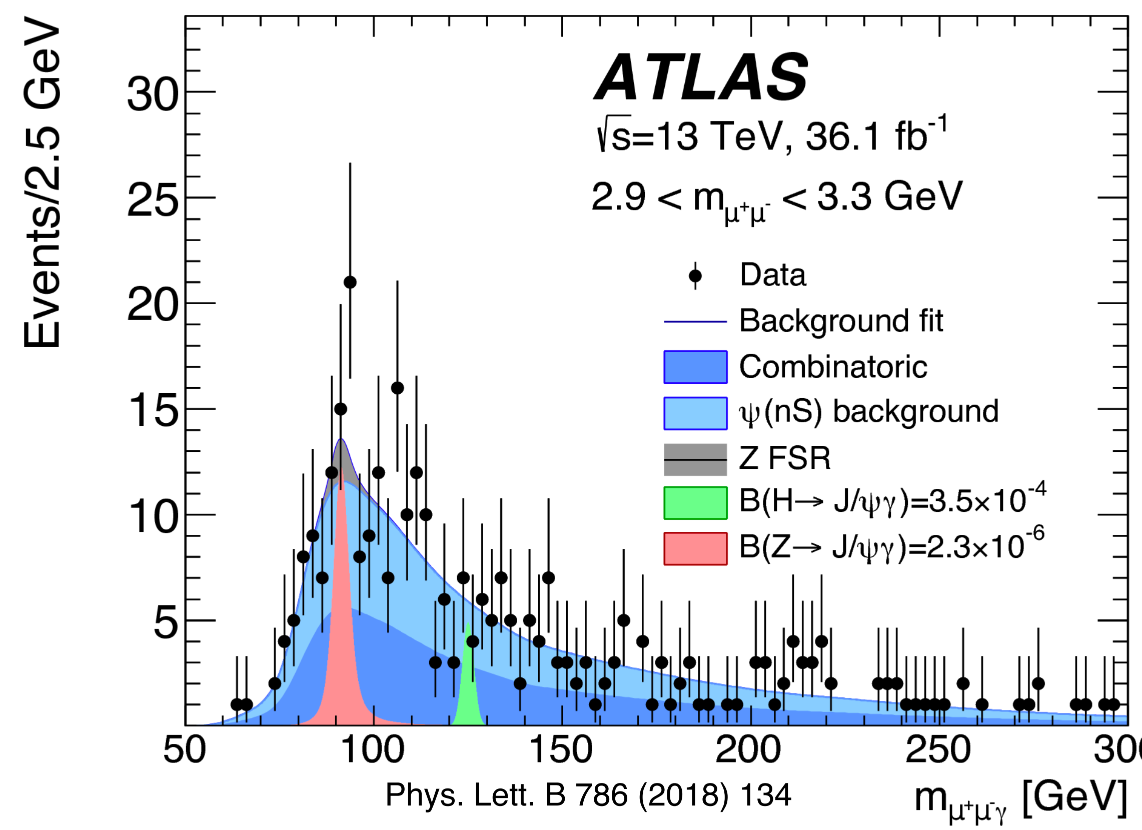
Non-Parametric Data-Driven Background Modelling using Conditional Probabilities

Konstantinos Nikolopoulos

University of Birmingham



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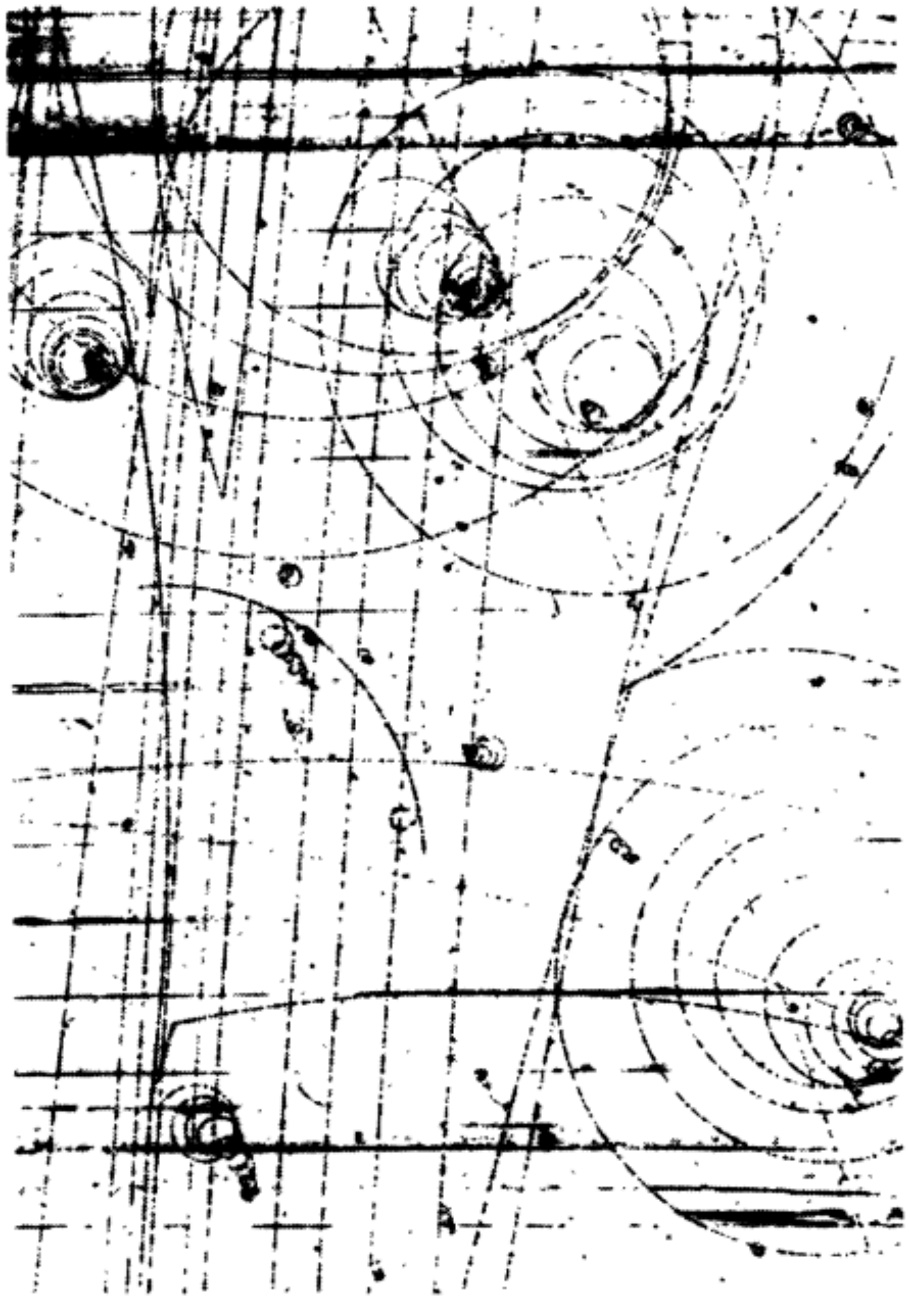

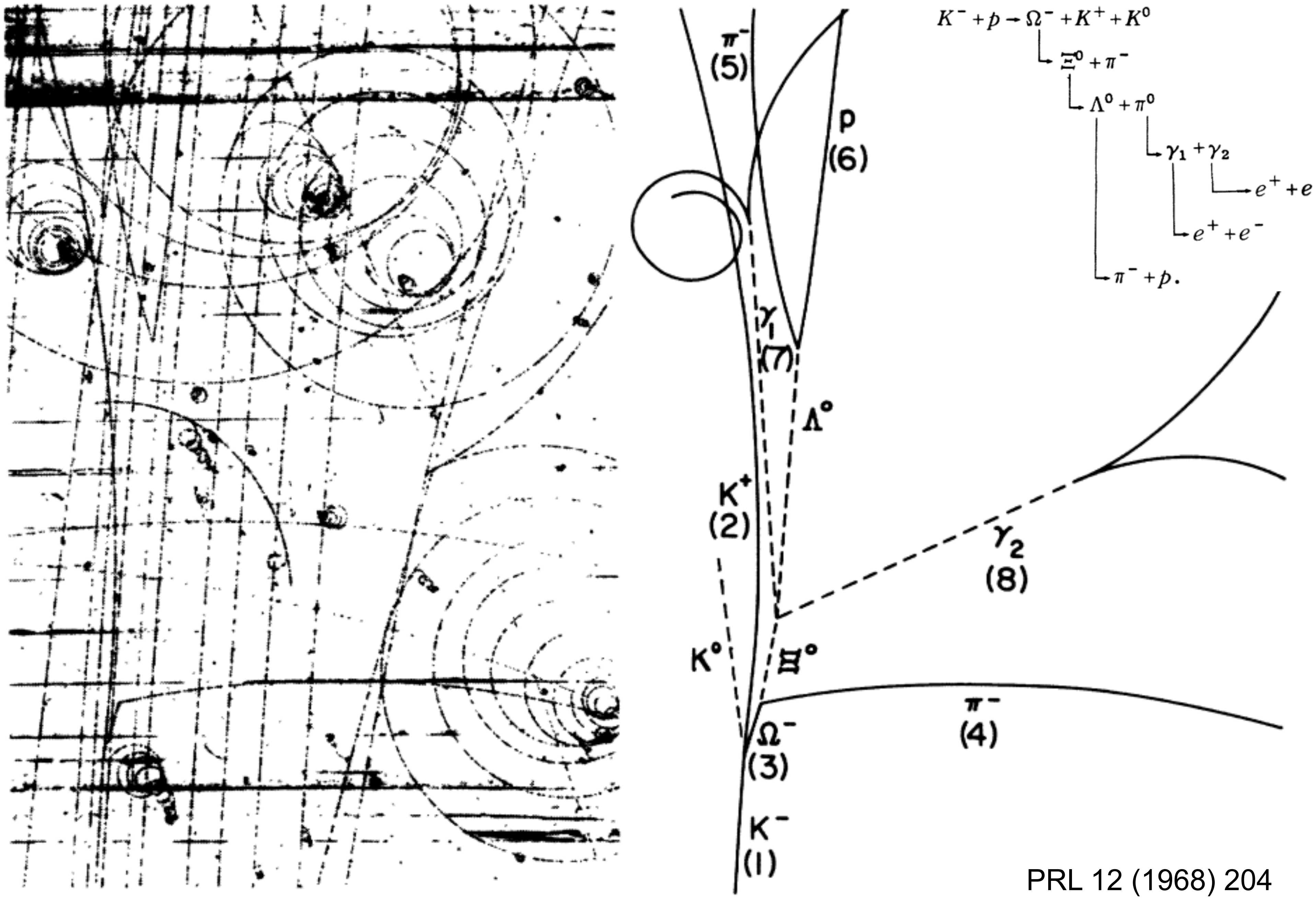

PRL 12 (1968) 204

Discoveries of new signals

…are all about controlling the backgrounds

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Construct the **profile likelihood ratio** test statistic: $\lambda\left(\mu\right) = \dfrac{L\left(\mu, \hat{\hat{\theta}}\right)}{L\left(\hat{\mu}, \hat{\theta}\right)}$

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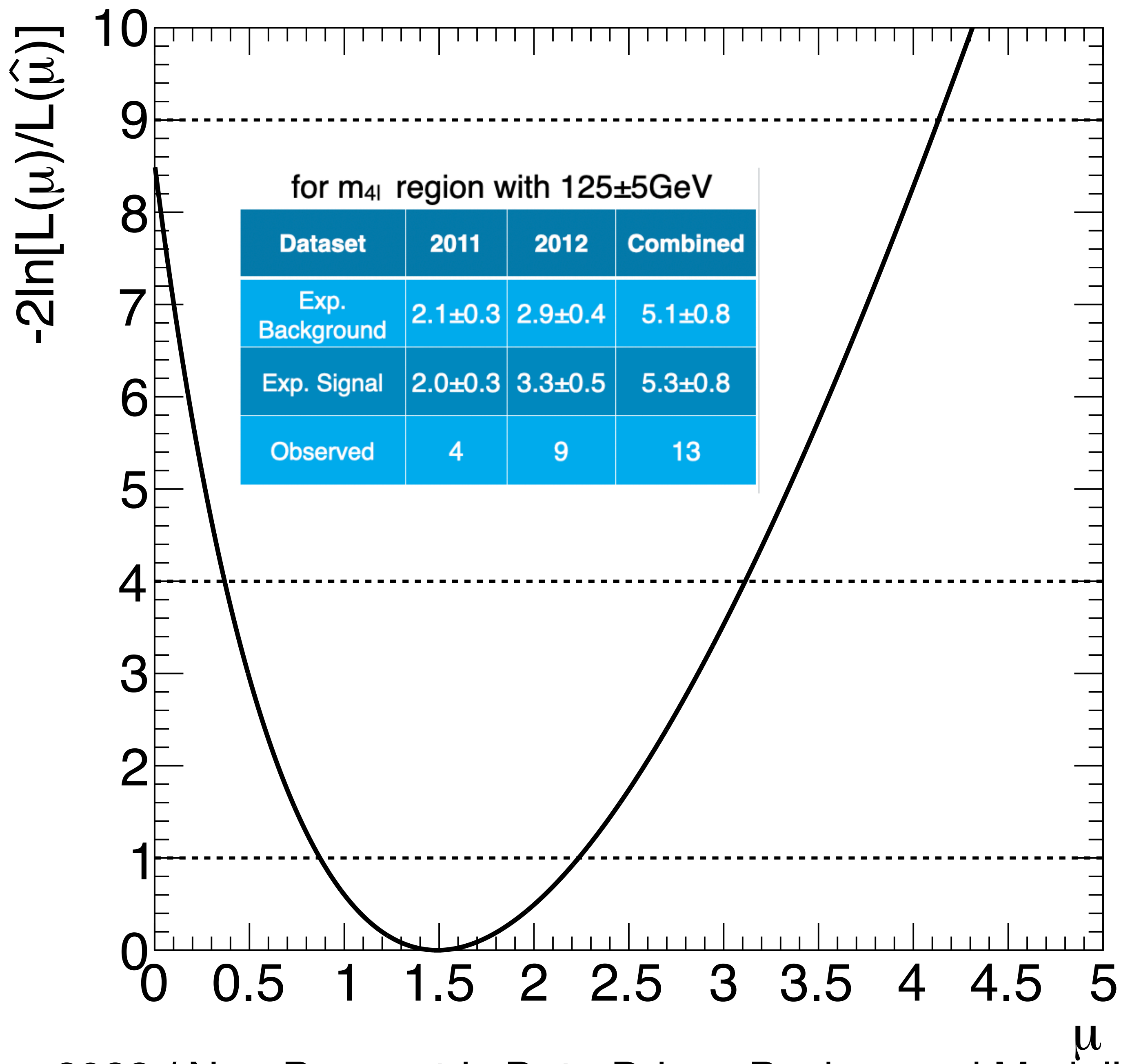

for m_{4l} region with 125±5GeV

Dataset	2011	2012	Combined
Exp. Background	2.1±0.3	2.9±0.4	5.1±0.8
Exp. Signal	2.0±0.3	3.3±0.5	5.3±0.8
Observed	4	9	13

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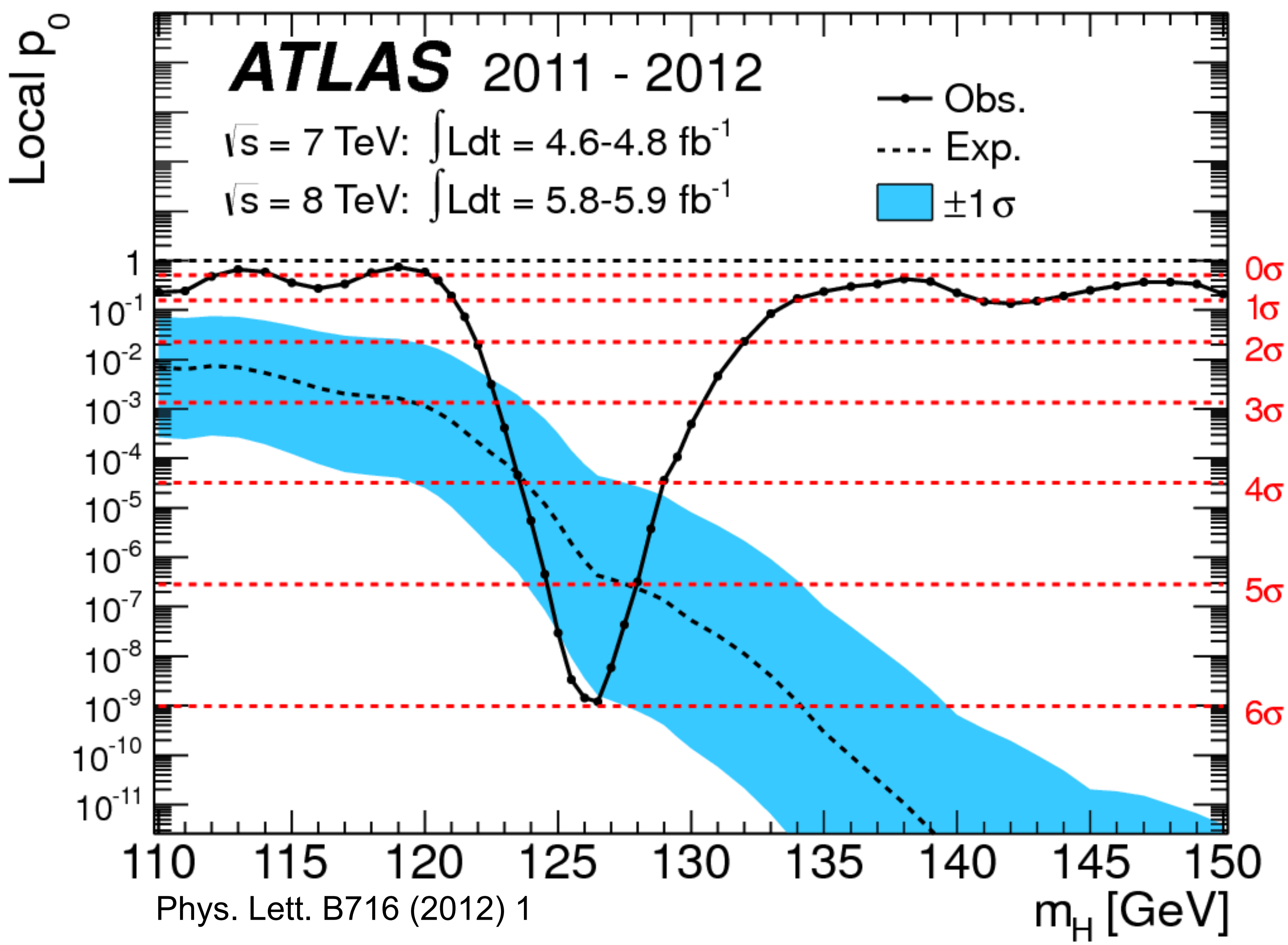

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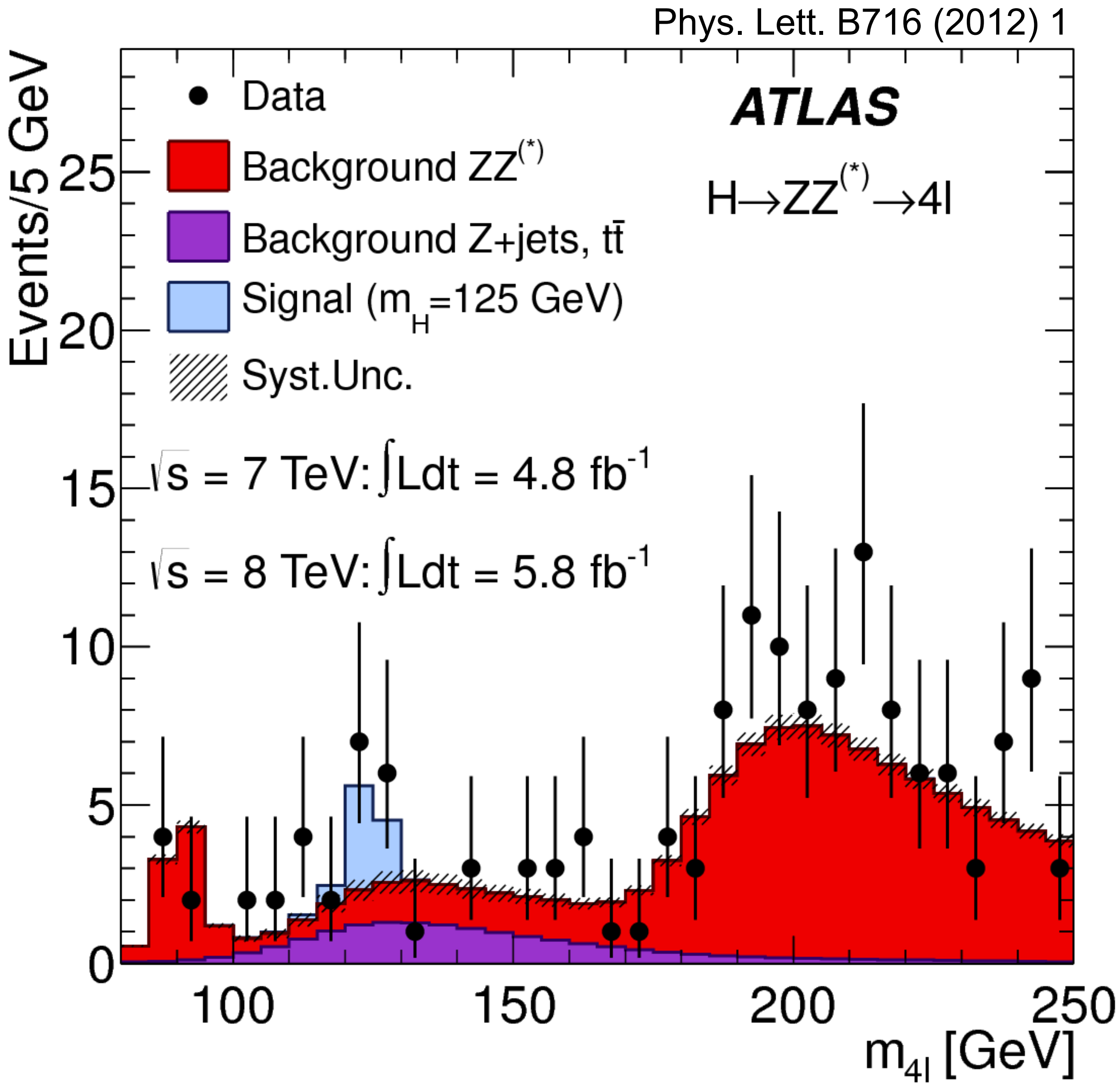
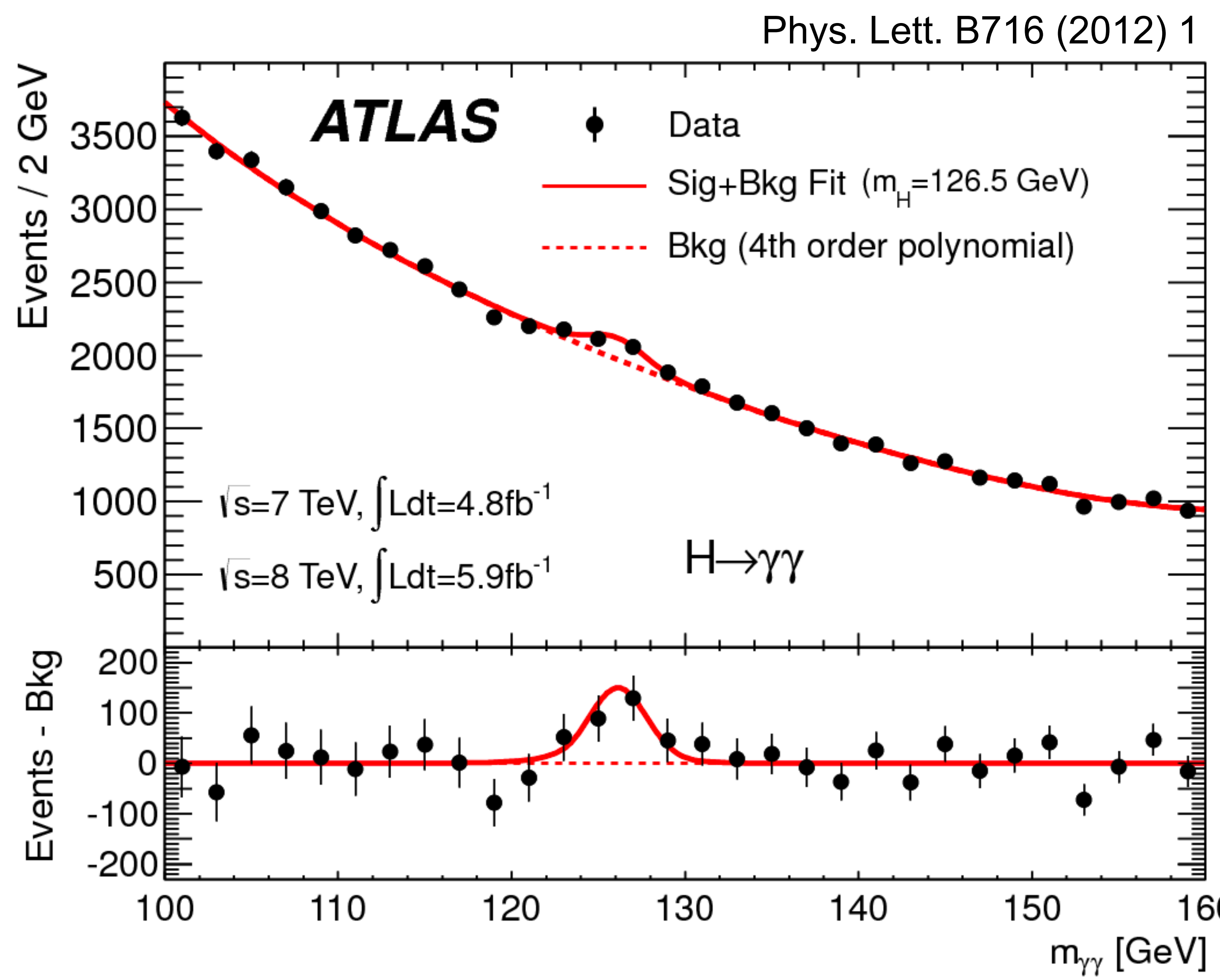
Observing the Higgs boson





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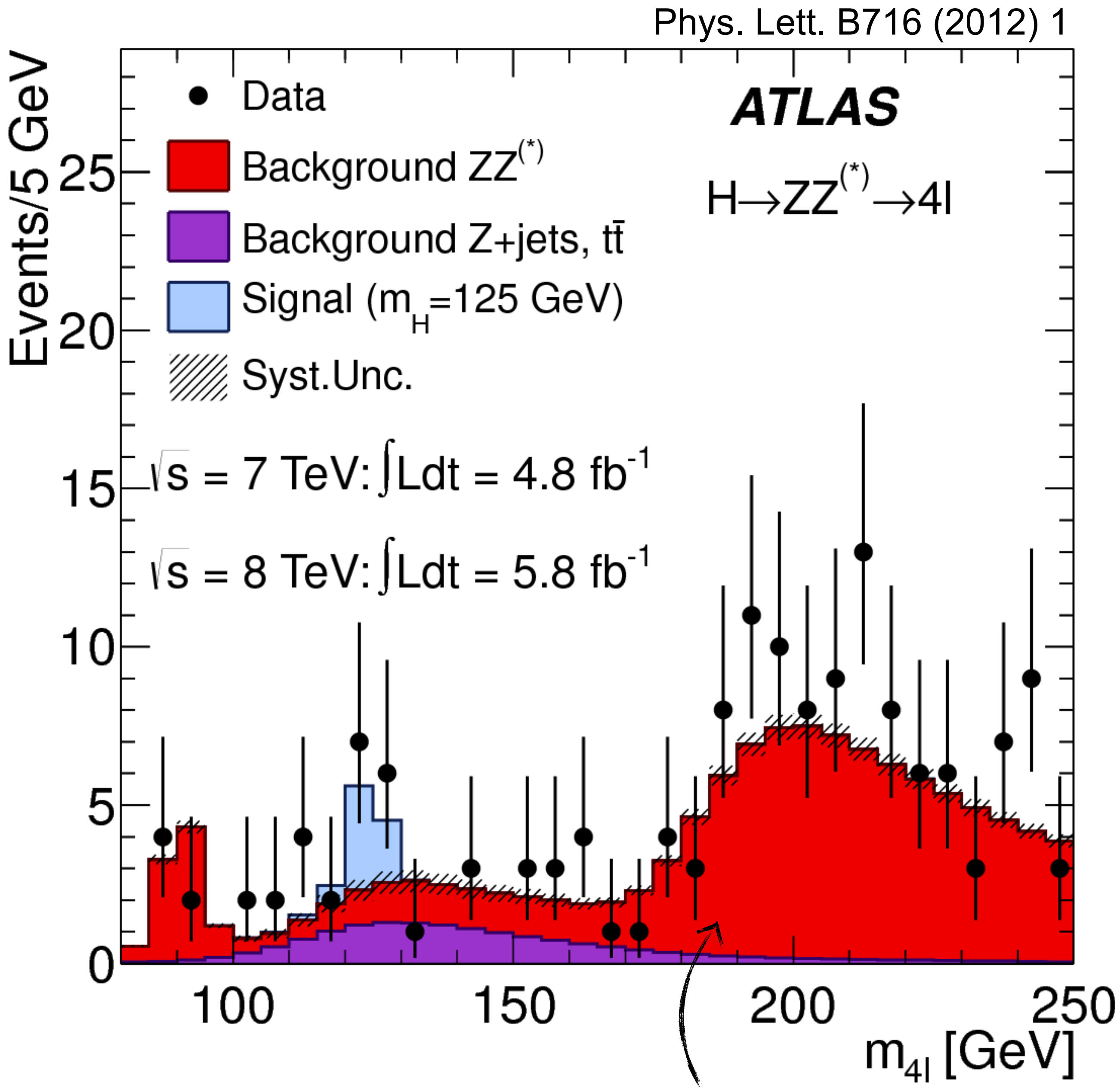

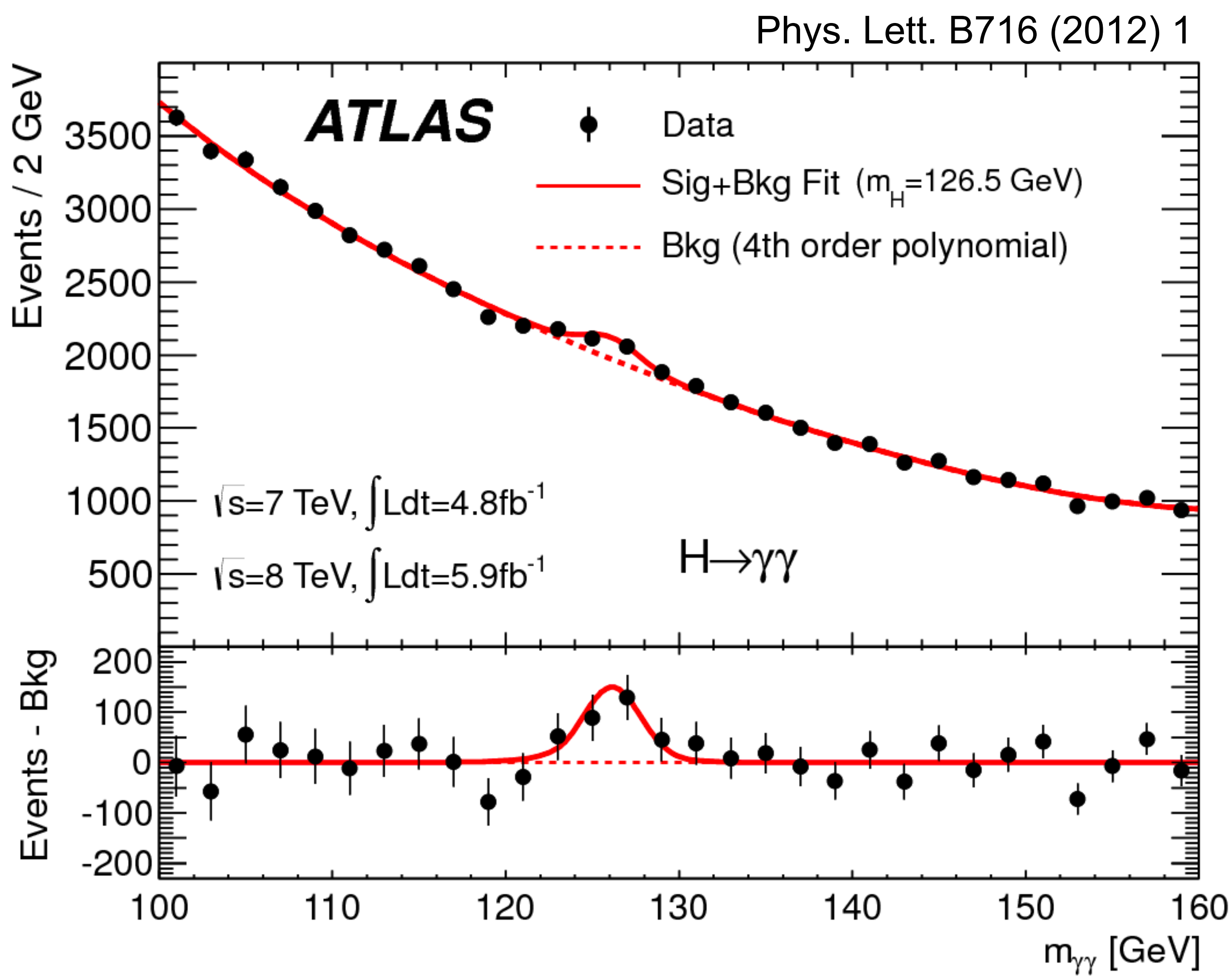

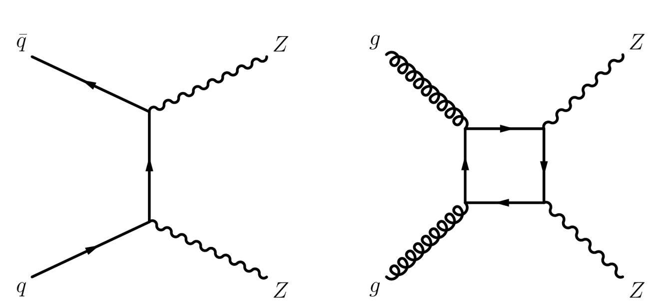

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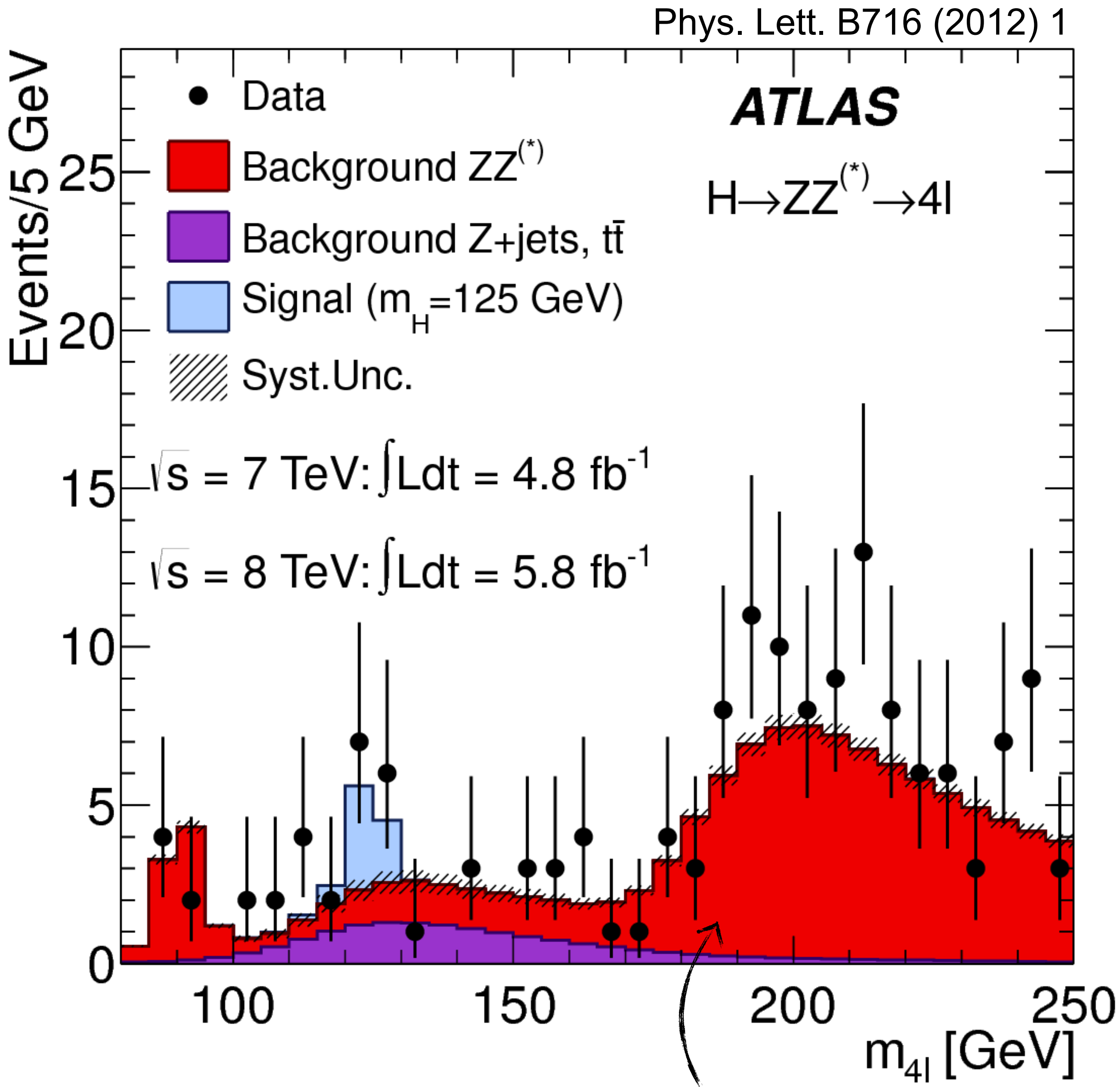
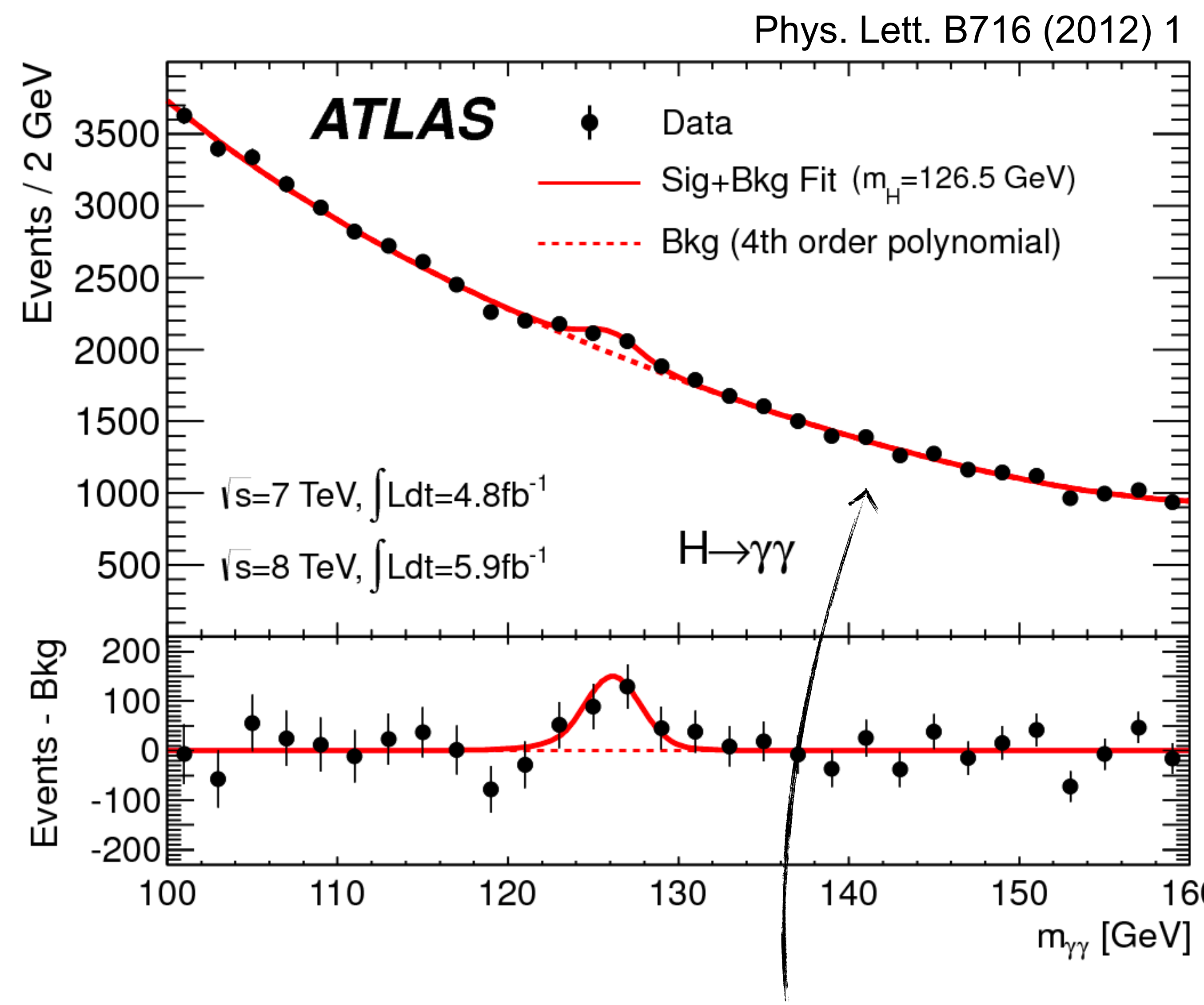
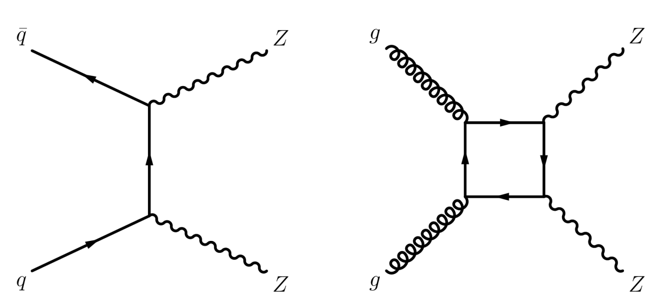
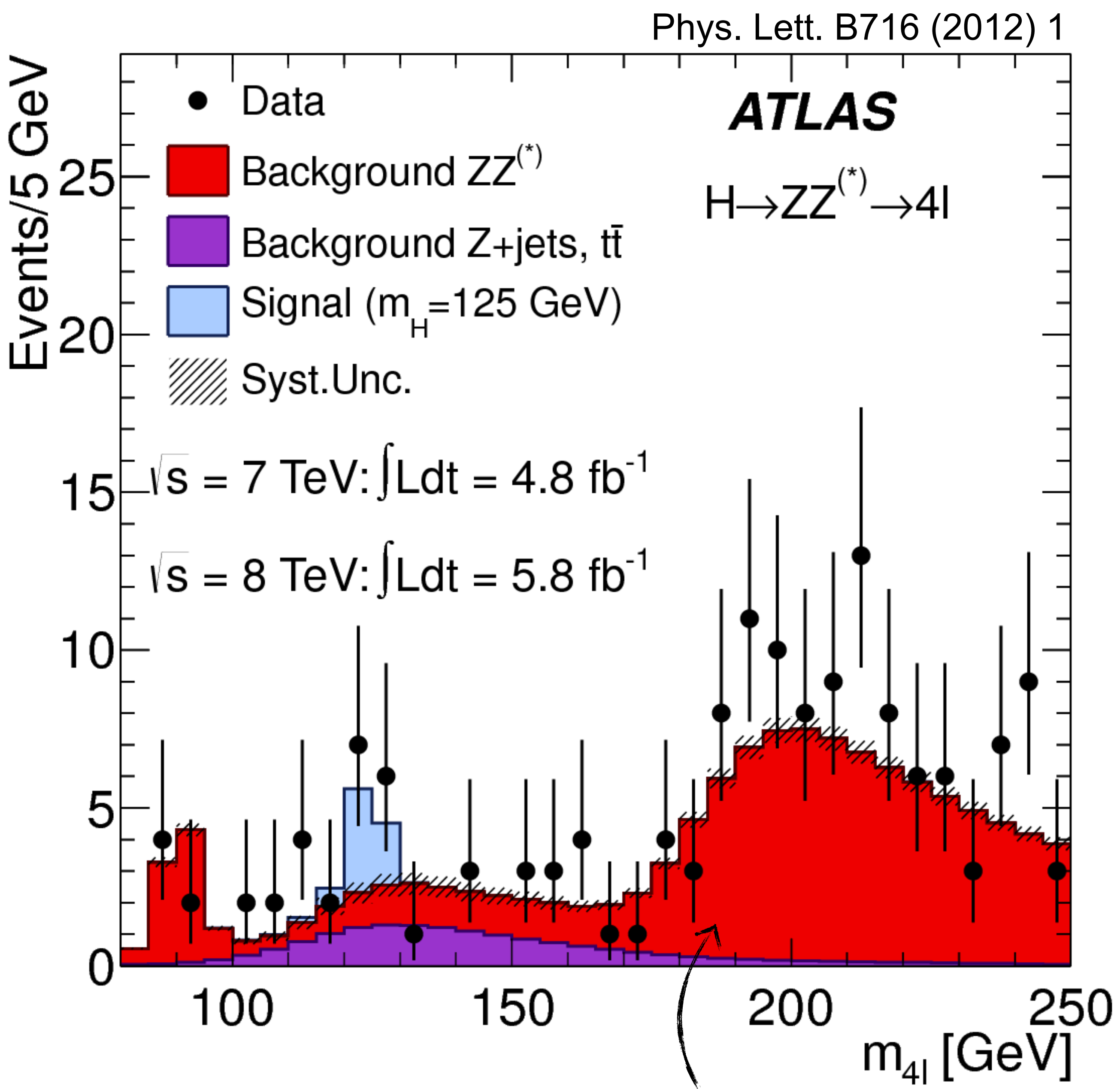


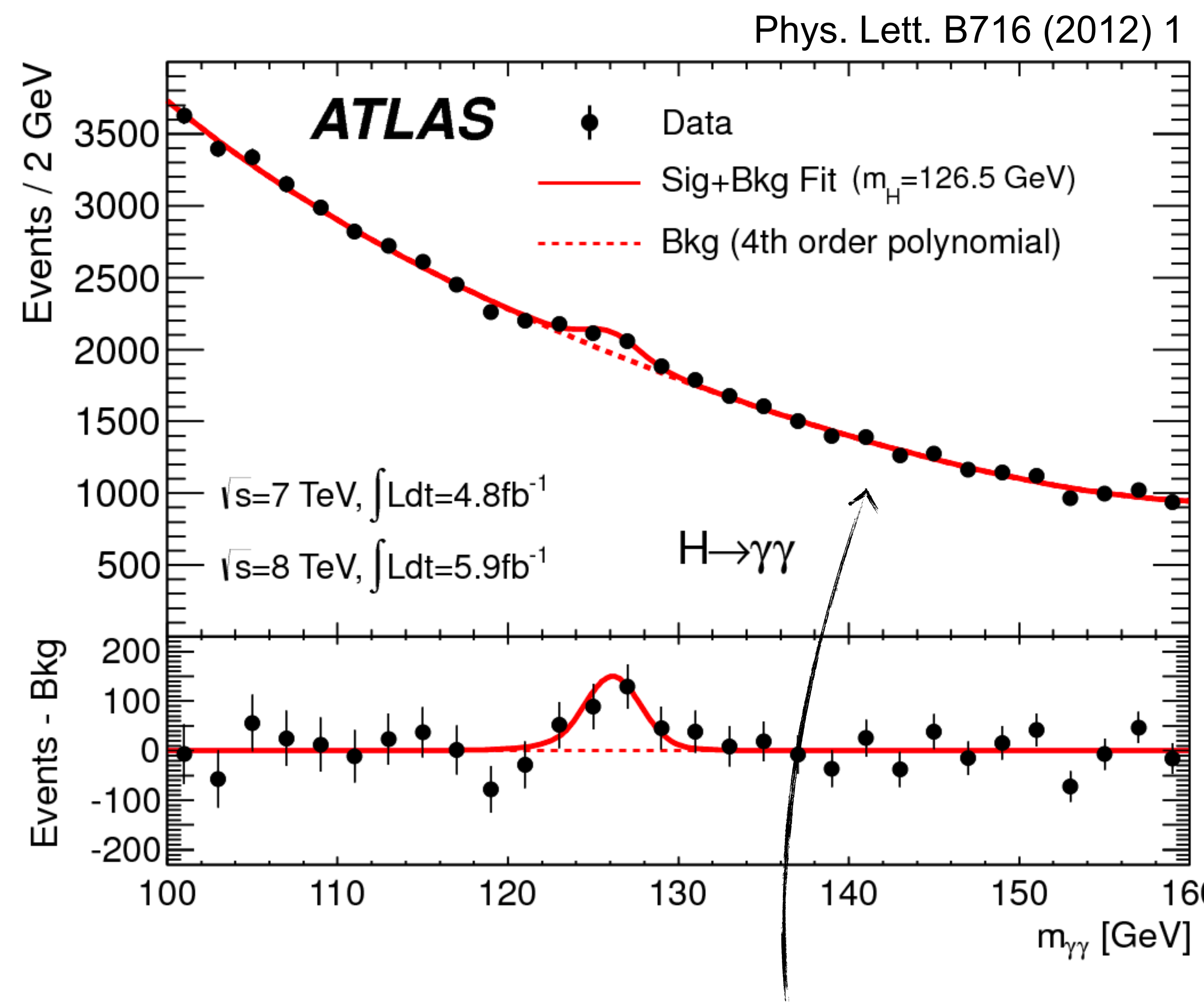


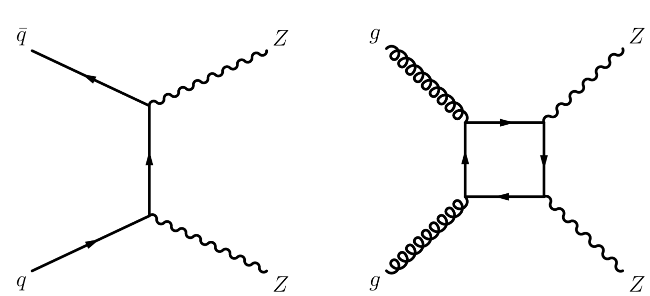


di-photon, photon+jet, jet+jet

Observing the Higgs boson







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Trying to maximise data-driven input, e.g. signal side-bands

Parametric methods

Both ATLAS and CMS $H \to \gamma\gamma$ use parametric methods

- Also $H \to \mu\mu$, $H \to Z\gamma$, $H \to bb\gamma\gamma$, etc

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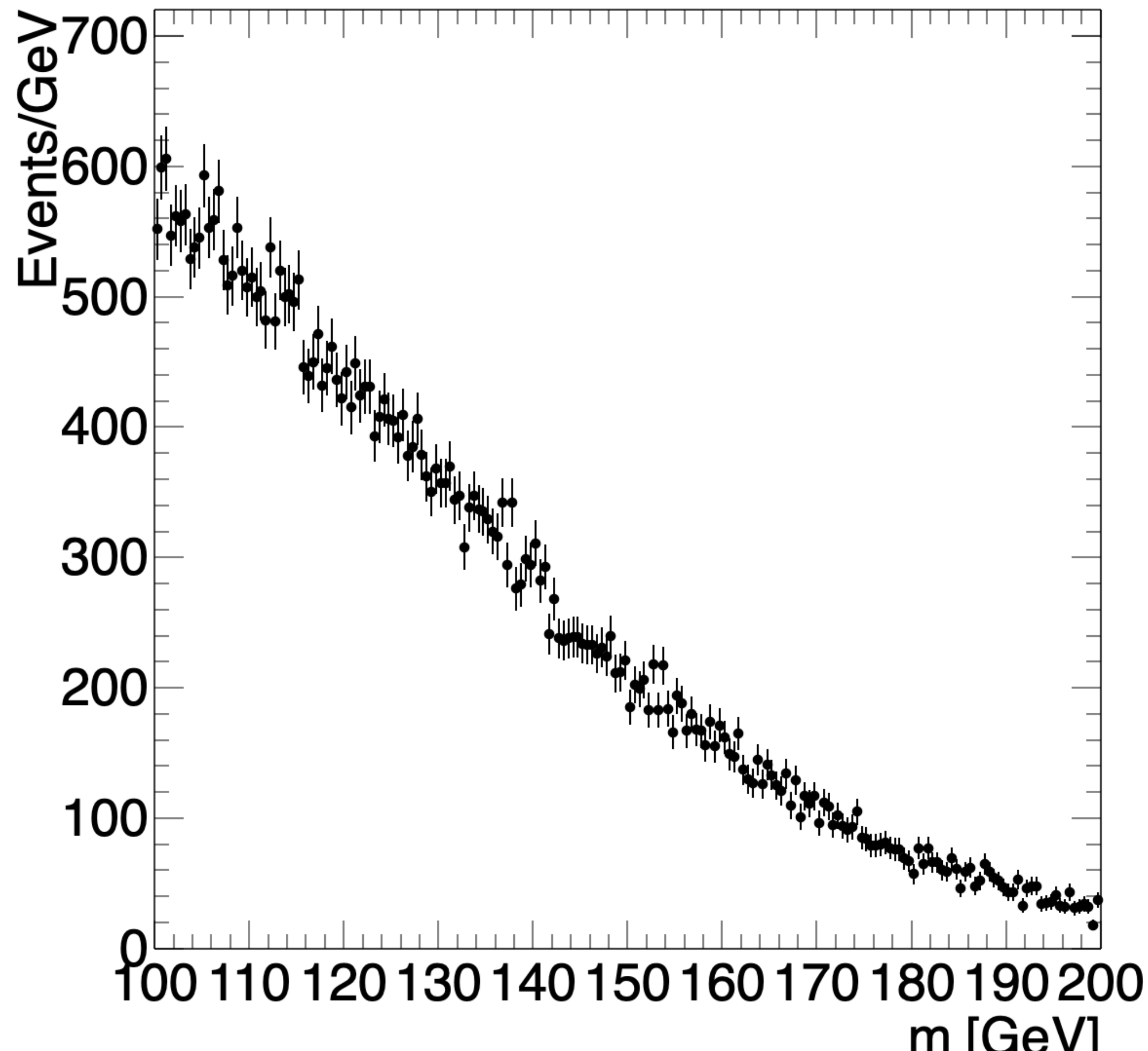

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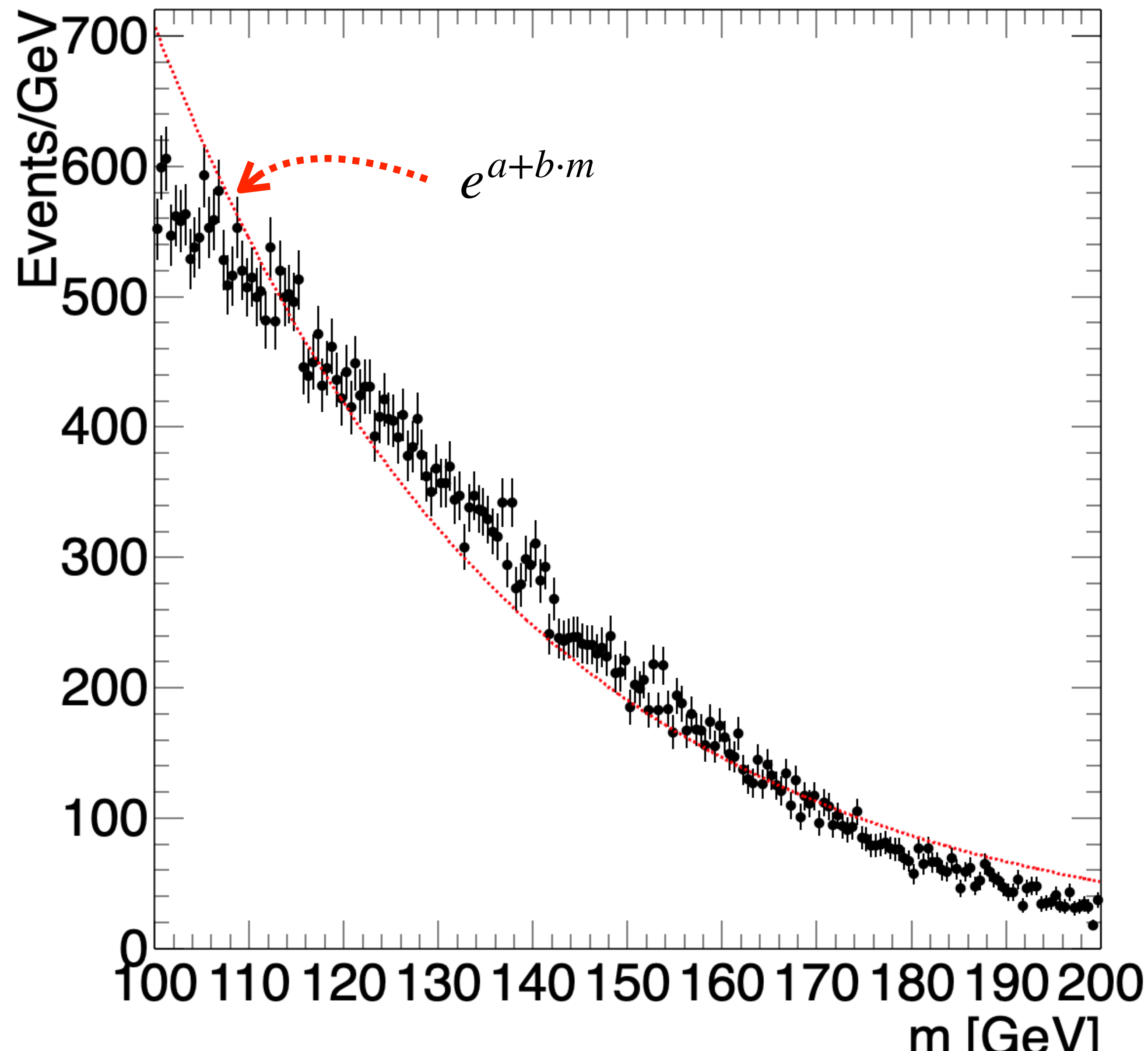

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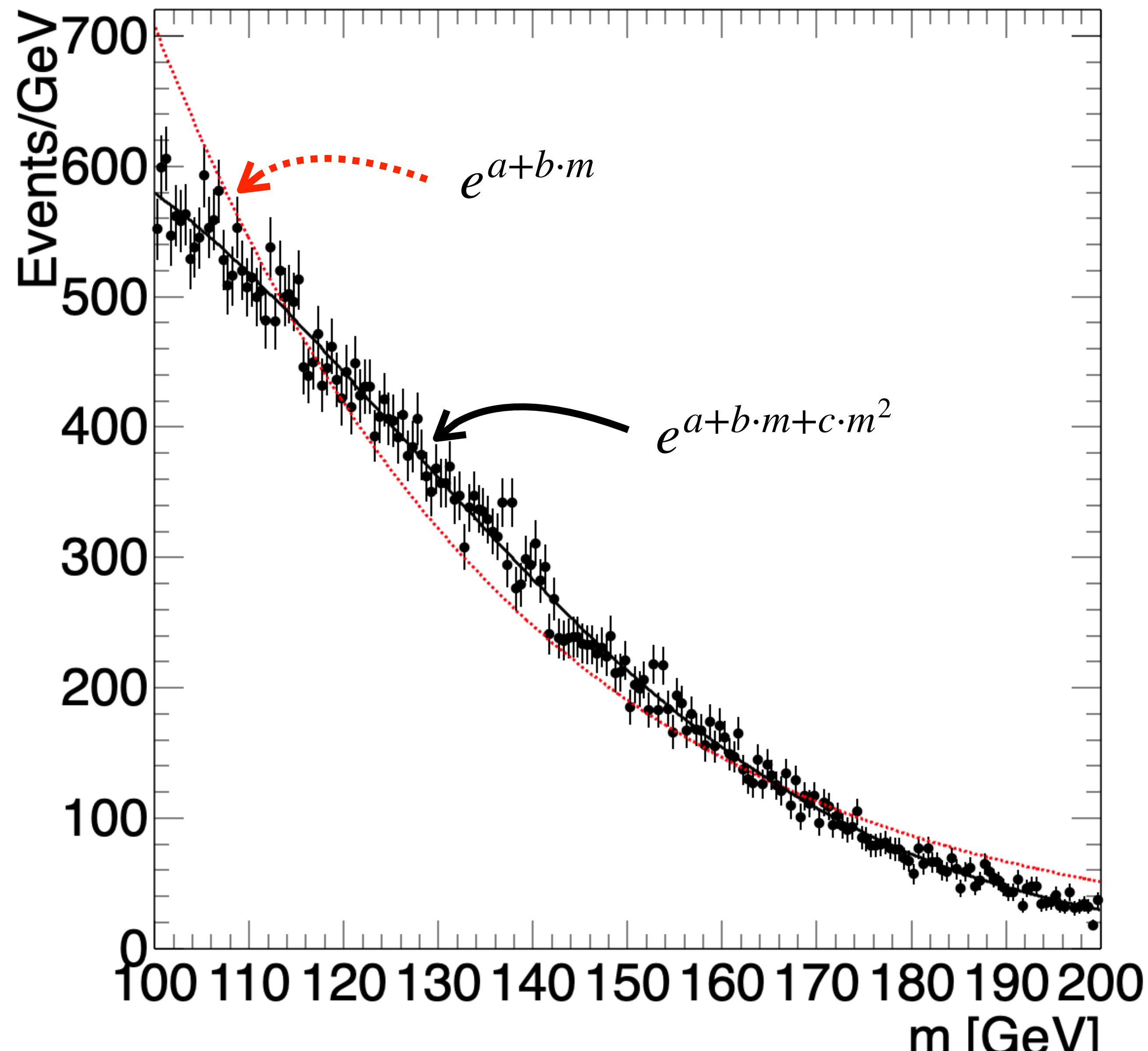

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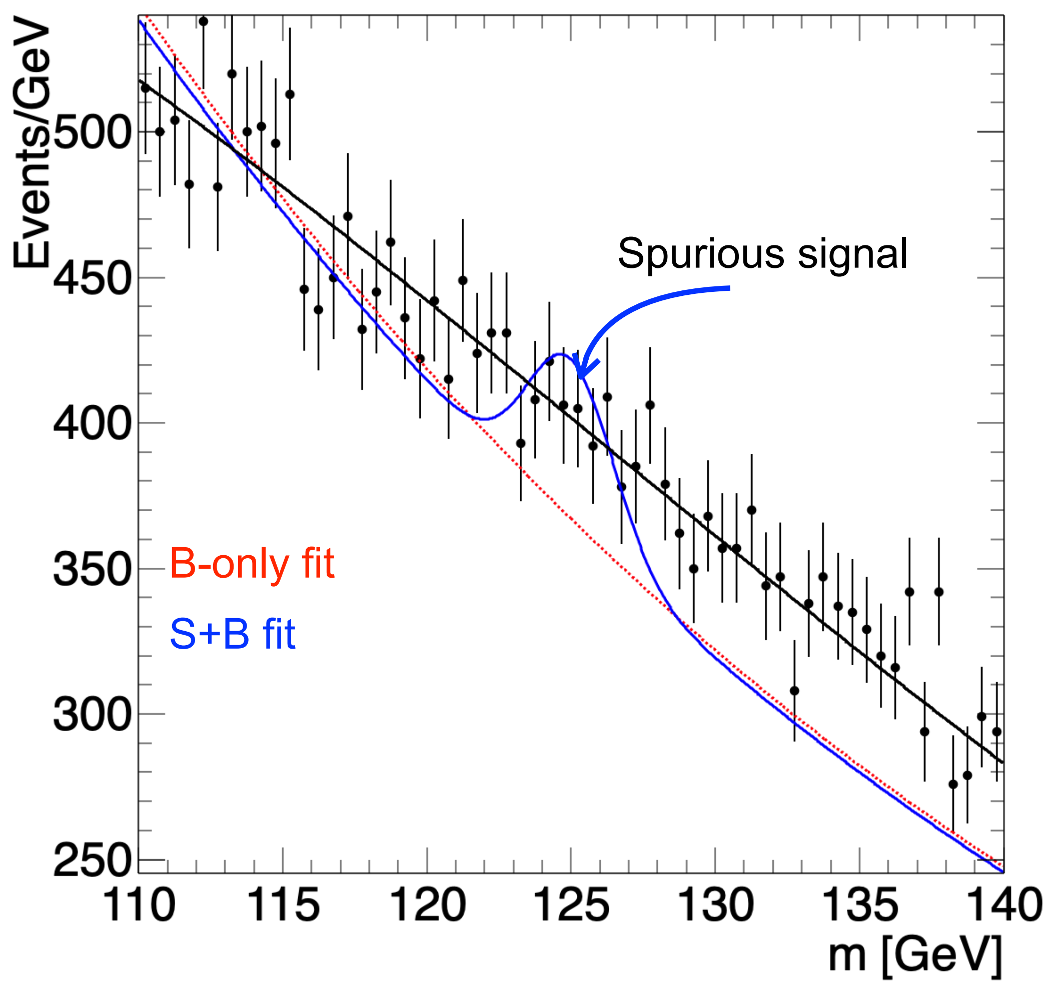

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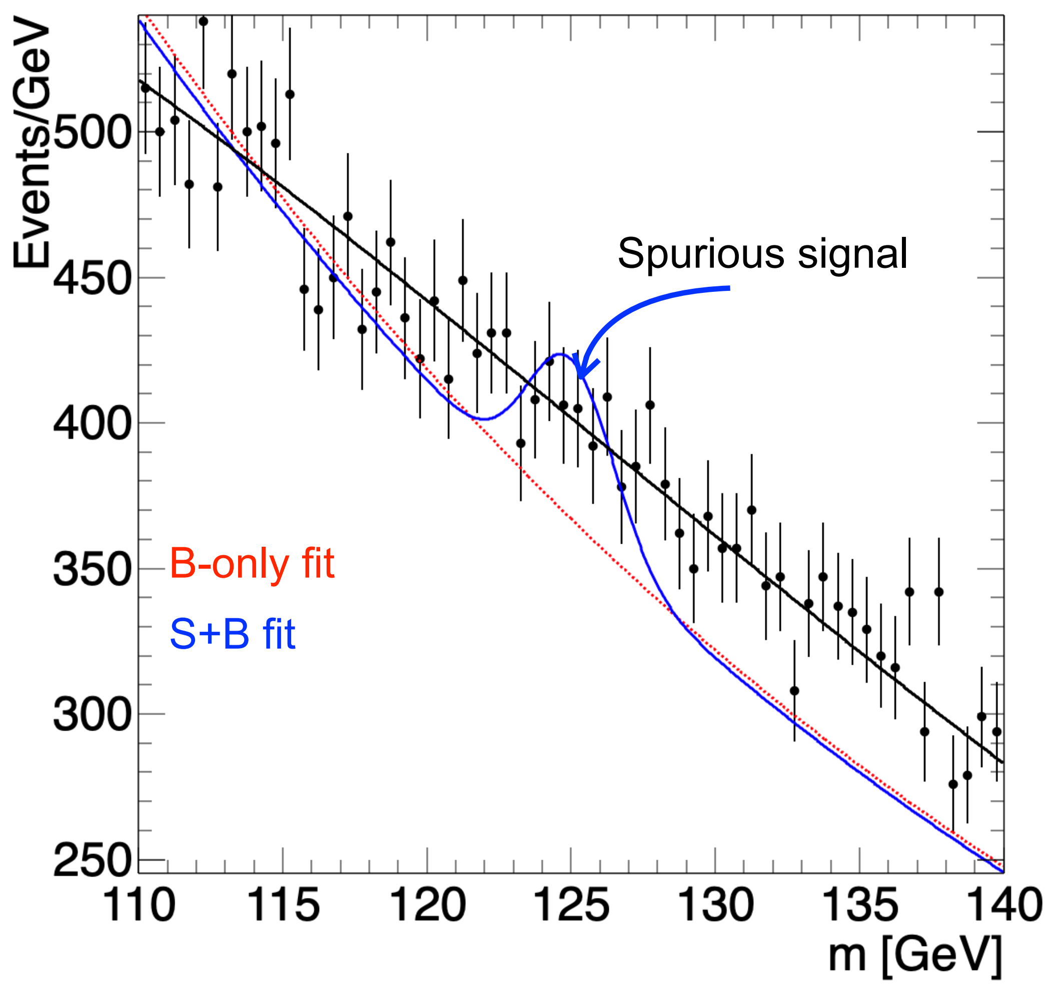

Challenges:

- **Conceptual:** use MC sample not deemed reliable for modelling the background
- **Practical:** required MC sample orders of magnitude larger than dataset of interest

Spurious signal

H→γγ inclusive fiducial cross section measurement uncertainties

Source	Uncertainty (%)
Fit (stat.)	10
Fit (syst.)	8.3
Photon energy scale & resolution	4.0
Background modeling (spurious signal)	7.3
Correction factor	5.2
Photon isolation efficiency	4.6
Pileup	1.9
Photon ID efficiency	1.3
Trigger efficiency	0.7
Dalitz Decays	0.4
Theoretical modeling	$^{+0.3}_{-0.4}$
Diphoton vertex selection	0.1
Photon energy scale & resolution	0.1
Luminosity	2.0
Total	14

ATLAS-CONF-2018-028

Higgs boson mass measurement with H→ZZ→4l and H→γγ

Source	Systematic uncertainty in m_H [MeV]
EM calorimeter response linearity	60
Non-ID material	55
EM calorimeter layer intercalibration	55
$Z \to ee$ calibration	45
ID material	45
Lateral shower shape	40
Muon momentum scale	20
Conversion reconstruction	20
$H \to \gamma\gamma$ background modelling	20
$H \to \gamma\gamma$ vertex reconstruction	15
e/γ energy resolution	15
All other systematic uncertainties	10

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Discrete Profiling Method

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- Combine different parametric models at the likelihood level
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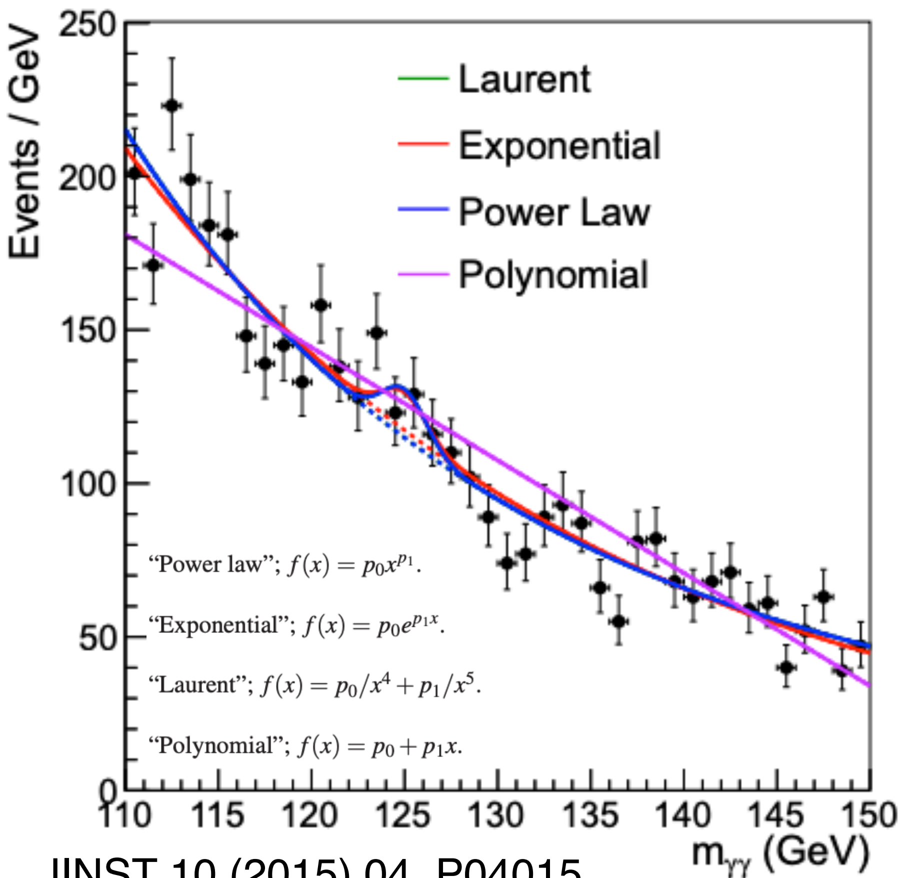

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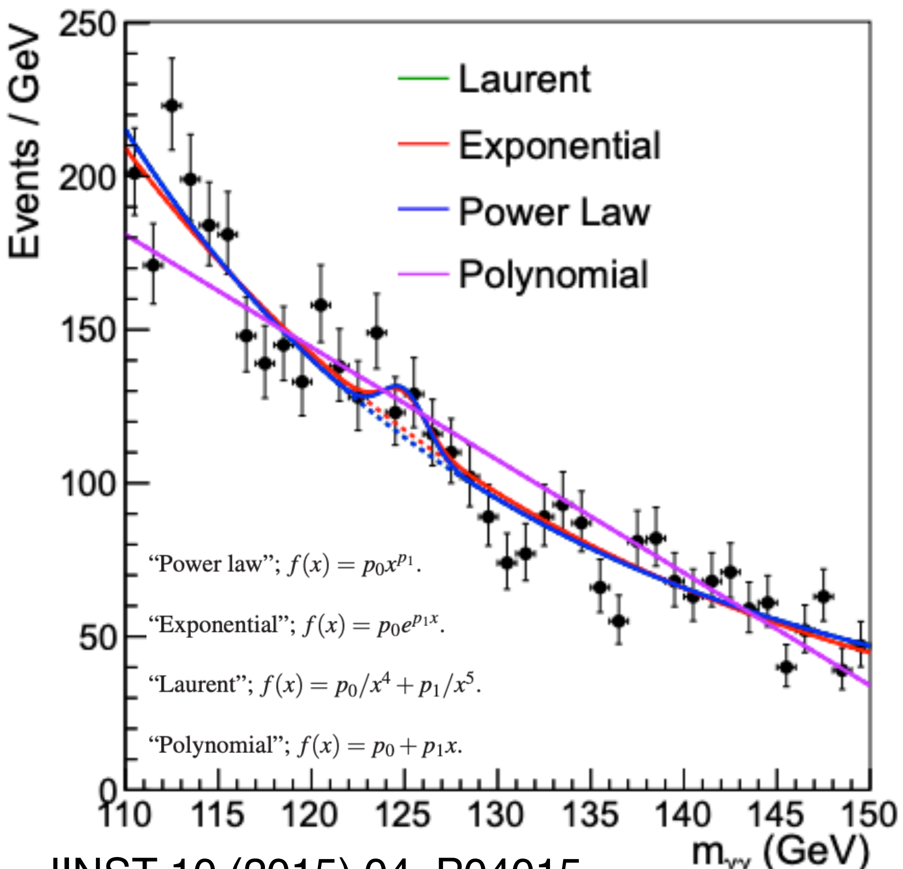

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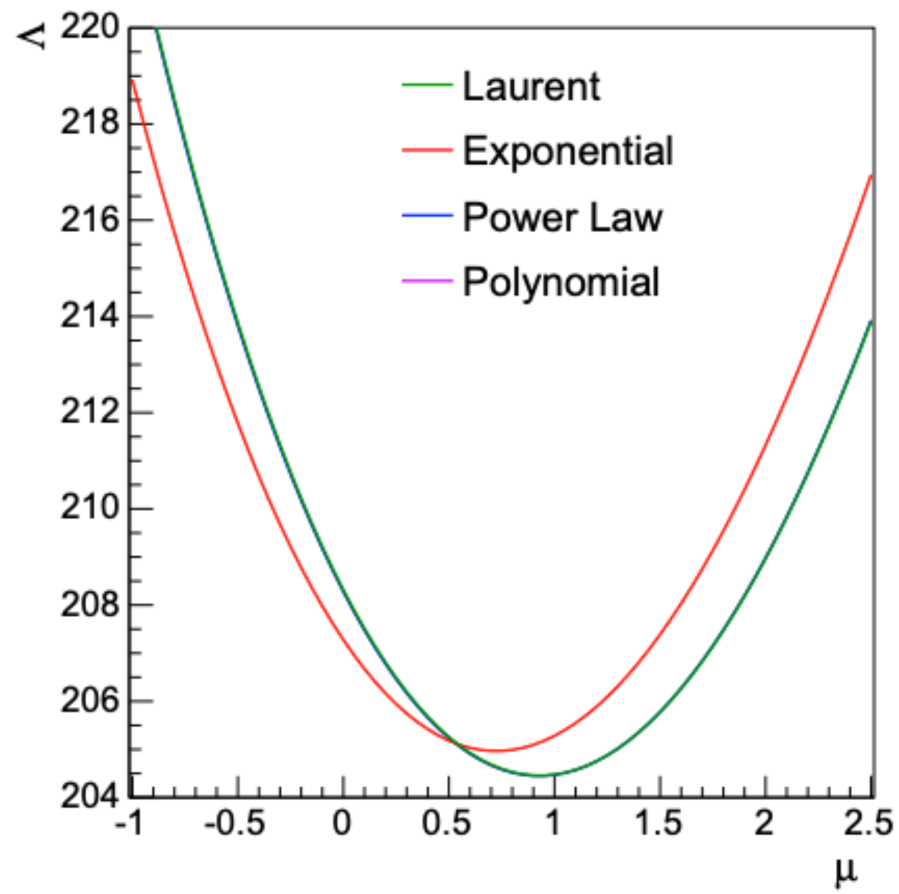

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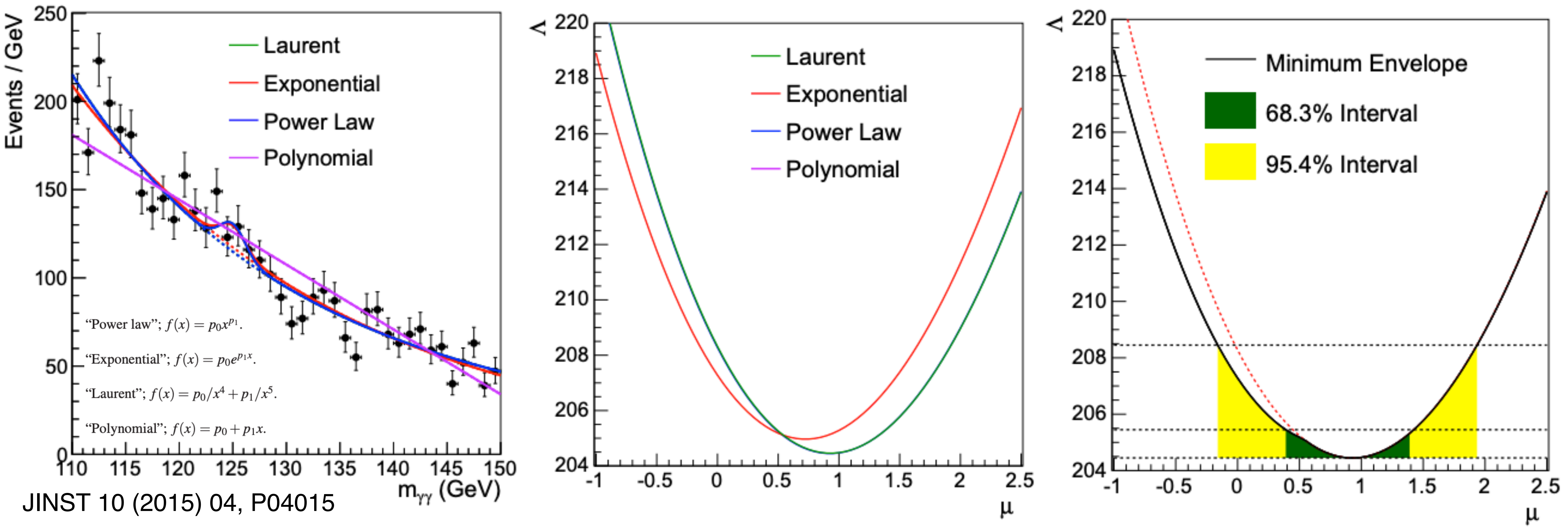

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Practical and conceptual complications when models have different N_{par}

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Correction: penalise functions with more parameters

- Inspired by p-value and Akaike information criterion
- Parametrised as $\Lambda_{corr} = \Lambda + cN_{par}$
- Bias vs coverage trade-off versus c studied case-by-case

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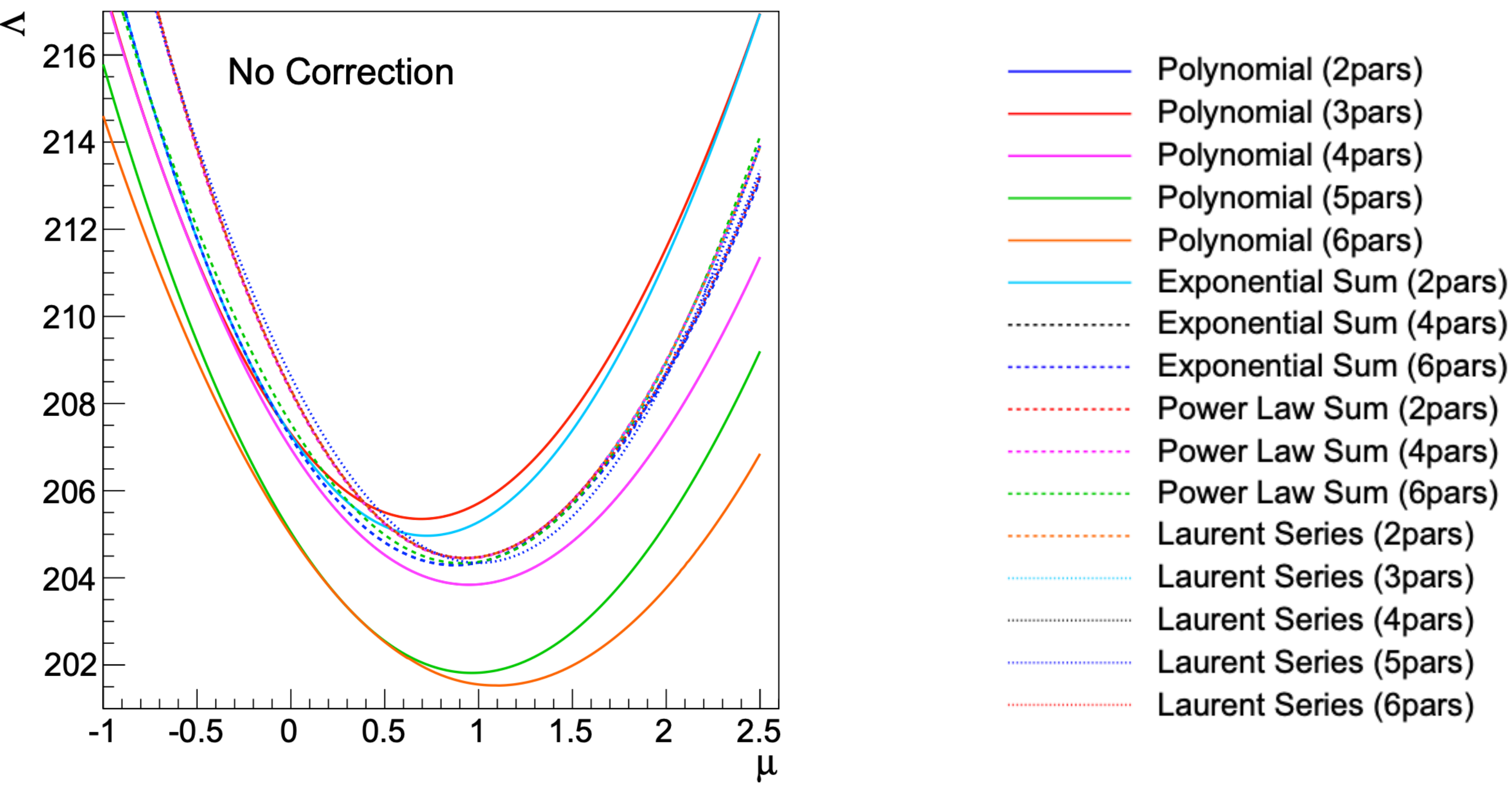

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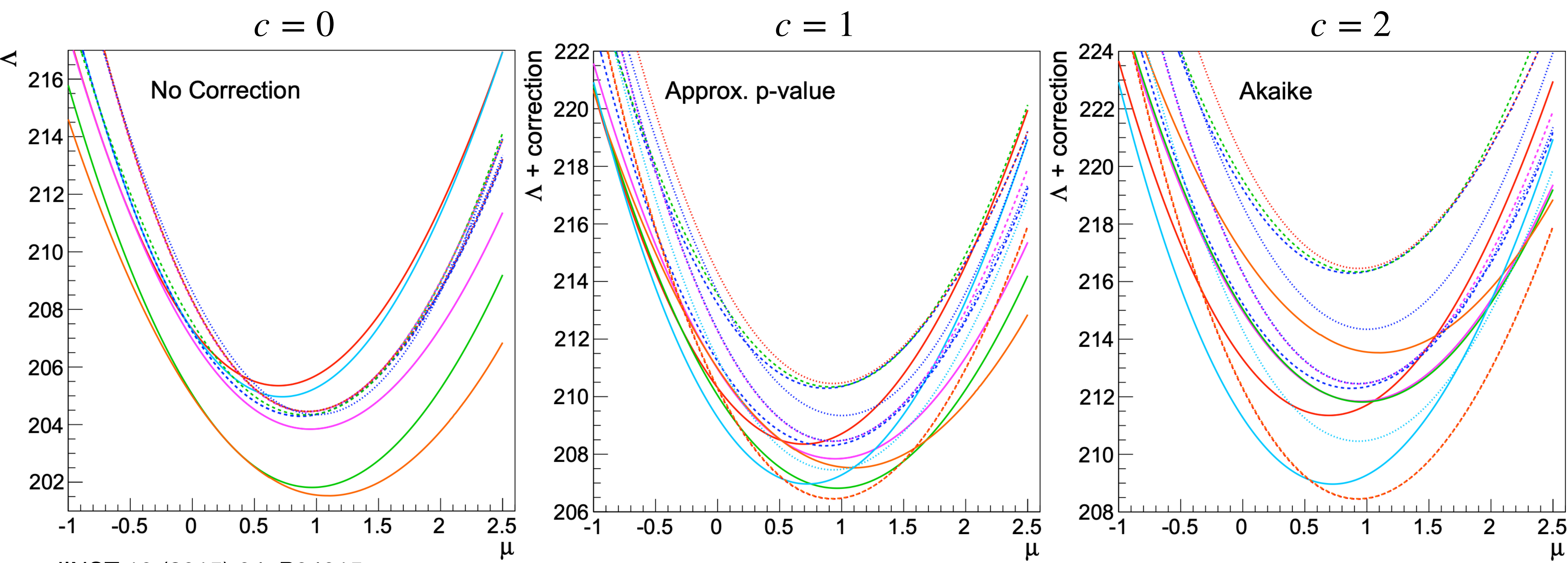

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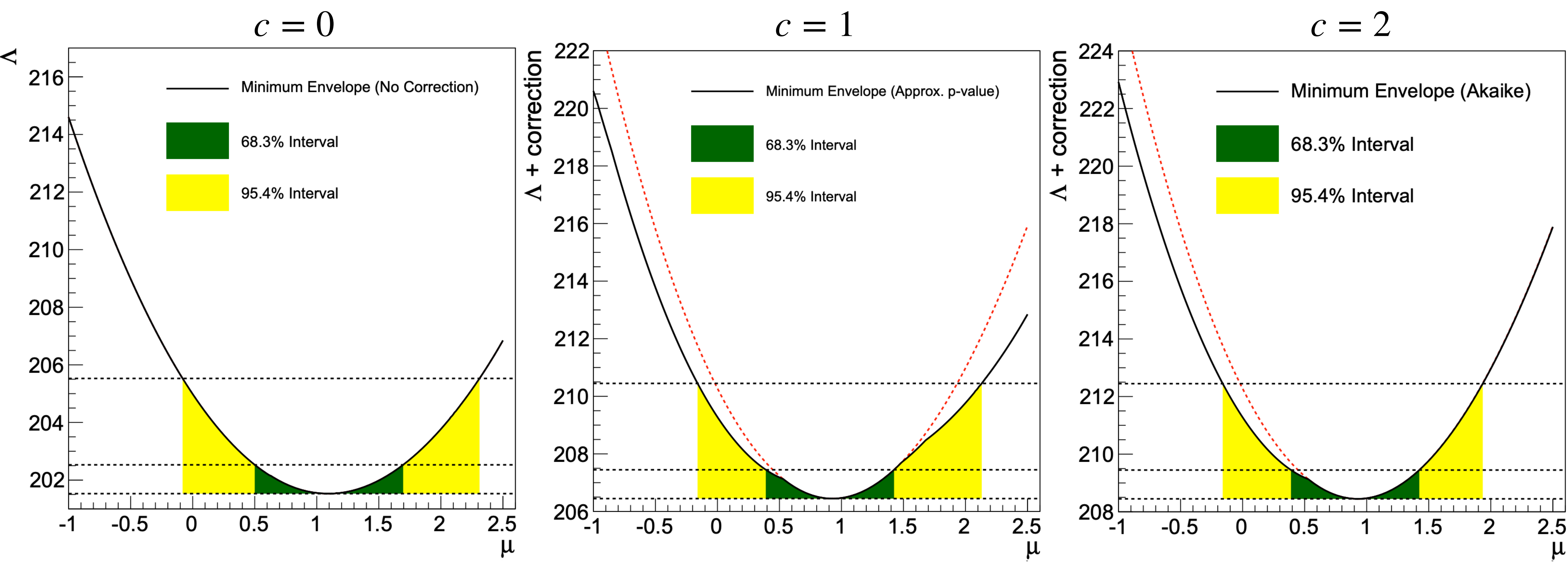

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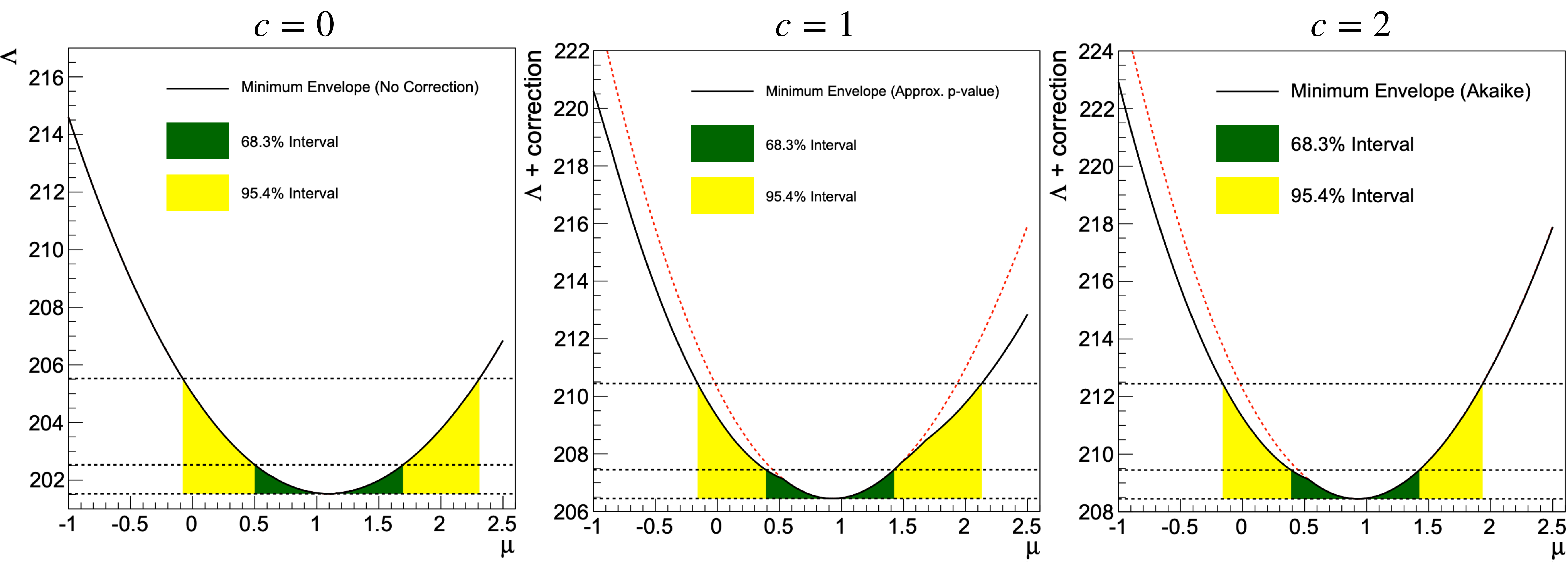

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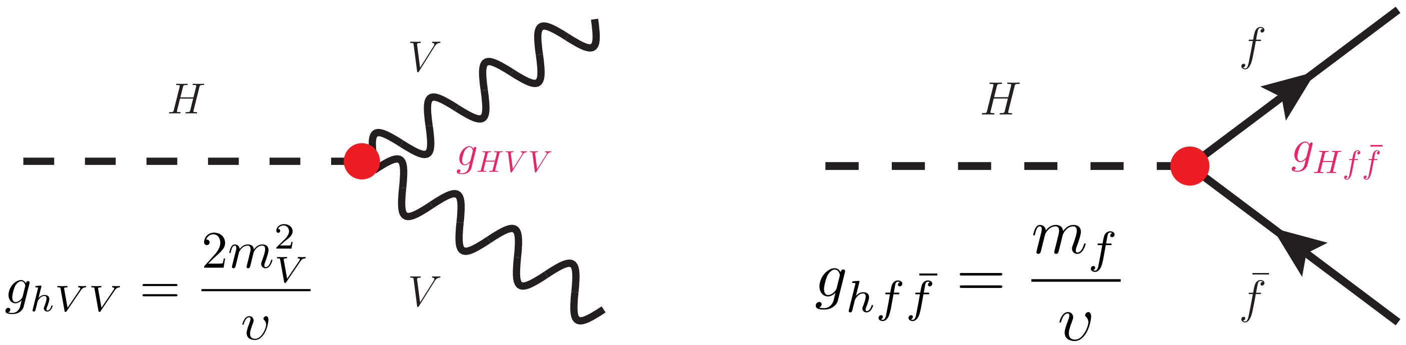
Common systematic effects across categories: All combinations of functions and nuisance parameters need to be scanned

→Naive implementation impractical and usually approximations used.

Higgs-fermion interactions

- **Higgs interactions to vector bosons:** defined by symmetry breaking
- **Higgs interactions to fermions:** ad-hoc hierarchical Yukawa couplings $\propto m_f$



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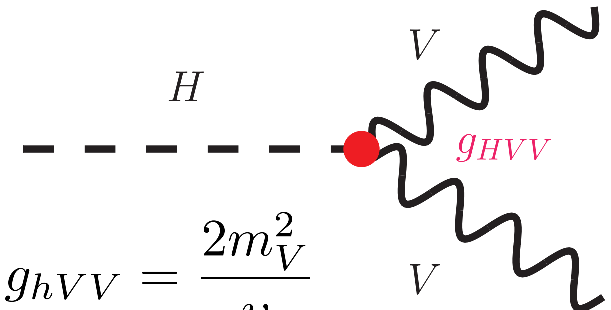

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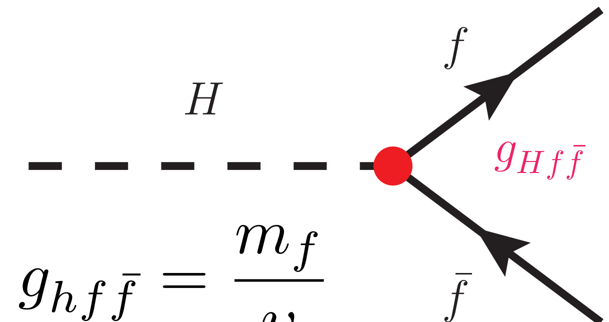

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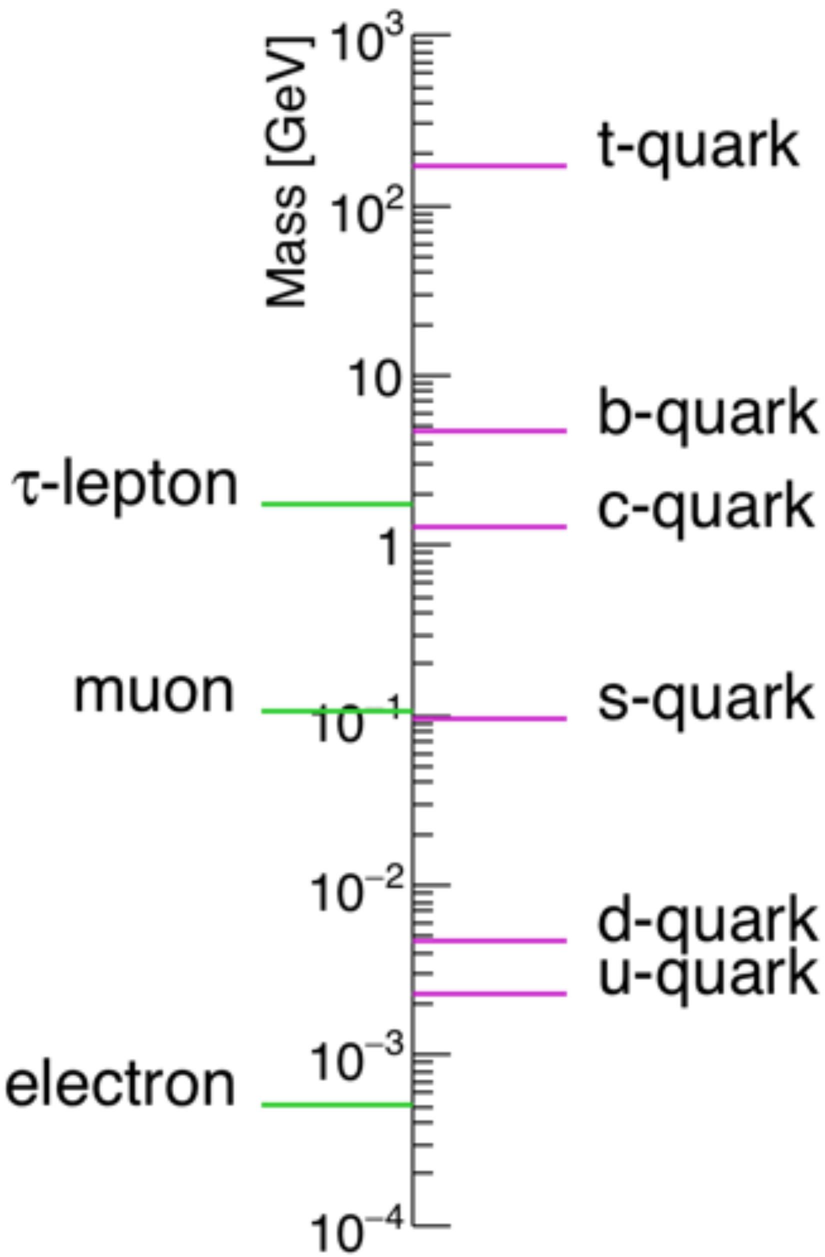

$$\frac{m_e}{m_t} \approx 3 \times 10^{-6}$$

- Yukawa couplings **not** imposed by fundamental principle
- Modified Higgs-fermion couplings in BSM scenarios
- Probing fermion mass generation scale→independent task

Standard Model successful

but matter particle mass

hierarchy unexplained!

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Extended Higgs sectors

- The Standard Model **Higgs sector is an $SU(2)_L$ doublet of complex scalar fields:** this is the most economic way to obtain spontaneous symmetry breaking
- **Extended Higgs sectors** are possible, and can potentially provide answers to a number of open questions
- The ρ parameter puts tight constraints on model viability
  - For SM ρ=1 (with small corrections)
  - Constraints naturally fulfilled for appropriate configurations of scalar singlets and doublets

$$\rho = \frac{M_W^2}{M_Z^2 \cos^2\theta_W} = 1.00039 \pm 0.00019$$

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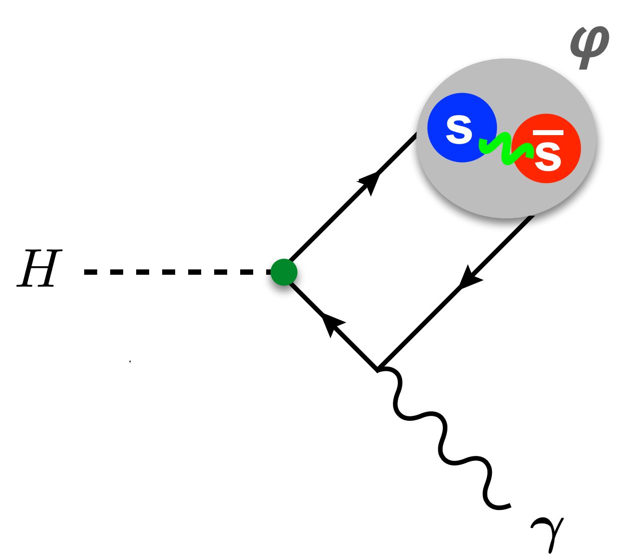
$$\rho = \frac{M_W^2}{M_Z^2 \cos^2\theta_W} = 1.00039 \pm 0.00019$$

- A number of possibilities with **rich phenomenology**:
  - Higgs double with one or more scalar singlets,
  - Two Higgs Doublets (2HDM),
  - 2HDM with additional scalar singlet (2HDM+S)
- Particularly interesting: additional scalar lighter than observed Higgs boson.
  - $h \to aa$
  - $h \to Za$

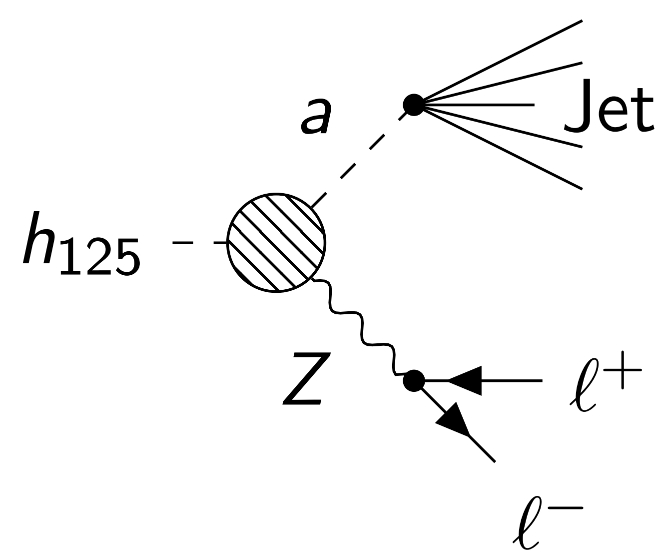
Searches for new physics

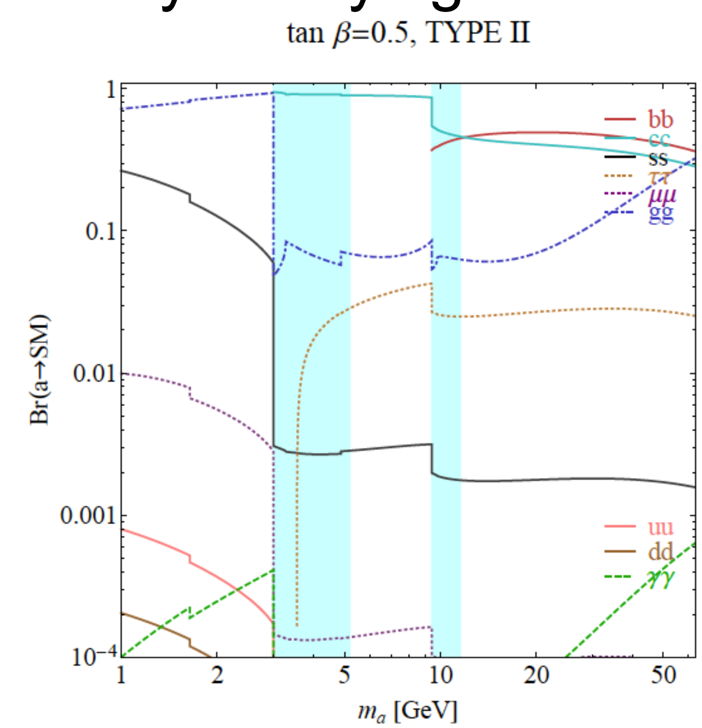
Exclusive Higgs decays



$$BR(h \to \phi\gamma) = (2.31 \pm 0.03_{f_\phi} \pm 0.11_{h\to\gamma\gamma}) \cdot 10^{-6}$$

Higgs decays to light hadronically decaying scalars





PRD 90 (2014) 7, 075004

These analyses share the challenge that the respective backgrounds are not straightforward to model with simulations.

Beyond Parametric Methods

Parametric methods have several advantages but also important issues

In the following: aim to develop **fully data-driven non-parametric background models**

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School of Physics and Astronomy, University of Birmingham, Birmingham, B15 2TT, United Kingdom

E-mail: andrew.chisholm@cern.ch, tom.neep@cern.ch, konstantinos.nikolopoulos@cern.ch, rhys.owen@cern.ch, elliot.reynolds@cern.ch, julia.manuela.silva@cern.ch

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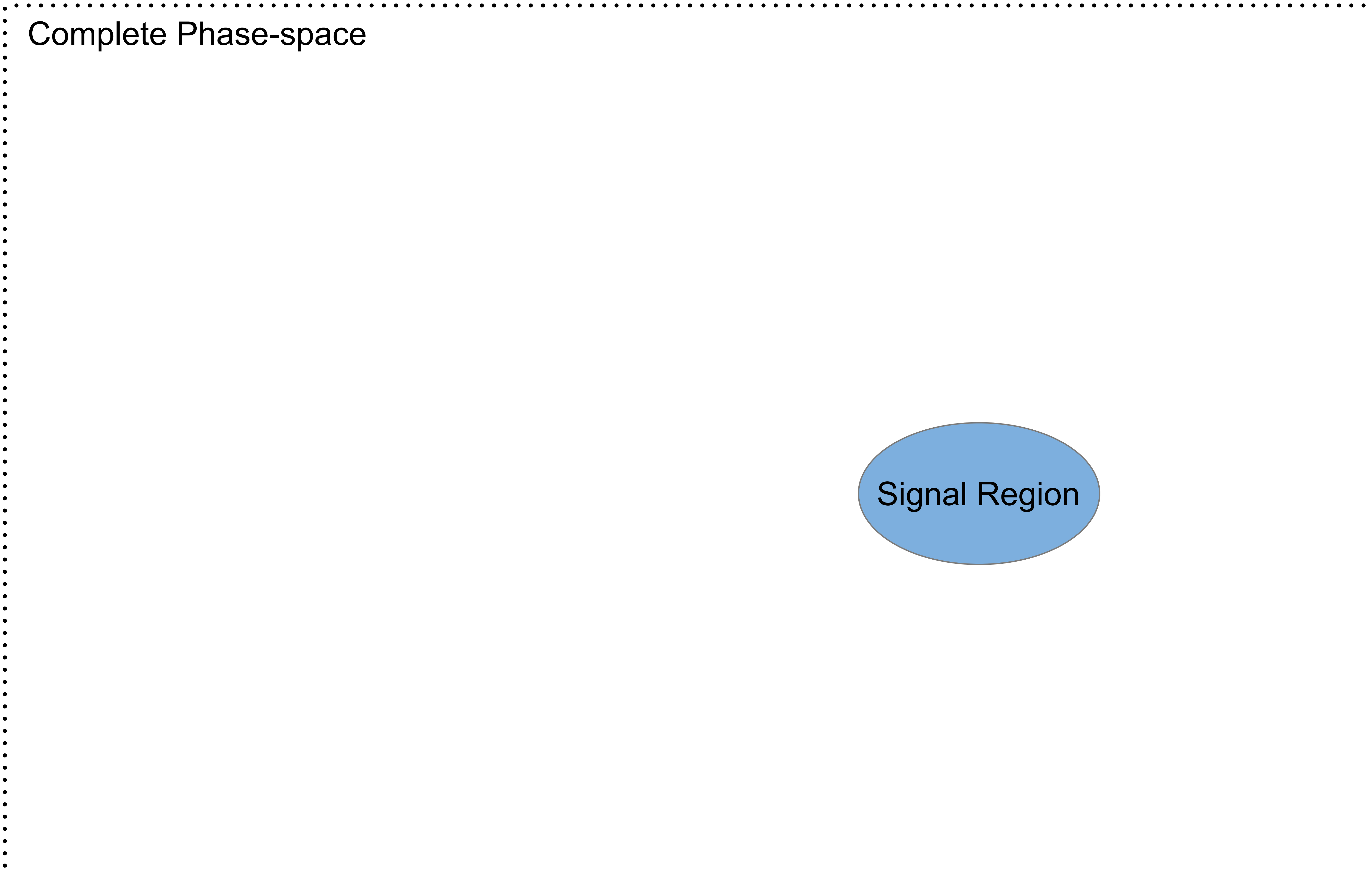
Methods motivated by specific analyses, but with wide applicability

The strategy

Complete Phase-space

The strategy



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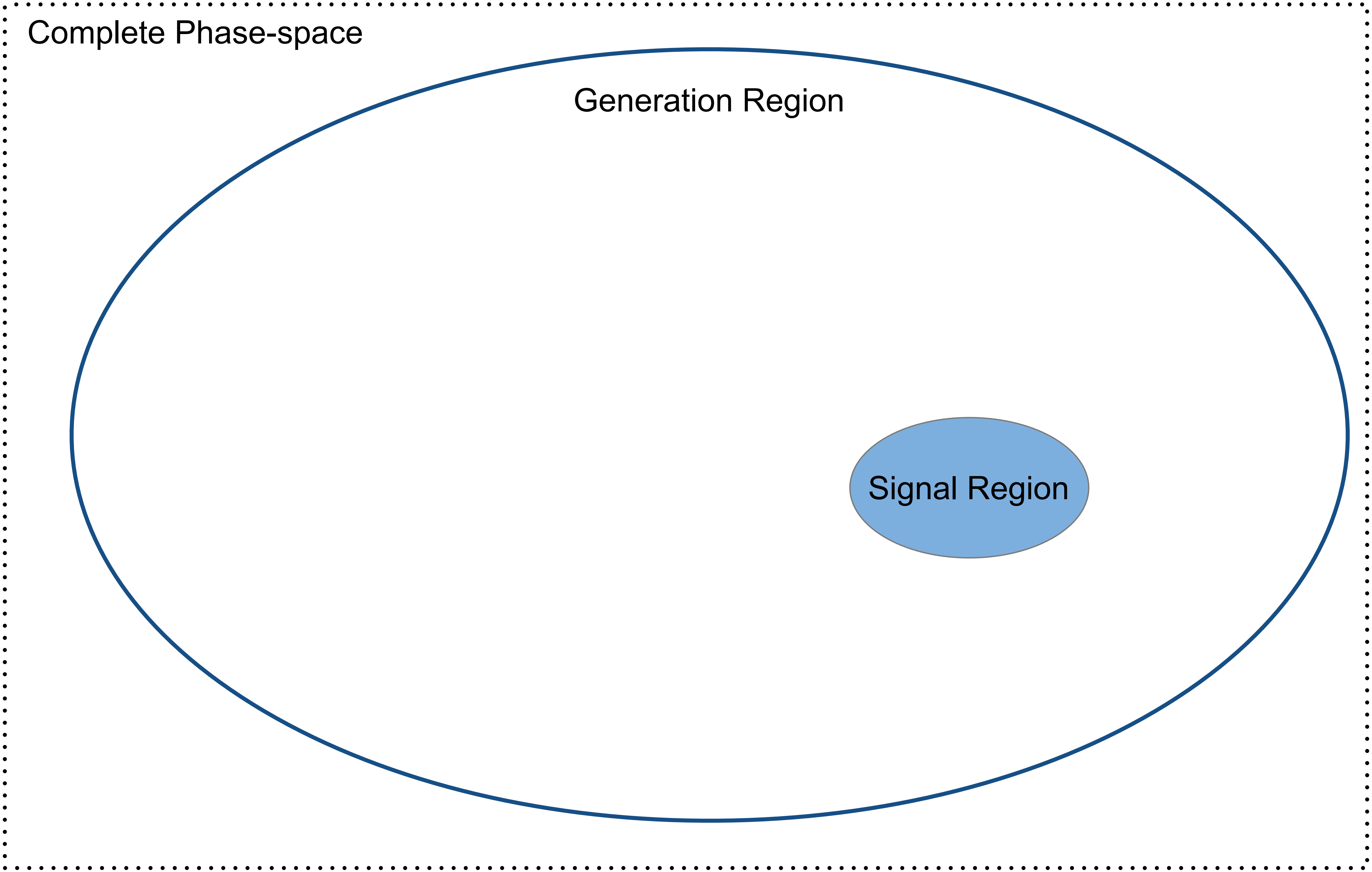

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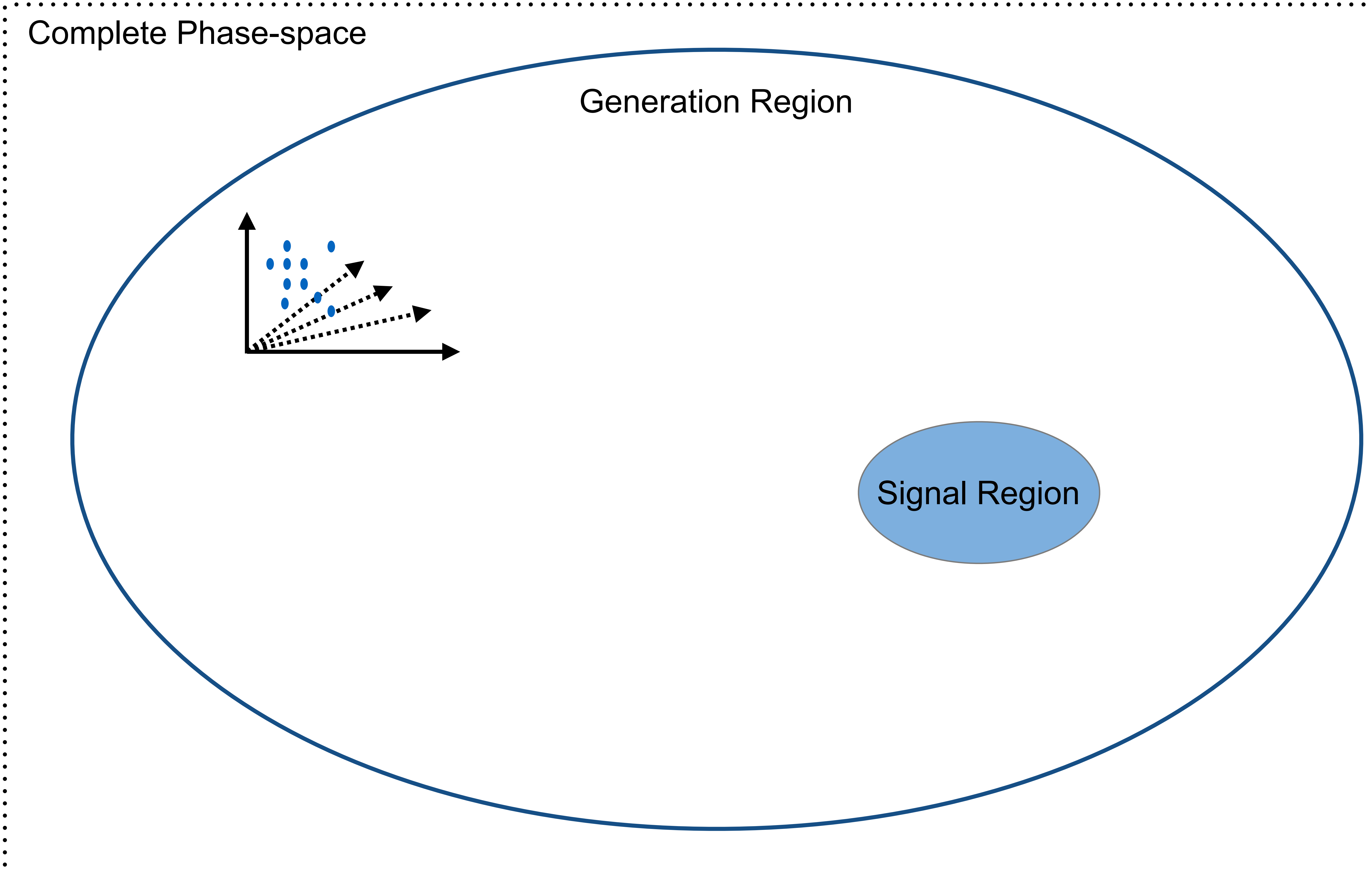

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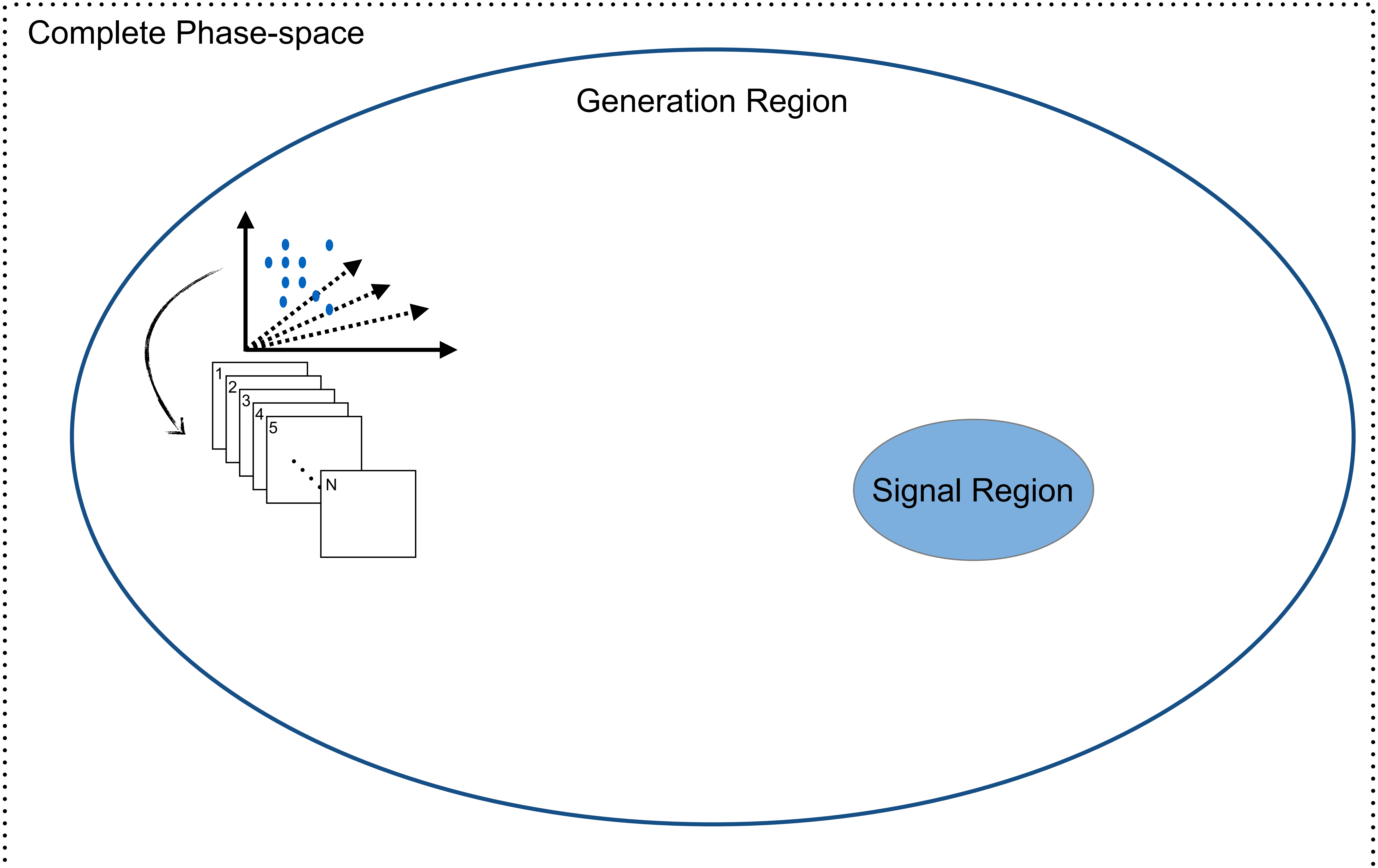

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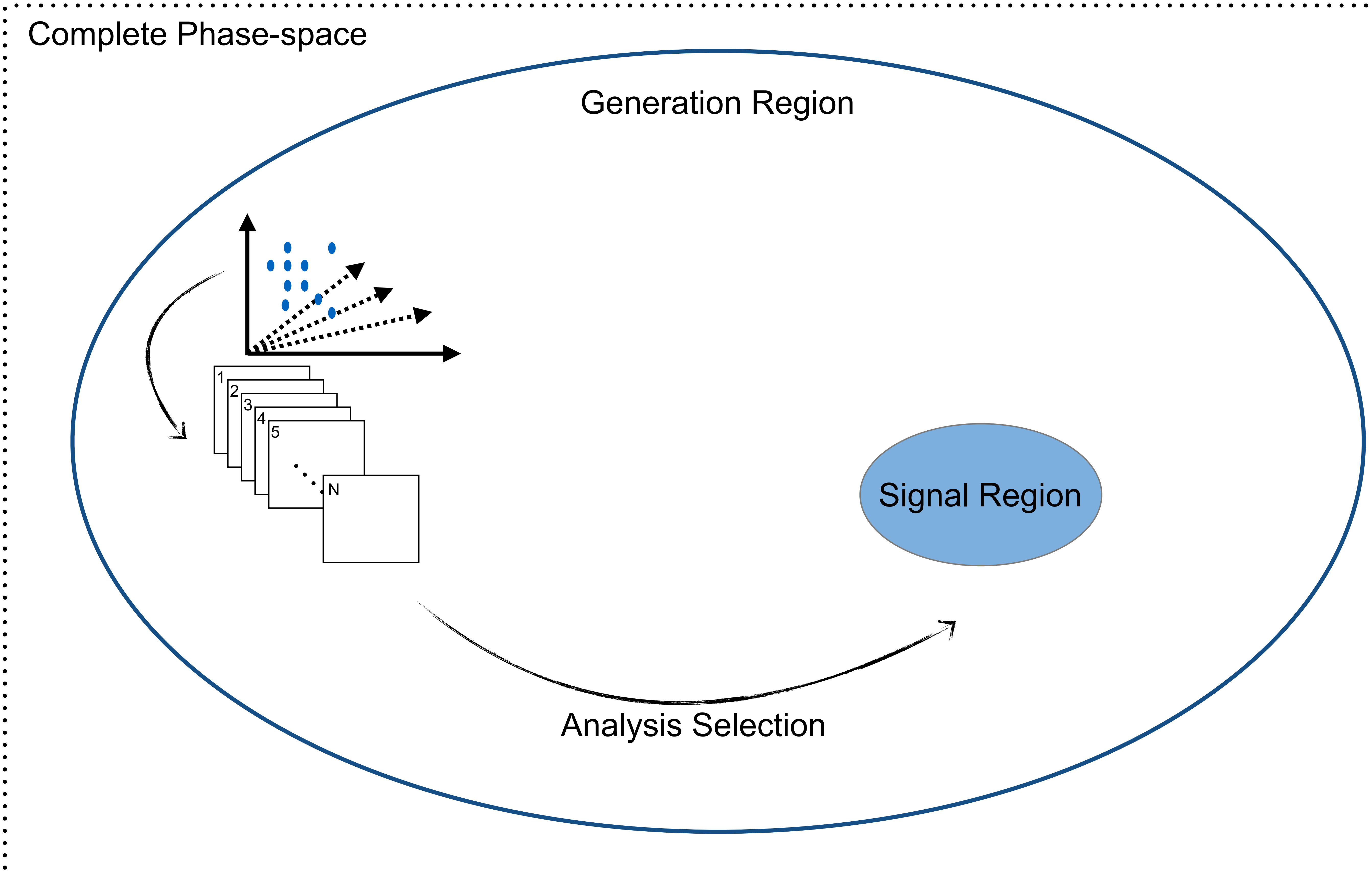

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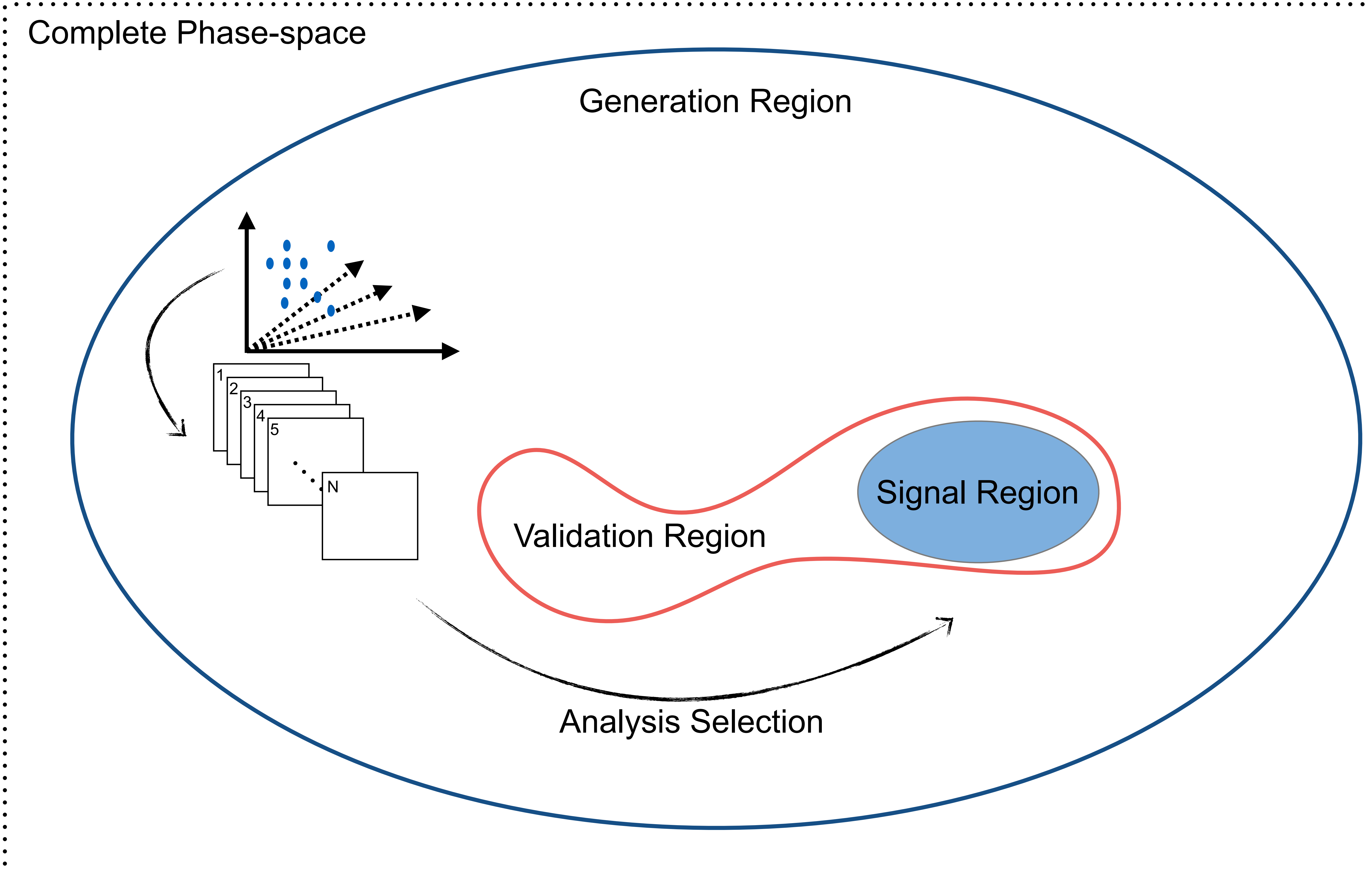

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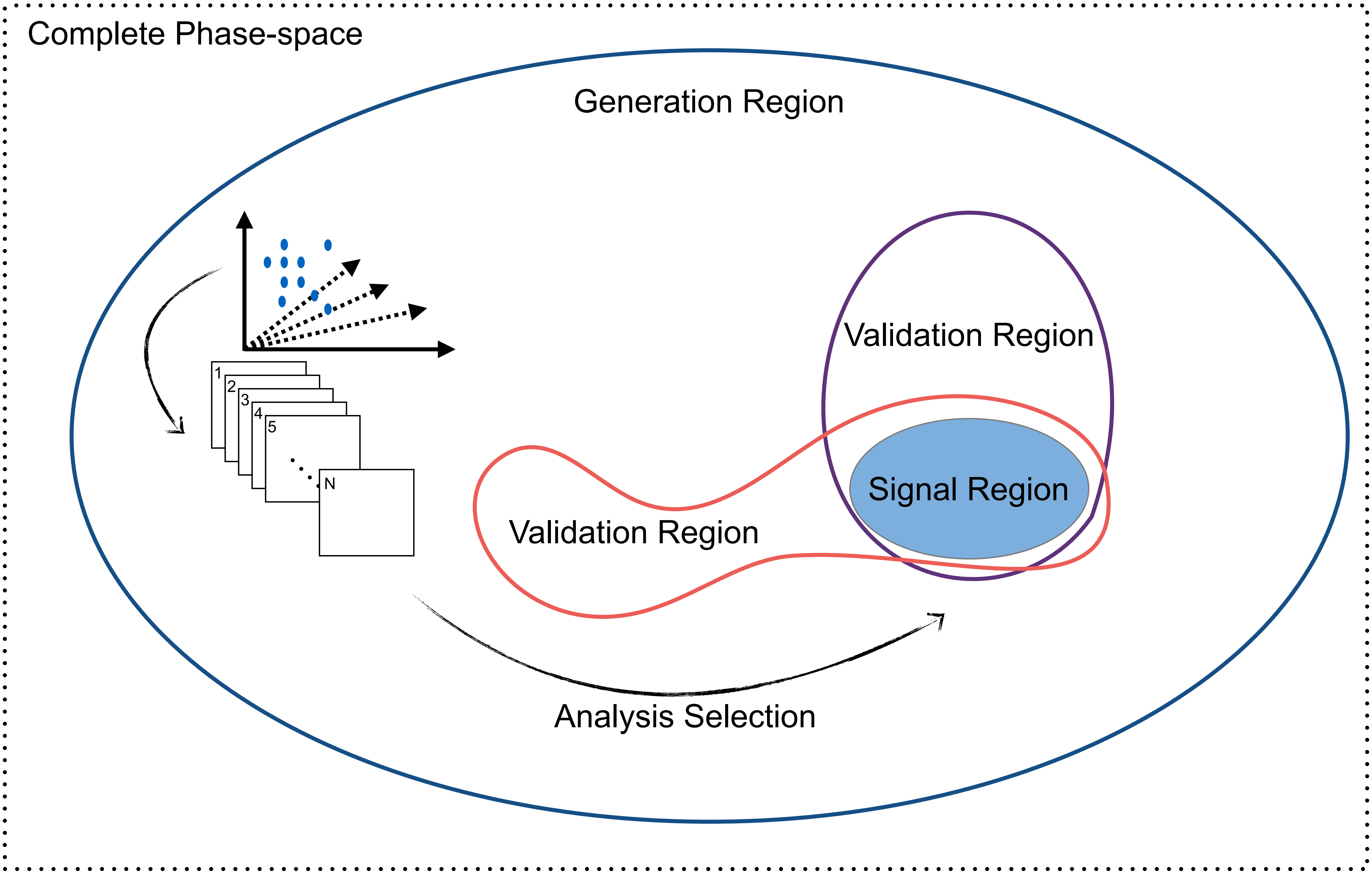

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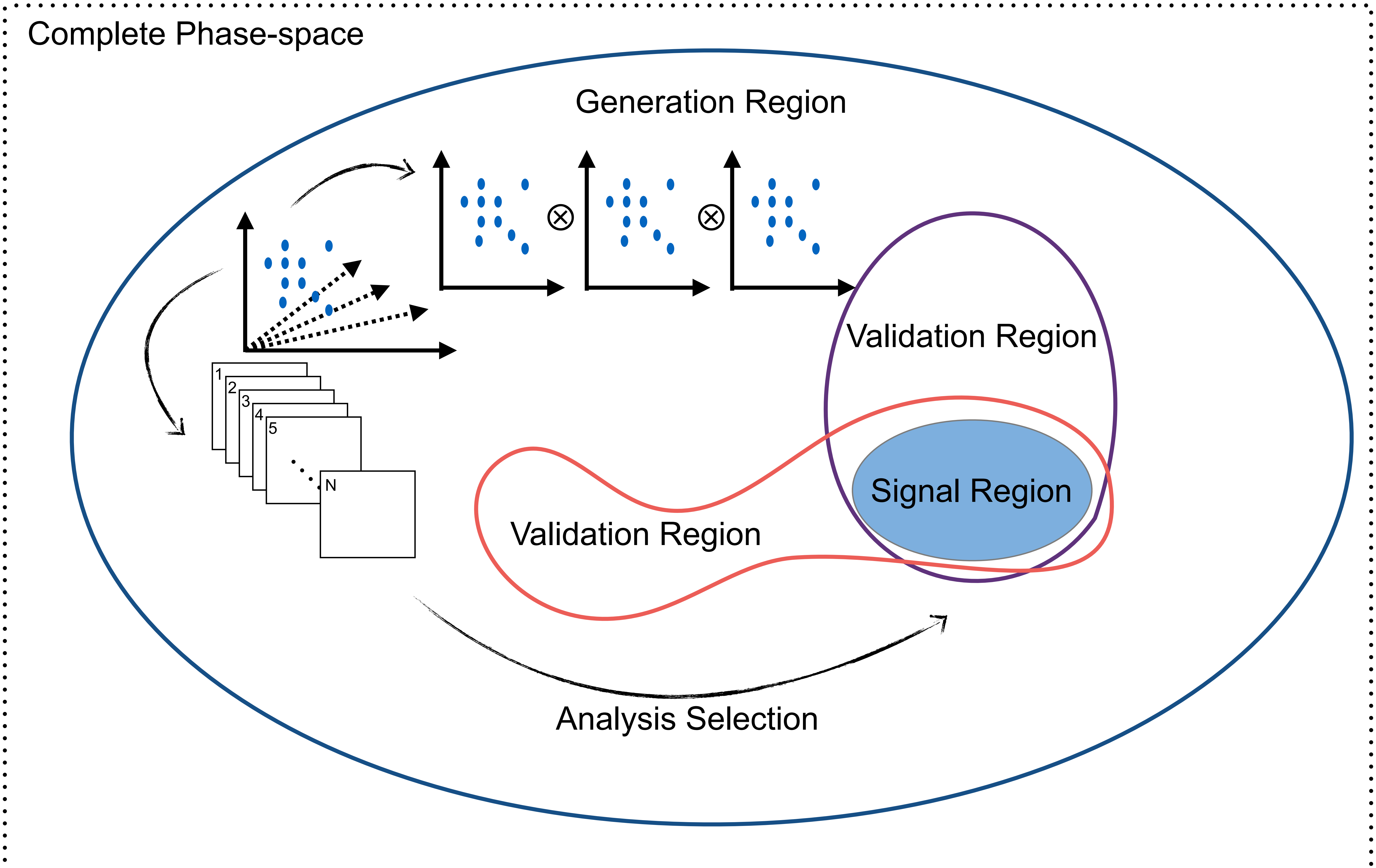

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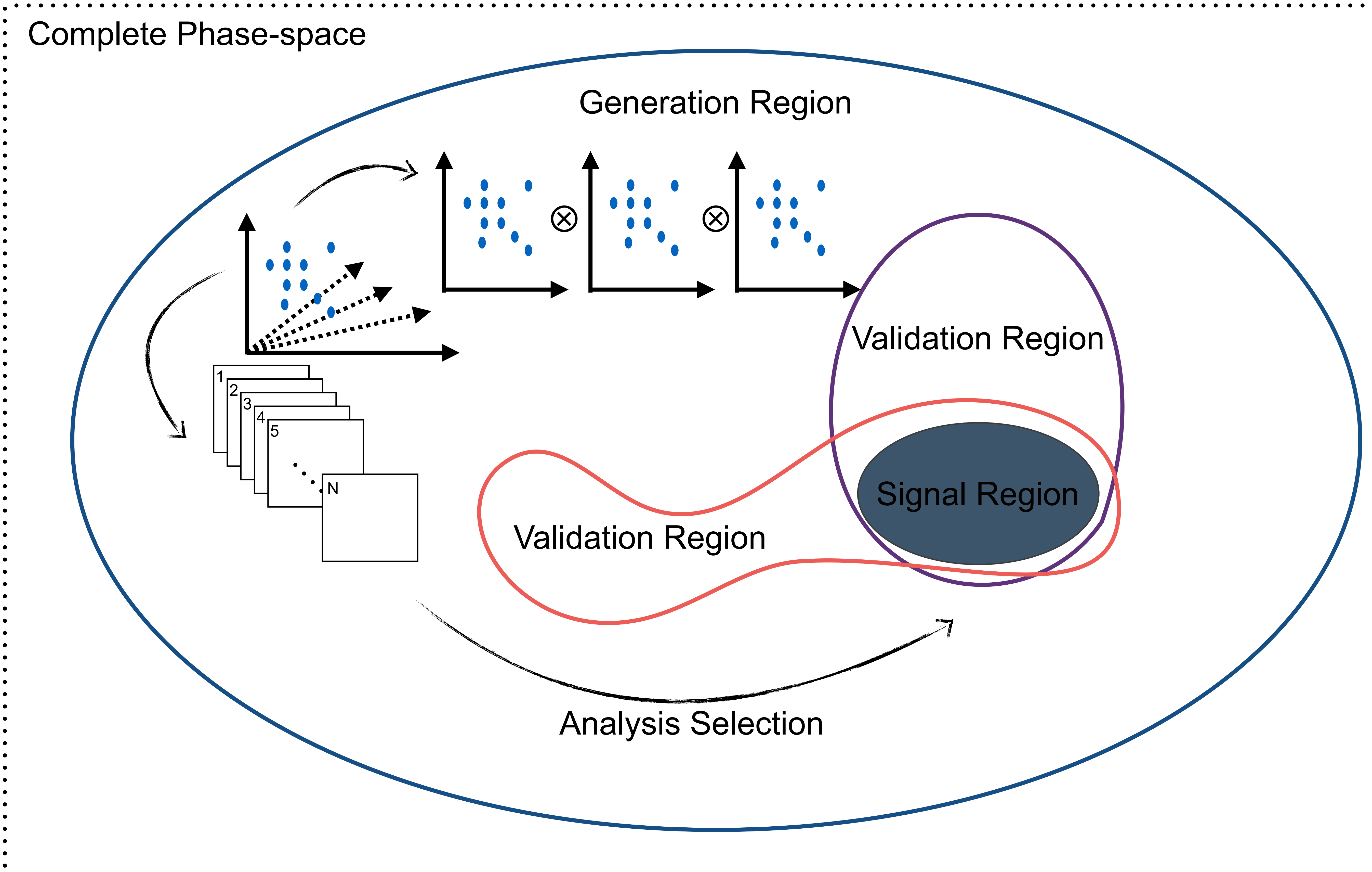
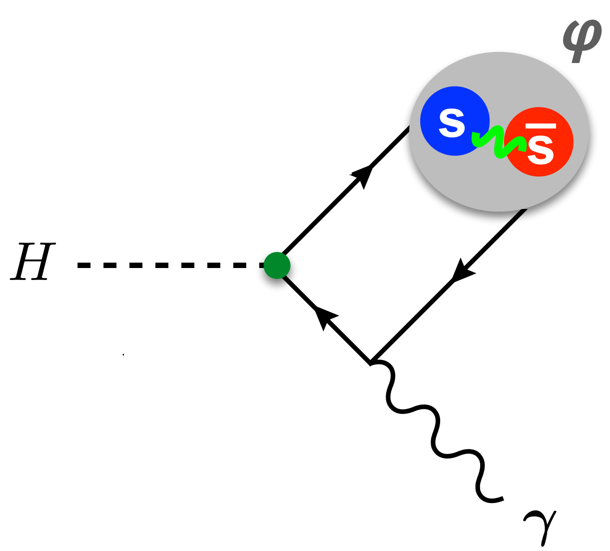


h/Z→ϕγ/ργ

Exclusive Higgs decays

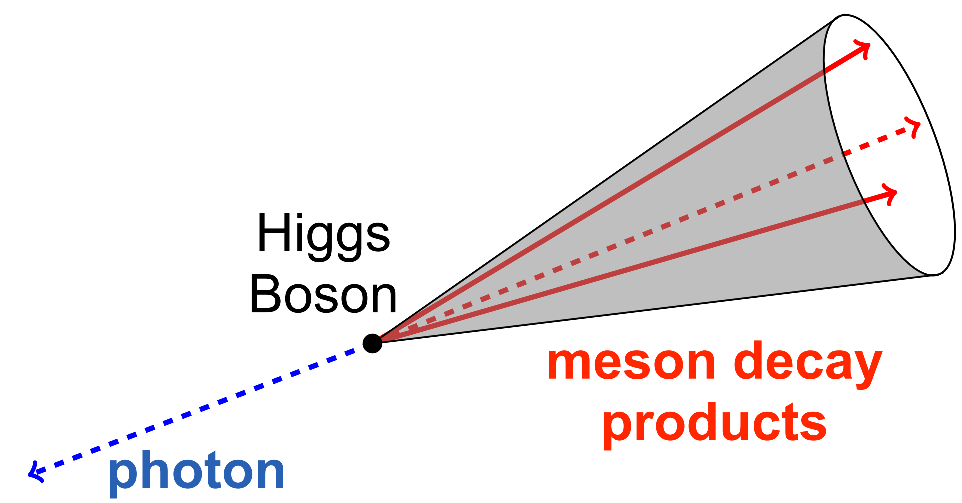


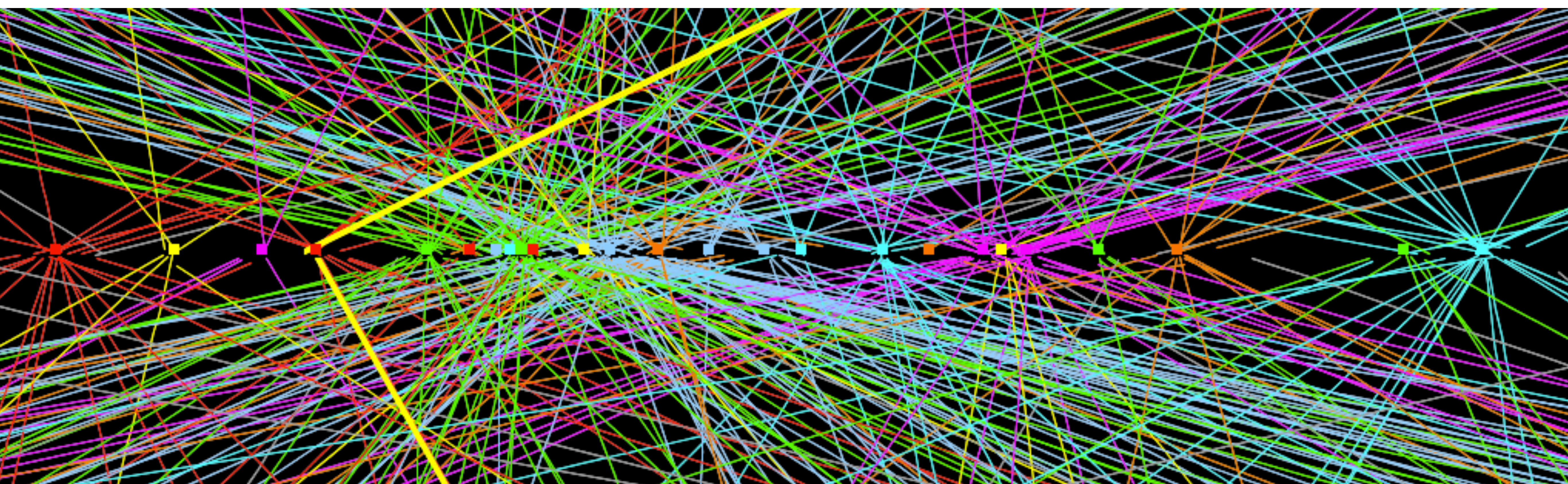
$$BR(h \to \phi\gamma) = (2.31 \pm 0.03_{f_\phi} \pm 0.11_{h\to\gamma\gamma}) \cdot 10^{-6}$$

h/Z→φγ/ργ

- **Exclusive decays → distinct experimental signature**
  - Pair of collimated high-pT isolated tracks

  recoils against high-pT isolated photon
- **Meson decays:**
  - **$\phi \to K^+K^-$**, BR=49%
  - **$\rho \to \pi^+\pi^-$**, BR~100%
- **Small opening angles between decay products**
  - Particularly for $\phi \to K^+K^-$
  - Tracking in dense environments





Z→μμ candidate with 25 reconstructed vertices from the 2012 run. Only good quality tracks with pT>0.4GeV are shown

h/Z→ϕγ/ργ

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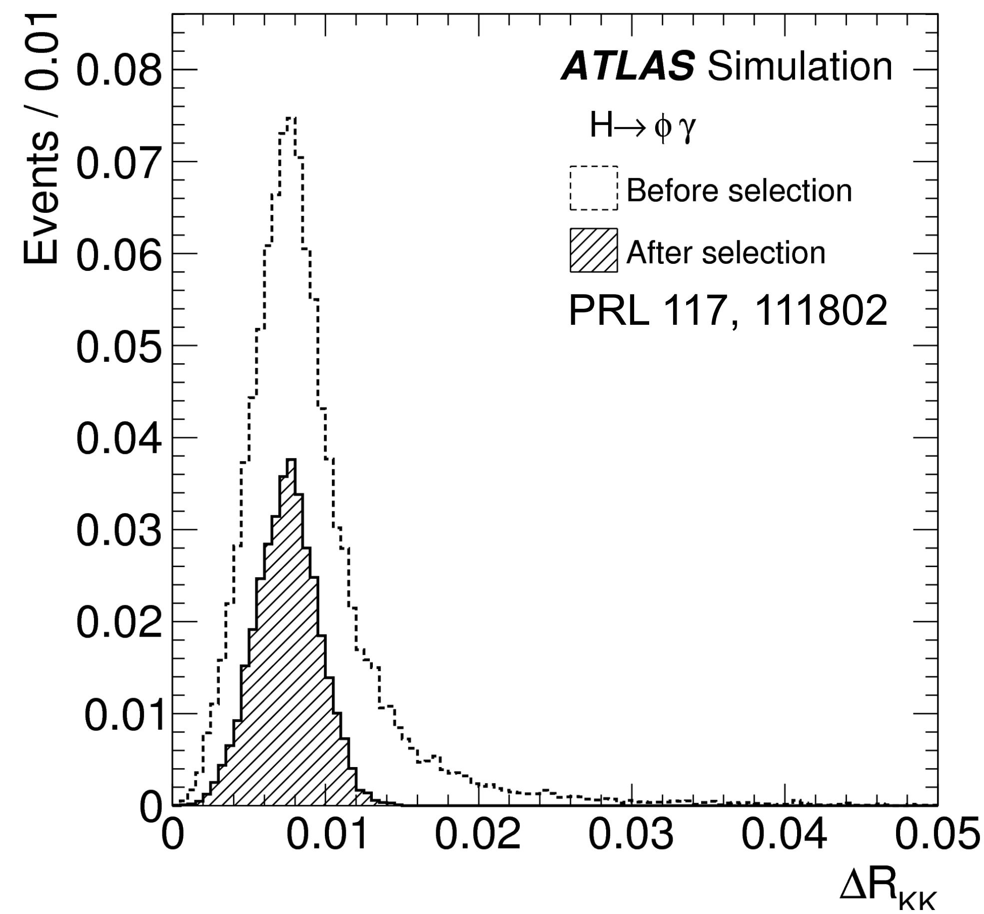
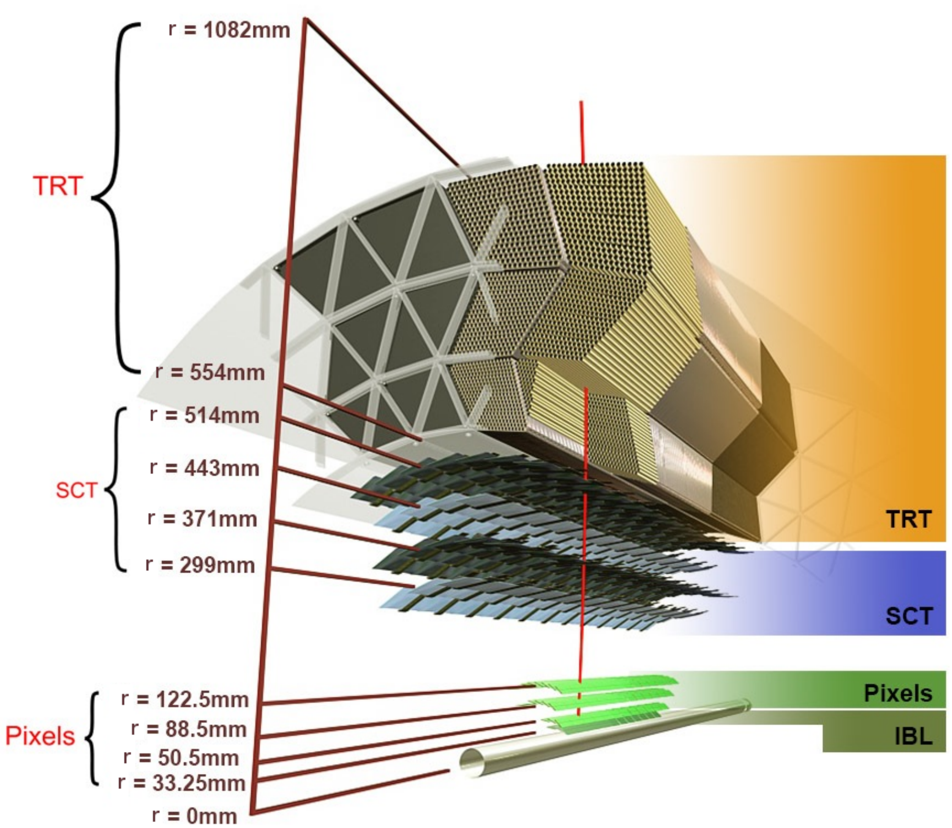
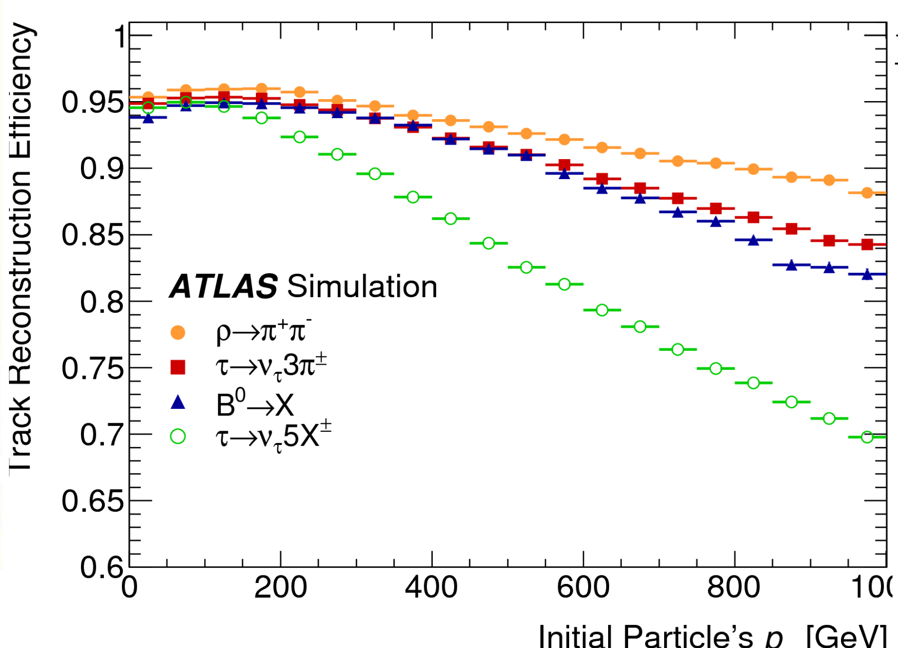
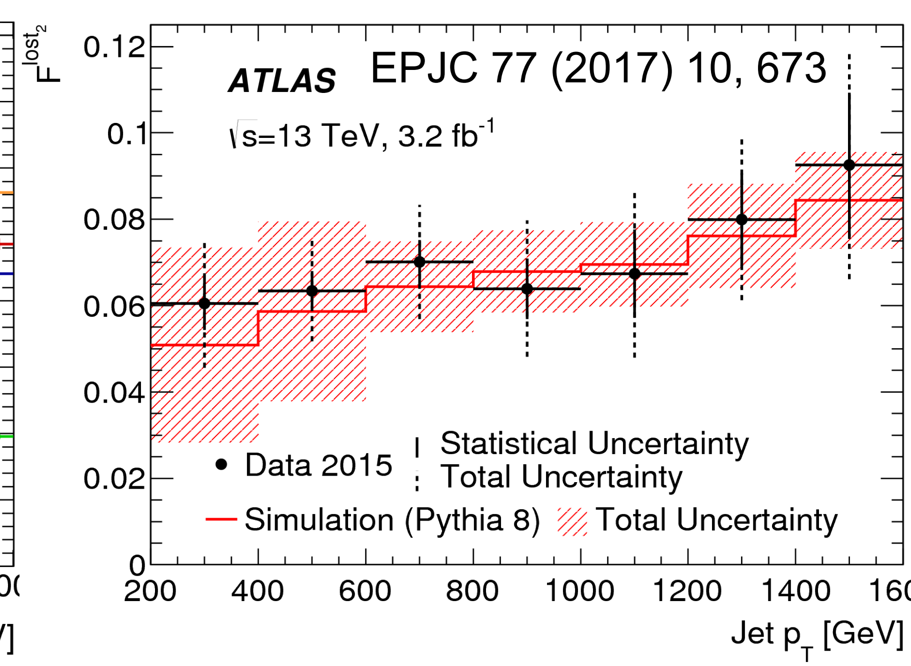
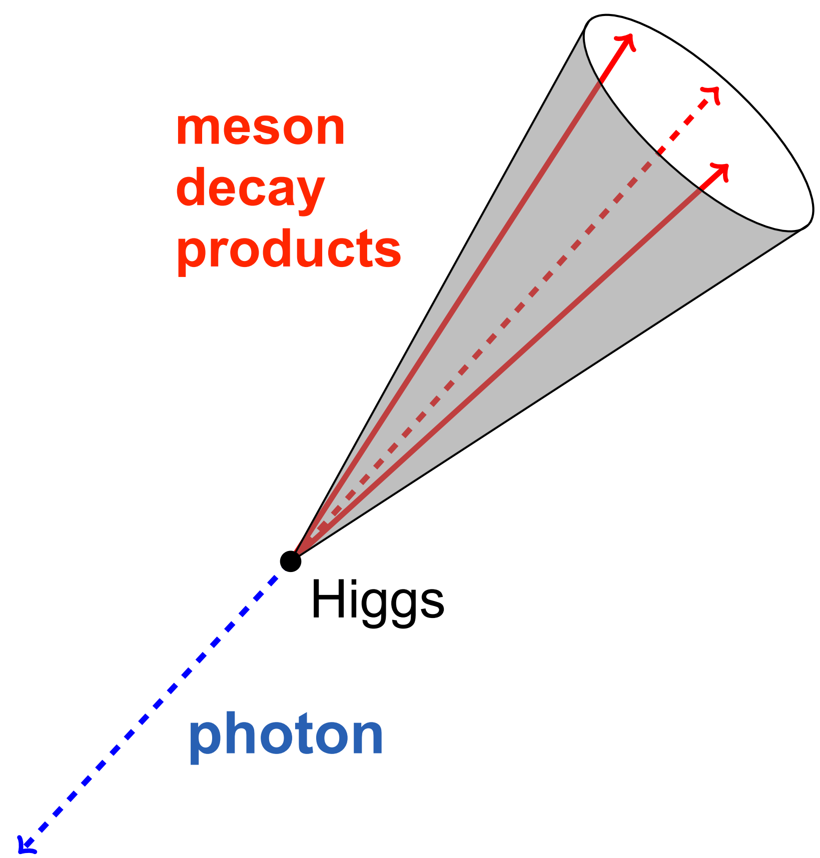


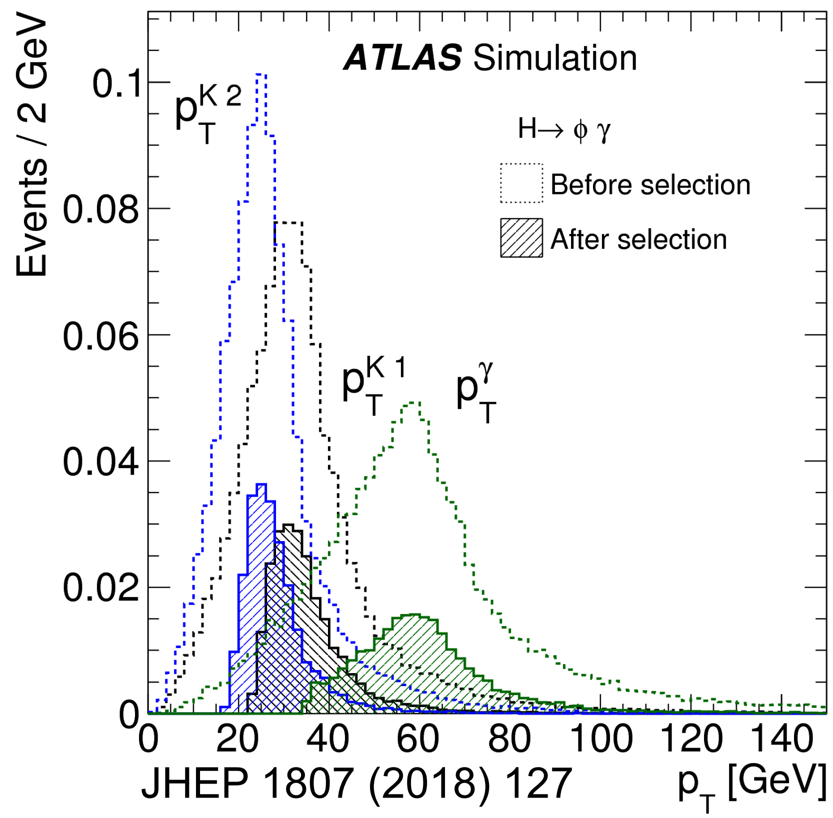






Event Selection





JHEP 1807 (2018) 127

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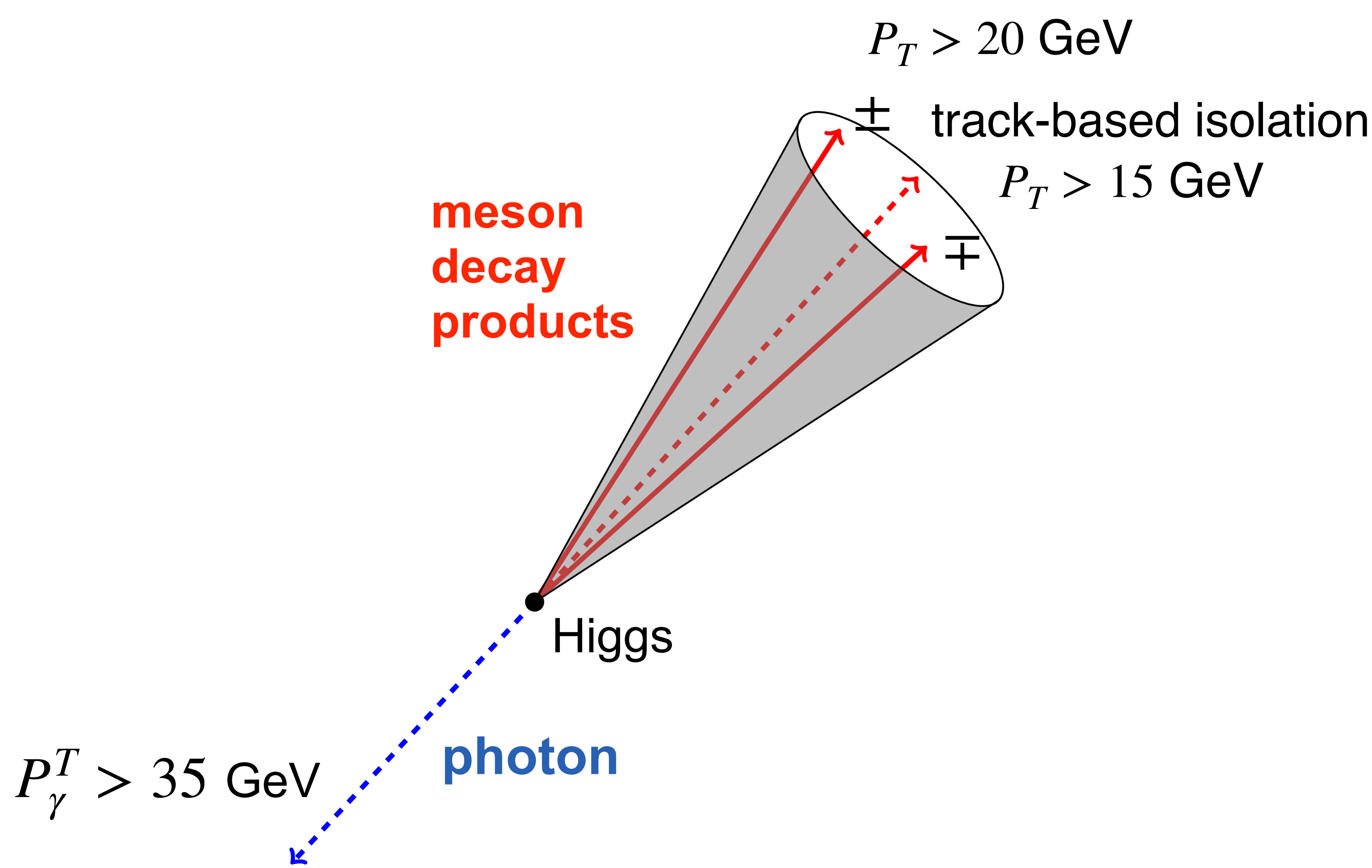
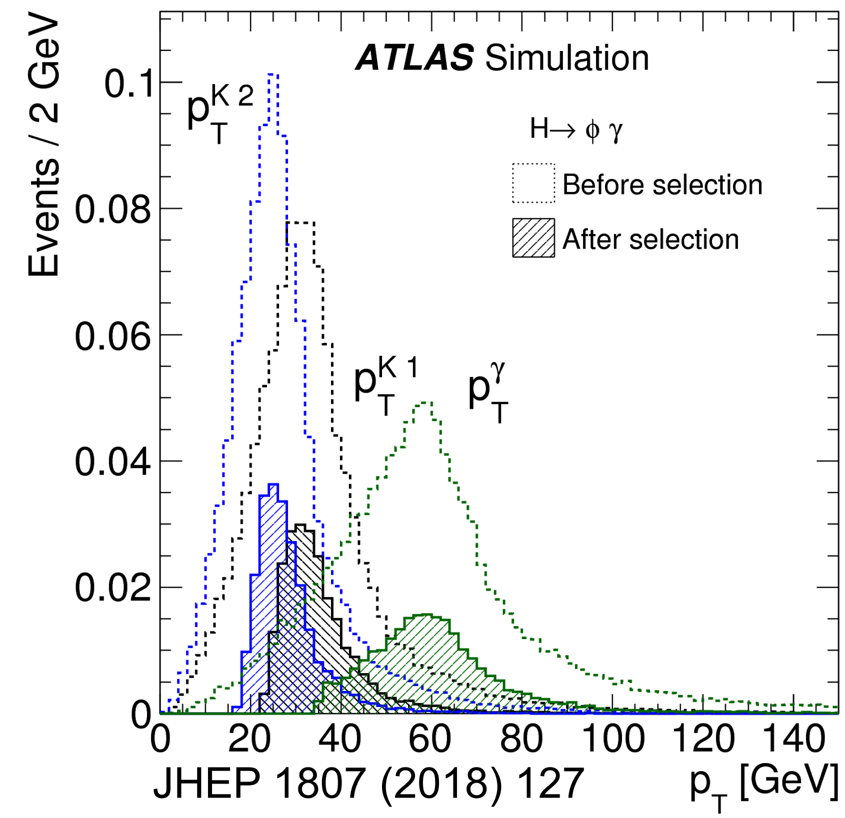


“Tight” identification criteria
Isolated (calorimeter- and track-based)



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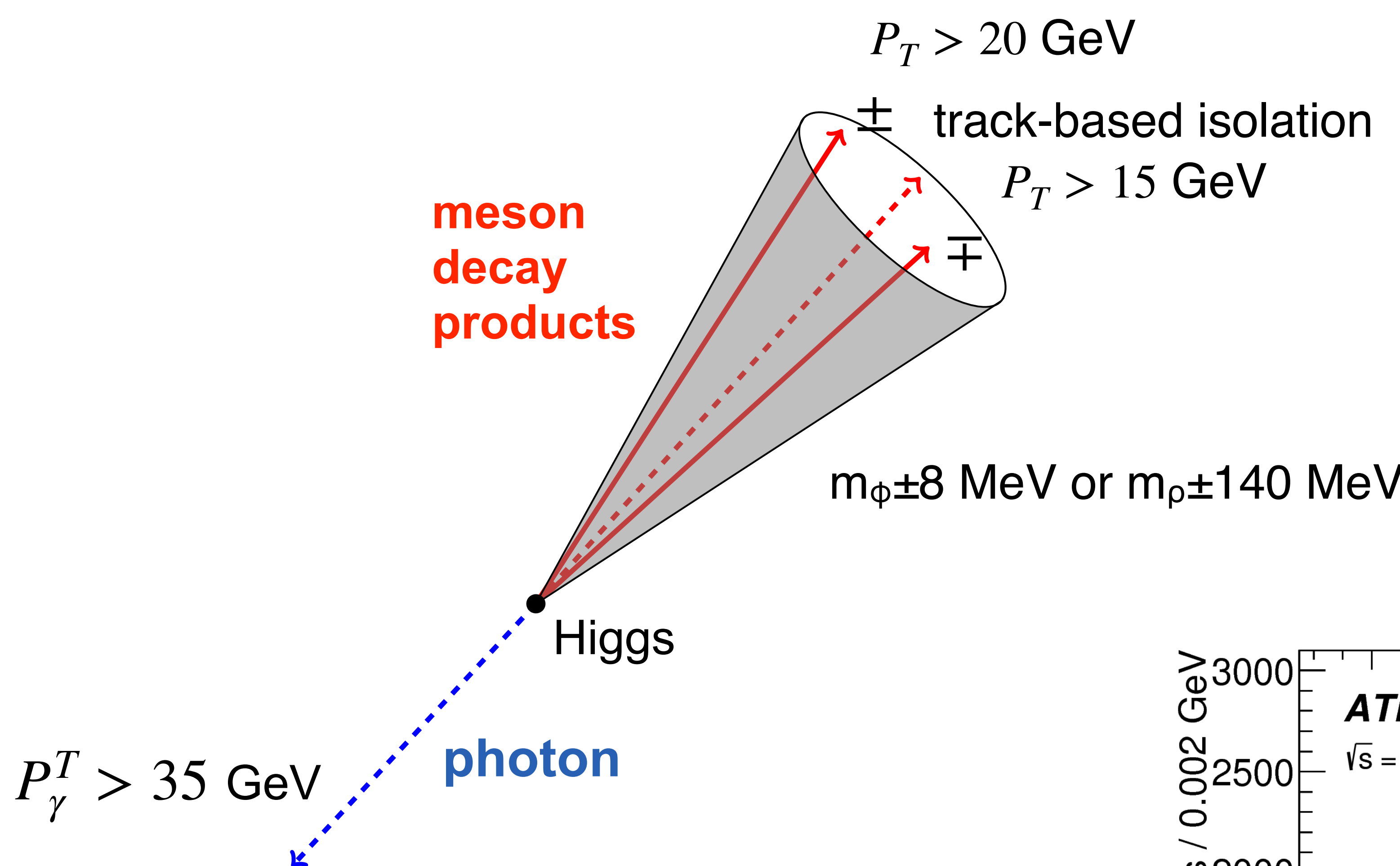

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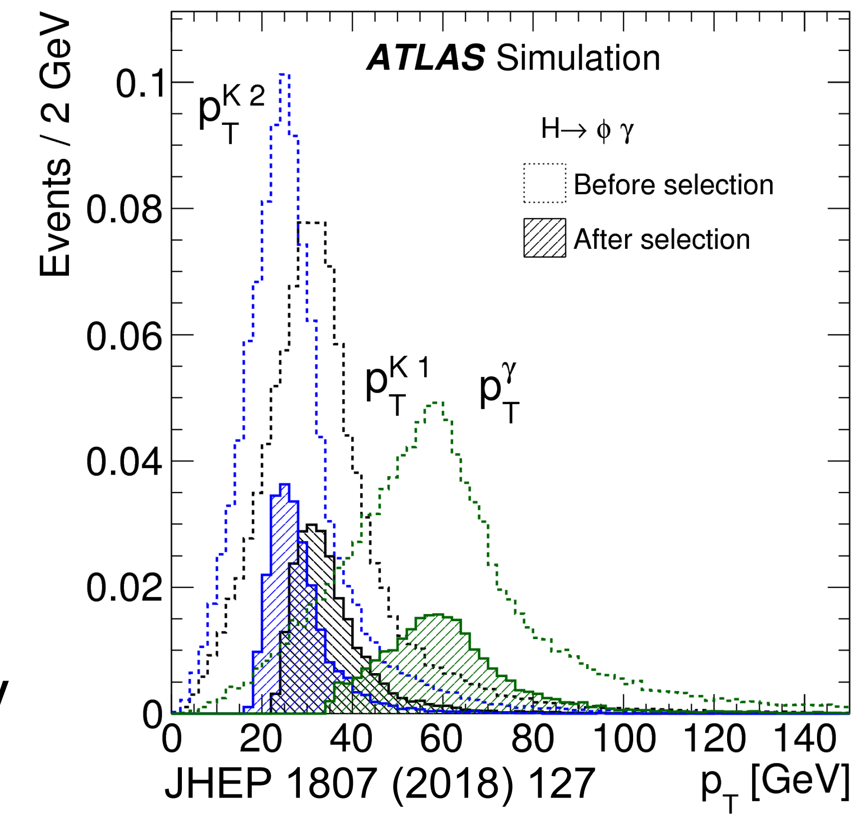

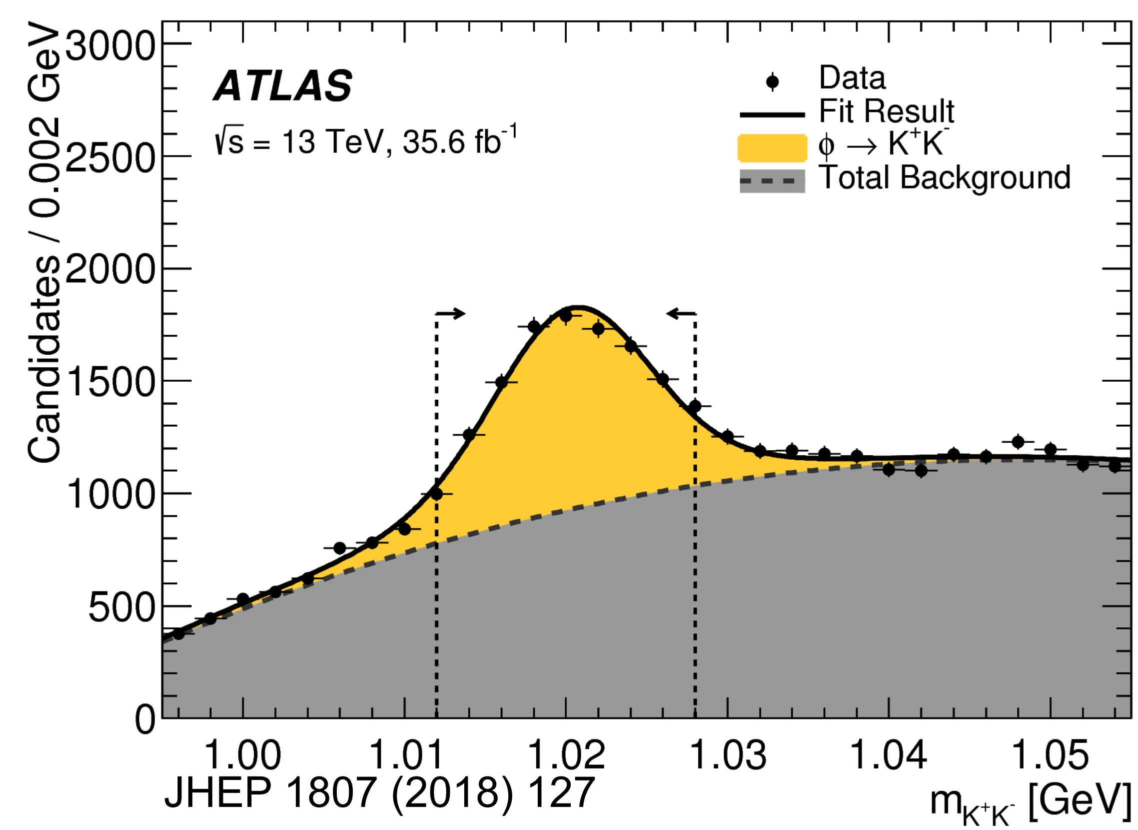

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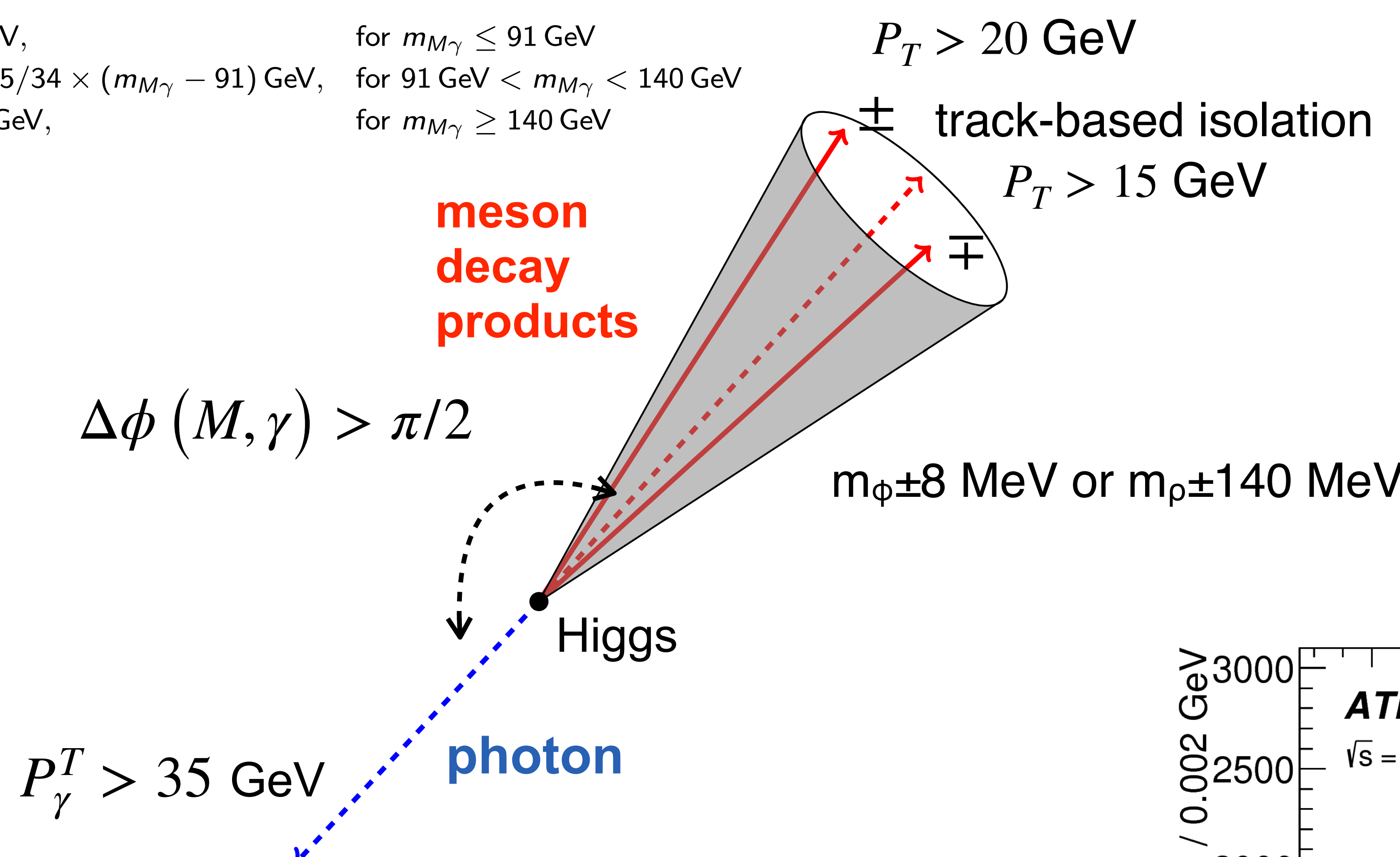

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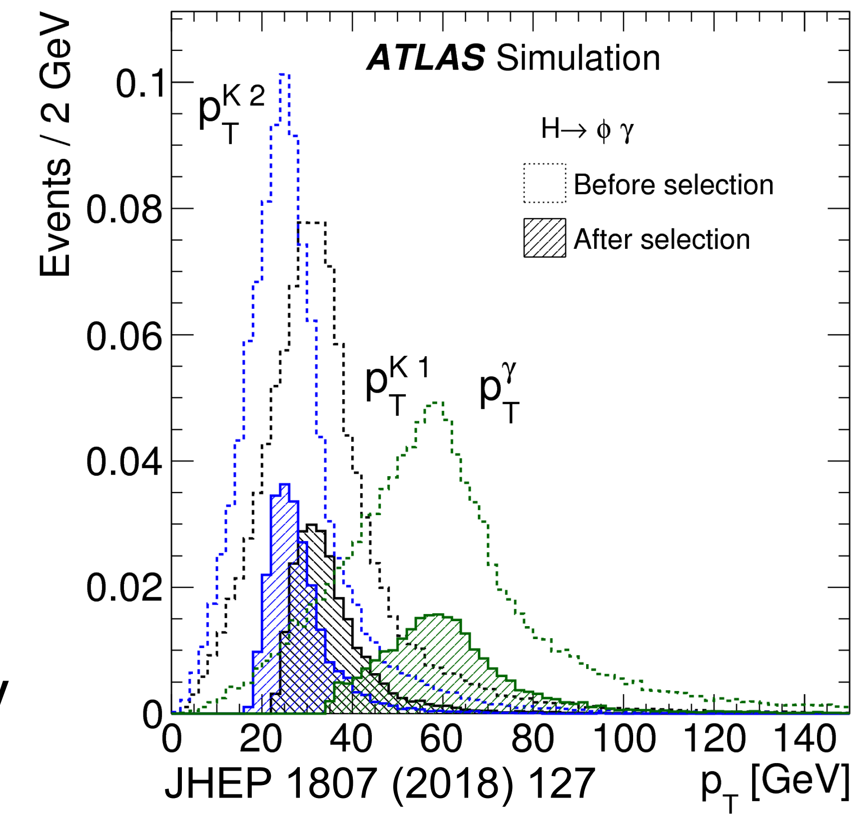

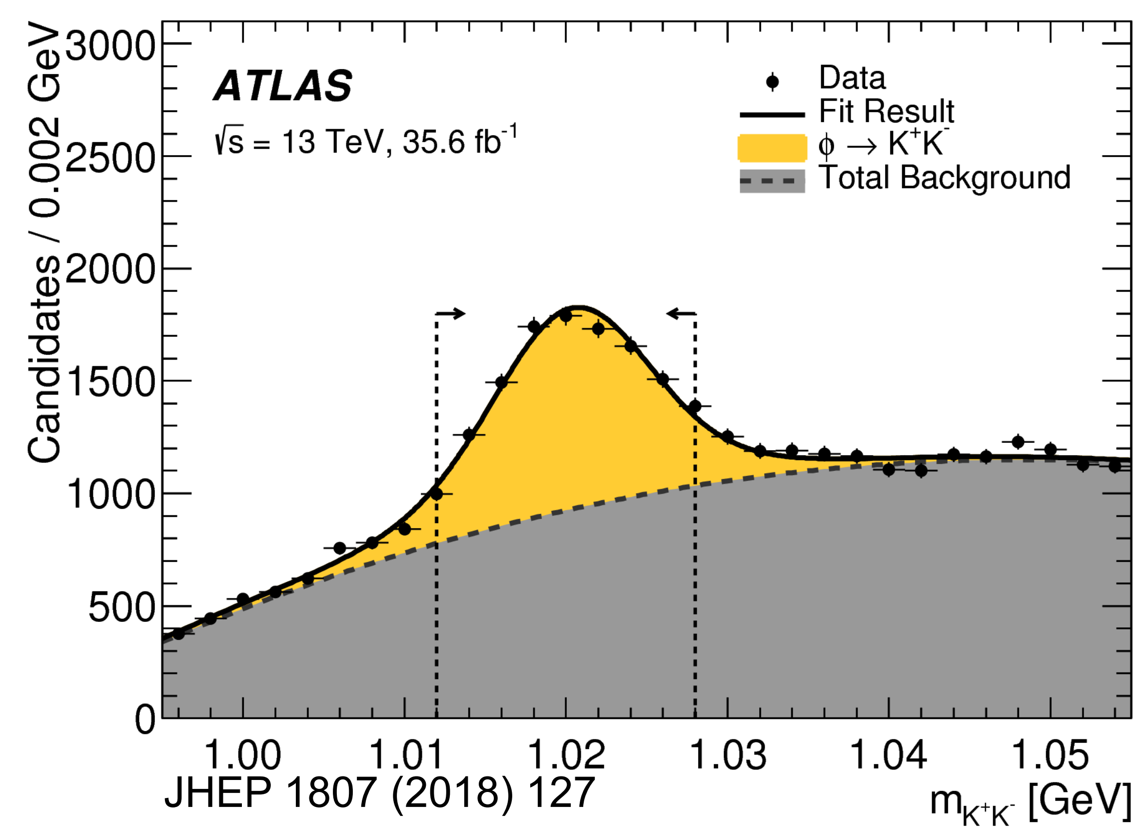

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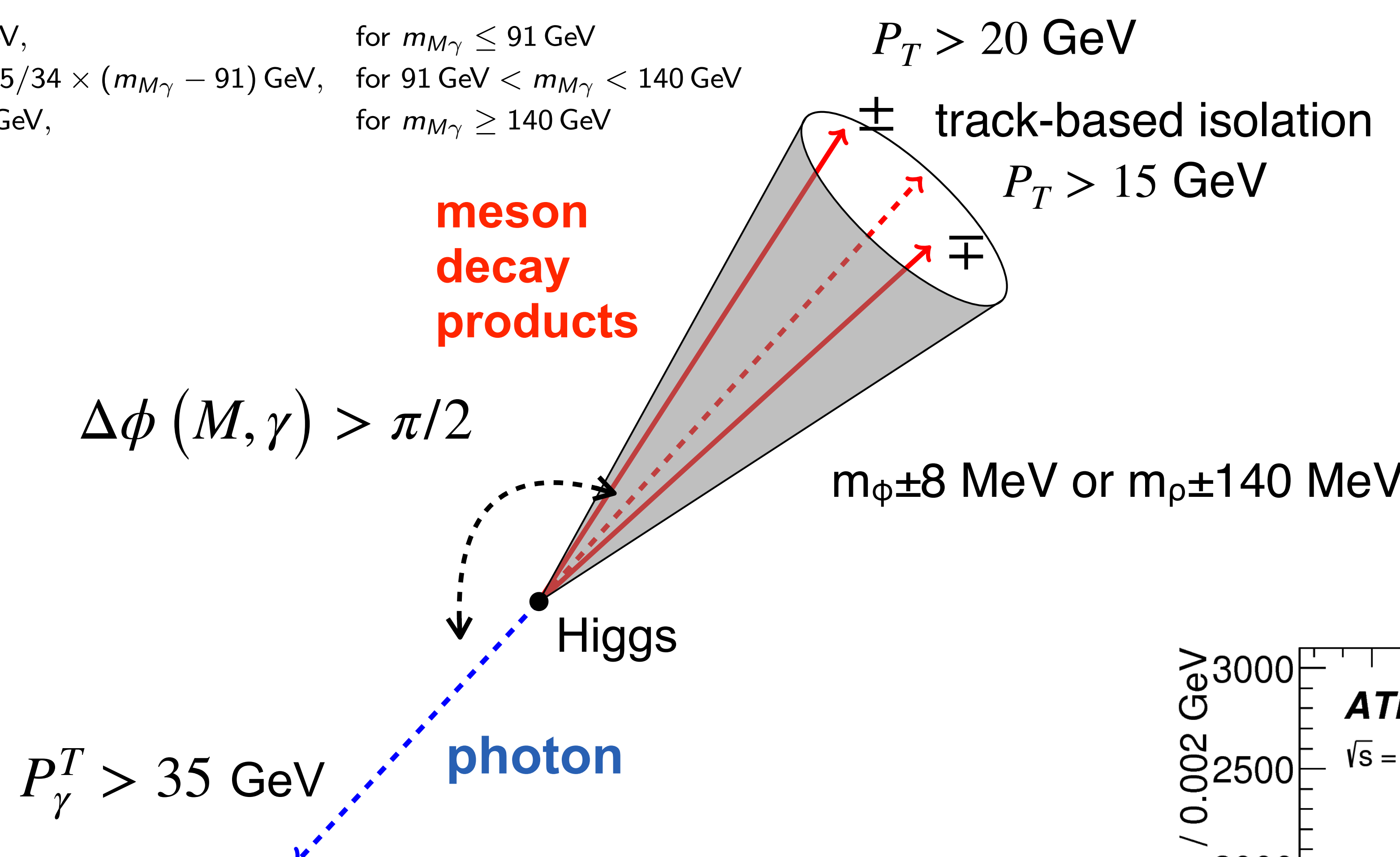

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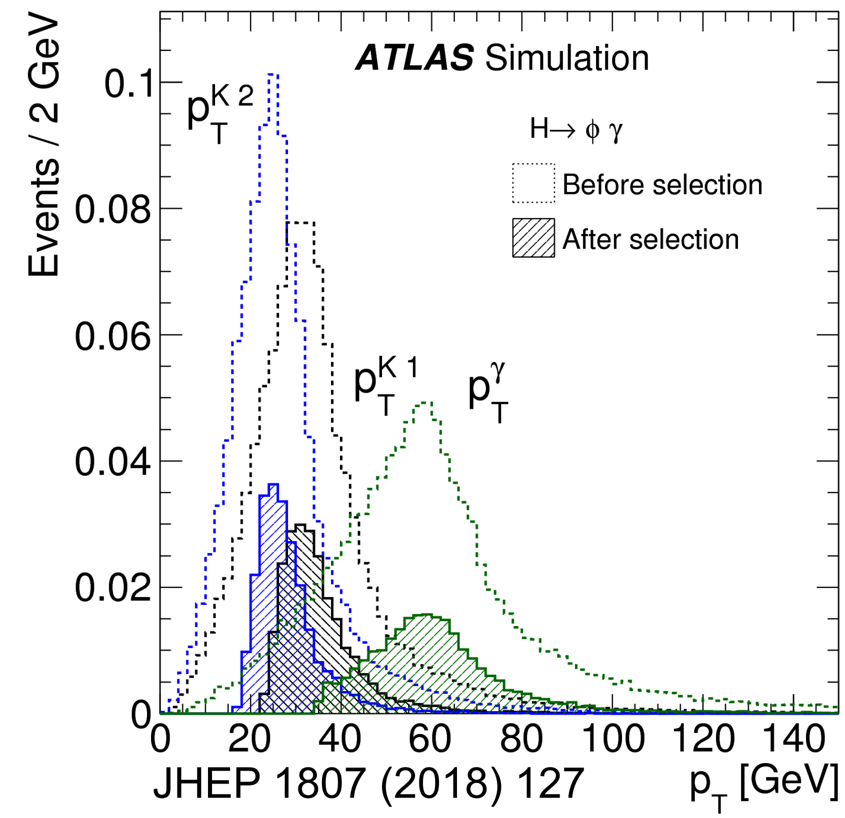

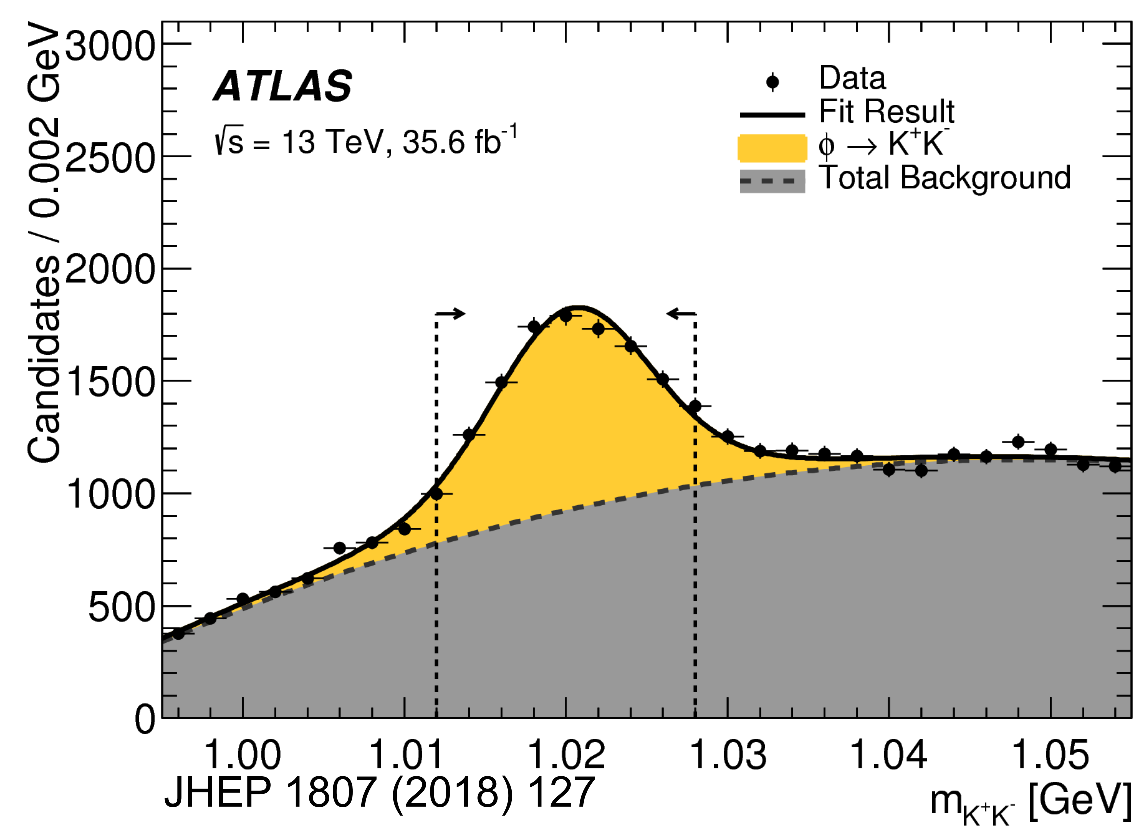

- **“Inclusive” backgrounds**
  - γ+jet, di-jet with jet “seen” as γ

Background Model

- **Non-parametric data-driven** background model based on **Ancestral Sampling**
  - Obtain loose sample of candidates
  - Model kinematic and isolation distributions
    - Conditional PDFs modelled using histograms
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- **Used in several analyses already!**

[Phys. Rev. Lett. 114 (2015) 121801, Phys. Rev. Lett. 117, 111802 (2016), JHEP 07 (2018) 127, Phys. Lett. B 786 (2018) 134]

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Example application on γ+jet MC sample

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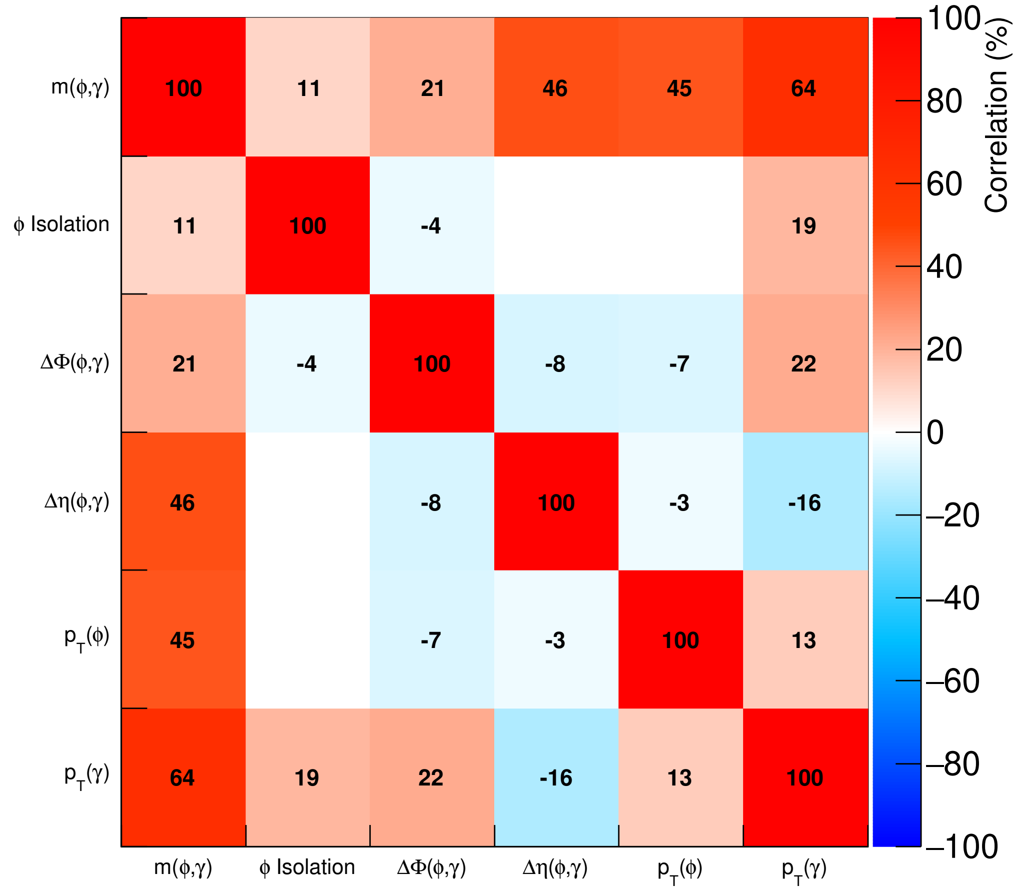

γ+jet MC

arXiv:2112.00650

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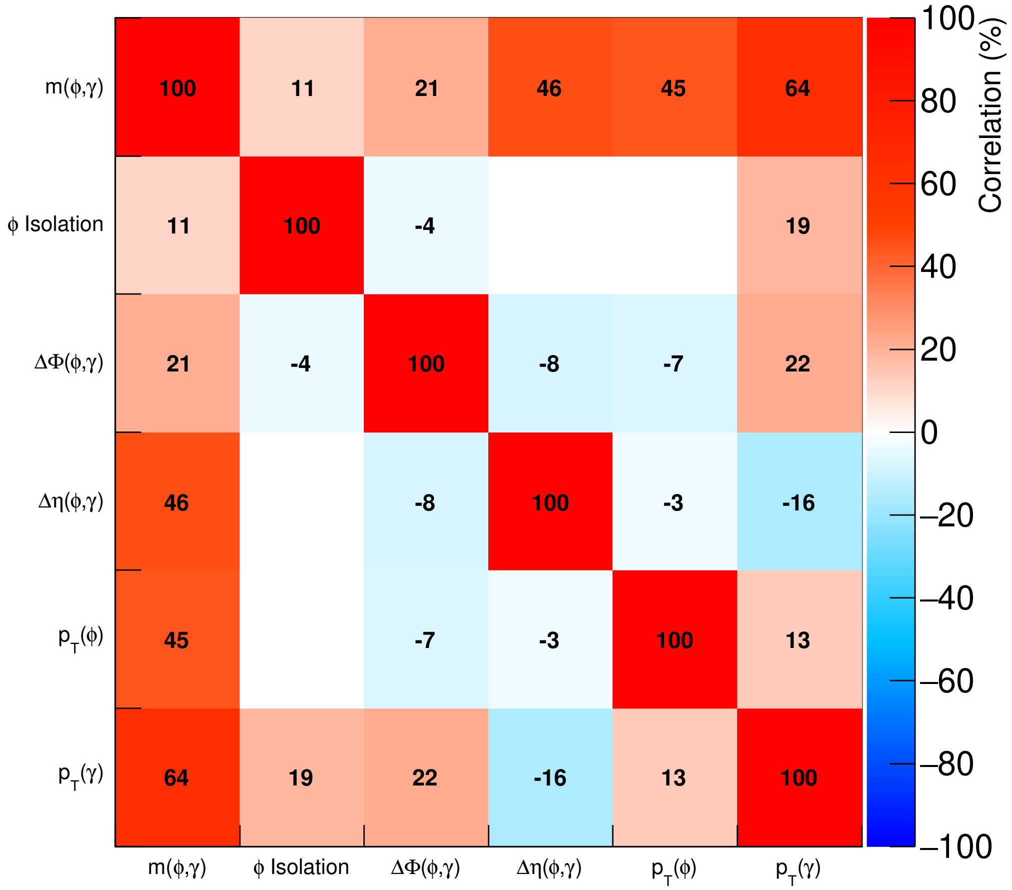

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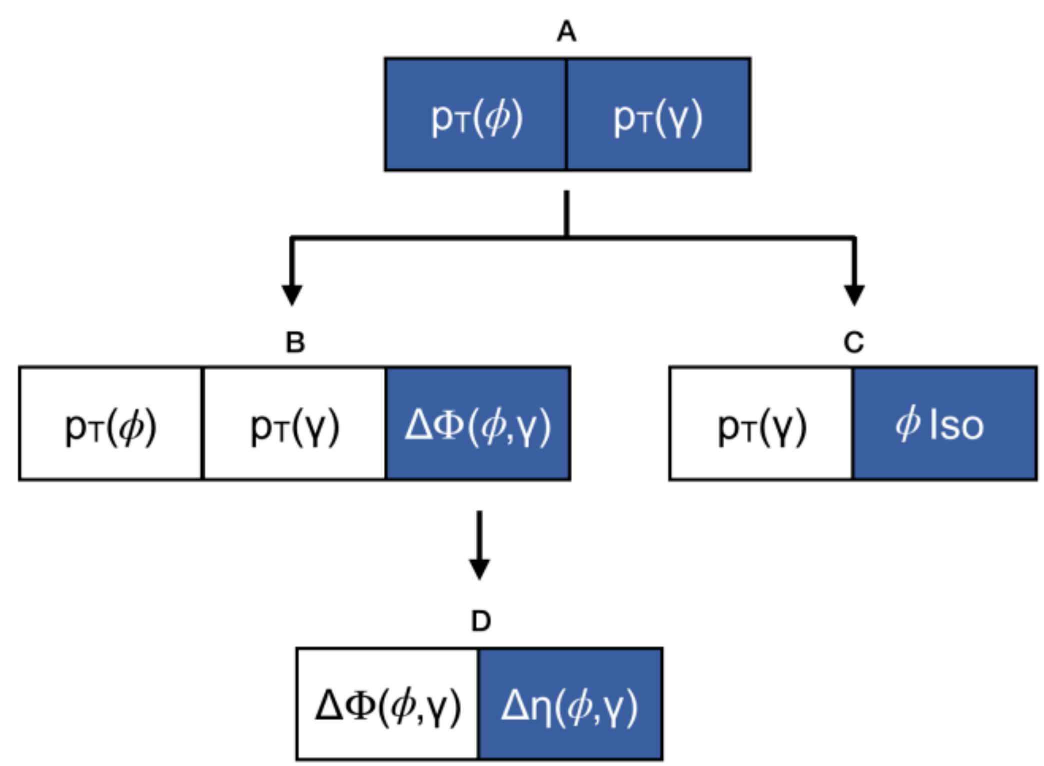

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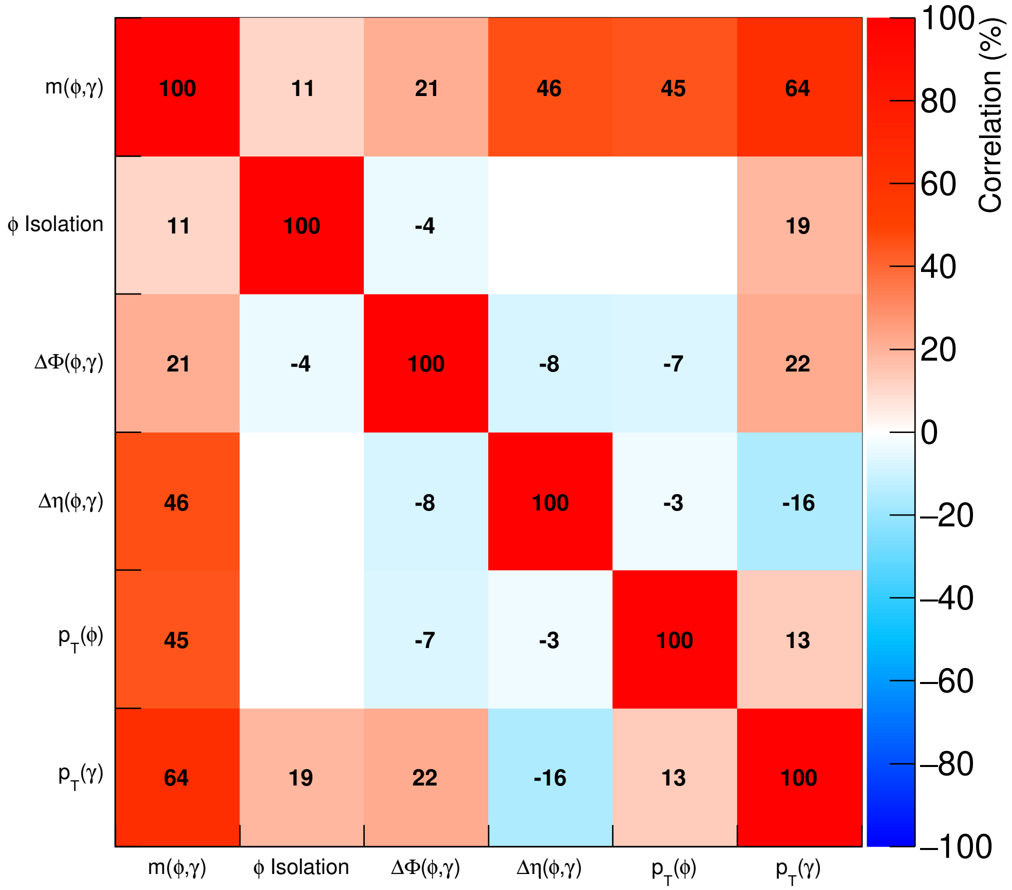

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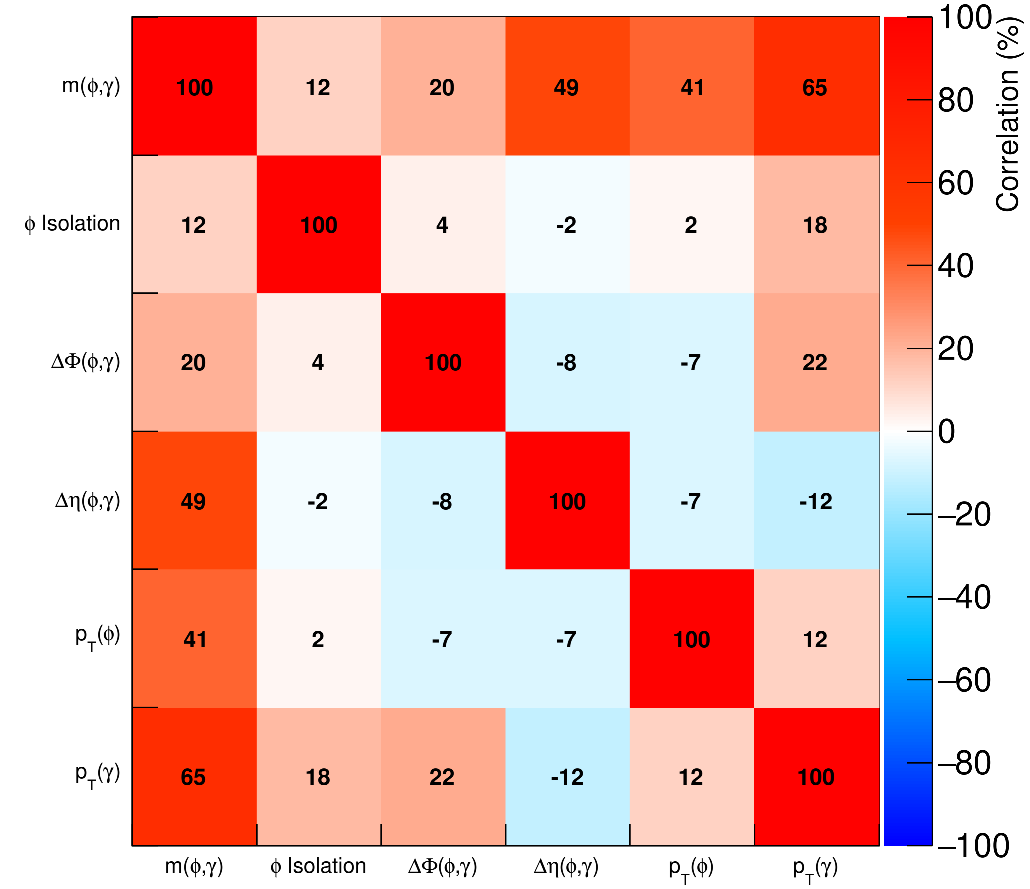

Model

arXiv:2112.00650

Background Model

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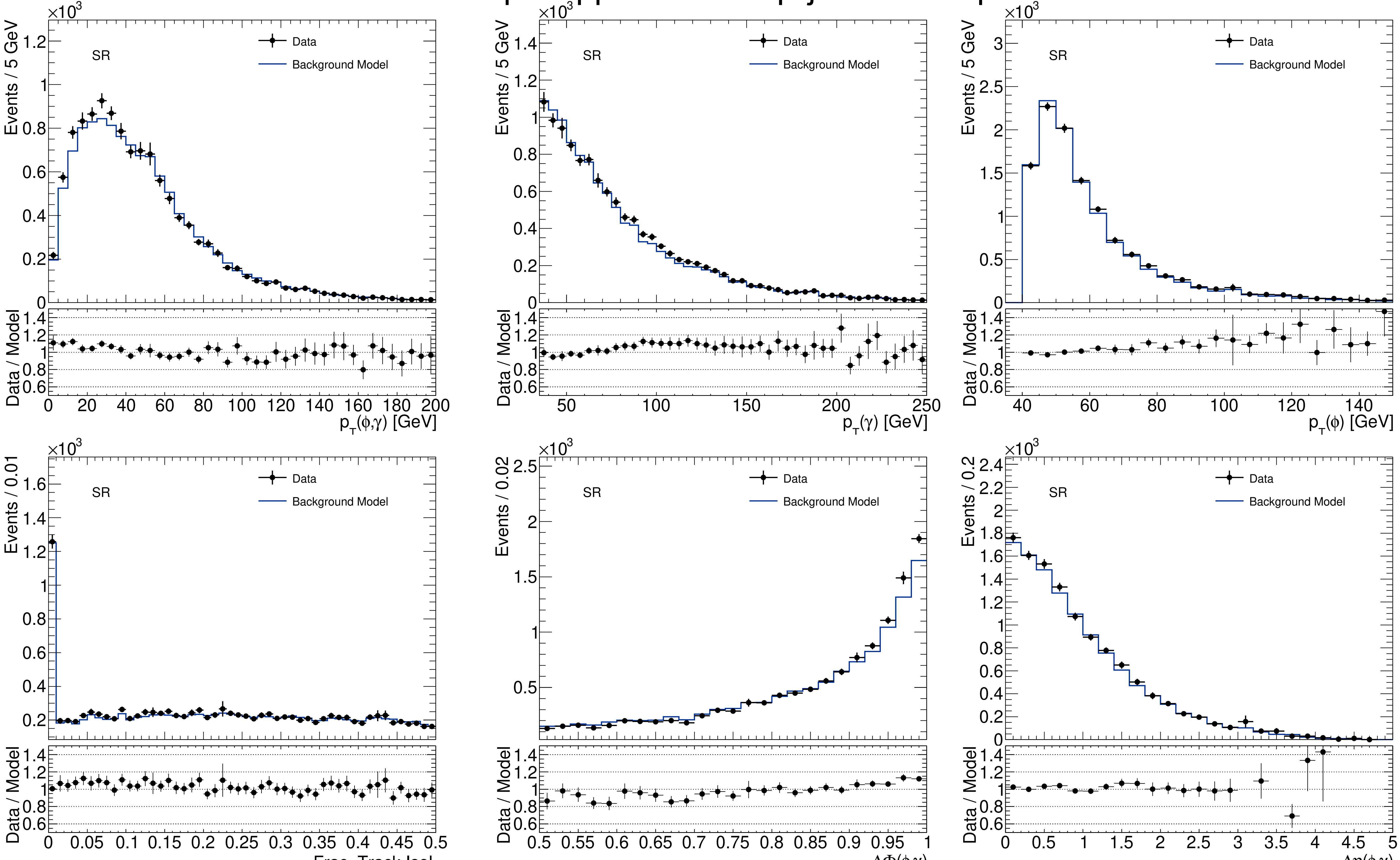

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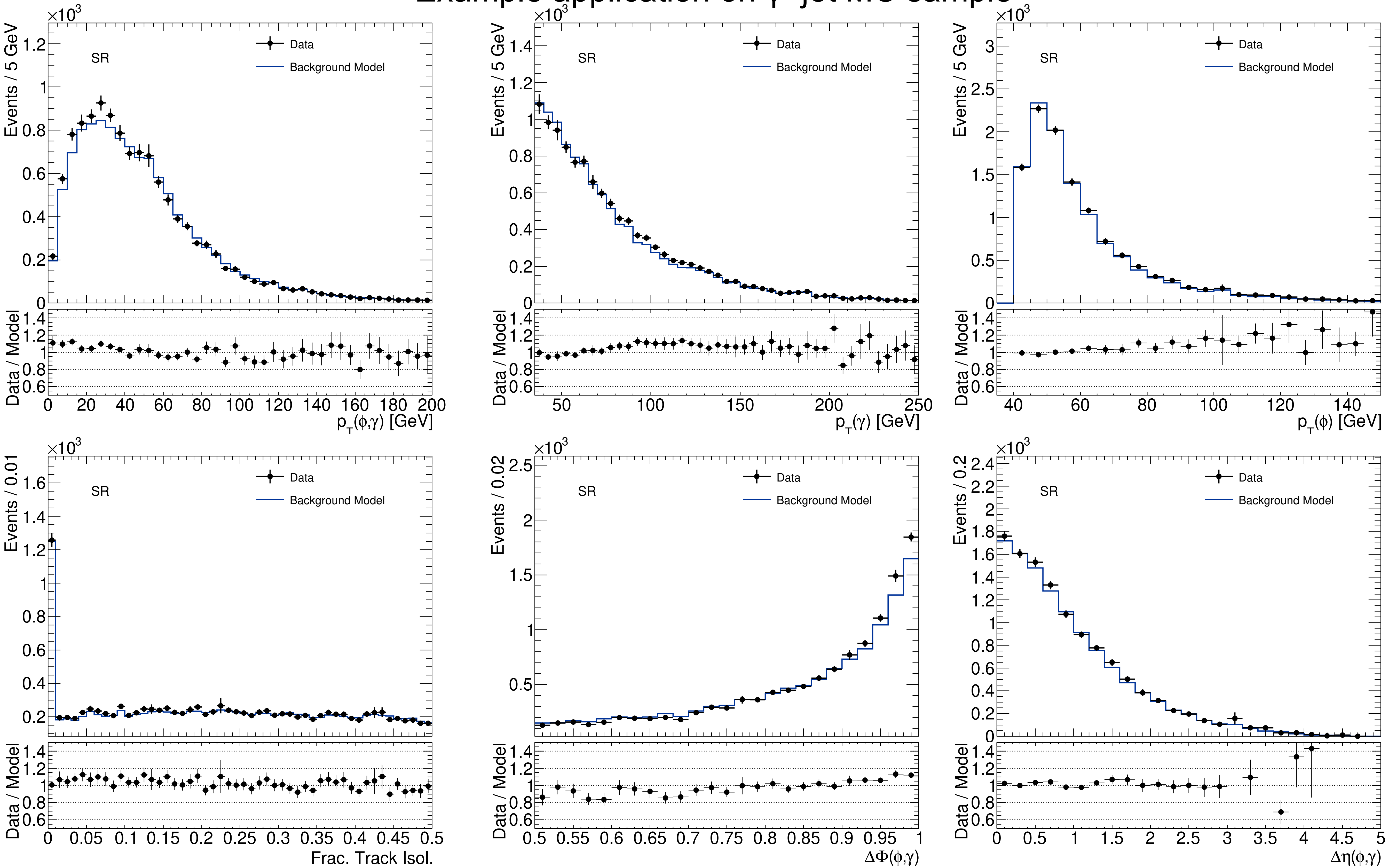
arXiv:2112.00650



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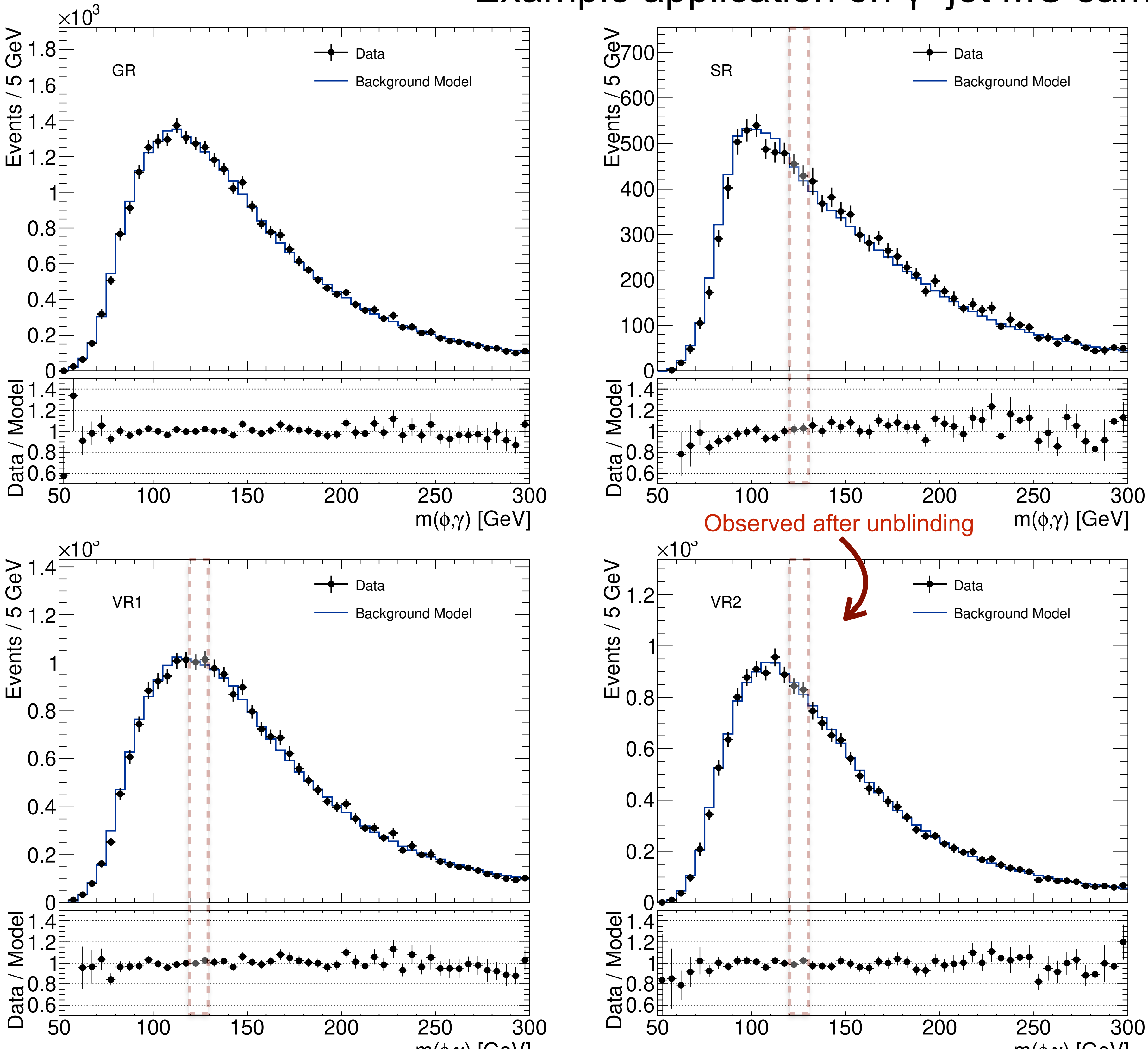

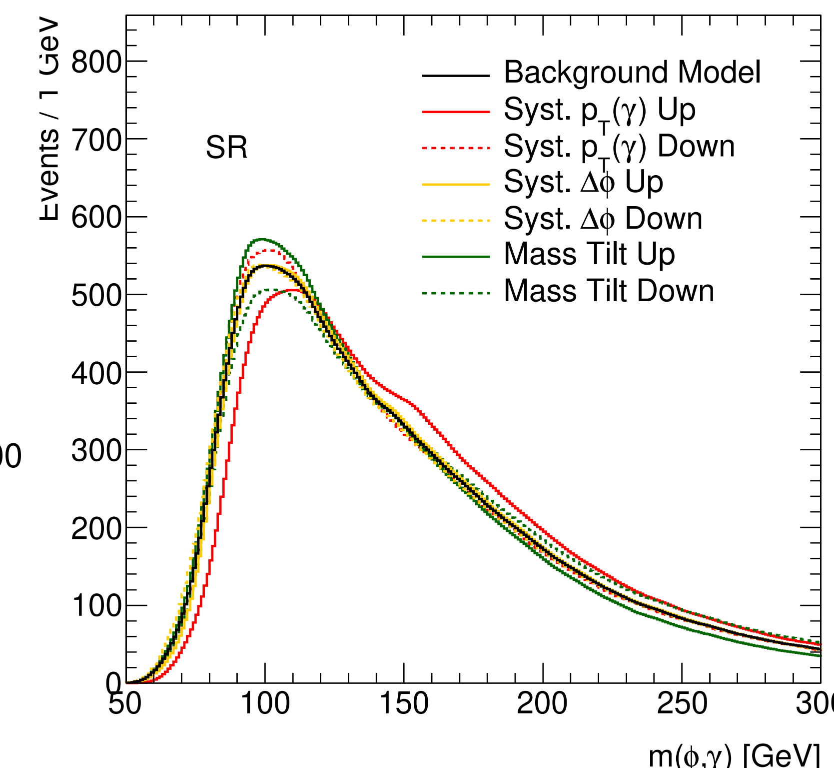

Shape variations

- Modifying sampling distributions
- Overall transformations of signal shape

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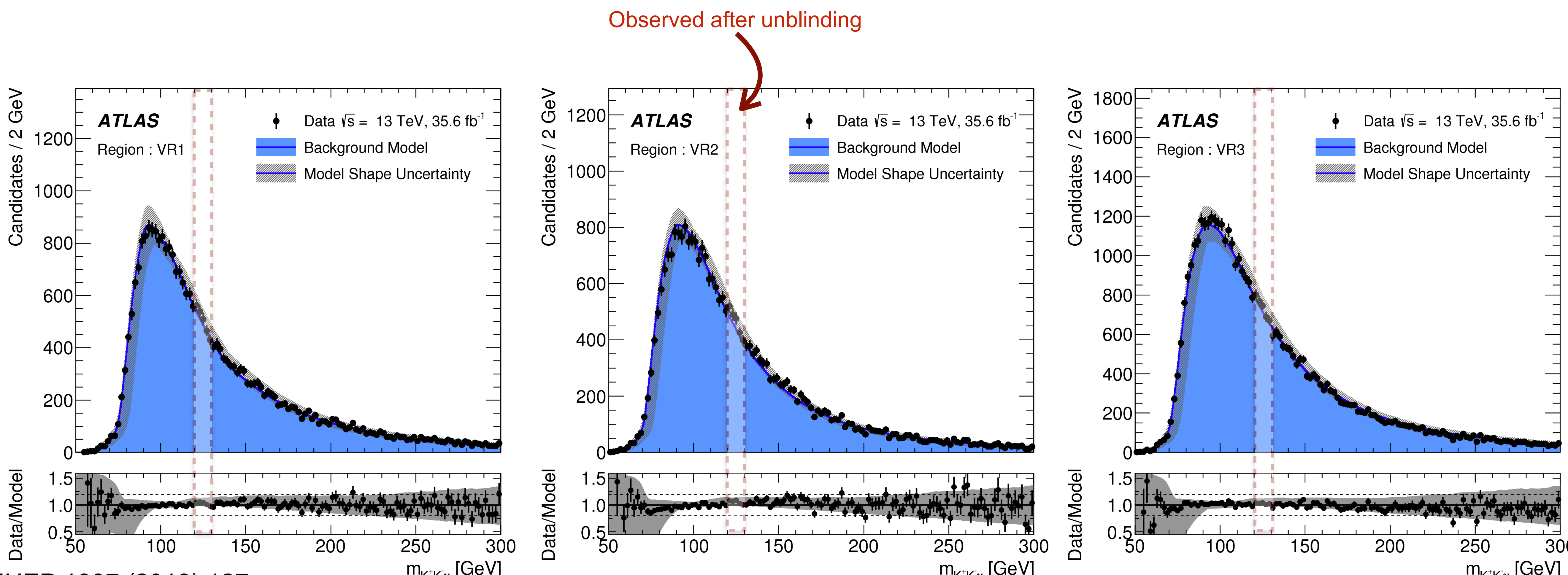
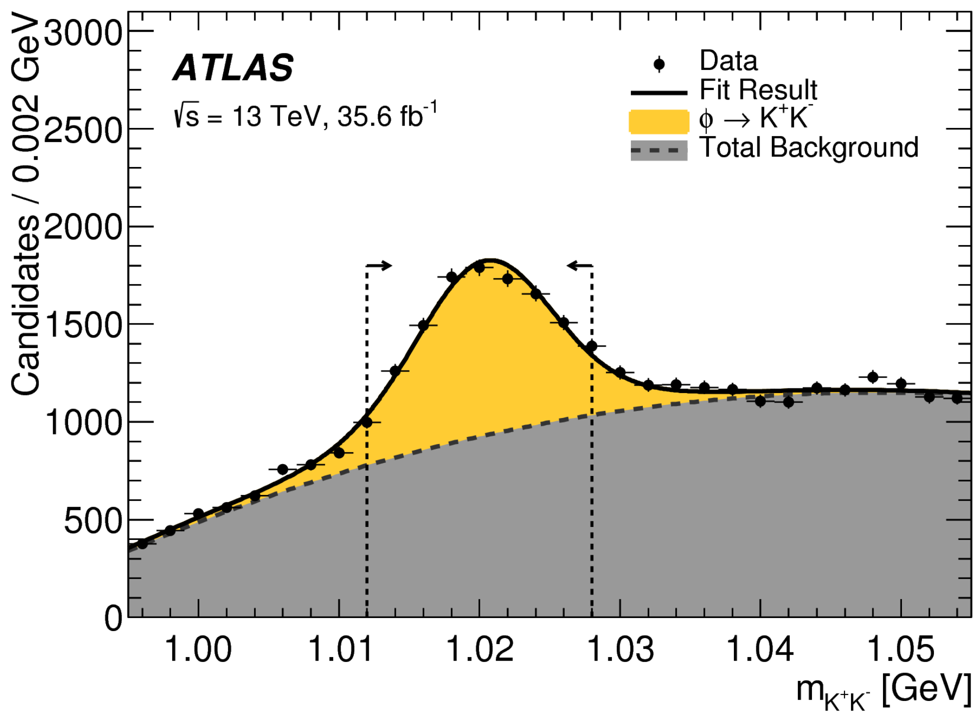
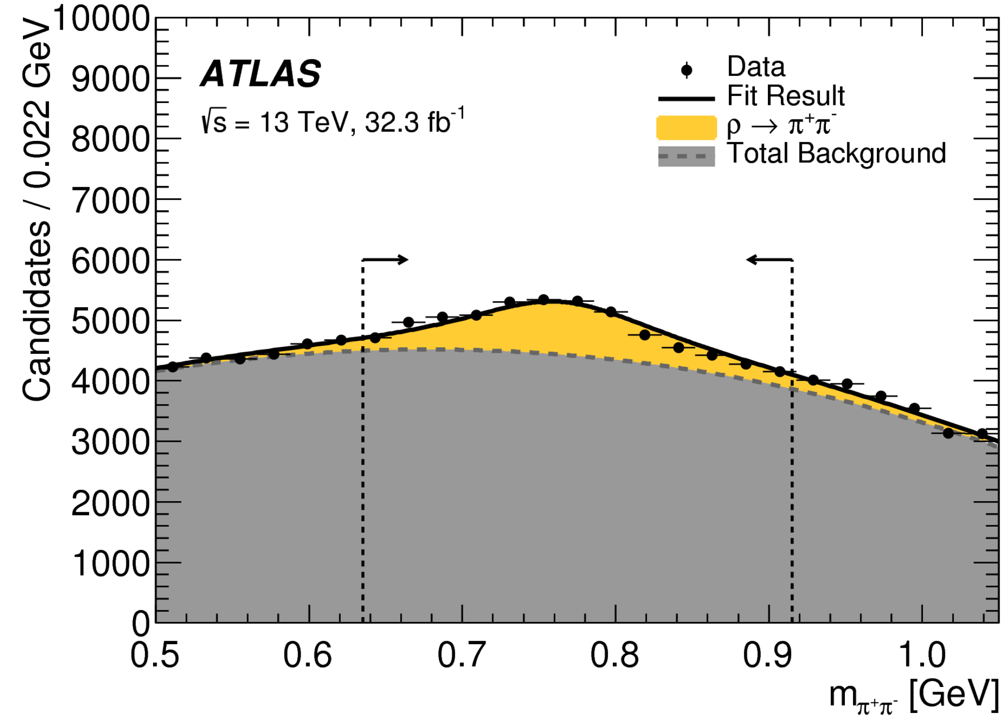


JHEP 1807 (2018) 127

Background Validation





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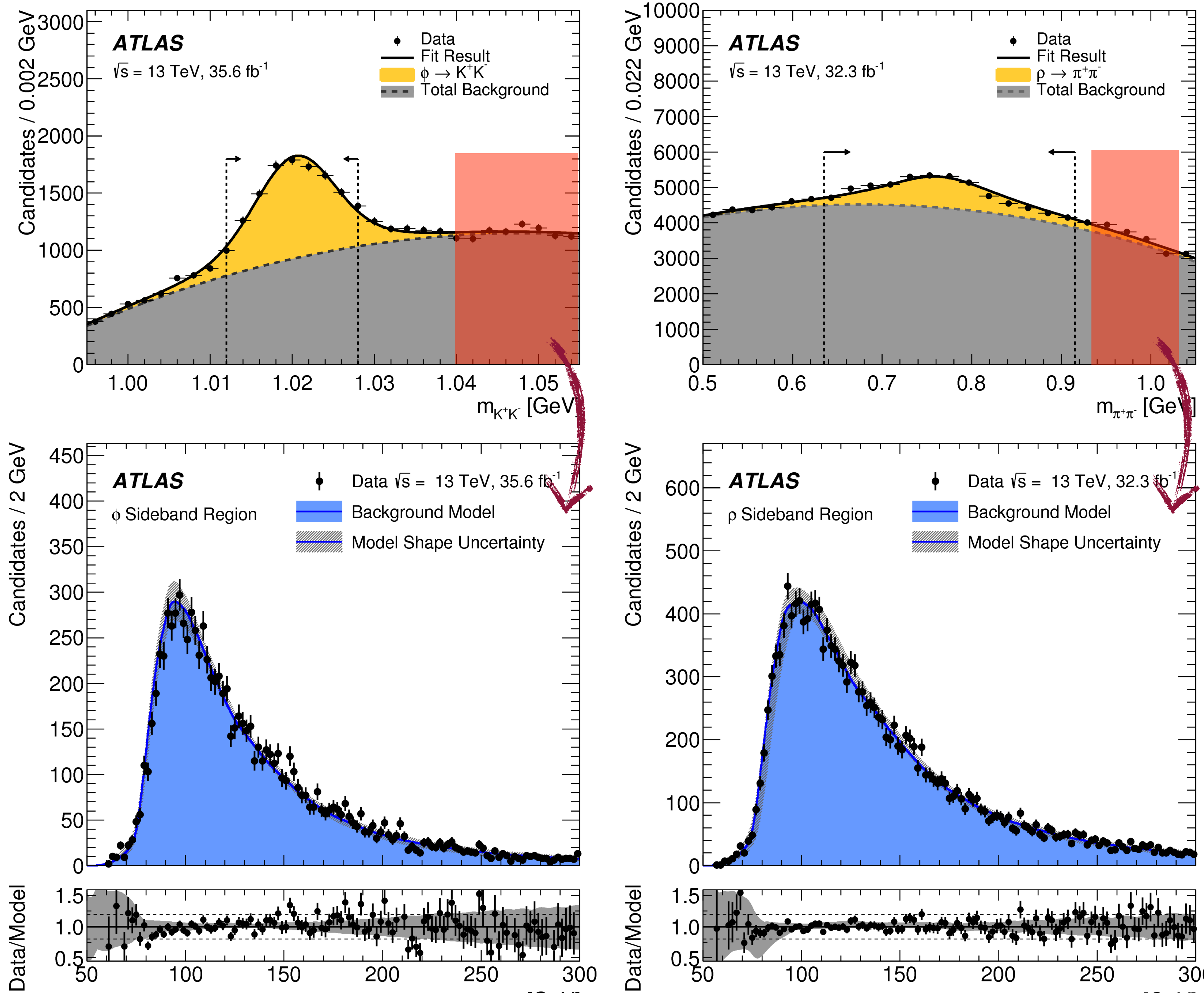
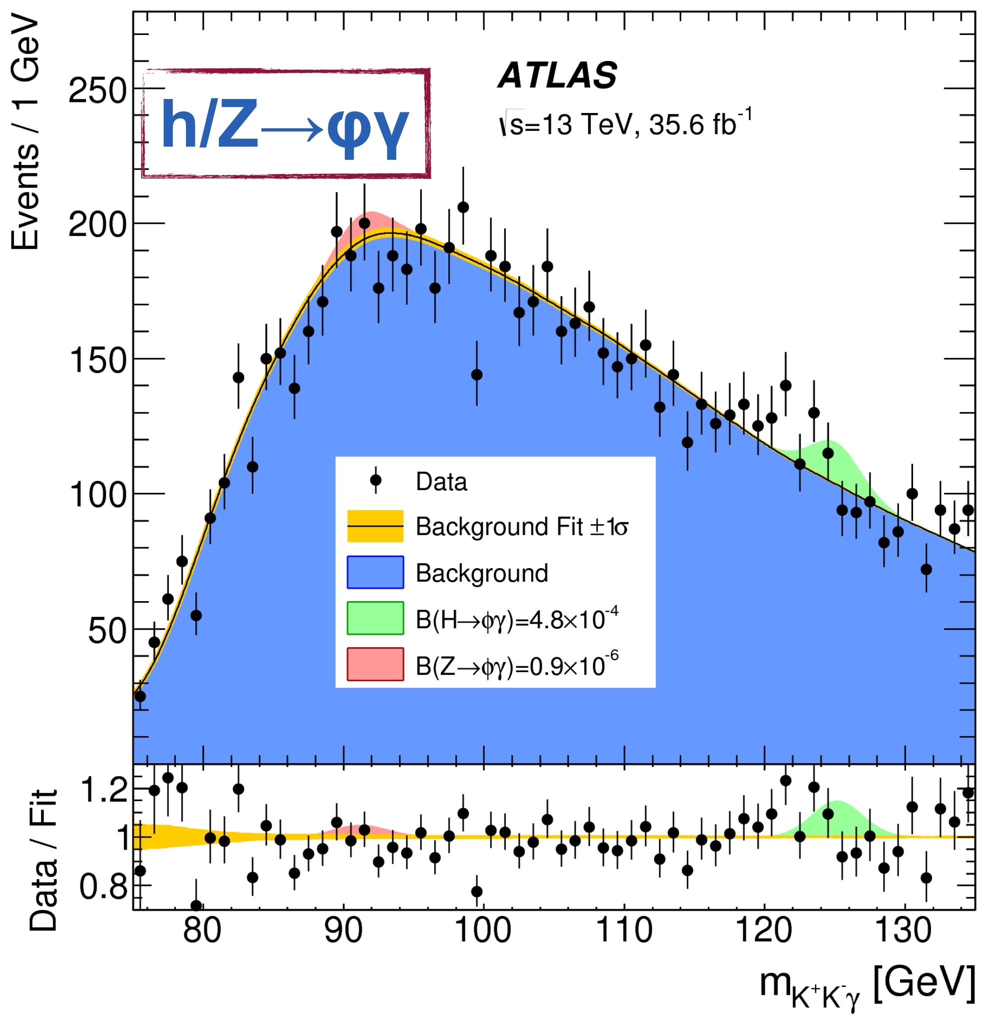
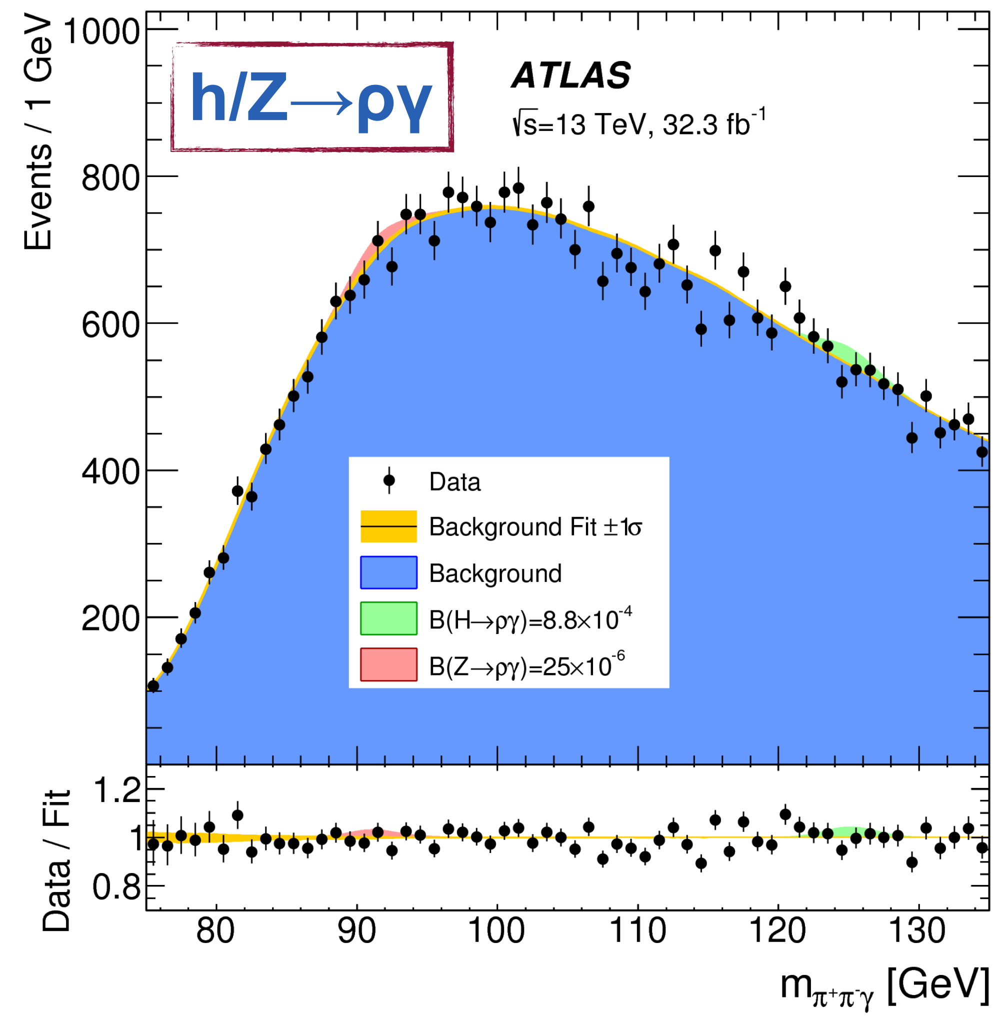


JHEP 1807 (2018) 127 JHEP 1807 (2018) 127

h/Z→φγ/ργ: Results





Final discriminant: $m_{KK\gamma}$ and $m_{\pi\pi\gamma}$

No significant signal observed

Branching Fraction Limit (95% CL)	Expected	Observed
$\mathcal{B}(H \to \phi\gamma)\ [10^{-4}]$	$4.2^{+1.8}_{-1.2}$	4.8
$\mathcal{B}(Z \to \phi\gamma)\ [10^{-6}]$	$1.3^{+0.6}_{-0.4}$	0.9
$\mathcal{B}(H \to \rho\gamma)\ [10^{-4}]$	$8.4^{+4.1}_{-2.4}$	8.8
$\mathcal{B}(Z \to \rho\gamma)\ [10^{-6}]$	33^{+13}_{-9}	25

JHEP 1807 (2018) 127

Model Robustness

- **Model describes main features of background**
  - Robust under signal contamination
  - Resonant backgrounds need to be considered separately

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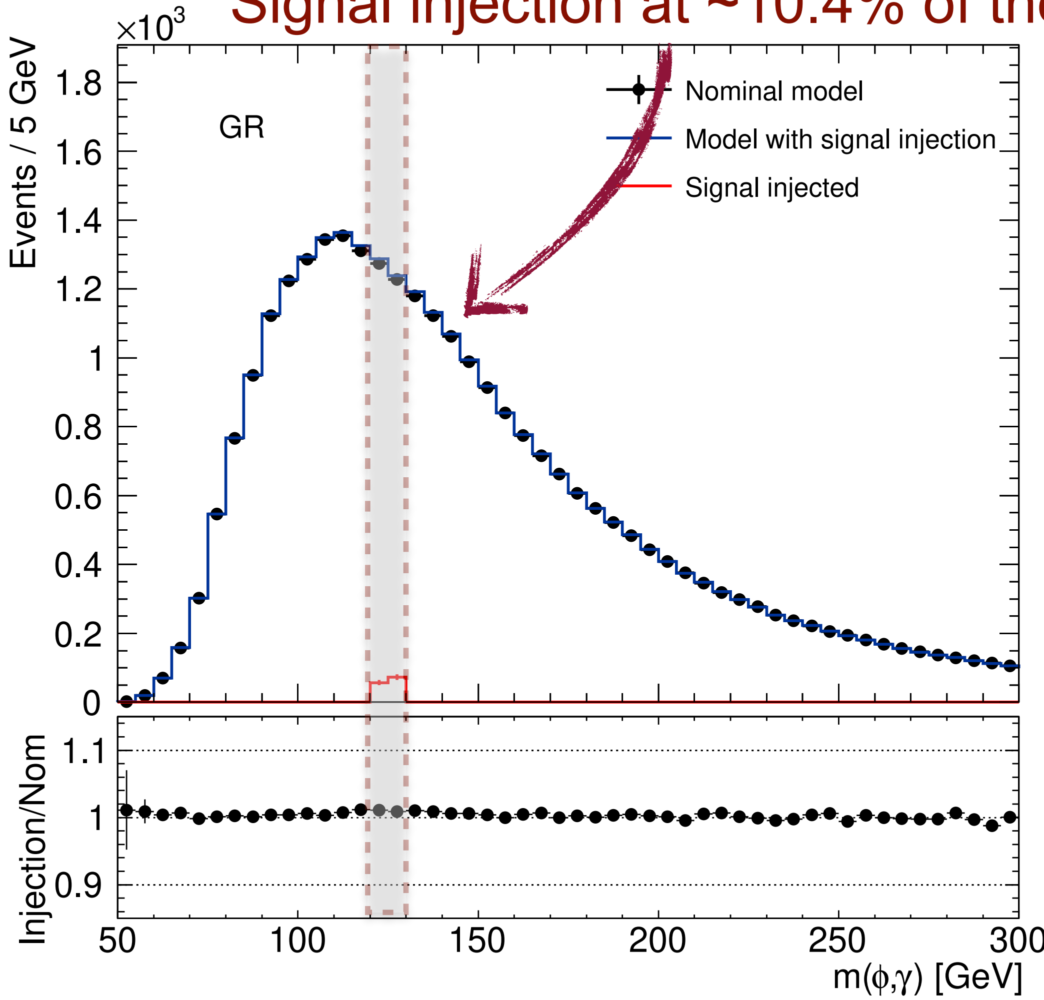
Signal injection at ~10.4% of the background



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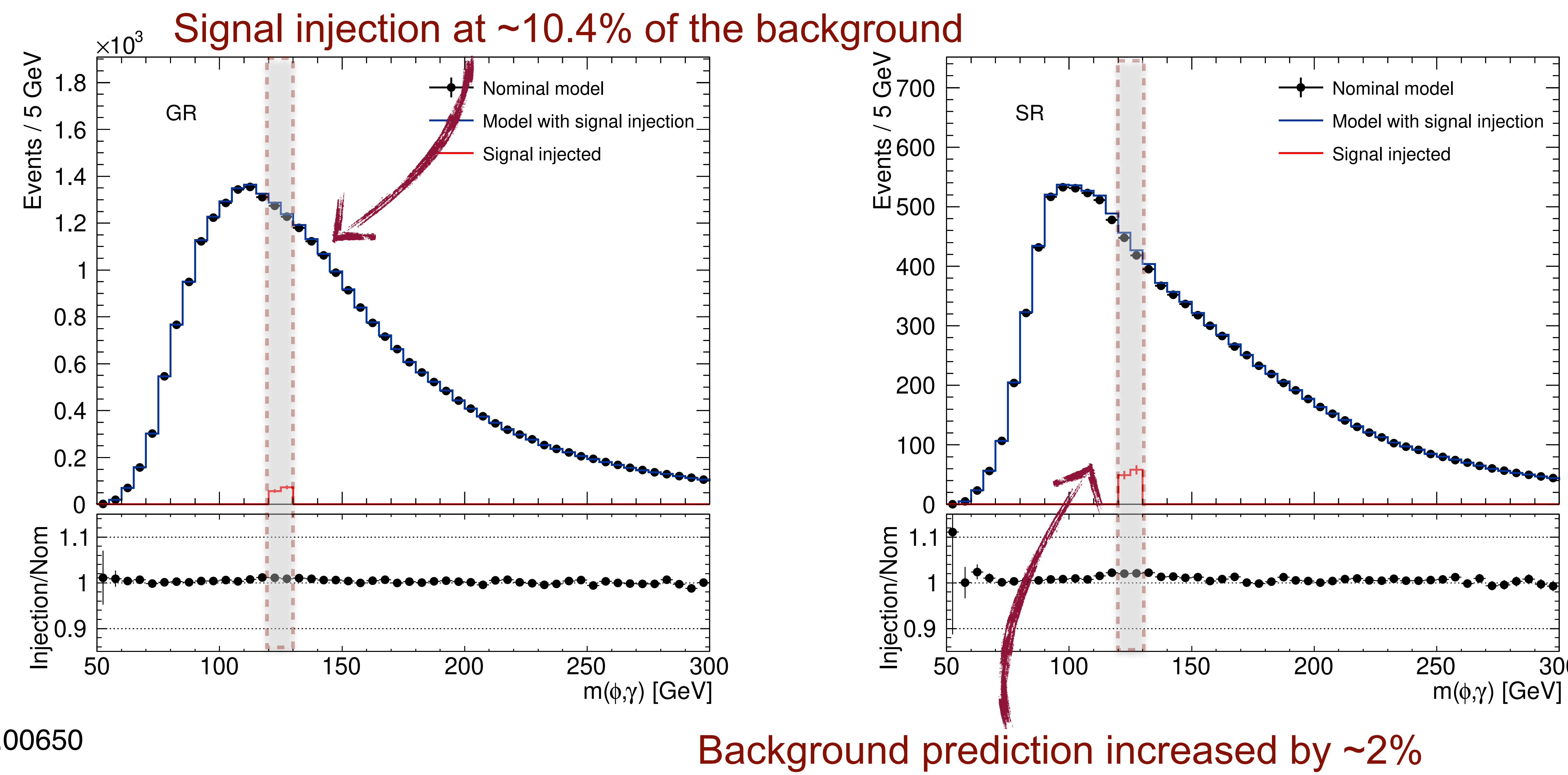

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h/Z→Qγ: Resonant Backgrounds

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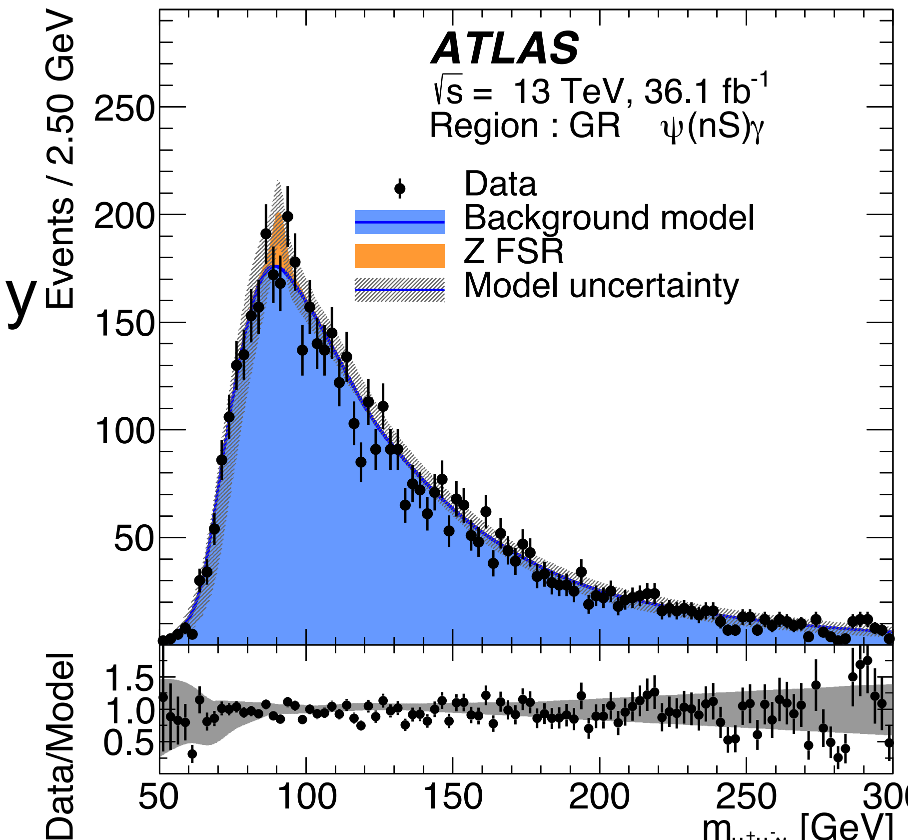
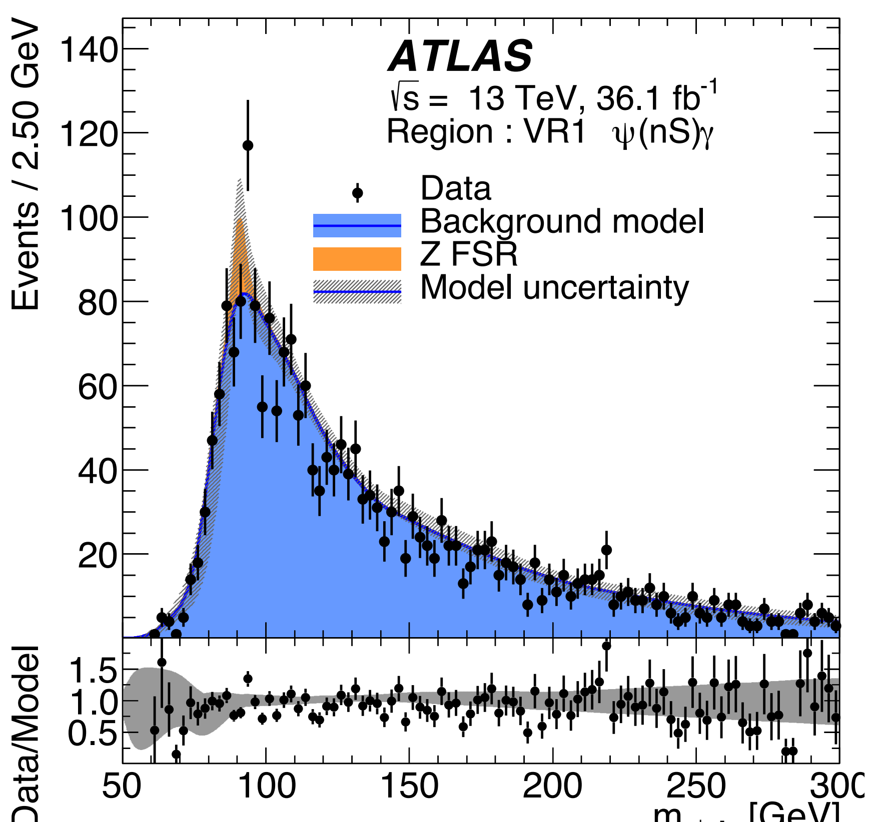
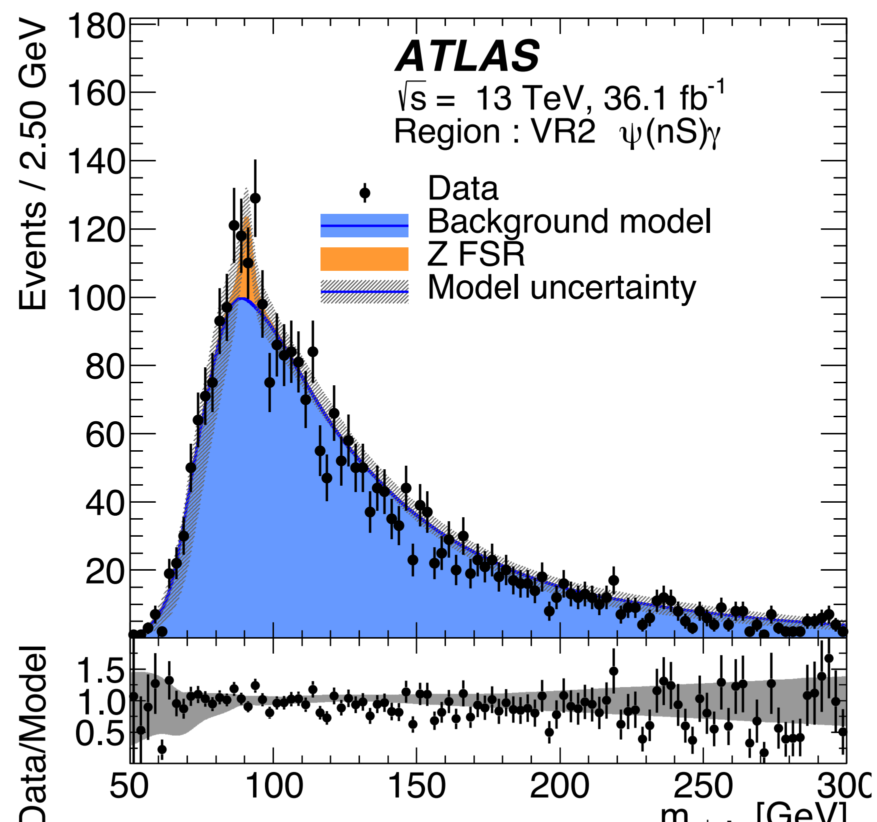
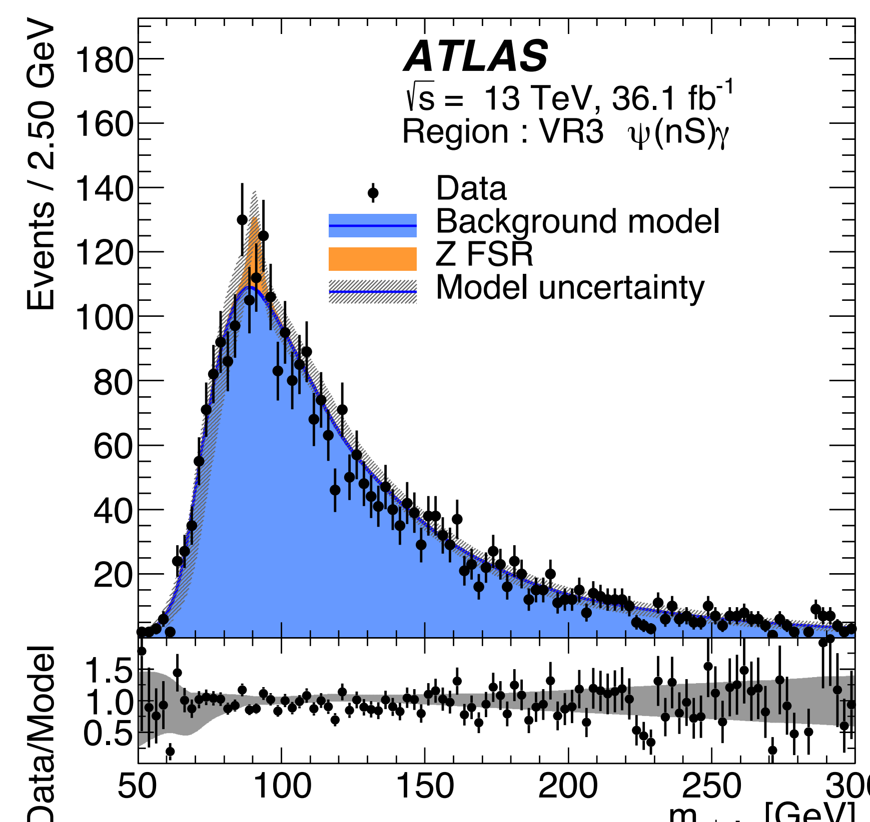


arXiv:1807.00802

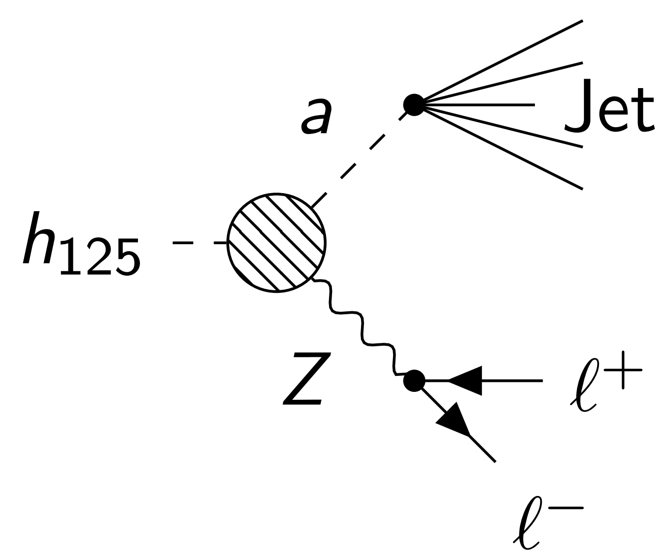


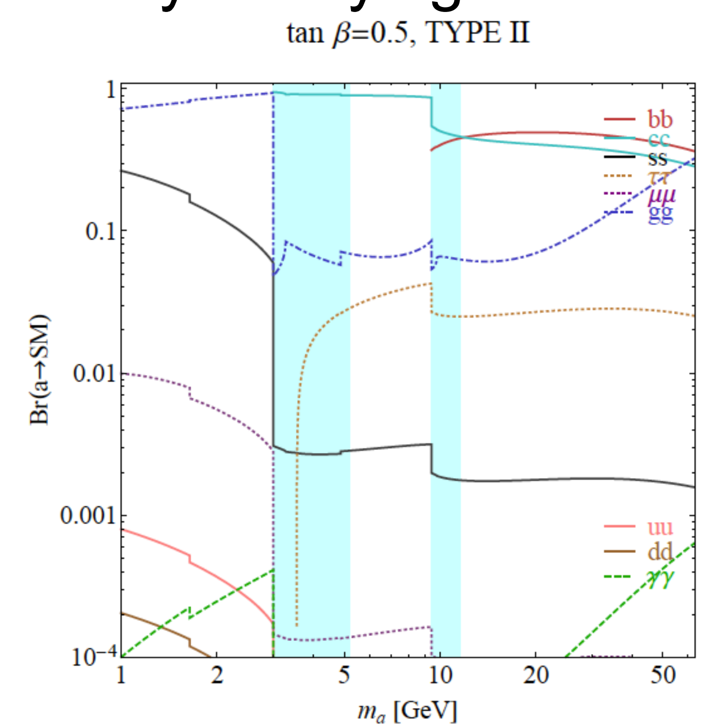




h→Za→ll+jet

Higgs decays to light hadronically decaying scalars





PRD 90 (2014) 7, 075004

h→Za→ll+jet

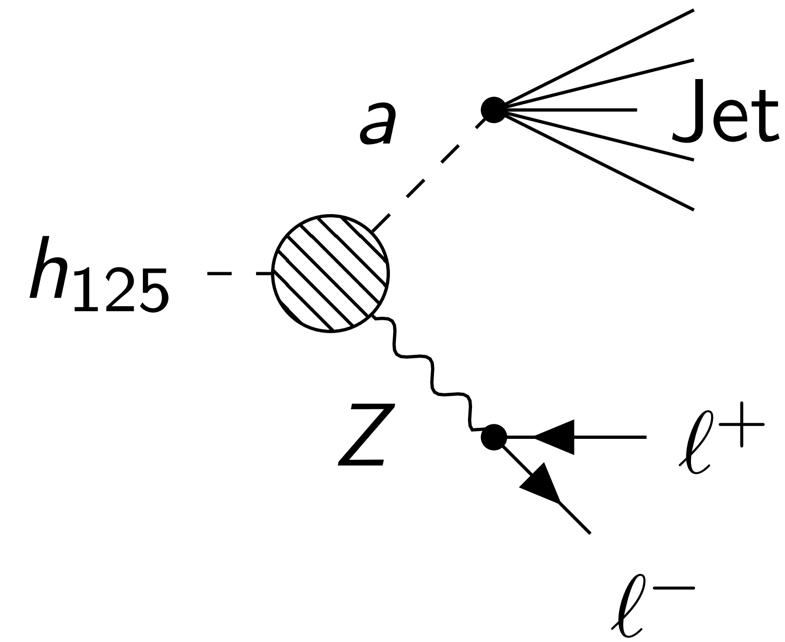
PRL 125 (2020) 22, 221802

Experimental focus mostly on:

- h→aa
- a→down-type fermions

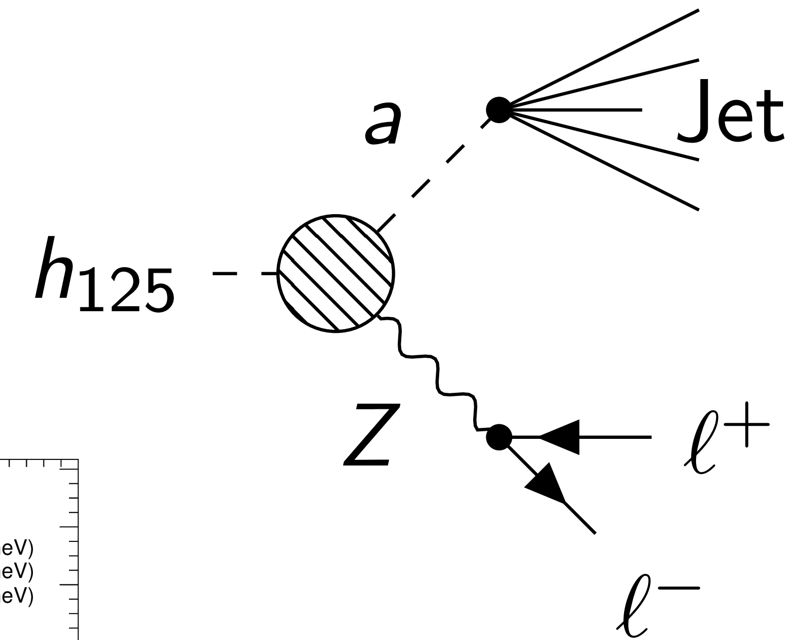
New search: h→Za with a→hadrons

- Overwhelming Z + jets background
- a→hadrons reconstruction using sub-structure techniques



h→Za→ll+jet

PRL 125 (2020) 22, 221802



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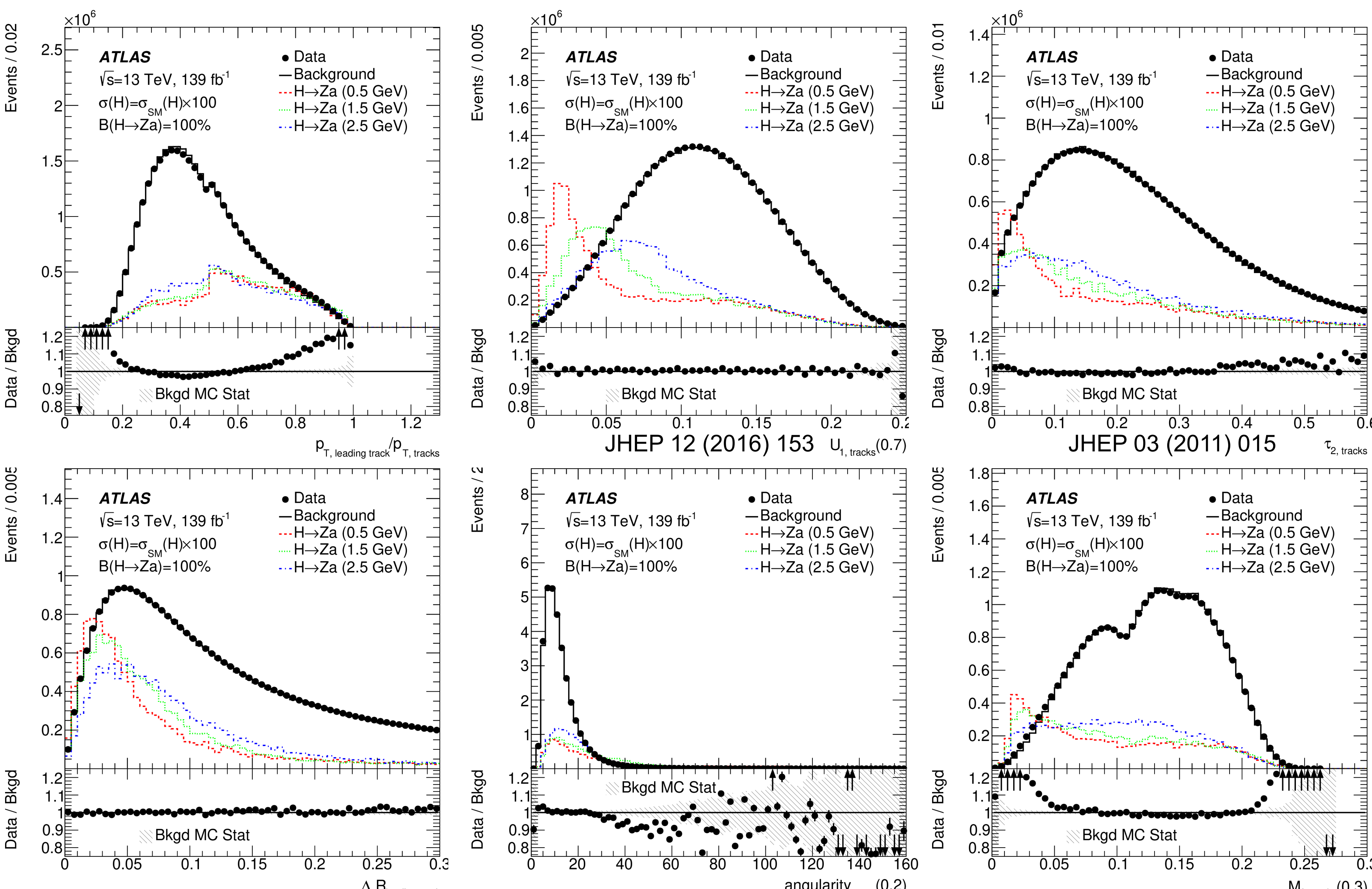


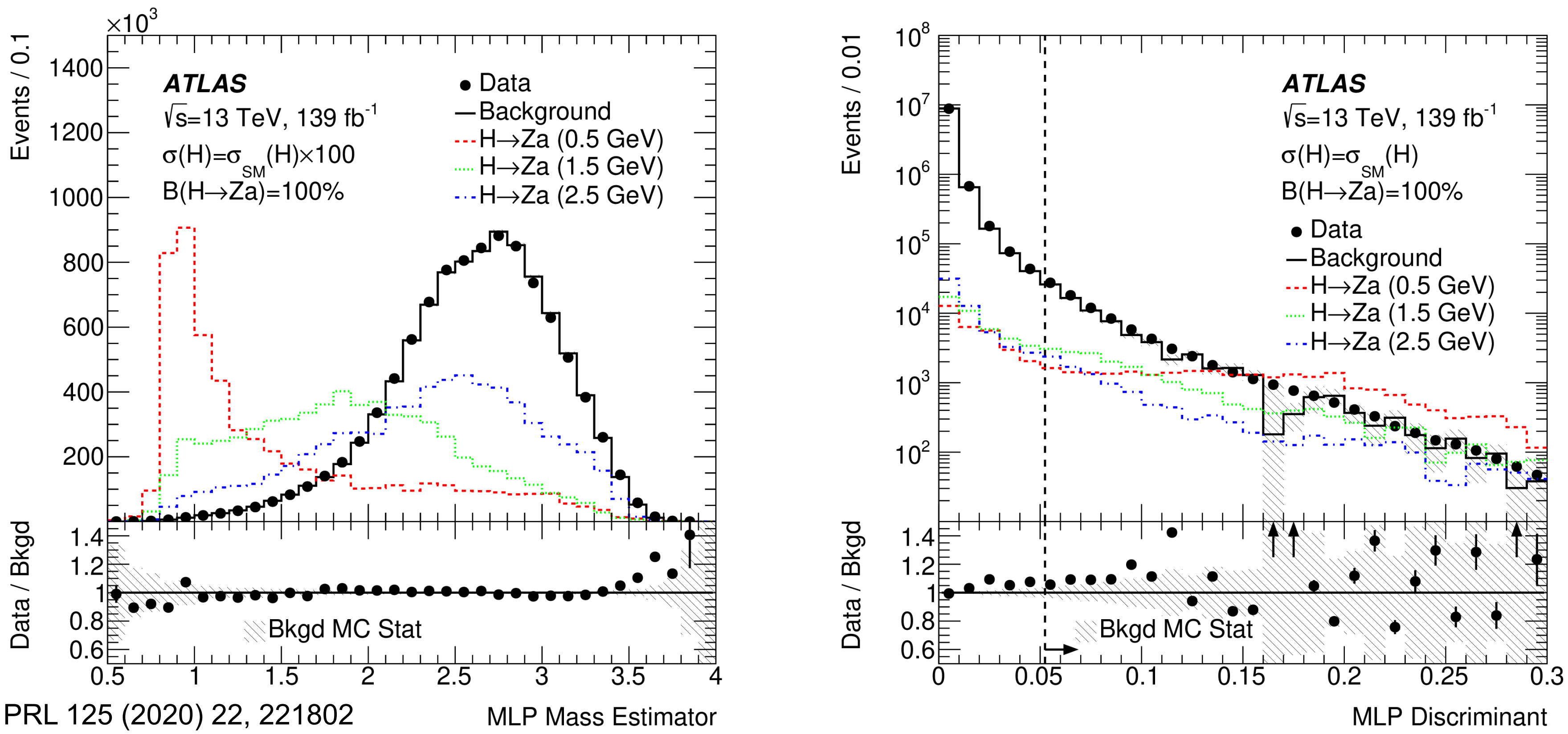
JHEP 12 (2016) 153

JHEP 03 (2011) 015

PRD 79 (2009) 074017

JHEP 12 (2016) 153

h→Za→ll+jet



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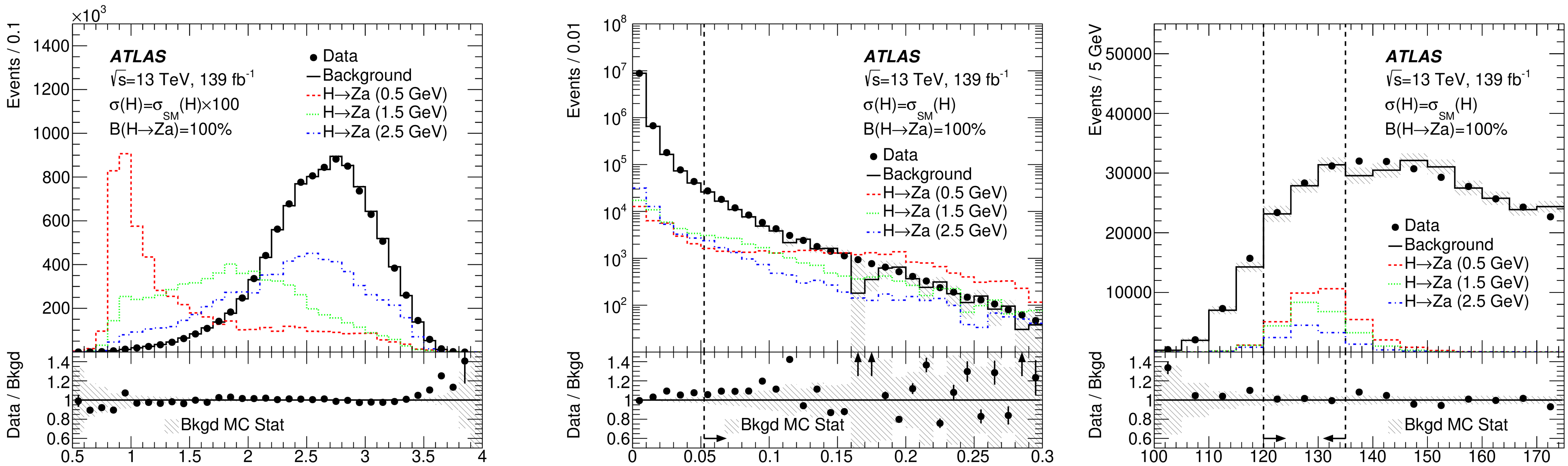
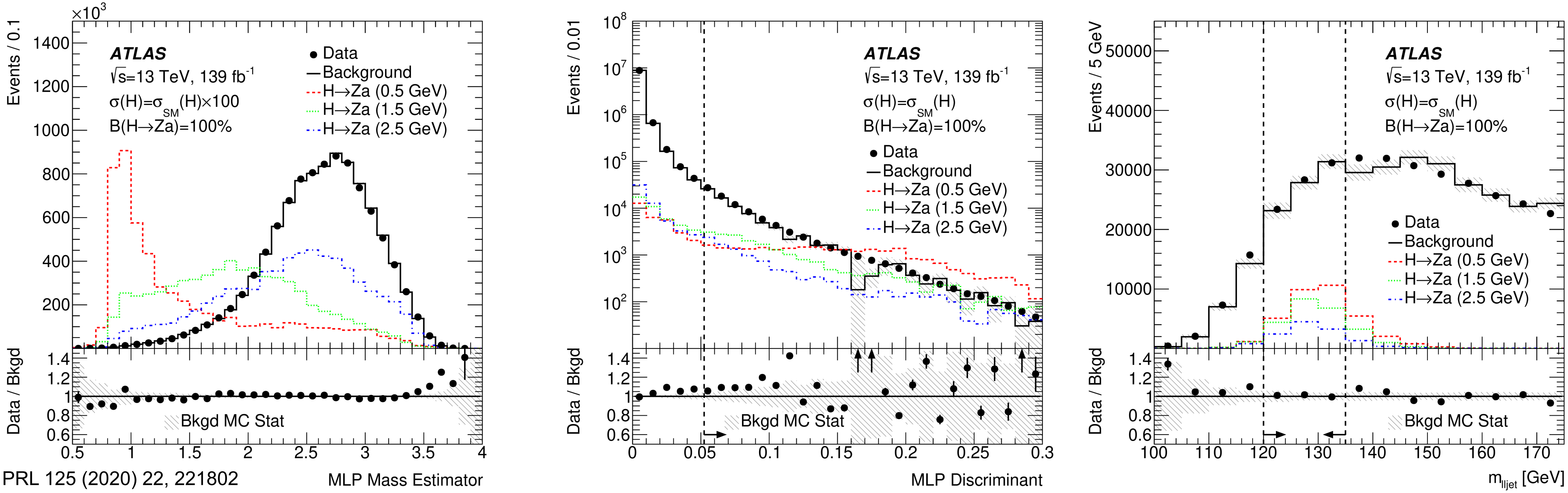


PRL 125 (2020) 22, 221802

Expected Bkg: 82400±3700
Observed: 82908

h→Za→ll+jet



PRL 125 (2020) 22, 221802

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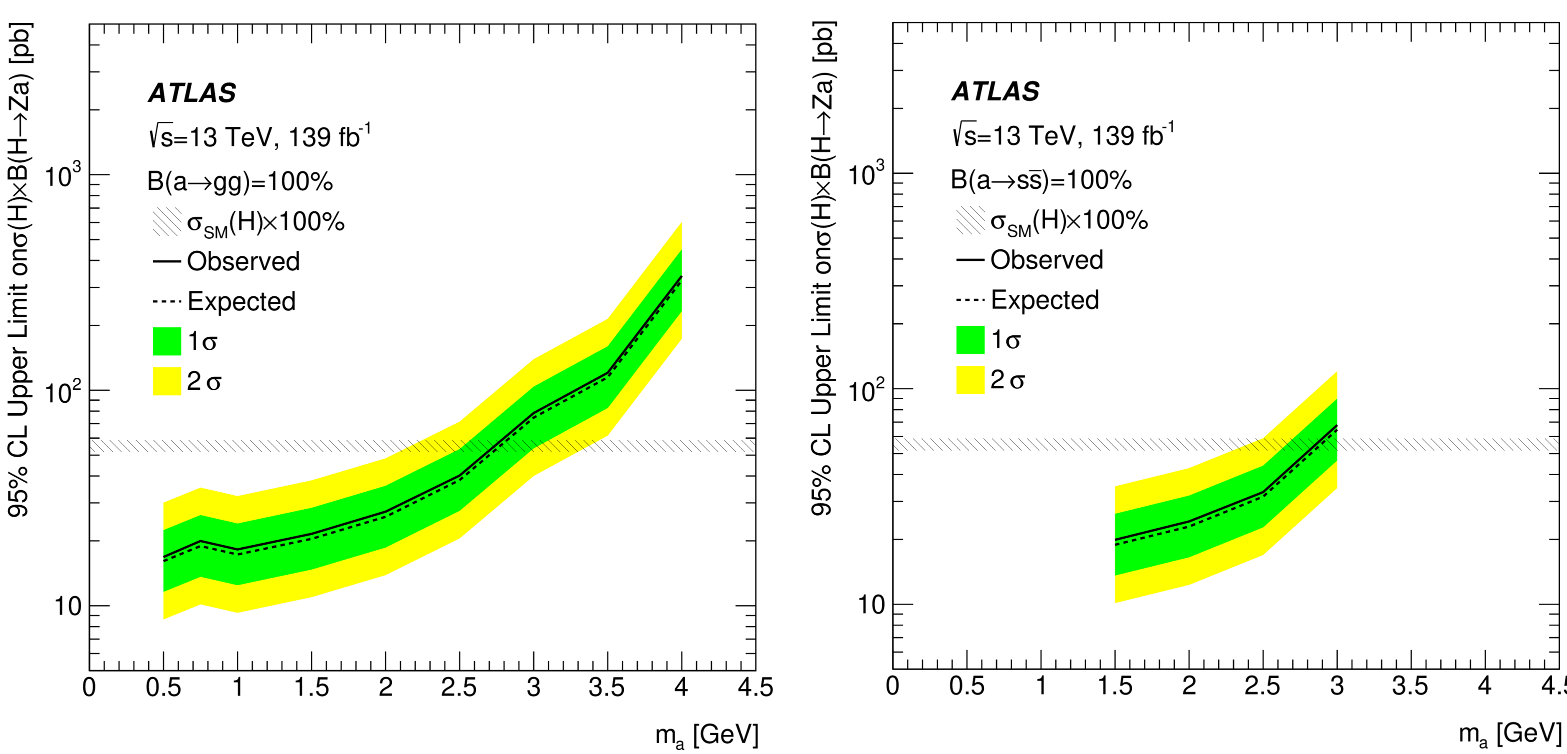
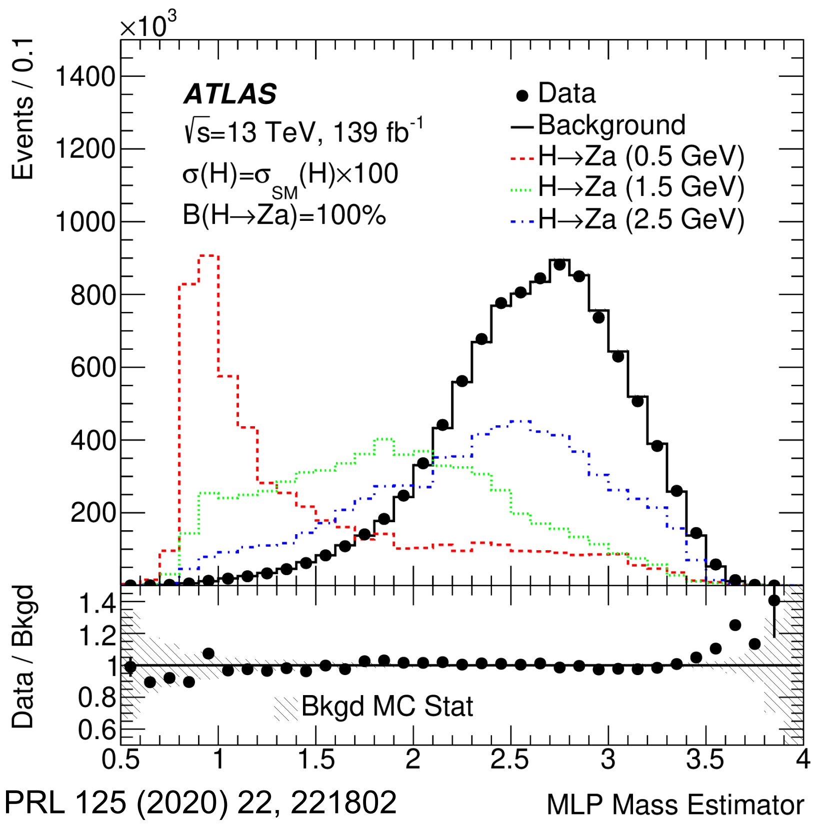


Expressed in $B(H \to Za) \times B(a \to \text{hadrons})$ limits start from BR<31%

h→Za→ll+jet



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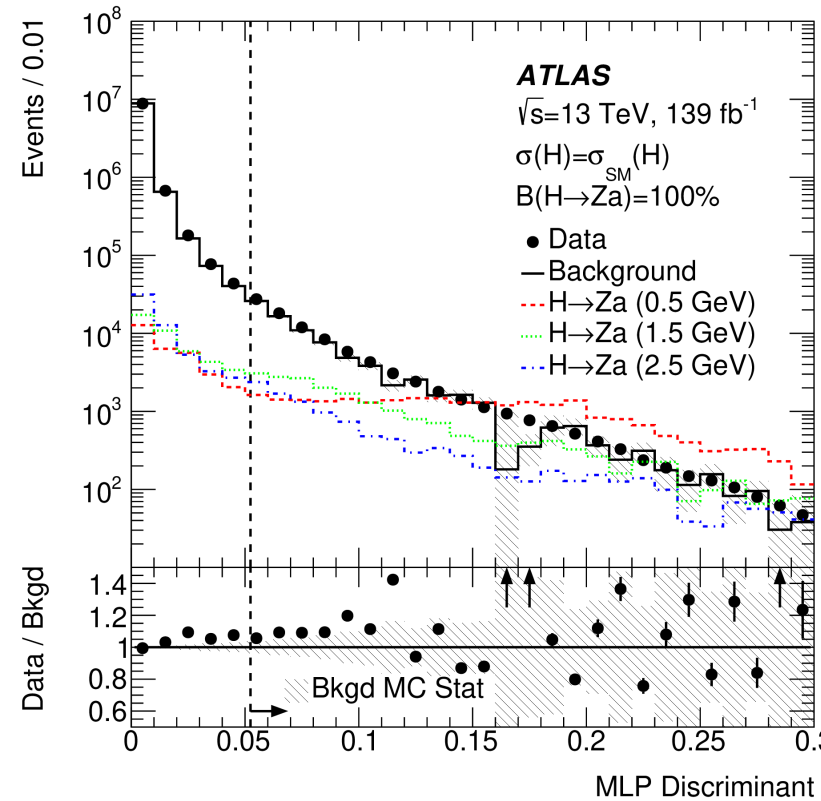

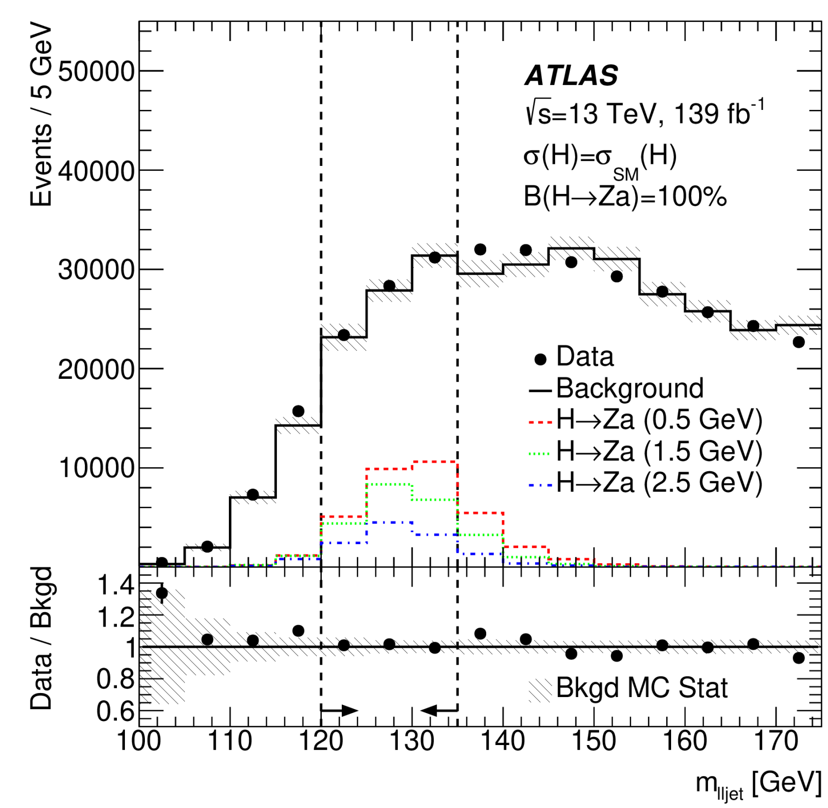

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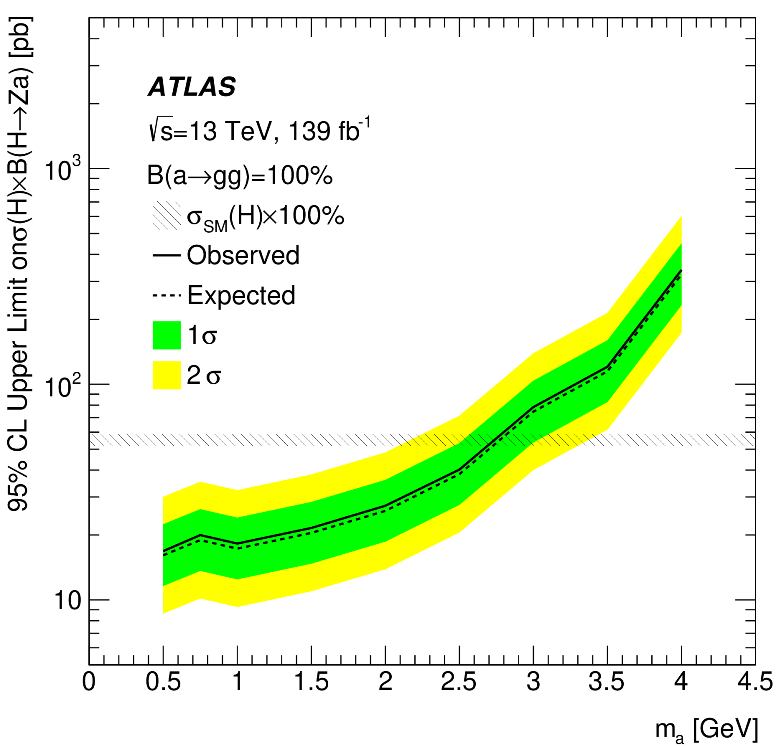

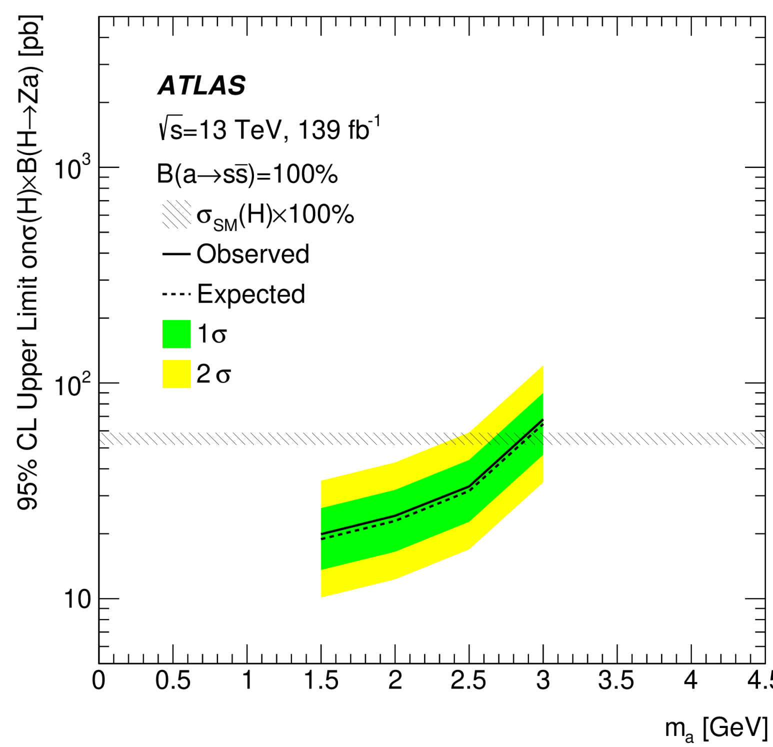

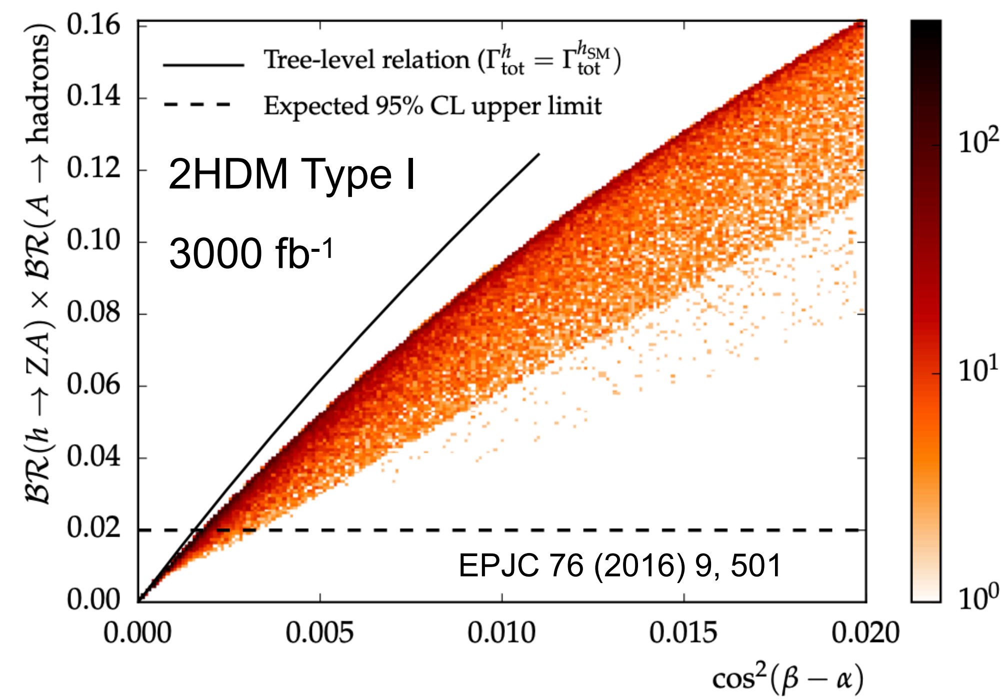

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h→Za→ll+jet

Background estimation: MC-corrected ABCD method using $m_{\ell\ell j}$ and MLP discriminant

- Accounts for 13% correlation between $m_{\ell\ell j}$ and MLP discriminant

$$A_{\text{SR}}^{\text{ABCD Est.}} = \underbrace{\frac{B_{\text{data}} C_{\text{data}}}{D_{\text{data}}}}_{\text{Data-driven ABCD Estimate}} \times \underbrace{\frac{A_{\text{MC}}}{\frac{B_{\text{MC}} C_{\text{MC}}}{D_{\text{MC}}}}}_{\text{MC-based ABCD Correction Factor}}$$

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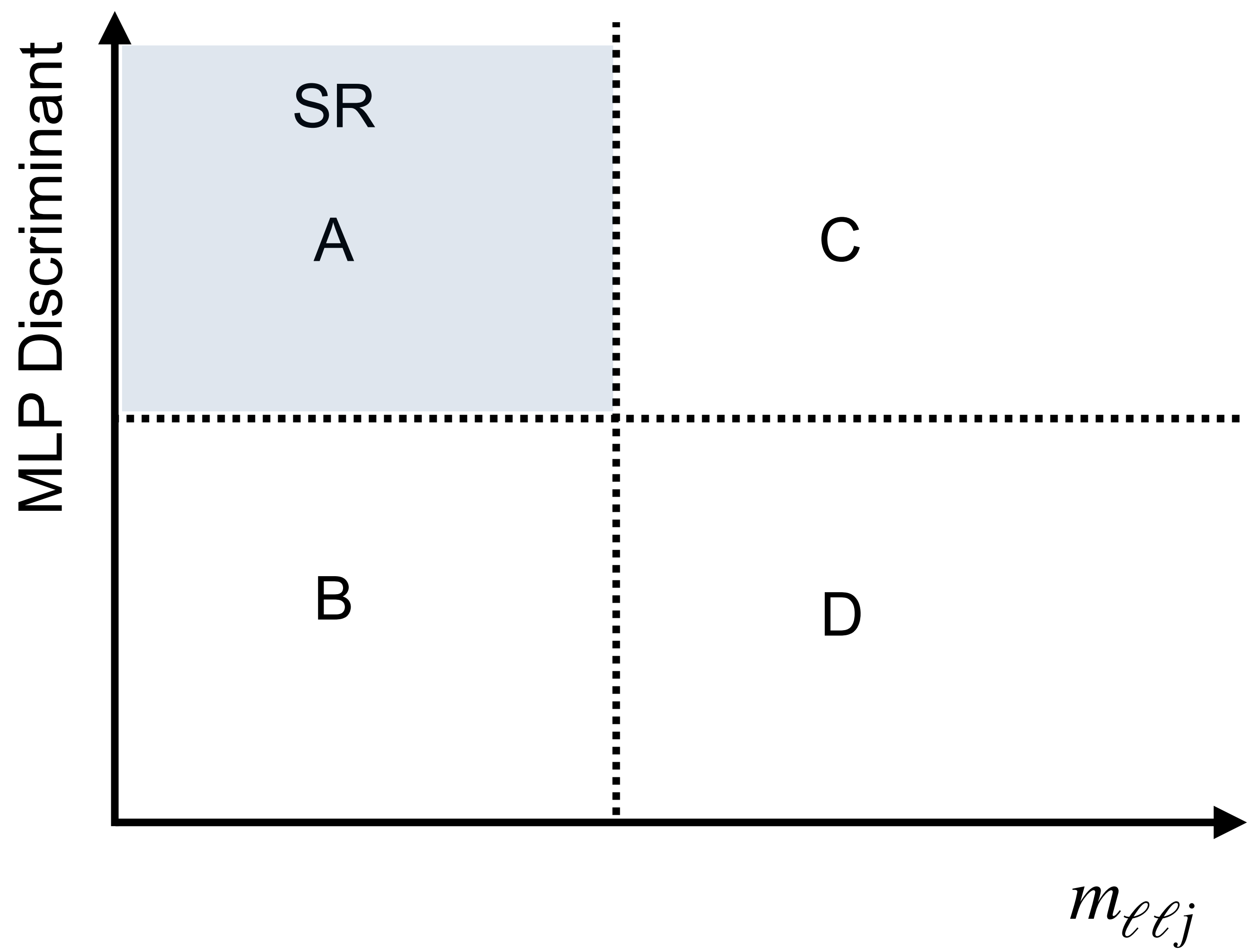

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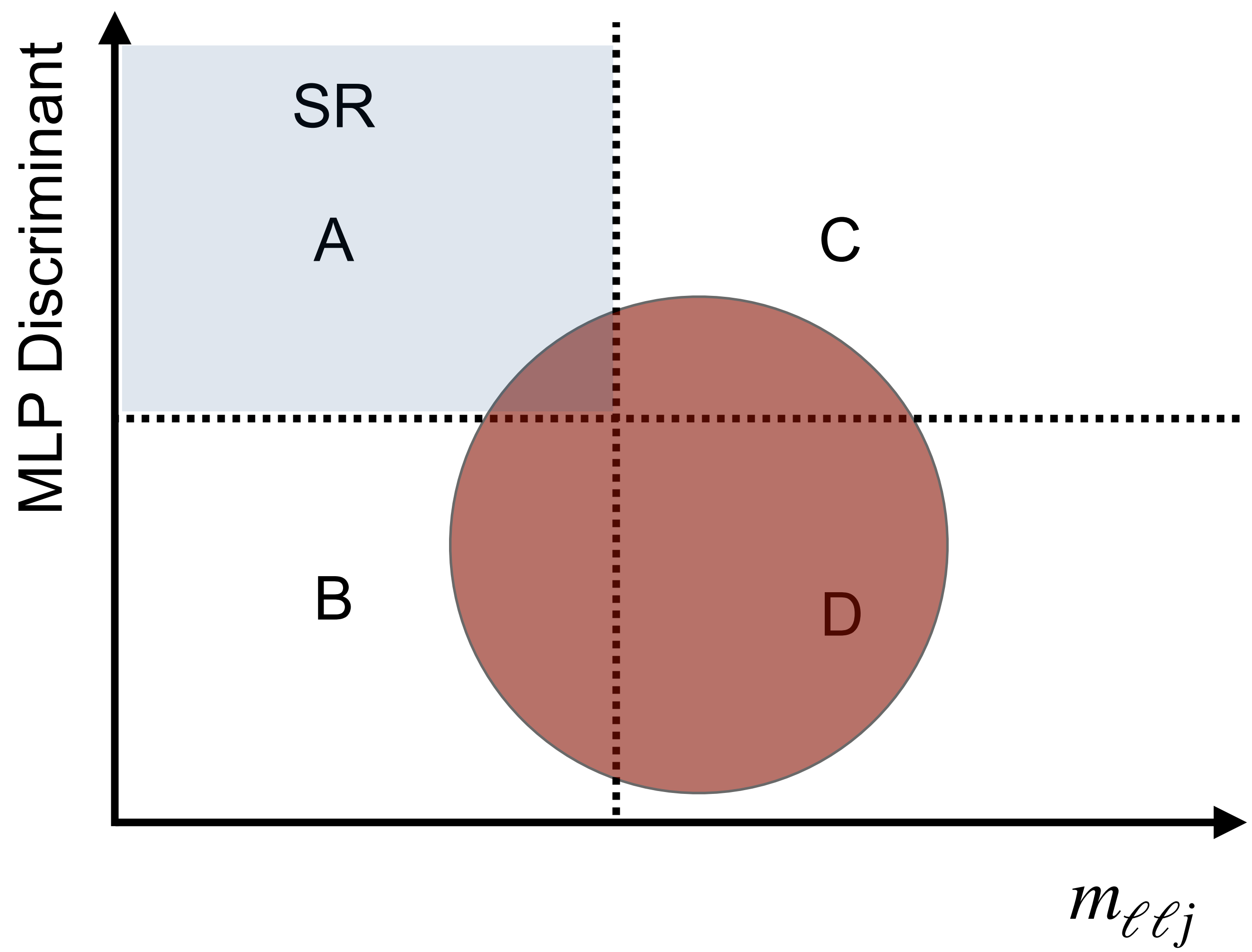

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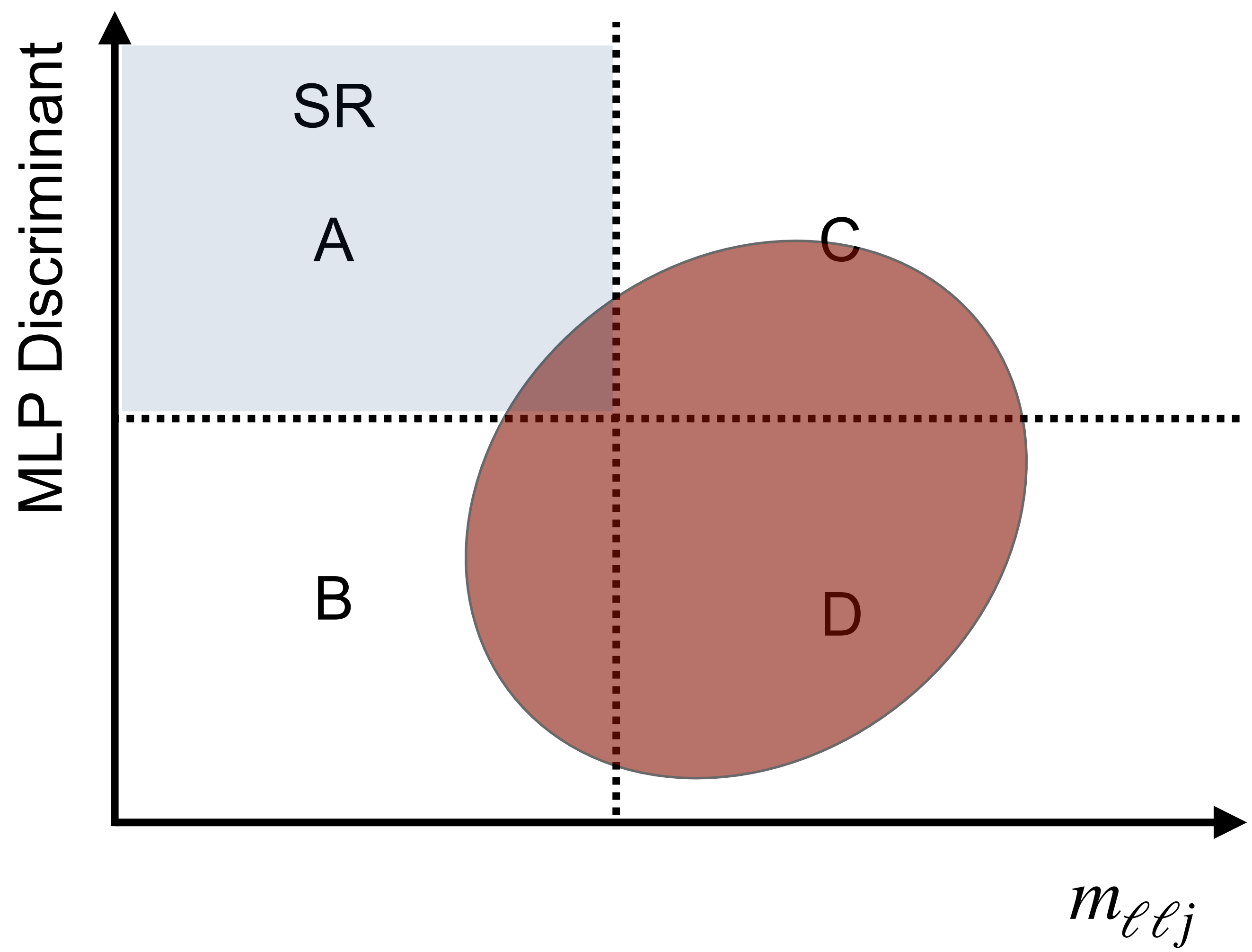

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a mass	0.5 GeV	1.5 GeV	2.5 GeV
Total Uncertainty	8.3	10.7	20.3
Total Statistical Uncertainty	0.6	0.8	1.6
Total Systematic Uncertainty	8.2	10.7	20.2
Signal Systematic Uncertainties			
Jet Energy Scale	1.3	1.5	1.5
Parton Shower	1.4	1.4	1.4
Luminosity, Pileup, Trigger, Leptons, & JVT	0.2	0.3	0.5
MC Statistics	0.2	0.2	0.6
Renormalization Scale	0.1	< 0.1	0.2
Acceptance	0.1	< 0.1	0.2
Background Systematic Uncertainties			
MC Statistics	6.4	8.4	15.8
Parton Shower and ME	3.9	5.1	9.6
Renormalization Scale	3.4	4.4	8.3

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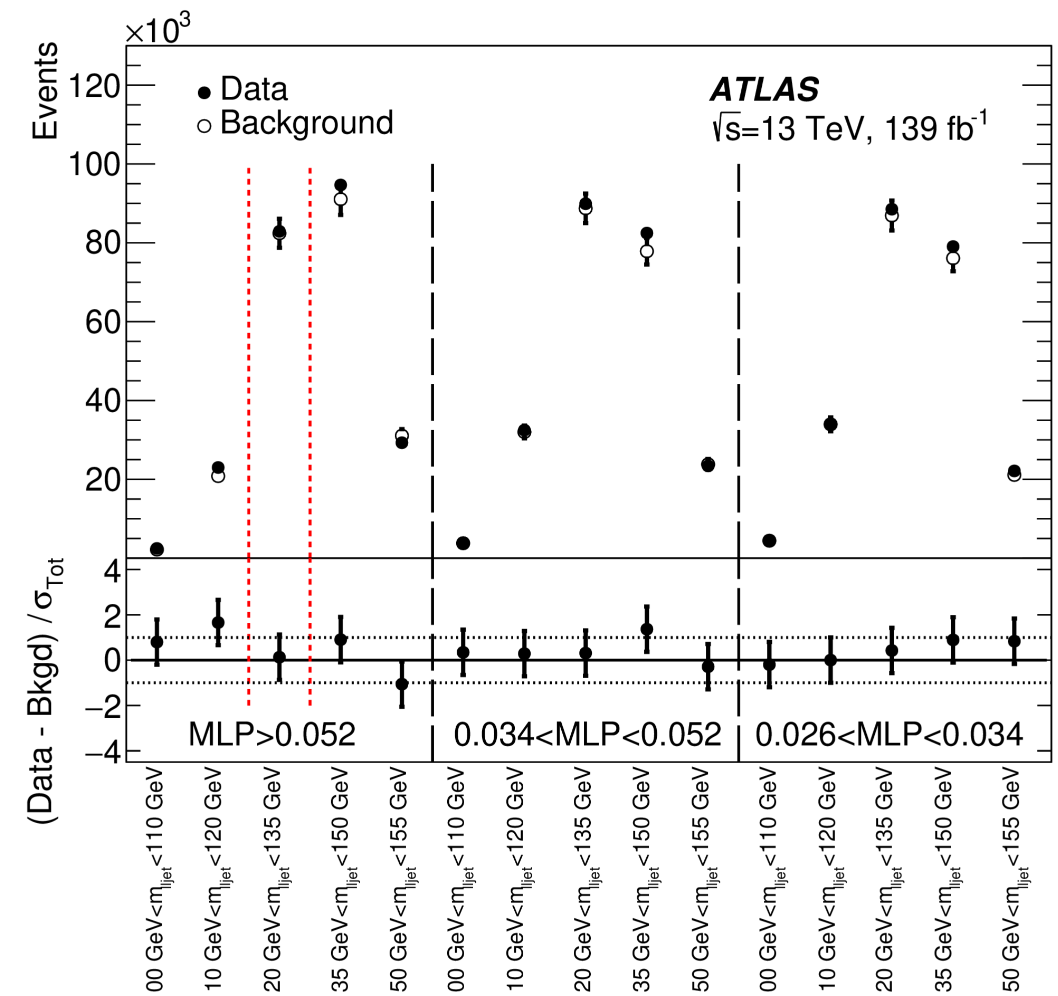

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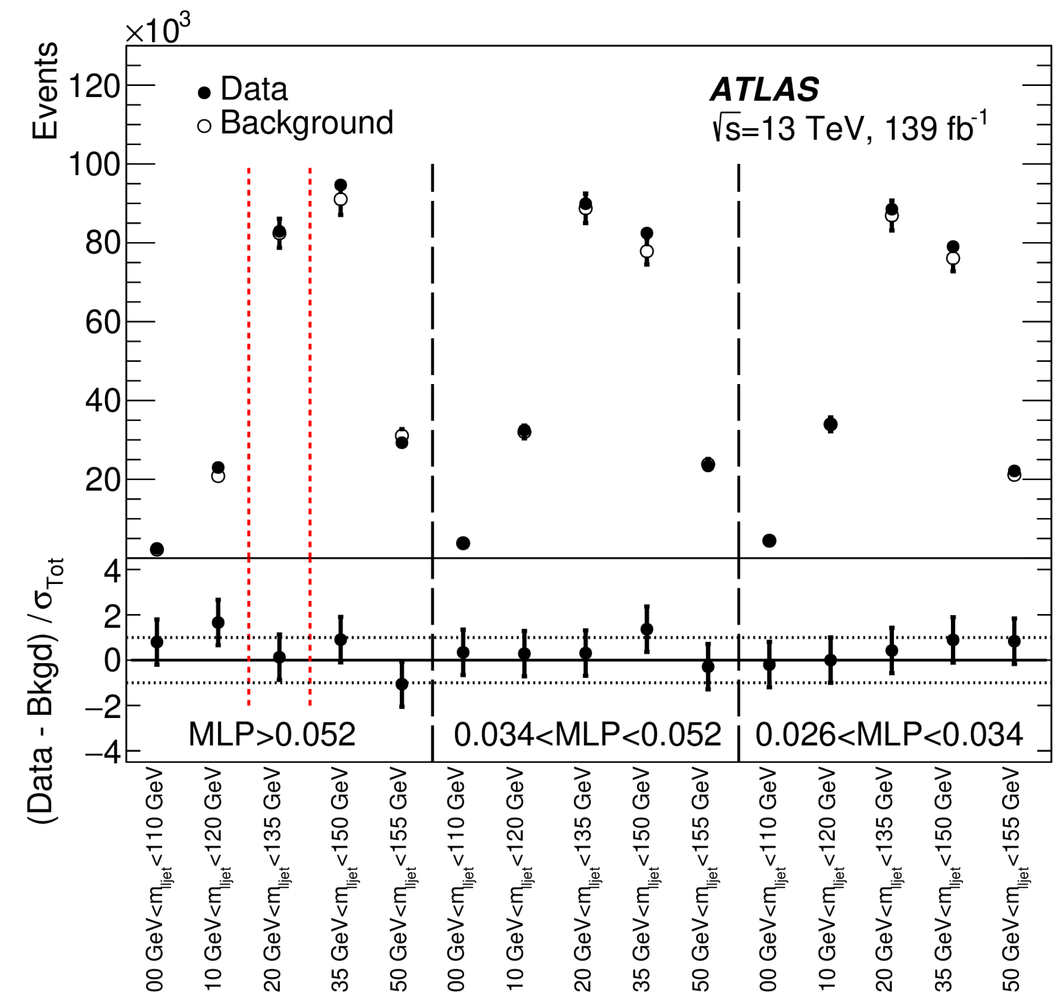

Suppressing MC statistical/modelling uncertainties would improve limit from 31% to 7.5%!

Generative Adversarial Network

To improve analysis sensitivity → improve background model

- Increase sample size
- Improve Generator-level modelling uncertainties

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Ancestral sampling procedure presented earlier is impractical

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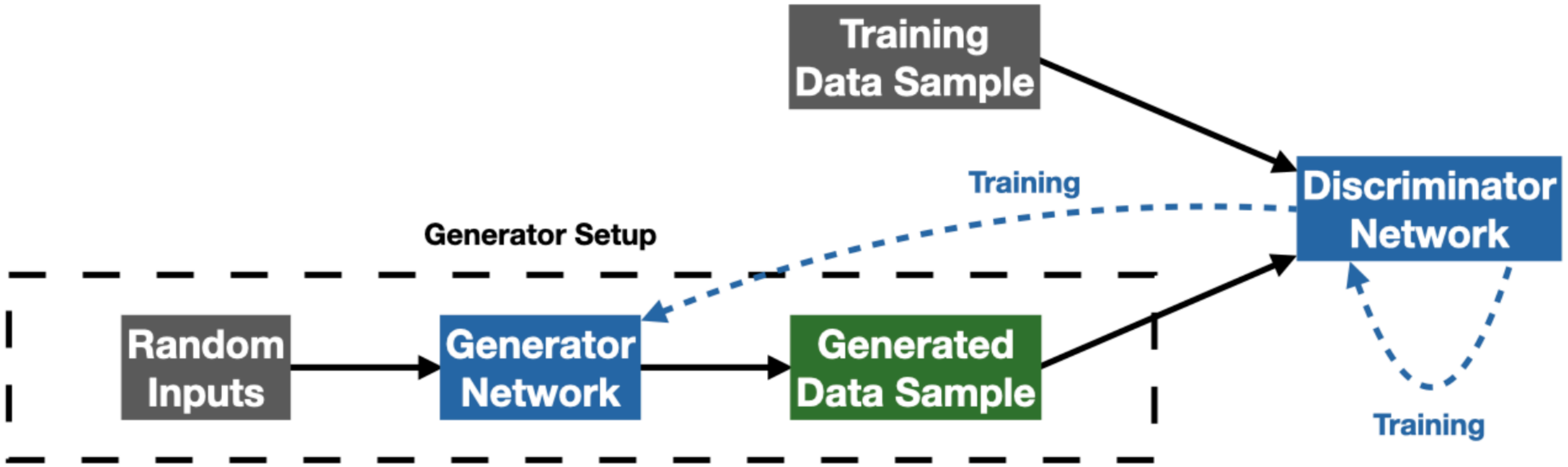

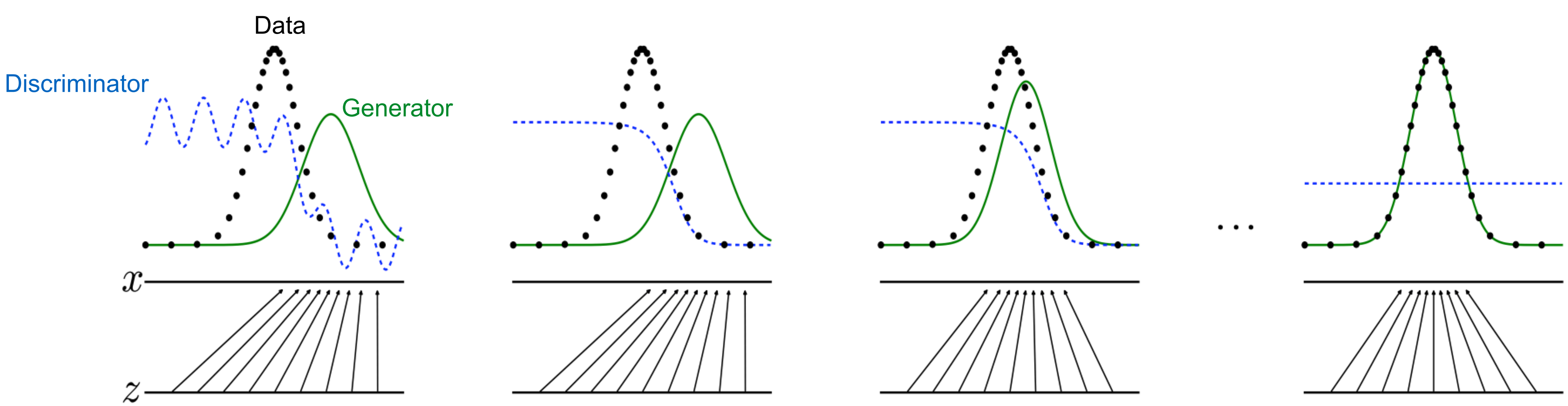

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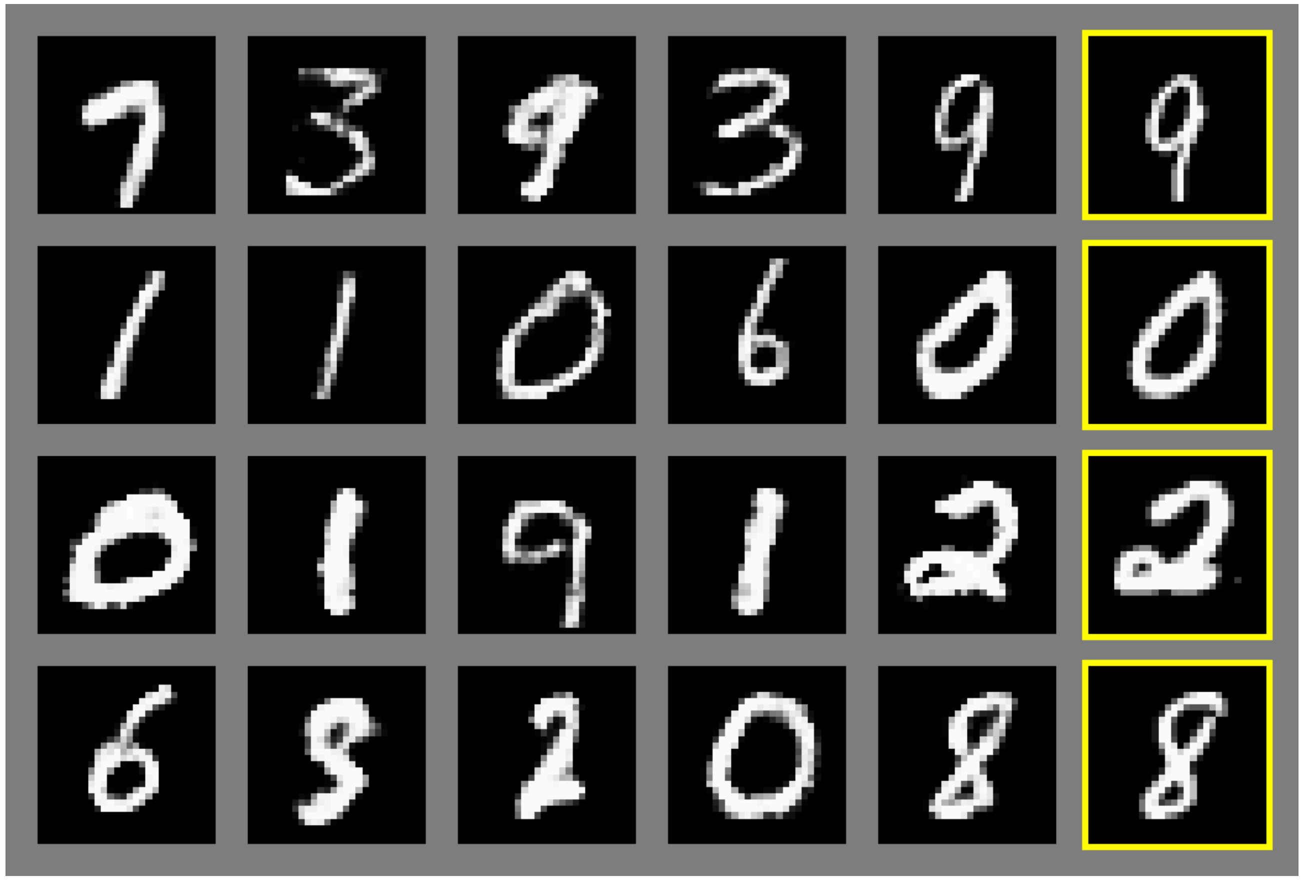
arXiv:1406.2661



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StyleGAN2 (Dec 2019) - Karras et al. and Nvidia

Novelty: directly use data in superset of signal region for model generation

- Resolves concerns about modelling uncertainties

conditioned-GAN

Complication: dataset used for model generation may be contaminated by signal

- Blind the Signal Region while training the GAN

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conditioned-GAN (cGAN): generator depends on **conditioning variable** → model can be interpolated

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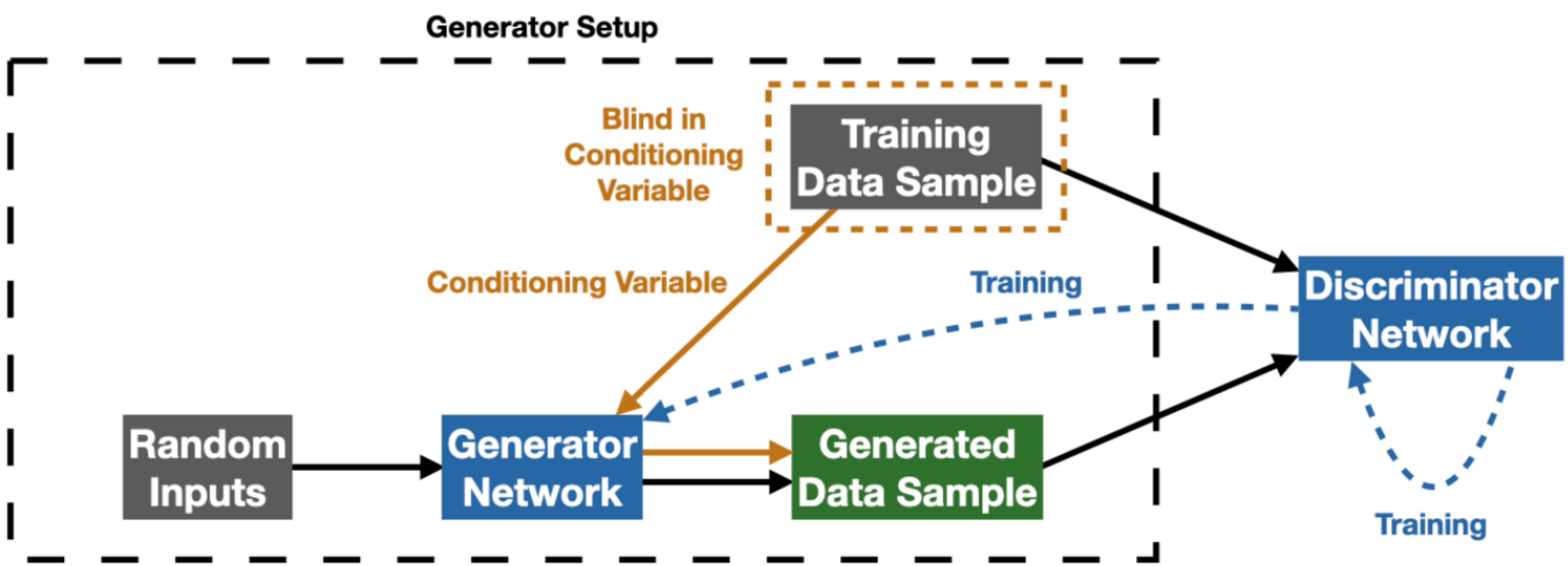


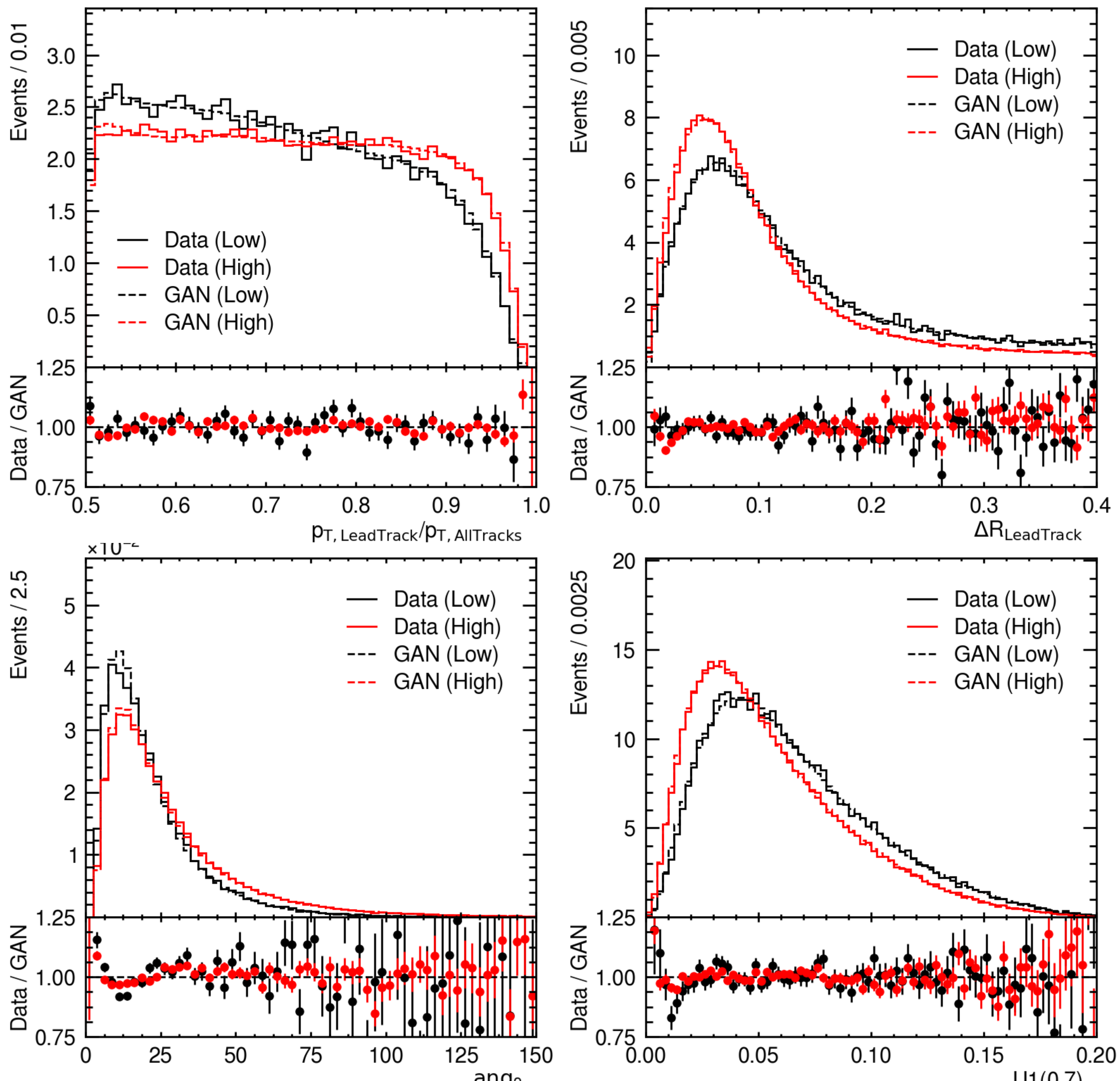
Generator and discriminator:

- 5 layers × 256 hidden nodes with leaky ReLU activation function
- Binary cross entropy loss function and L2 regularisation

cGAN: Modelling of variables

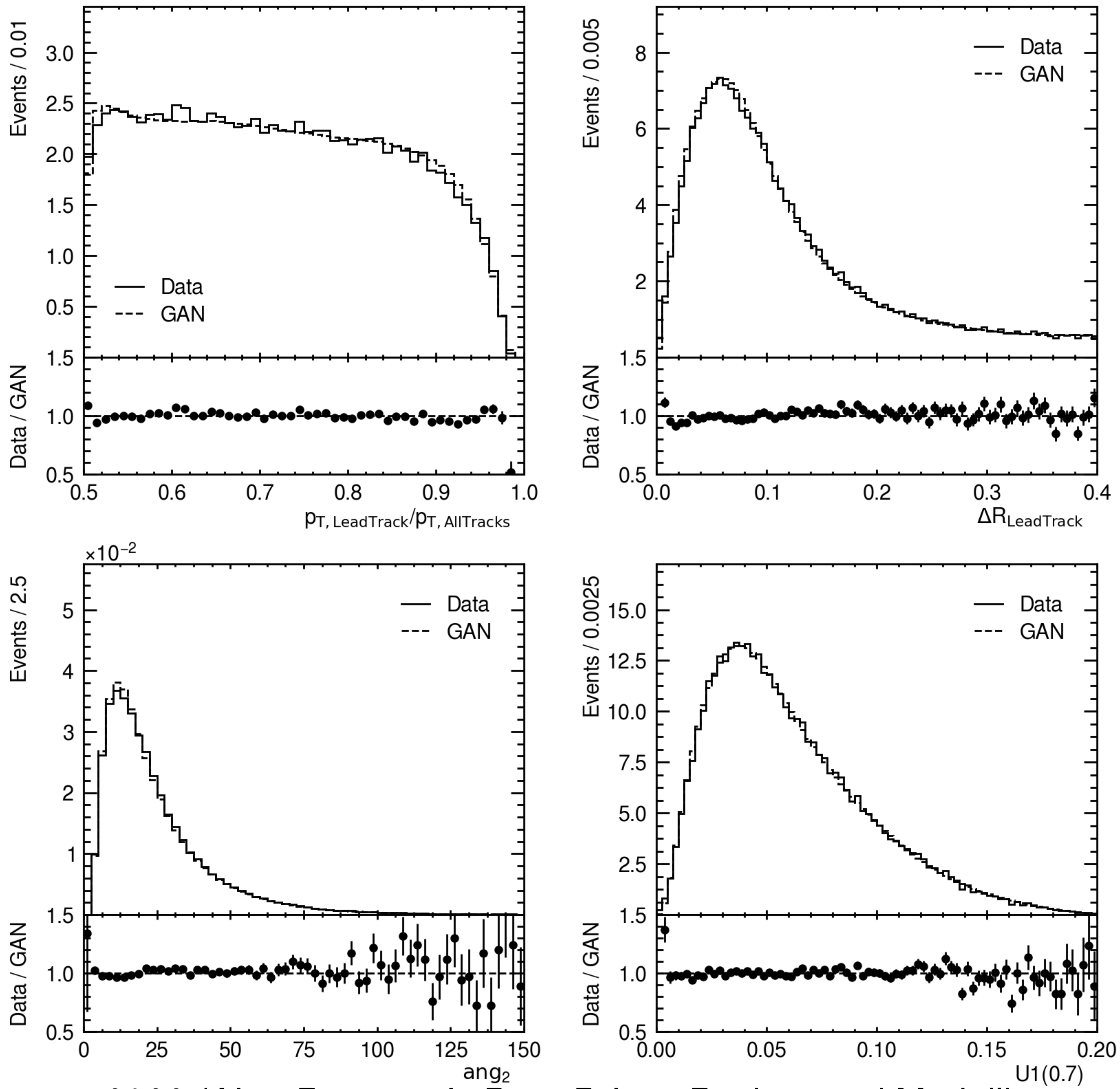
Trained 100 cGANs with random hyper-parameters

- Ensemble of top 5 cGANs, based on χ^2, retained



cGAN: Modelling of variables

$$123 \text{ GeV} < m_{\ell\ell j} < 135 \text{ GeV}$$



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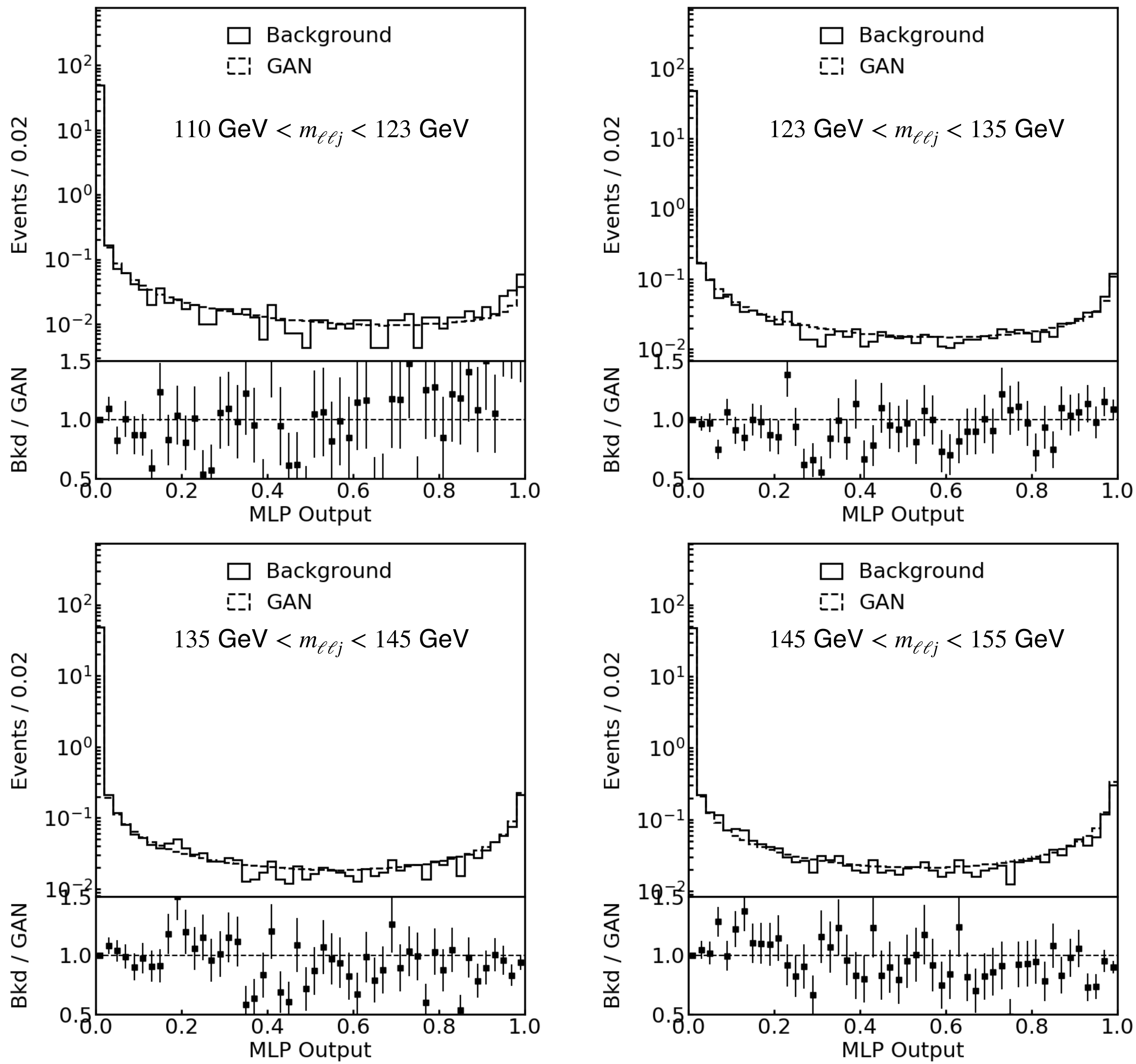

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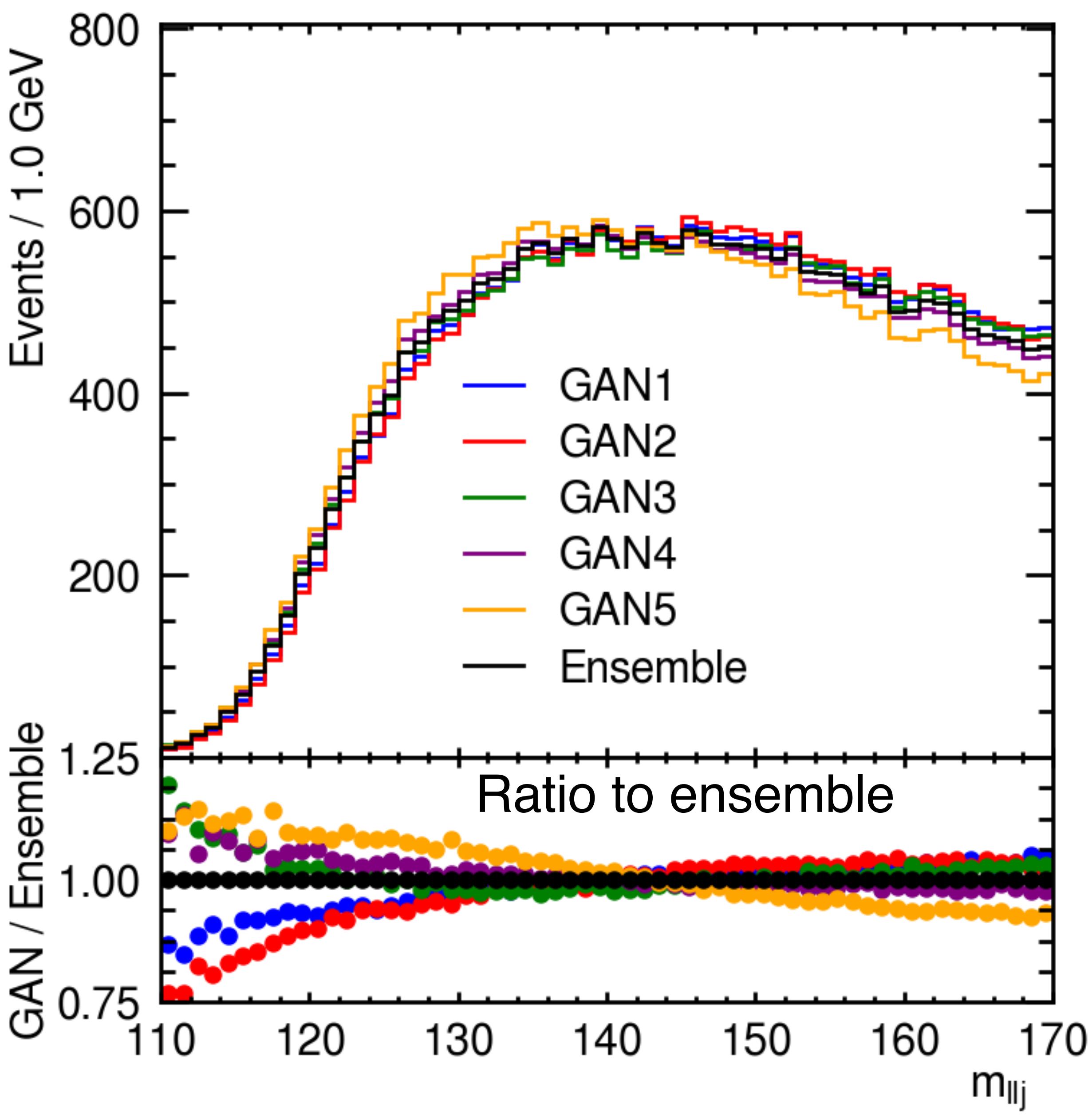
cGAN: Ensemble and Shape Variations

Shape variations:

- Perform Principal Component Analysis on differences of individual cGANs to ensamble



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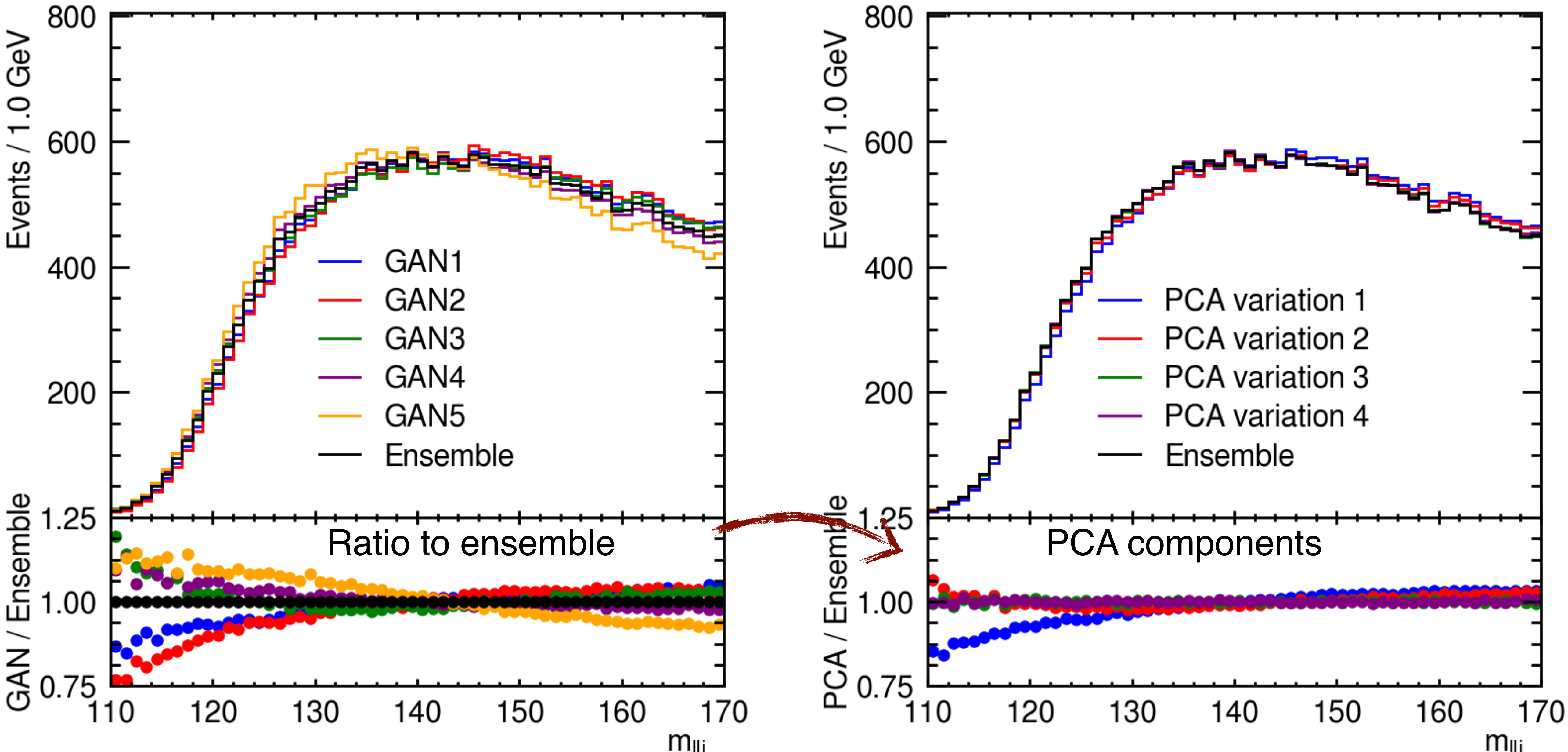
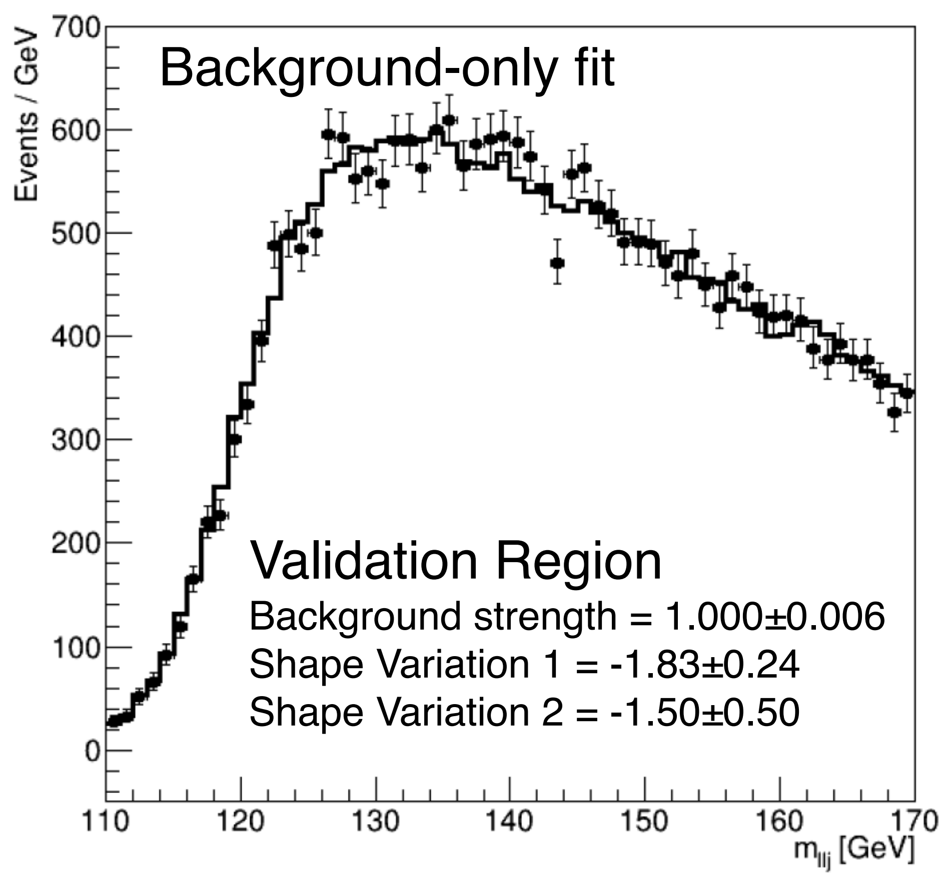


PCA components account for: 89%, 9.6%, 0.55%, and 0.40% of variance

cGAN: Fitting the "data"



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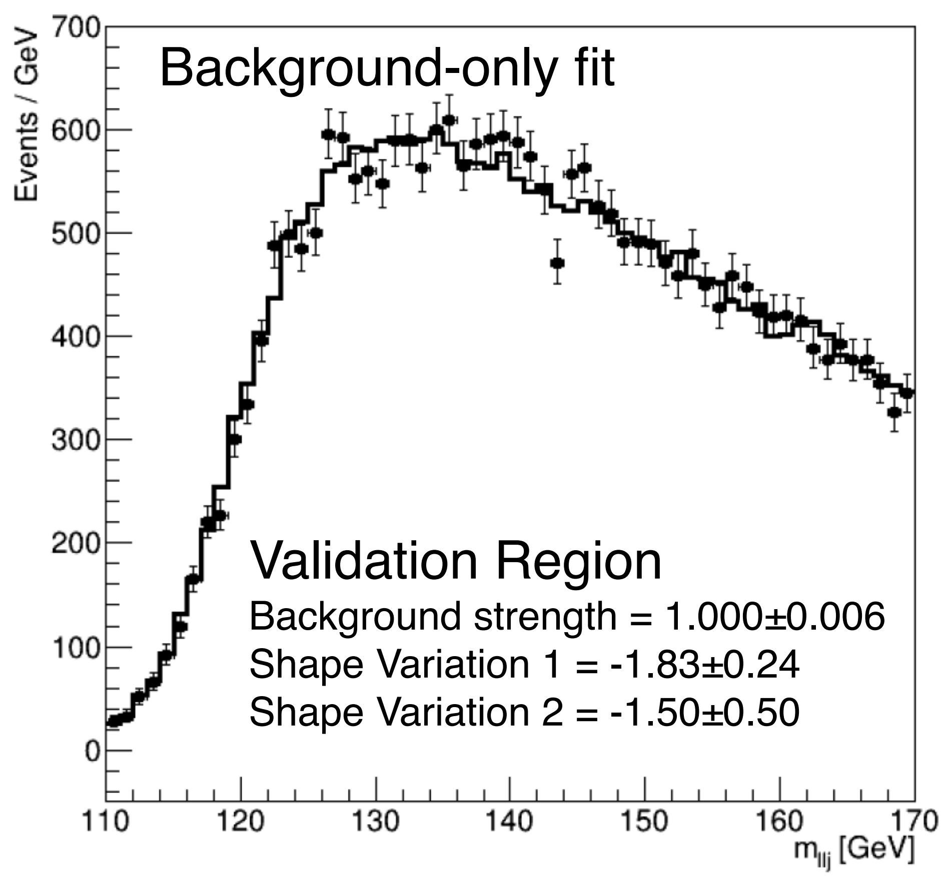

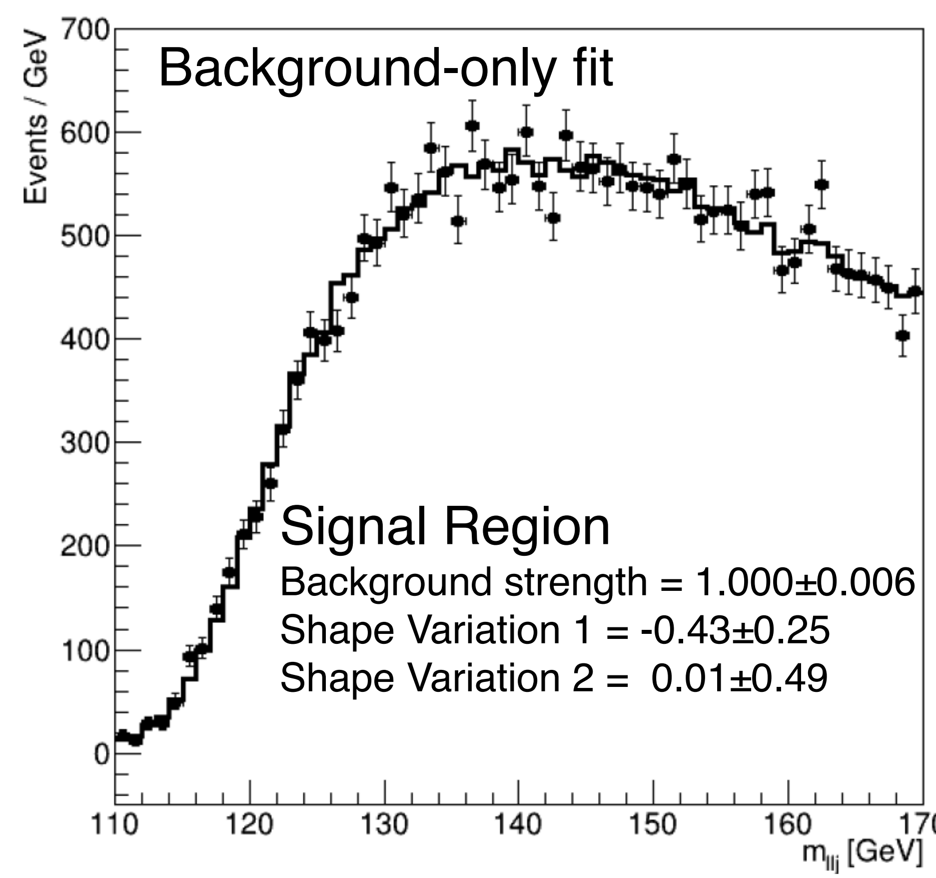

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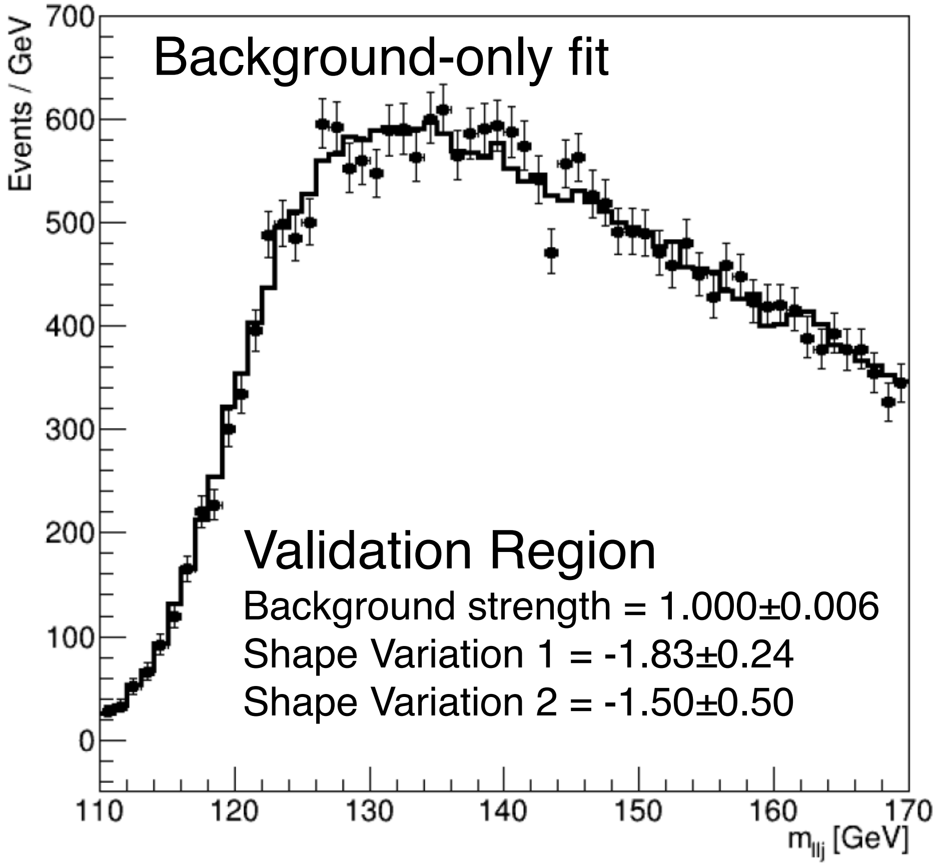
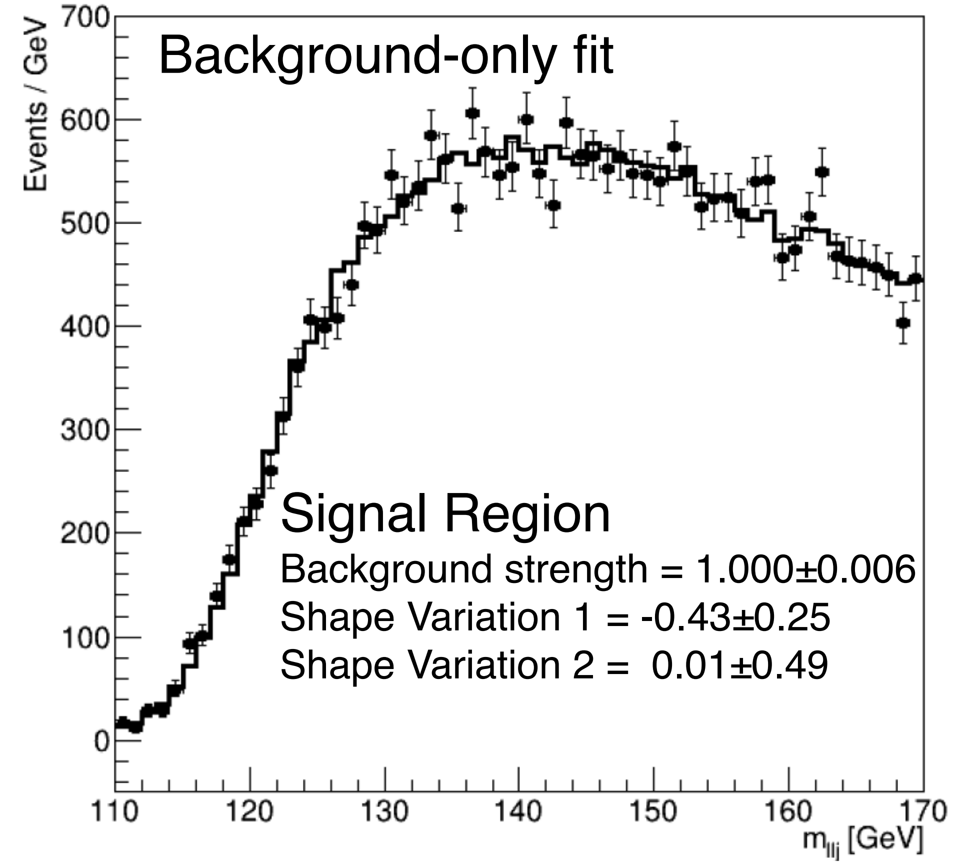
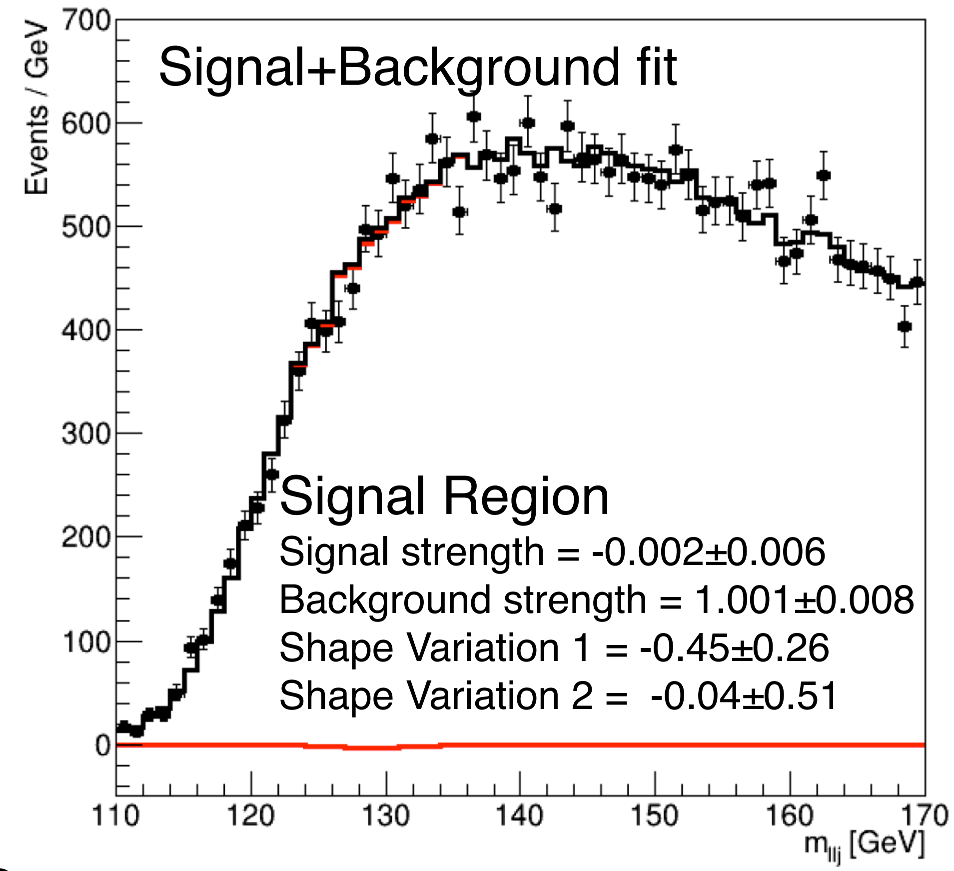






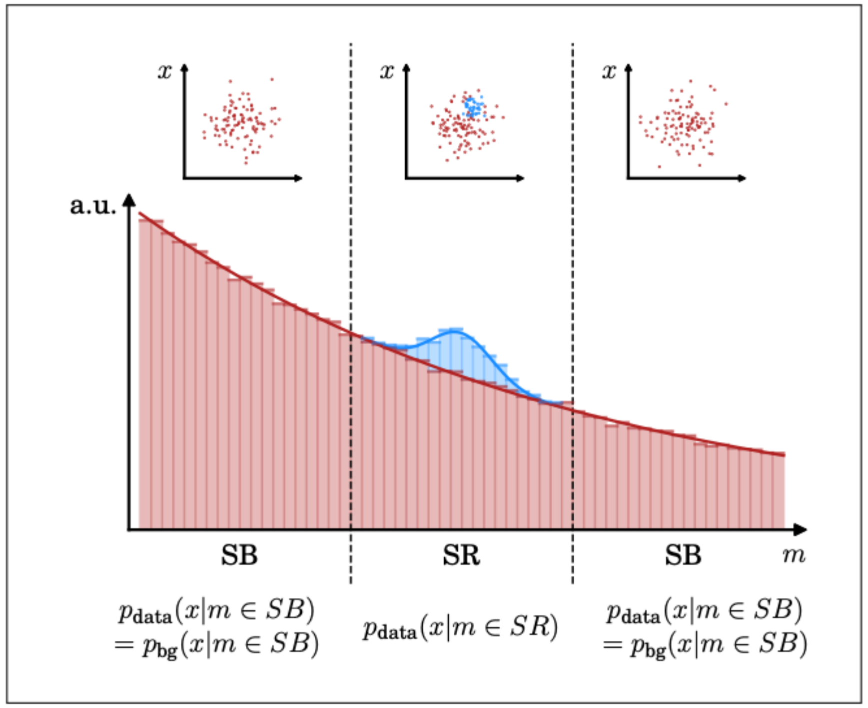
Signal+Background fit behaves as expected

- Obtained signal compatible with 0

CATHODE

- CATHODE: Classifying Anomalies Through Outer Density Estimation
  - Training a conditional density estimator (Masked Autoregressive Flow) on the discriminant variables in the side-band
  - Interpolating it into the signal region and sampling from it
  - Train classifier: separate SR data from produced "background" sample
  - Anomaly detection: Apply the trained classifier to data in SR
- In real life: the CATHODE method would need to be combined with a background estimation procedure

arXiv:2109.00546



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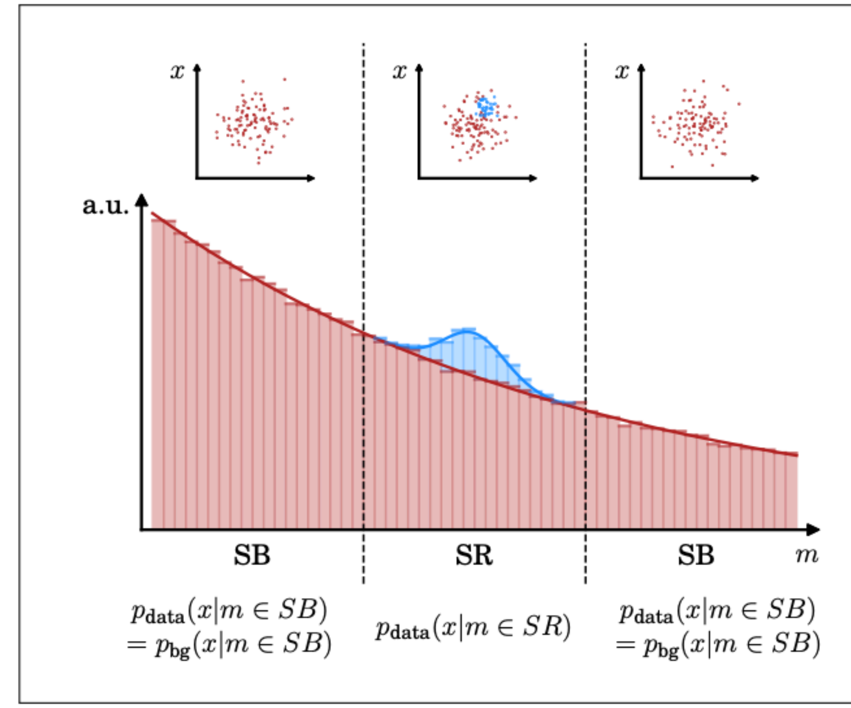

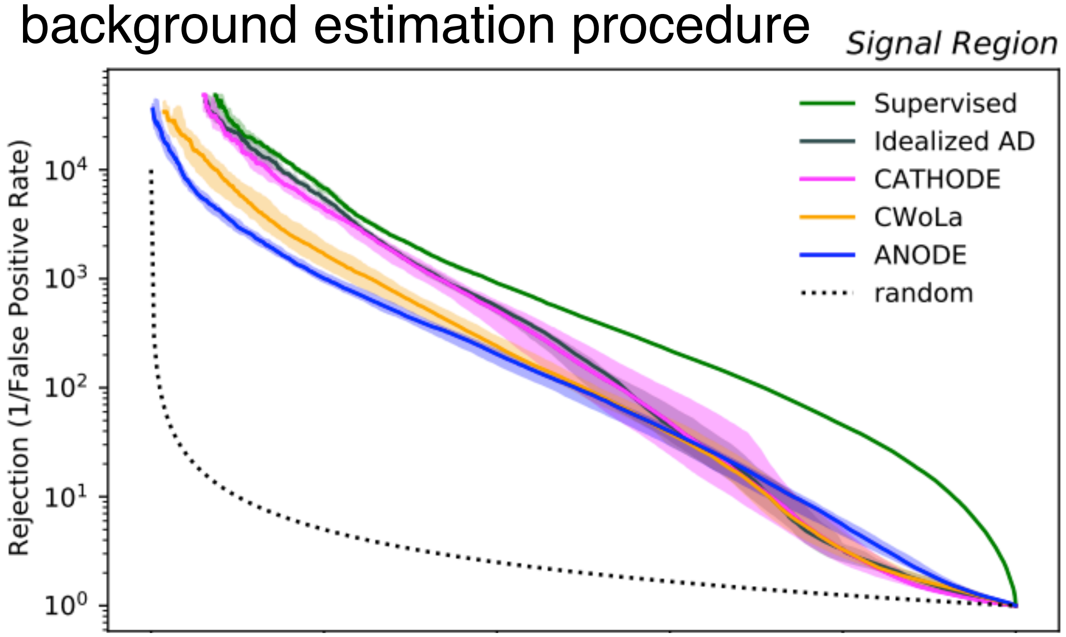

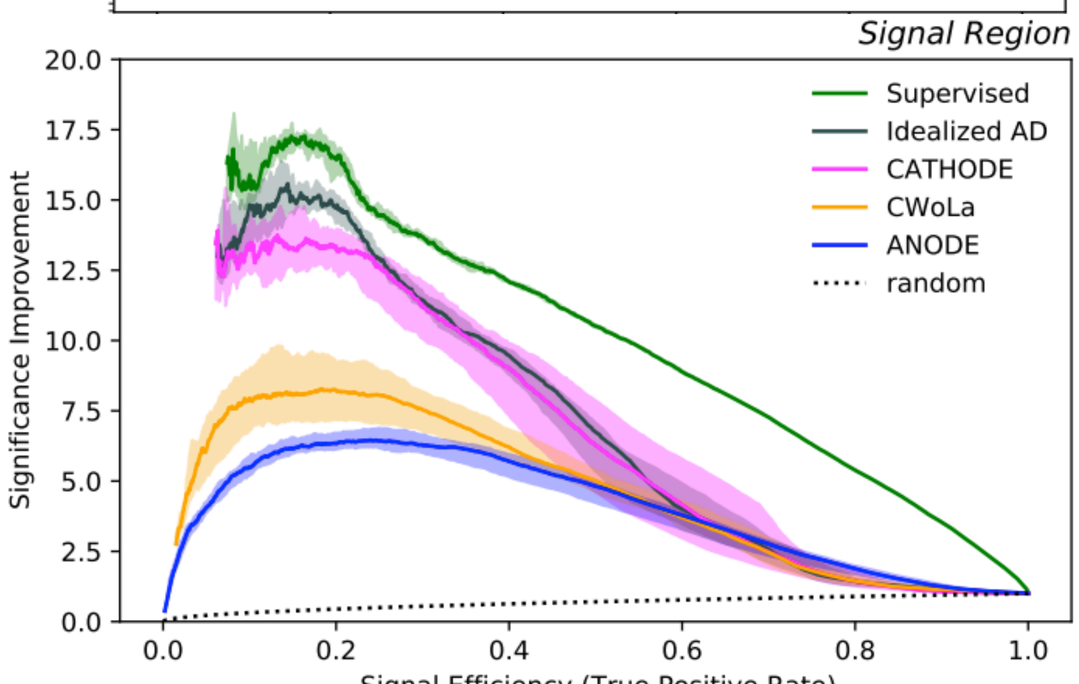

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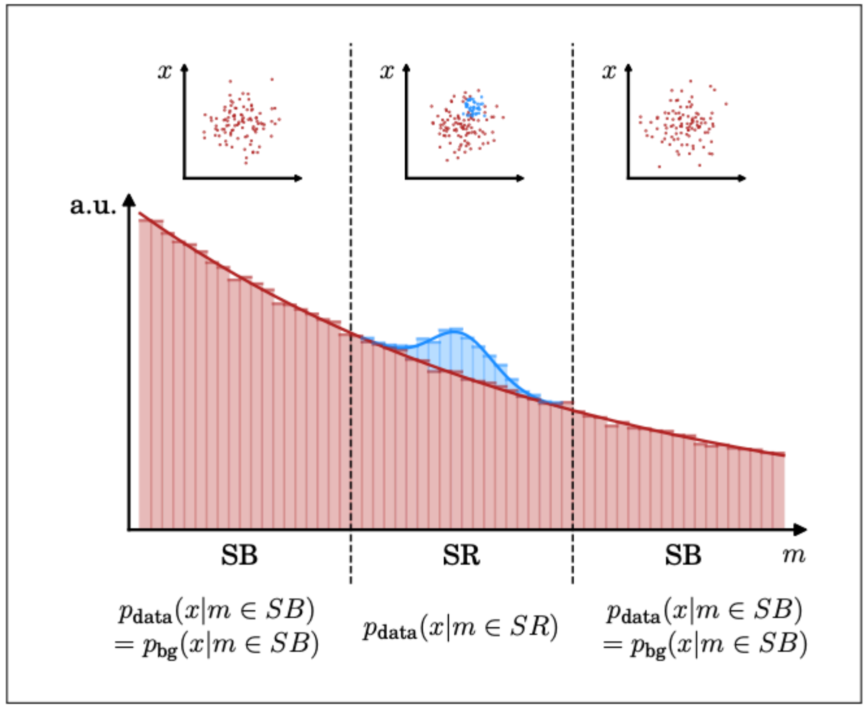
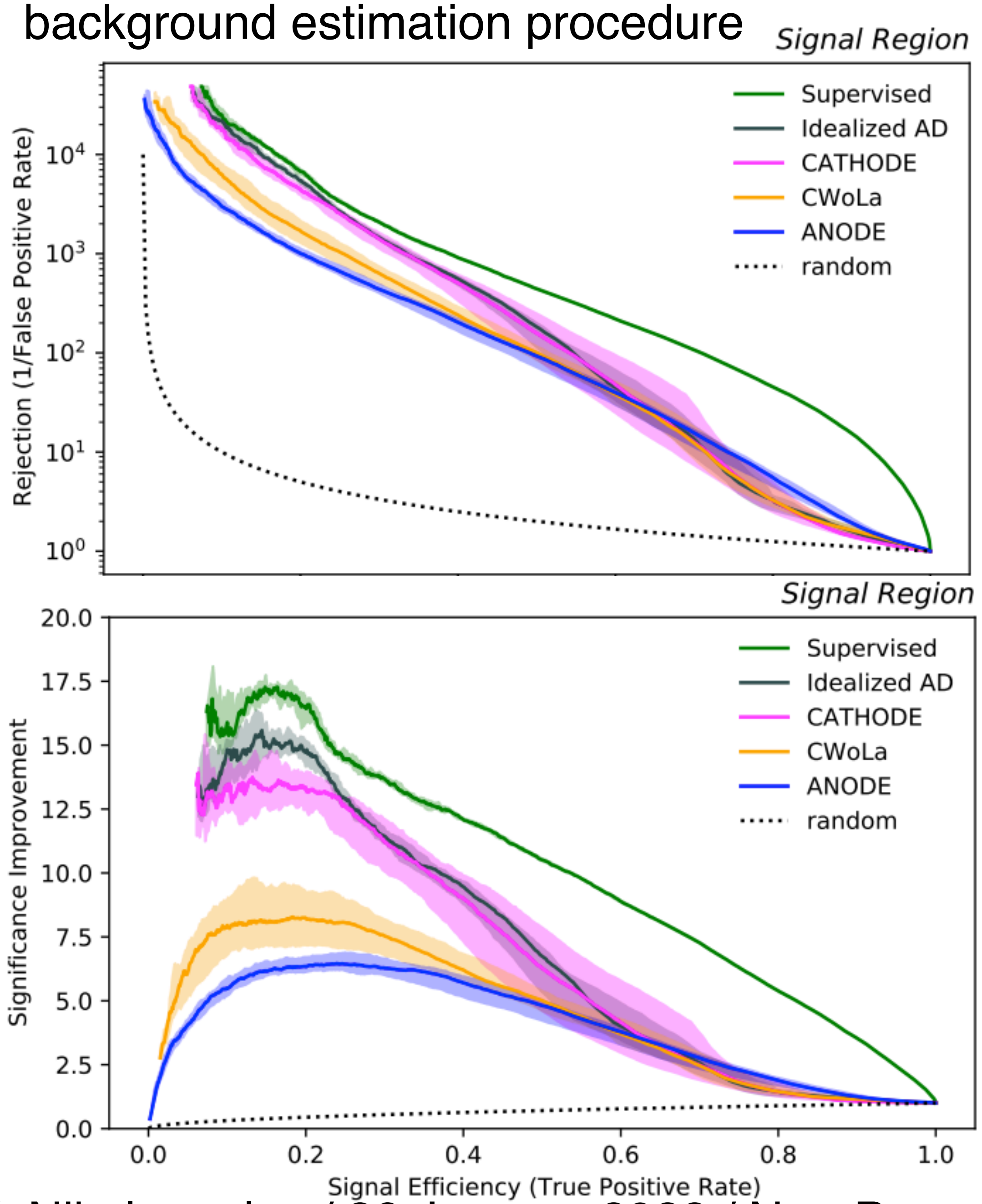
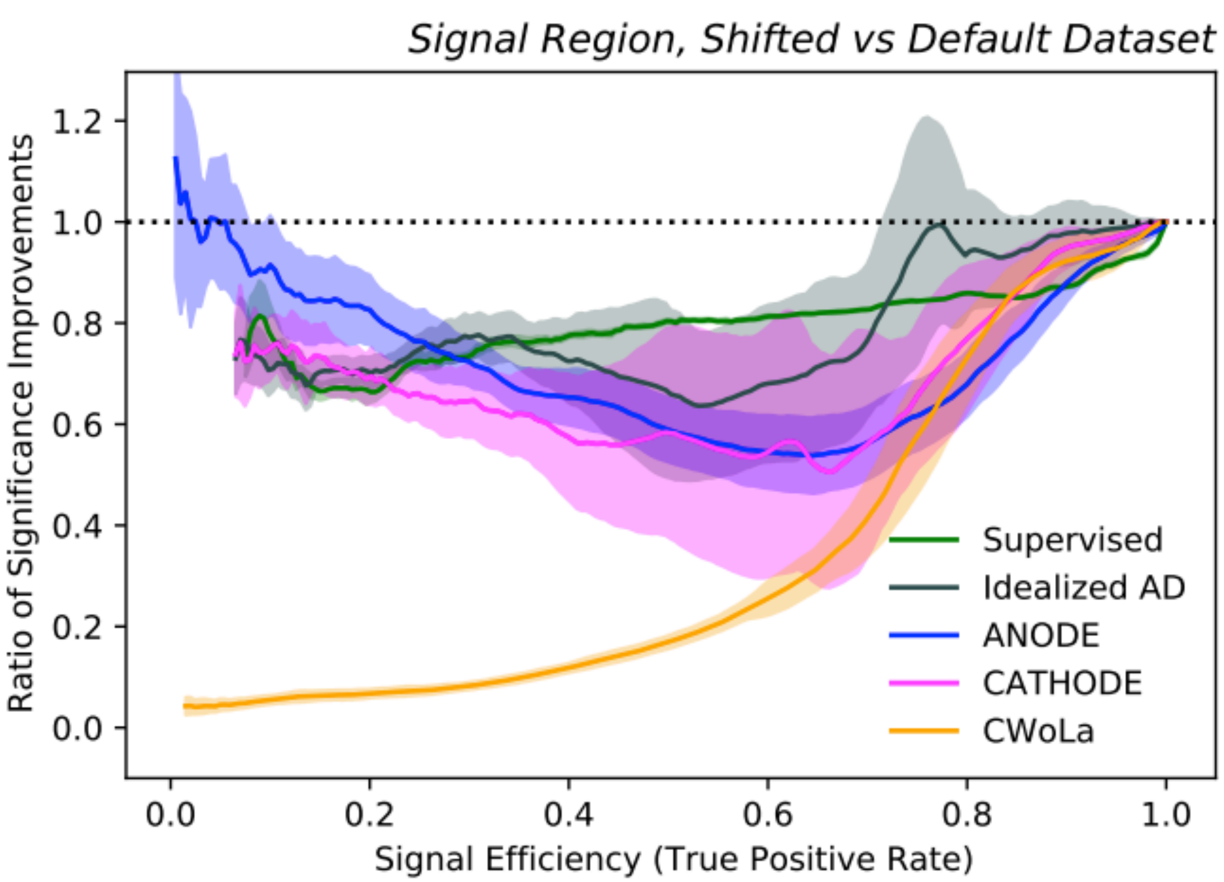




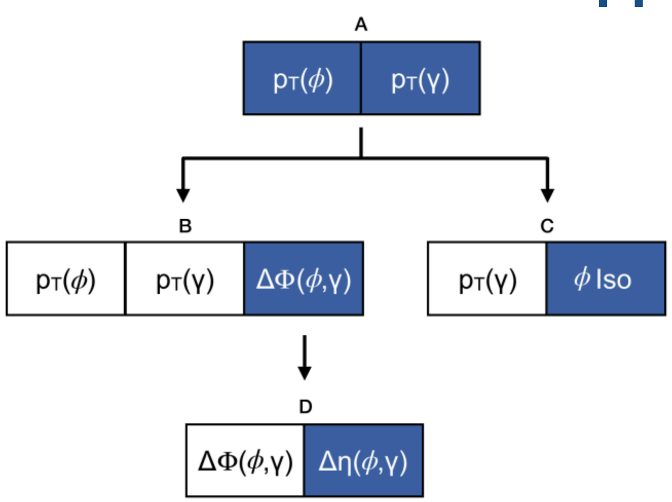


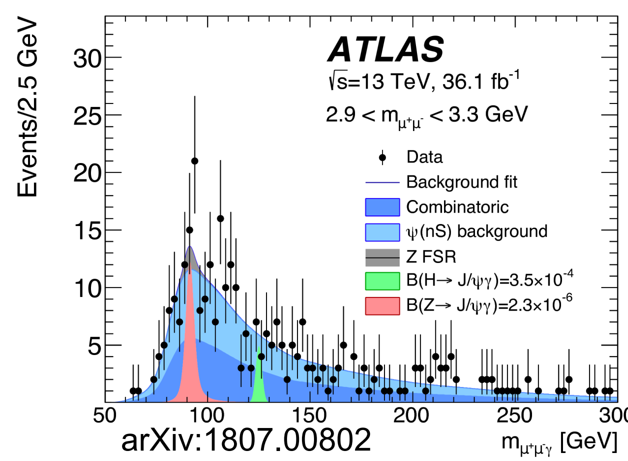
Summary

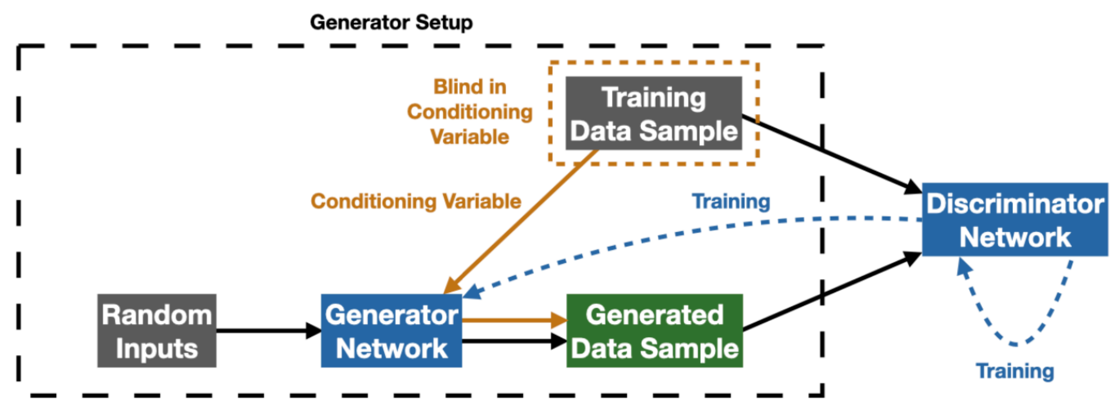
Background modelling crucial in searches for new physics and precision measurements
- Variety of methods has been developed
- Many rely on availability of large, reliable, simulated data samples
- Parametric methods suffer "spurious signal" type of effects

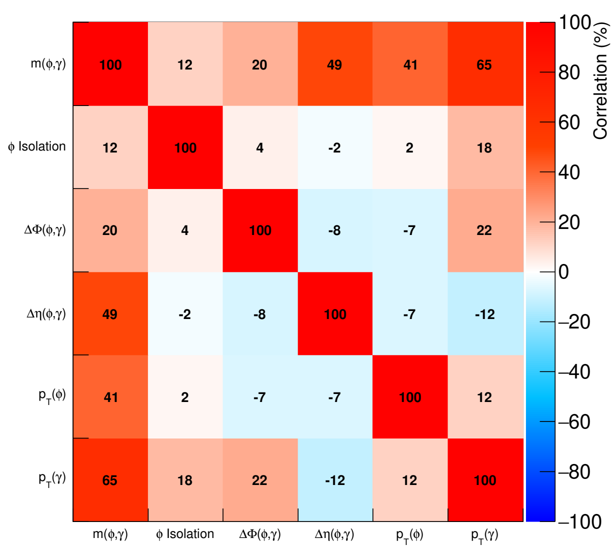
Developed **non-parametric, conditional probability-based, methods for data-driven modelling**:
- Histogram-based ancestral sampling method
- Machine learning technique using conditioned-Generative Adversarial Network

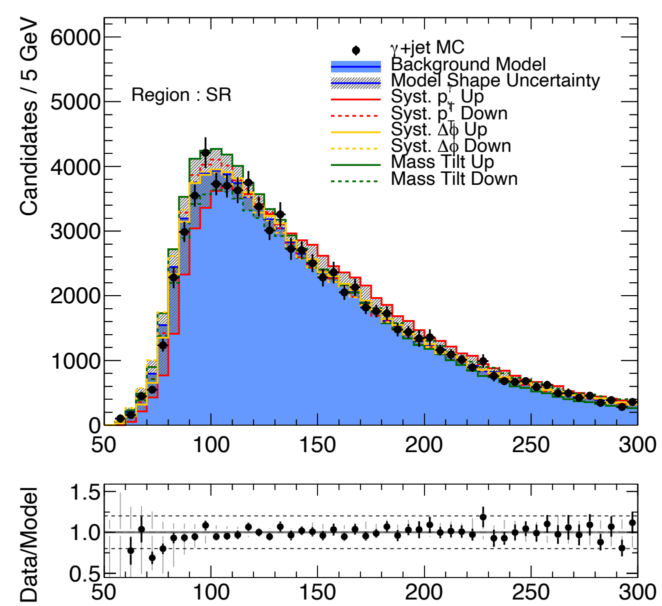
Presented methods applicable to any analysis!

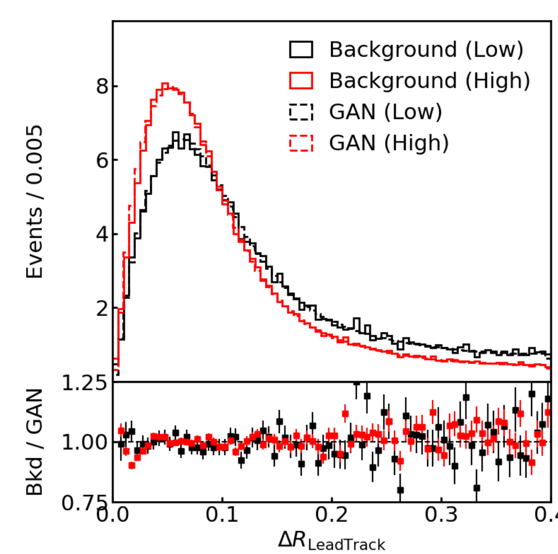


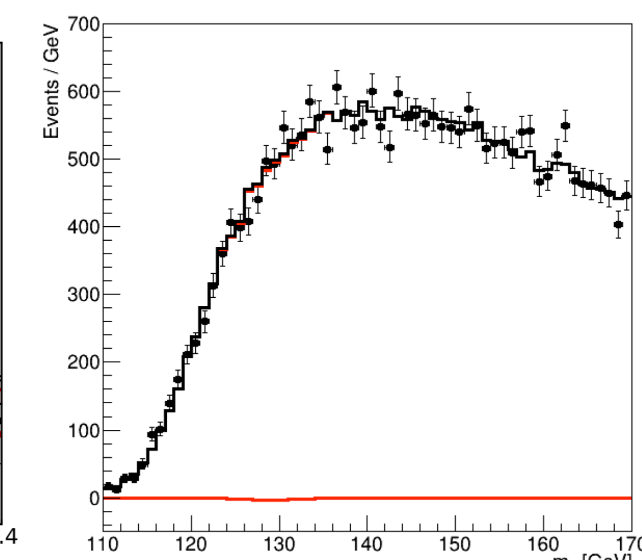












This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme under grant agreement 714893 (ExclusiveHiggs) and under Marie Skłodowska-Curie agreement 844062 (LightBosons)