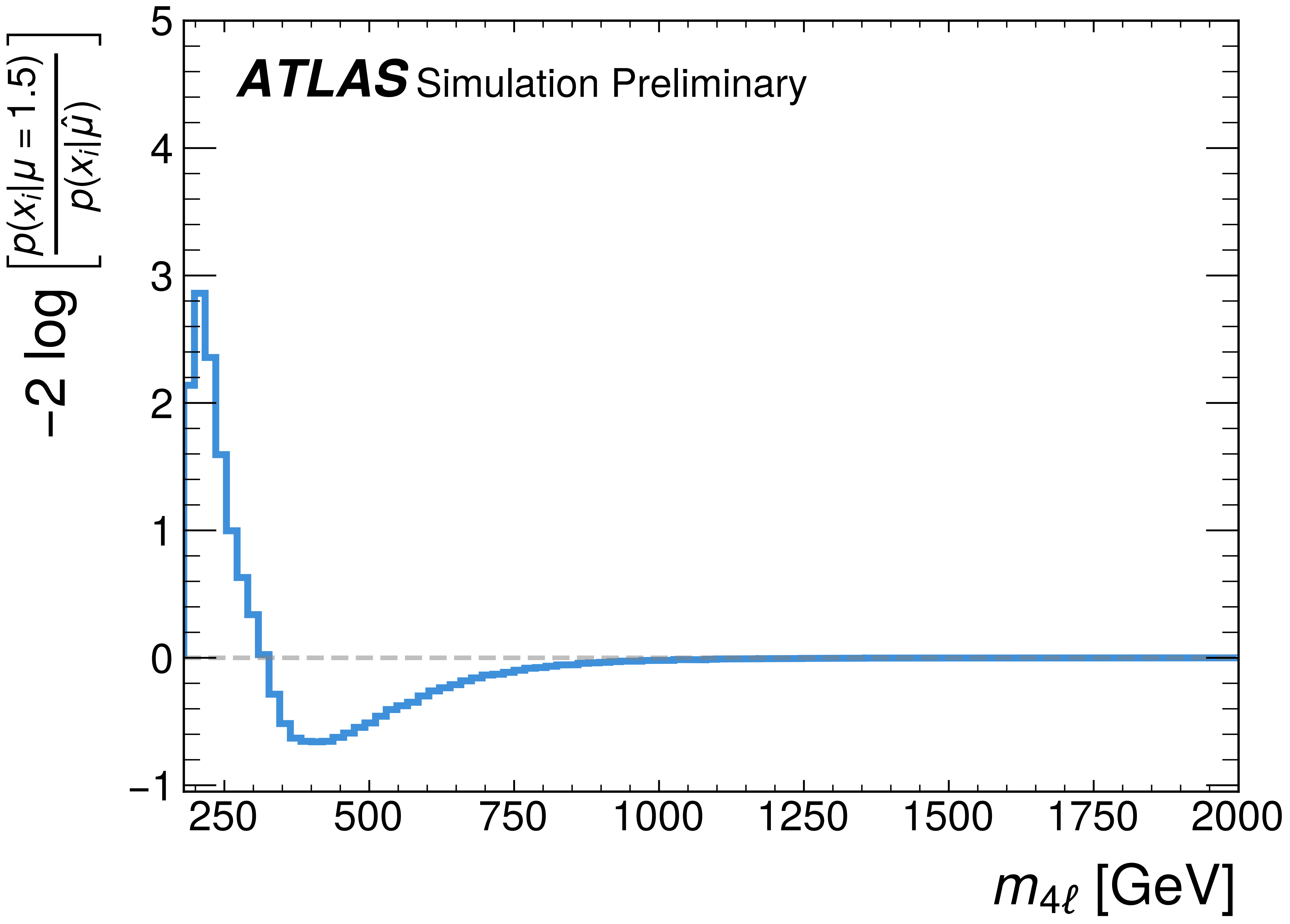

Ensemble prediction

Interpretability:
Which phase space favours one hypothesis over another?

$$-2 \cdot log\frac{P(x_i|\mu = 0.5)}{P(x_i|\mu = 1)}$$

$$-2 \cdot log\frac{P(x_i|\mu = 1.5)}{P(x_i|\mu = 1)}$$



# Negative Weighted Events

1. Start from a positive weighted reference sample instead
2. Re-weight to intended parameter point
3. Throw toys from this sample

$$w_i^{\text{rwt-ref}} \to w_i^{\text{Asimov}}(\mu) = \frac{\nu(\mu)}{\nu_{\text{rwt-ref}}} \cdot \frac{p(x_i\,|\,\mu)}{P_{\text{rwt-ref}}(x_i)} \cdot w_i^{\text{rwt-ref}}$$

# Estimating the variance on mean: Bootstrapping

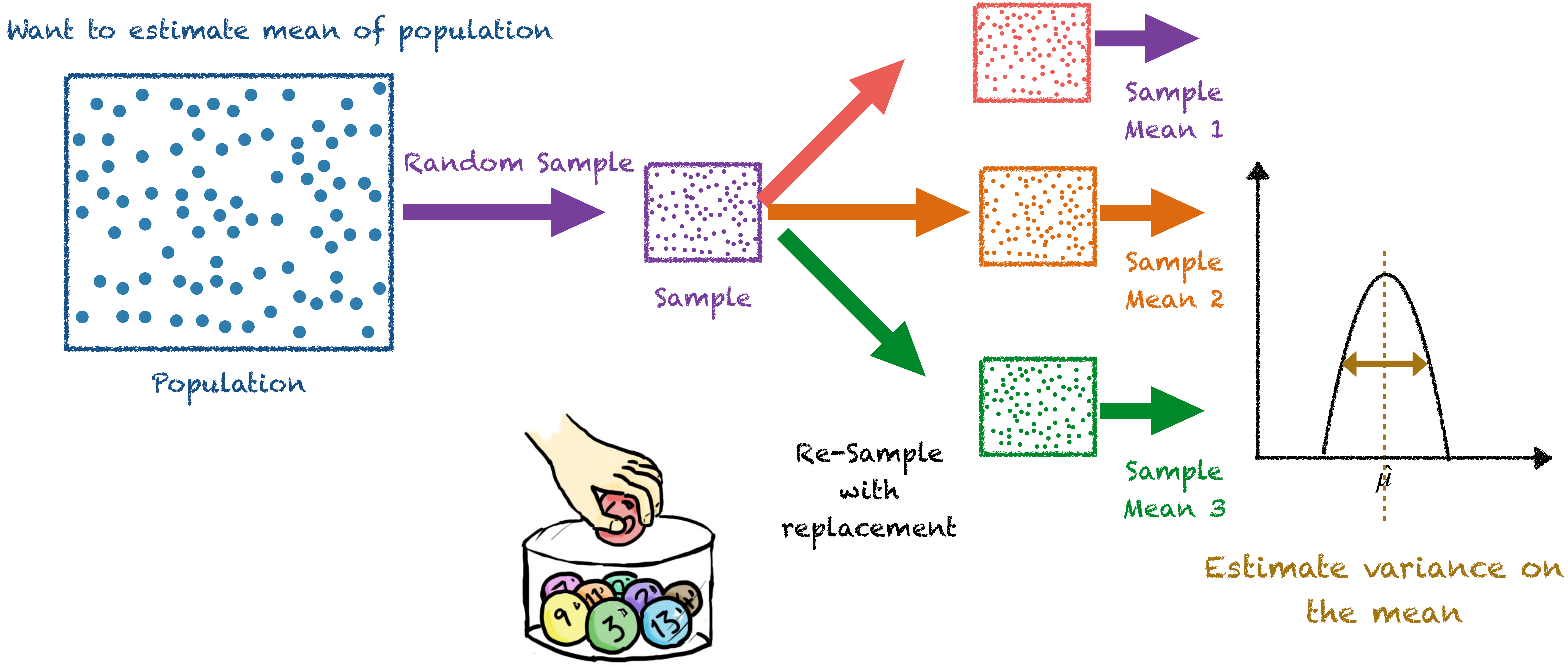



Image: Source

# Quantifying uncertainty on estimated density ratio

$$w_i \to w_i \cdot Pois(1)$$

- Train an ensemble of networks, **each on a Poisson fluctuated version of the training dataset**
- Ensemble average used as final prediction, **estimate the variance on mean from bootstrapped ensembles**

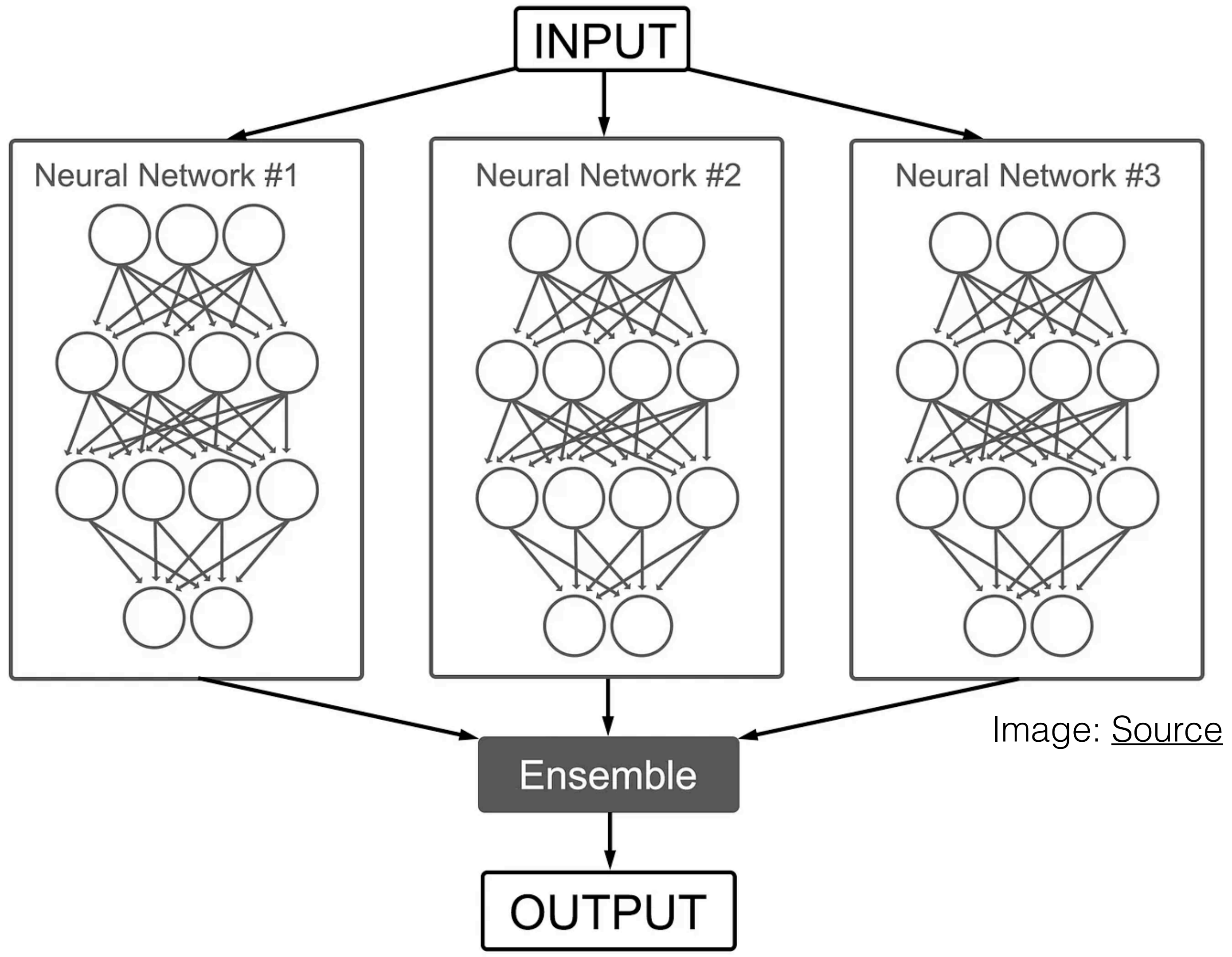



Image: Source

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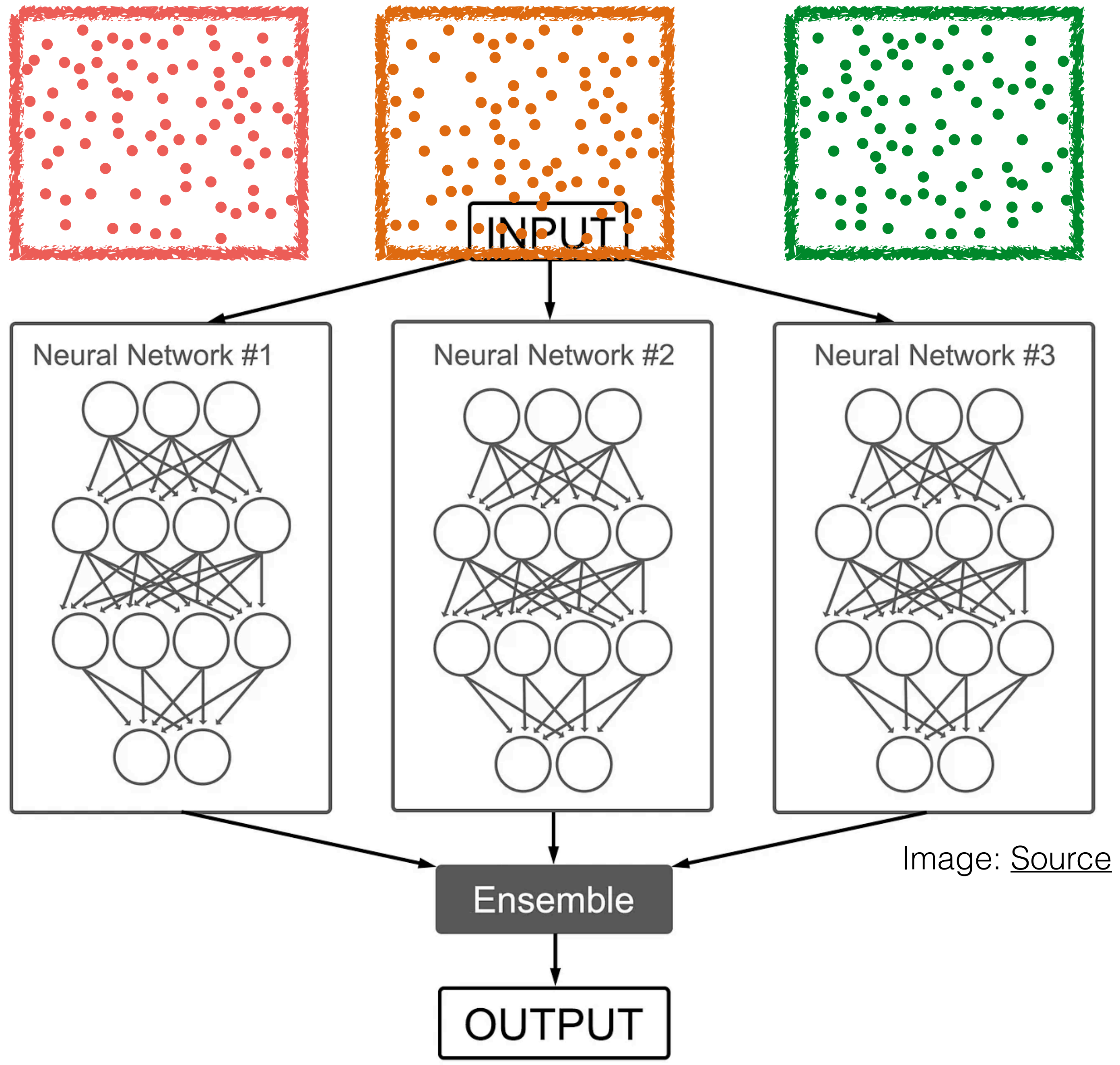


Image: Source

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- Train an ensemble of networks, **each on a Poisson fluctuated version of the training dataset**
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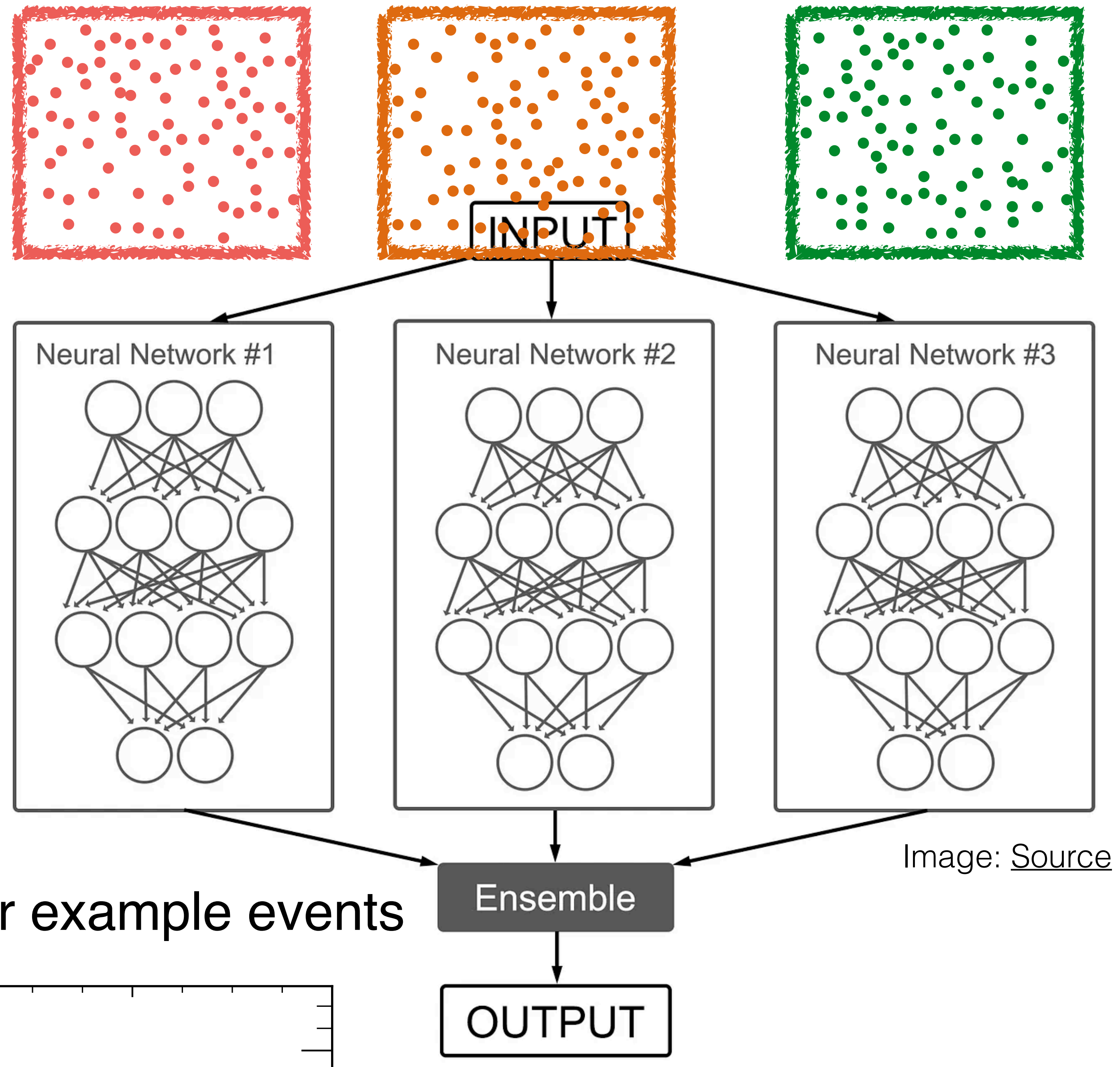
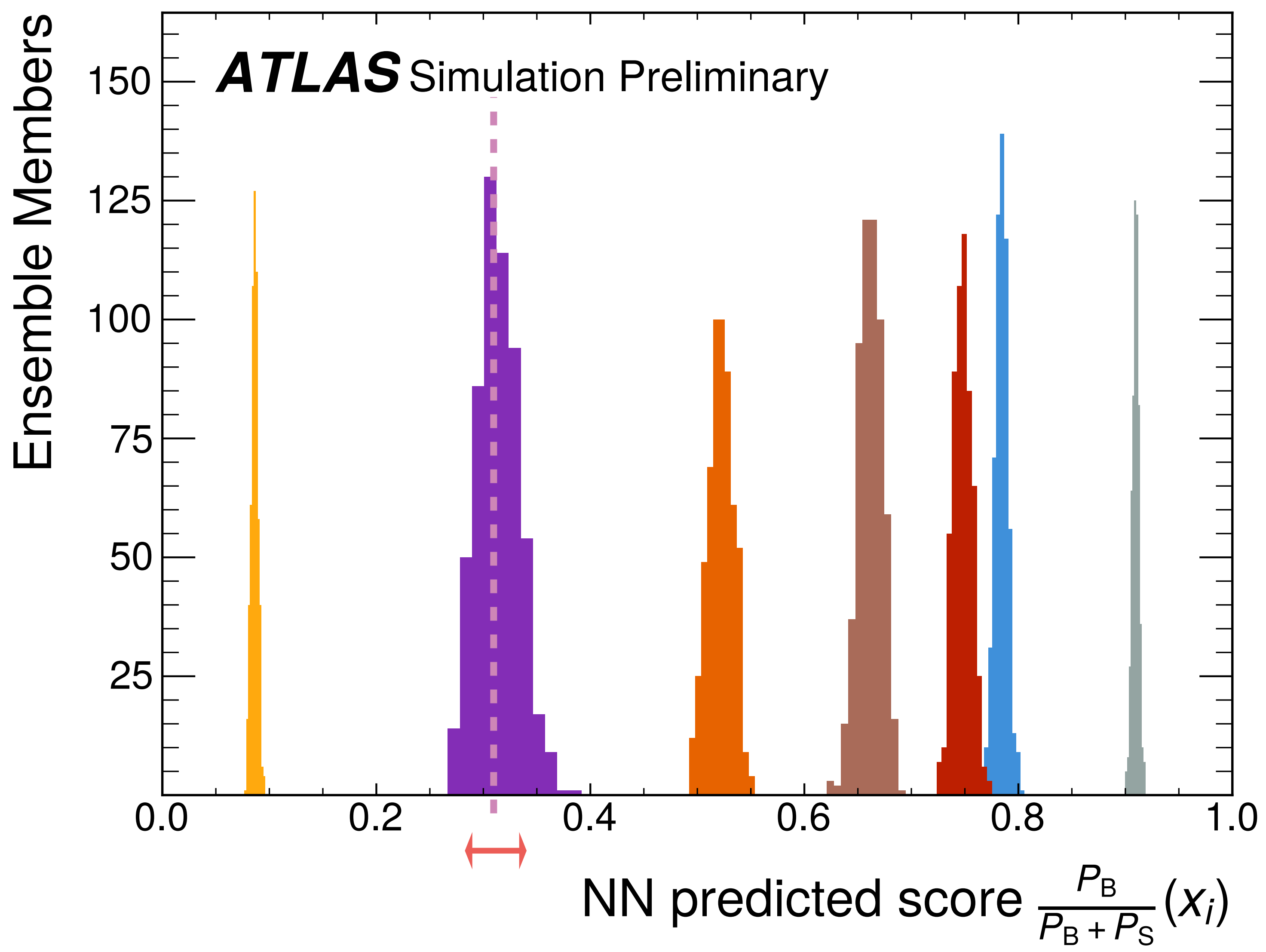



Image: Source

Distribution of NN predictions for example events



# Quantifying uncertainty on estimated density ratio

$$w_i \to w_i \cdot Pois(1)$$

- Train an ensemble of networks, **each on a Poisson fluctuated version of the training dataset**

- Ensemble average used as final prediction, **estimate the variance on mean from bootstrapped ensembles**

- Propagate with spurious signal method

$$f_j(\mu) \to f_j(\mu + \alpha \cdot \Delta\hat{\mu}(\mu))$$

Constraint term: $Gauss(0,1)$

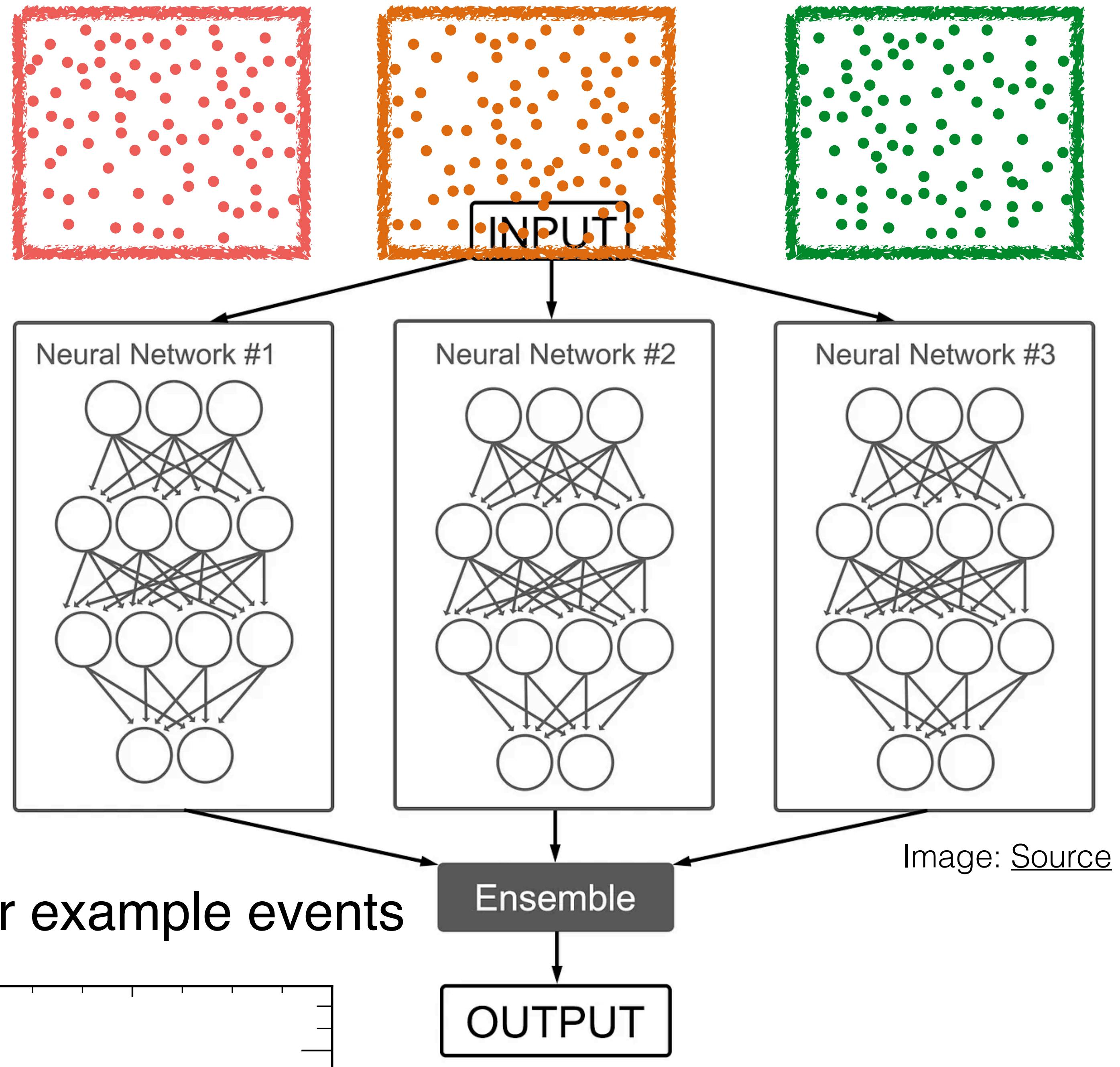
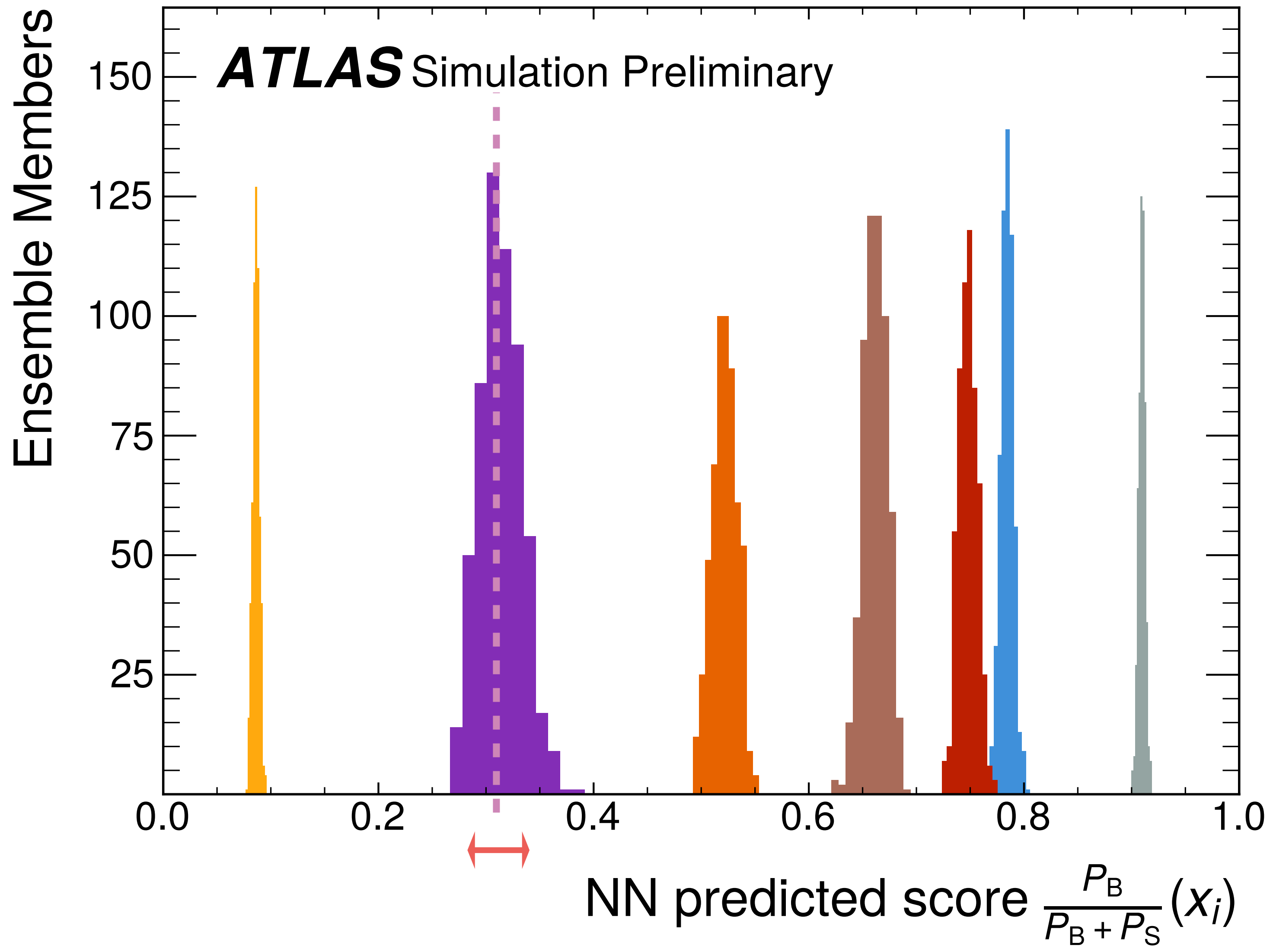



Image: Source

Distribution of NN predictions for example events



# Simulated Samples

- PoI: Signal strength $\mu$
- Simplified, unphysical dataset:
  - Processes: S: $gg \to H^* \to 4l$ & B: $gg \to ZZ \to 4l$, SBI: full process
  - No VBF processes or qqZZ background
  - Two systematics: ggF NLO K-factor uncertainty (shape + norm) & luminosity uncertainty (norm only)

Input variables

| **Variable** | **Definition** |
|---|---|
| Production Kinematics | |
| $m_{4\ell}$ | Four-lepton invariant mass |
| $p_T^{4\ell}$ | Four-lepton transverse momentum |
| $\eta^{4\ell}$ | Four-lepton pseudo-rapidity |
| Decay Kinematics | |
| $m_{Z1}$ | $Z_1$ mass |
| $m_{Z2}$ | $Z_2$ mass |
| $\cos\theta^*$ | Higgs decay angle |
| $\cos\theta_1$ | $Z_1$ decay angle |
| $\cos\theta_2$ | $Z_2$ decay angle |
| $\phi$ | Angle between $Z_1, Z_2$ decay planes |
| $\phi_1$ | $Z_1$ decay plane angle |

# Combination with histogram analyses

$$\frac{L_{\text{comb}}(\mu, \alpha)}{L_{\text{ref}}} = \frac{L_{\text{full}}(\mu, \alpha)}{L_{\text{ref}}} \; L_{\text{hist}}(\mu, \alpha)$$

# Calculating pulls and impacts in JAX

$$\lambda(\mu, \alpha) = -2 \ln(L_{full}(\mu, \alpha)/L_{ref})$$

Hessian:

$$C_{nm} = \left[ \frac{1}{2} \frac{\partial^2 \lambda}{\partial \alpha_n \partial \alpha_m} (\widehat{\mu}, \widehat{\alpha}) \right]^{-1}$$

Pulls:

$$\frac{\widehat{\alpha}_k - \alpha_k^0}{\sqrt{C_{kk}}}.$$

Post-fit Impact:

$$\Gamma_k = \frac{\partial \widehat{\mu}}{\partial \alpha_k} \times \sqrt{C_{kk}}$$

$$= -\left[ \frac{\partial^2 \lambda}{\partial^2 \mu} (\widehat{\mu}, \widehat{\alpha}) \right]^{-1} \frac{\partial^2 \lambda}{\partial \mu \partial \alpha_k} (\widehat{\mu}, \widehat{\alpha}) \times \sqrt{C_{kk}},$$

# Vertical interpolation

$$G_j(\alpha_k) = \begin{cases} \left(\frac{\nu_j(\alpha_k^+)}{\nu_j(\alpha_k^0)}\right)^{\alpha_k} & \alpha_k > 1 \\ 1 + \sum_{n=1}^{6} c_n \alpha_k^n & -1 \le \alpha_k \le 1 \\ \left(\frac{\nu_j(\alpha_k^-)}{\nu_j(\alpha_k^0)}\right)^{-\alpha_k} & \alpha_k < -1 \end{cases}$$

$$g_j(x_i, \alpha_k) = \begin{cases} \left(g_j(x_i, \alpha_k^+)\right)^{\alpha_k} & \alpha_k > 1 \\ 1 + \sum_{n=1}^{6} c_n \alpha_k^n & -1 \le \alpha_k \le 1 \\ \left(g_j(x_i, \alpha_k^-)\right)^{-\alpha_k} & \alpha_k < -1 \end{cases}$$

With some continuity requirements