

Efficient Search for New Physics Using Active Learning in the ATLAS Experiment

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NYU



ATLAS
EXPERIMENT

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[ATL-PHYS-PUB-2022-045](#)

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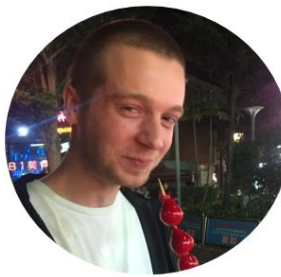
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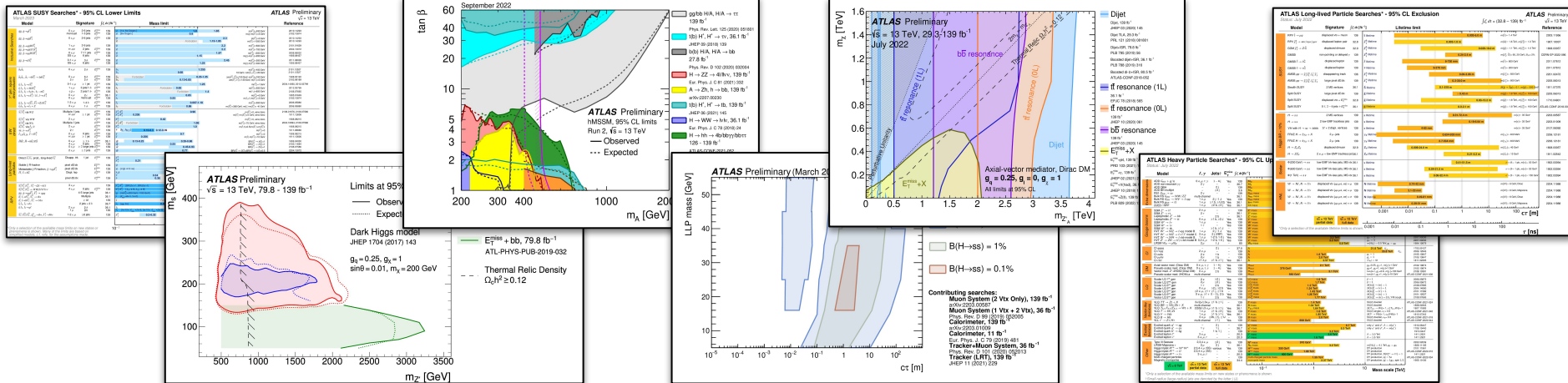


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1000's of New Physics Papers



- Proliferation of new physics models with a multitude of parameters
 - Need to raise efficiency in limit setting
- How do we increase efficiency in Beyond Standard Model parameters limit setting?
 - Active learning of exclusion contours

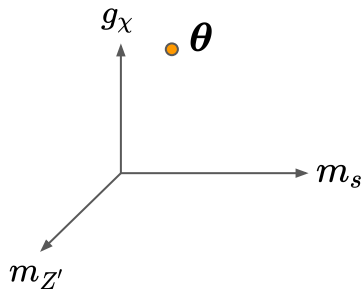
[I. Espejo et al. RIF 2022](#)
[P. Rieck et al. ACAT 2022](#)

https://atlaspo.cern.ch/public/summary_plots/

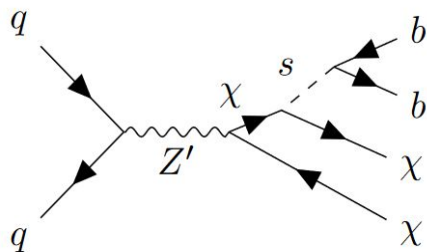
Limit Setting at ATLAS

Full Pipeline

$$\mathcal{L}_{SM} + \mathcal{L}_{BSM}(\theta)$$



$$\sigma(pp \rightarrow bg, sig)$$

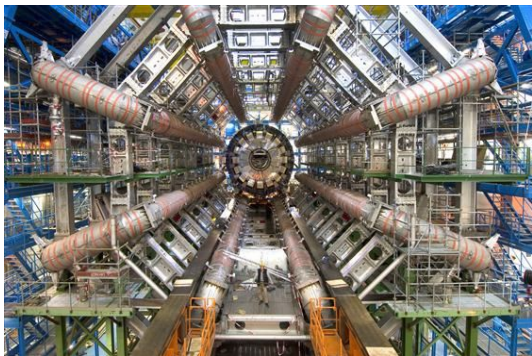


MC Event Simulation

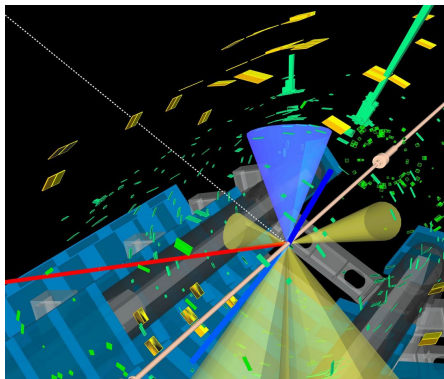
1. Event Generation
2. Showering/Hadronization
3. Detector Simulation
4. Digitization

MadGraph, Pythia, Herwig, Geant4, ...

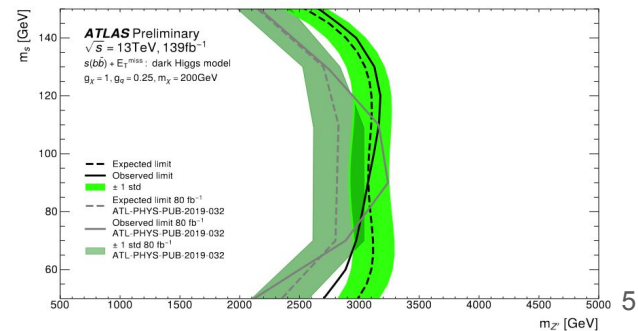
+ ATLAS Data



Event Reconstruction



Analysis and Inference



Determining Exclusion Contours

f , the full pipeline is expensive to evaluate:

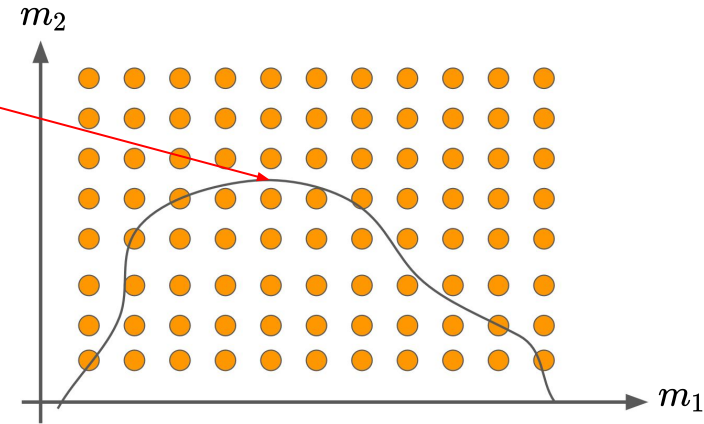
$$f : \boldsymbol{\theta} \rightarrow \mathbf{y} := (\log \mu_{exp}^{UL}(\boldsymbol{\theta}), \log \mu_{+1\sigma}^{UL}(\boldsymbol{\theta}), \log \mu_{-1\sigma}^{UL}(\boldsymbol{\theta}), \log \mu_{obs}^{UL}(\boldsymbol{\theta}))$$

And afterwards, we perform a regression across our grid on the signal strength upper limit:

$$\mu = \frac{\sigma^{excluded}}{\sigma^{theory}}$$

The exclusion contour is what we are interested in:

$$y(\boldsymbol{\theta}) = 0 \Rightarrow \mu_{exp}^{UL} = 1 \Rightarrow \sigma(\boldsymbol{\theta}) \approx \sigma_{BSM}(\boldsymbol{\theta})$$



[L. Heinrich et al. ACAT 2019](#)

Indiscriminate

“Arbitrary” 4D cartesian grid, e.g.:

11 m_1 , 8 m_2 , 10 m_3 , 4 g_1 : 3500 points

1 shot parallelized

Compromise on density?

Compromise on dimensionality?

Informed

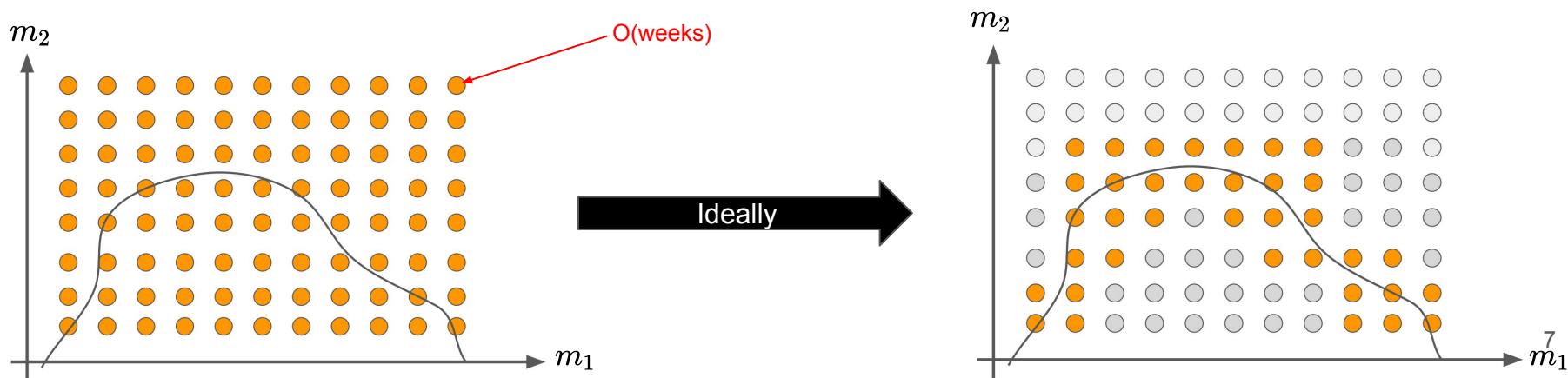
Start with prior knowledge:

Reduce total number of points

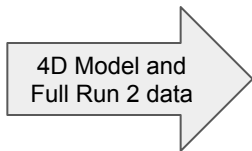
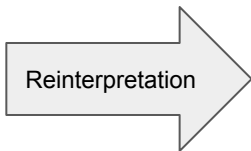
Iterative **and** parallelized

High density near contour & vice versa

Maintain full theory dimensionality



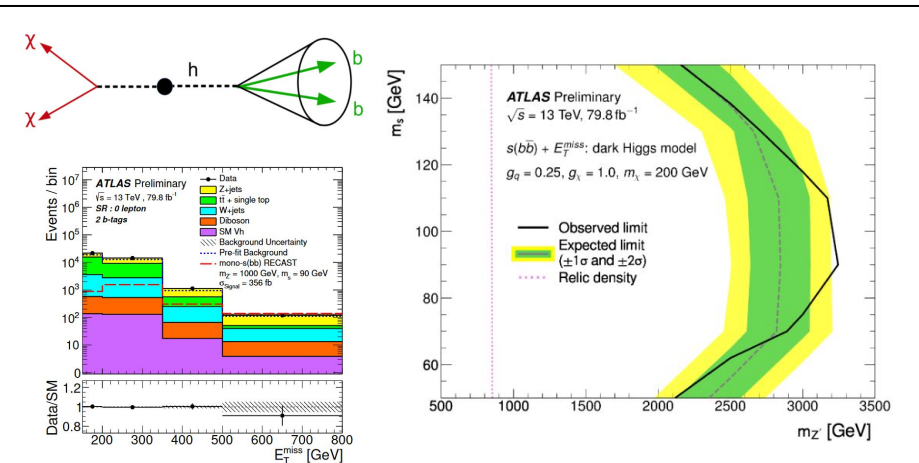
Dark Matter Search



Search for Dark Matter Produced in Association with a Higgs Boson decaying to $b\bar{b}$ at $\sqrt{s} = 13$ TeV with the ATLAS Detector using 79.8 fb^{-1} of proton-proton collision data

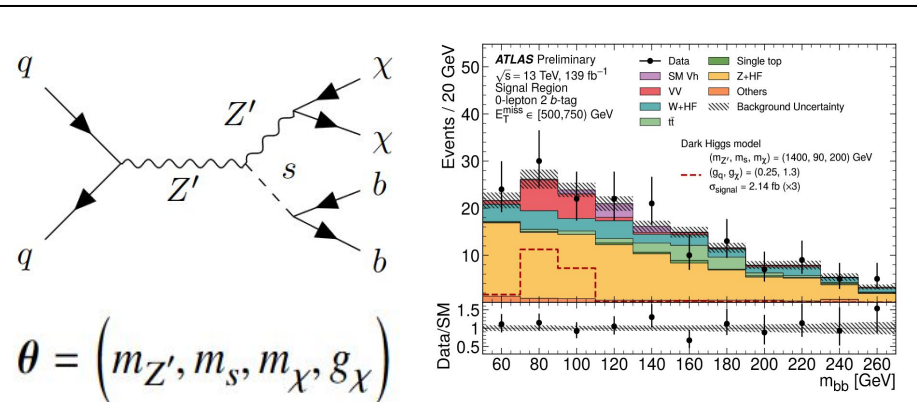
RECAST framework reinterpretation of an ATLAS Dark Matter Search constraining a model of a dark Higgs boson decaying to two b -quarks

Active Learning reinterpretation of an ATLAS Dark Matter search constraining a model of a dark Higgs boson decaying to two b -quarks



● From 2D Reinterpretation

- Sophisticated reconstruction techniques: Large-Radius jets with b-tagged subjects as Higgs boson decay candidates
- Numerous signal and control regions



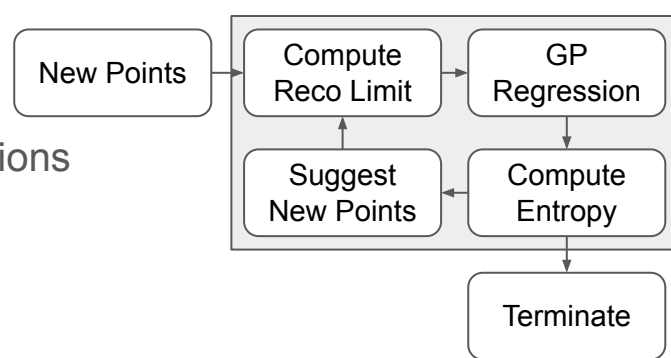
● To a Complete 4D Search

- Efficient parameter space sampling with Active Learning
- Full Run 2 139 fb^{-1} data

The Active Learning Approach

Overview of Active Learning

→ Follow up on [ACAT 2017](#), [ACAT 2019](#) & [ACAT 2022](#) presentations



for each new batch of BSM parameter points $\{\theta_i\}$:

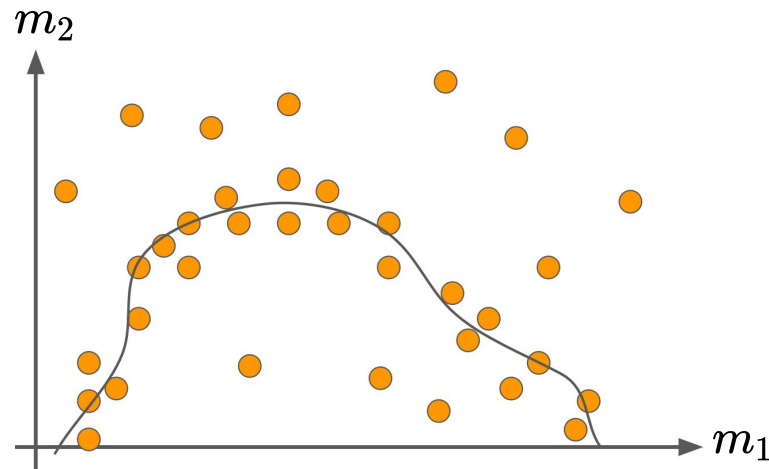
compute the reco limits $\mu_i = \mu(\theta_i)$

estimate the function $\mu(\theta)$ using [GP regression](#) given all $\{\mu_k\}$

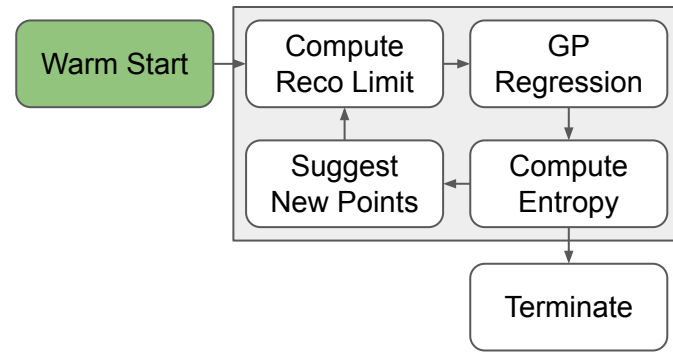
compute exclusion entropy

if the surface $\mu == 1$ is not yet sharp:
suggest new points $\{\theta_j\}$ where exclusion
is most uncertain

else:
break

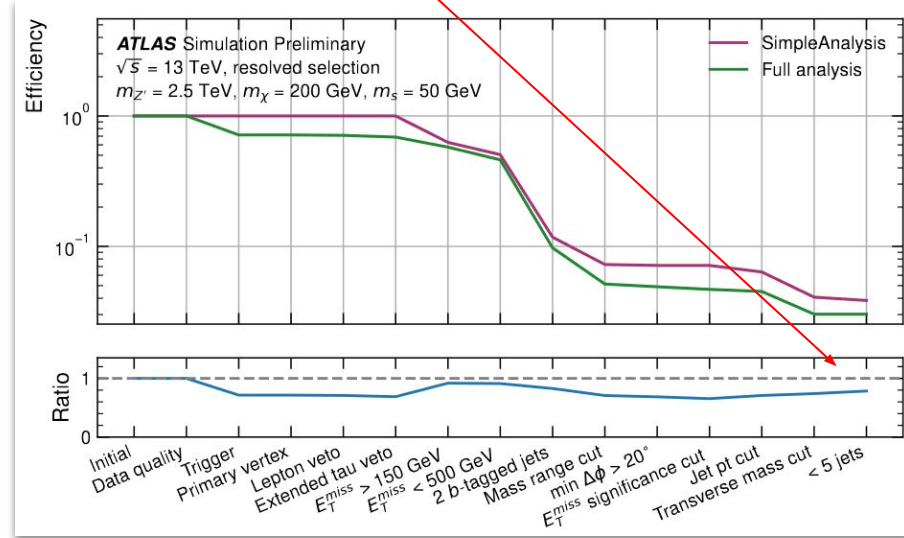


- Simplest measure: total cross-section
 - Exclusion limits $O(1 \text{ fb})$ for Run 2 Mono-H(bb)
 - Calculated during first steps in MC simulation



- Next level of accuracy: [SimpleAnalysis](#)
 - Approximate efficiencies and smearing functions applied on generator-level MC events
 - Grid of 5k points
 - Discrepancies compared to full reinterpretation:
 - Resolved regime : E_T^{miss} significance cut
 - Merged regime : large-R jet substructure

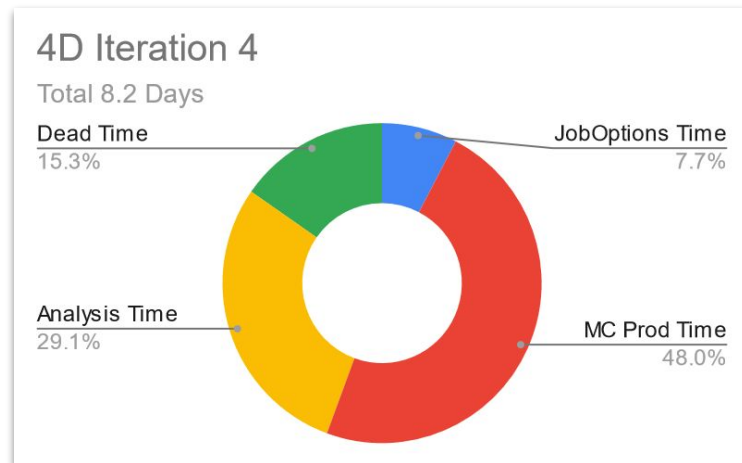
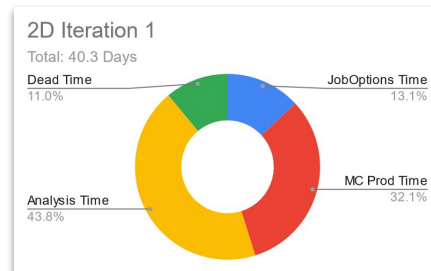
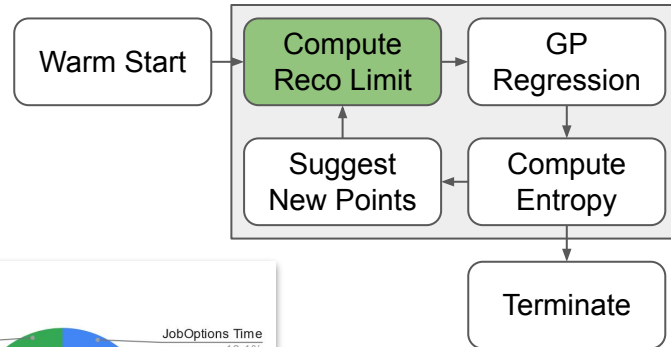
~20% discrepancy in selection efficiency



- Full accuracy achieved with [RECAST](#) efficiently, running the captured original workflow in a Docker container on CERN's reusable analysis platform ([reana](#))

- Improvements automating MC production:
 - Auto approval of JobOptions through GitLab
 - API based clone MC Production submission
 - First Iteration: ~40 Days for 15 points
 - Last Iteration: ~8 Days for 200 points

recast **reana**



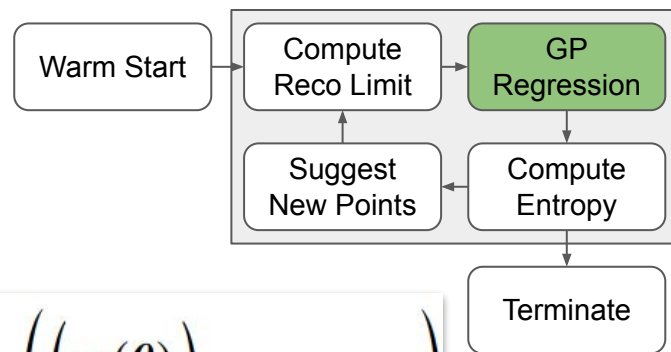
2-Task Gaussian Process

- SimpleAnalysis derived limits on a regular, fine grid support the limit determination
- SimpleAnalysis limit y_s and RECAST limit y_r

Training: 10 parameters determined from SimpleAnalysis and RECAST data (maximum likelihood)

Inference: Gaussian Process prediction of limits and their uncertainties

[Python GP library](#)



$$\begin{pmatrix} y_s(\boldsymbol{\theta}) \\ y_r(\boldsymbol{\theta}') \end{pmatrix} \sim \mathcal{GP} \left(\begin{pmatrix} m(\boldsymbol{\theta}) \\ m(\boldsymbol{\theta}') \end{pmatrix}, \Sigma_{sr}(\boldsymbol{\theta}, \boldsymbol{\theta}') \right)$$

$$m(\boldsymbol{\theta}) = \mathbf{w}^T \boldsymbol{\theta} + b$$

$$\Sigma_{sr}(\boldsymbol{\theta}, \boldsymbol{\theta}') = \begin{pmatrix} k_{ss}(\boldsymbol{\theta}, \boldsymbol{\theta}) & k_{sr}(\boldsymbol{\theta}, \boldsymbol{\theta}') \\ k_{sr}(\boldsymbol{\theta}, \boldsymbol{\theta}') & k_{rr}(\boldsymbol{\theta}', \boldsymbol{\theta}') \end{pmatrix}$$

$$k_{ij}(\boldsymbol{\theta}, \boldsymbol{\theta}') = k(\boldsymbol{\theta}, \boldsymbol{\theta}') \kappa_{ij} + \epsilon^2 \delta(\boldsymbol{\theta}, \boldsymbol{\theta}')$$

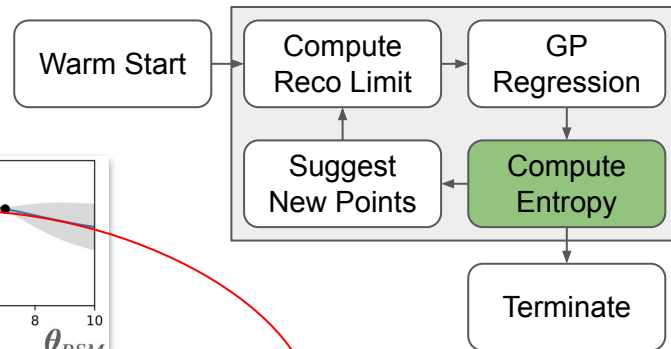
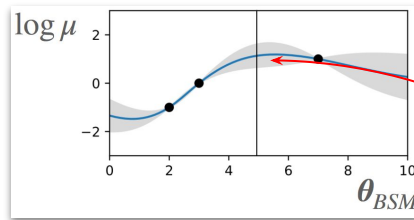
$$k(\boldsymbol{\theta}, \boldsymbol{\theta}') = \exp\left(-\frac{\|\boldsymbol{\theta} - \boldsymbol{\theta}'\|^2}{2l^2}\right)$$

$$\kappa_{ij} = \begin{cases} \sigma_s & \text{if } i = j = s \\ \sigma_r & \text{if } i = j = r \\ \sigma_{sr} & \text{if } i \neq j \end{cases}$$

$$\delta(\boldsymbol{\theta}, \boldsymbol{\theta}') = \begin{cases} 1, & \text{if } \boldsymbol{\theta} = \boldsymbol{\theta}' \\ 0, & \text{else} \end{cases}$$

Exclusion probability / Uncertainty Estimate

$$p_{\text{excl}}(\boldsymbol{\theta}) = \int_{-\infty}^0 g(y | \mu(\boldsymbol{\theta}), \sigma(\boldsymbol{\theta})) dy$$

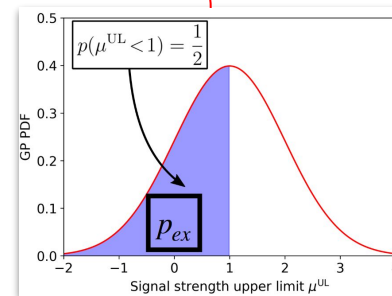


Exclusion entropy for each new point

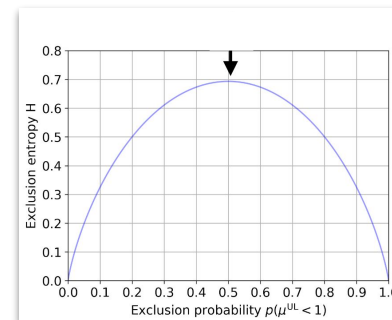
$$H_{\text{excl}}(\boldsymbol{\theta}) = -p_{\text{excl}}(\boldsymbol{\theta}) \log p_{\text{excl}}(\boldsymbol{\theta}) - (1 - p_{\text{excl}}(\boldsymbol{\theta})) \log (1 - p_{\text{excl}}(\boldsymbol{\theta}))$$

Is exclusion entropy across parameter space low?

$$p_{\text{excl}} = 0 \quad p_{\text{excl}} = 1$$

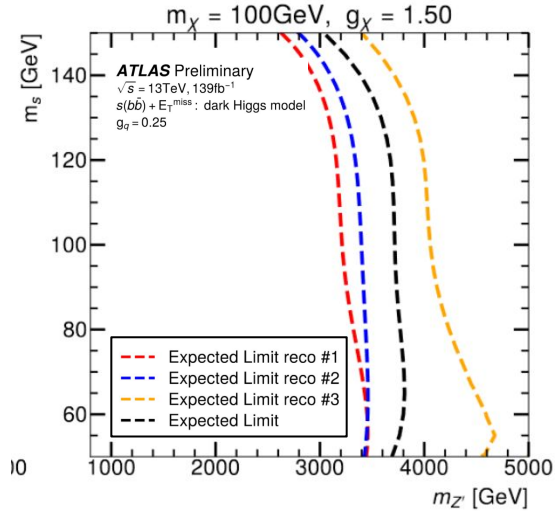


Acquire new points such that H_{excl} is reduced

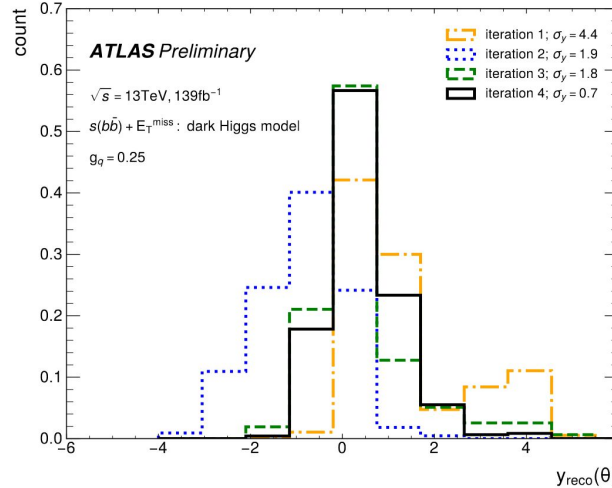


GP Convergence and Performance

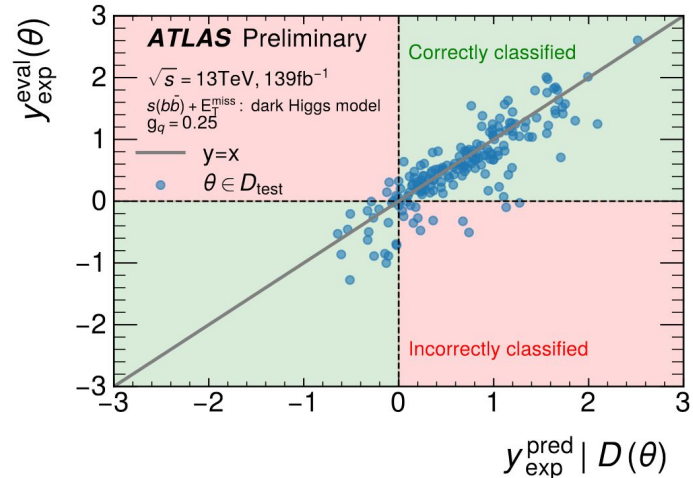
- 4 iterations of RECAST, approx. 200 new points θ each
 - Selecting 50% of new points according to max exclusion entropy and 50% [Poisson discs](#) around the expected exclusion contour



Stabilization of Limits



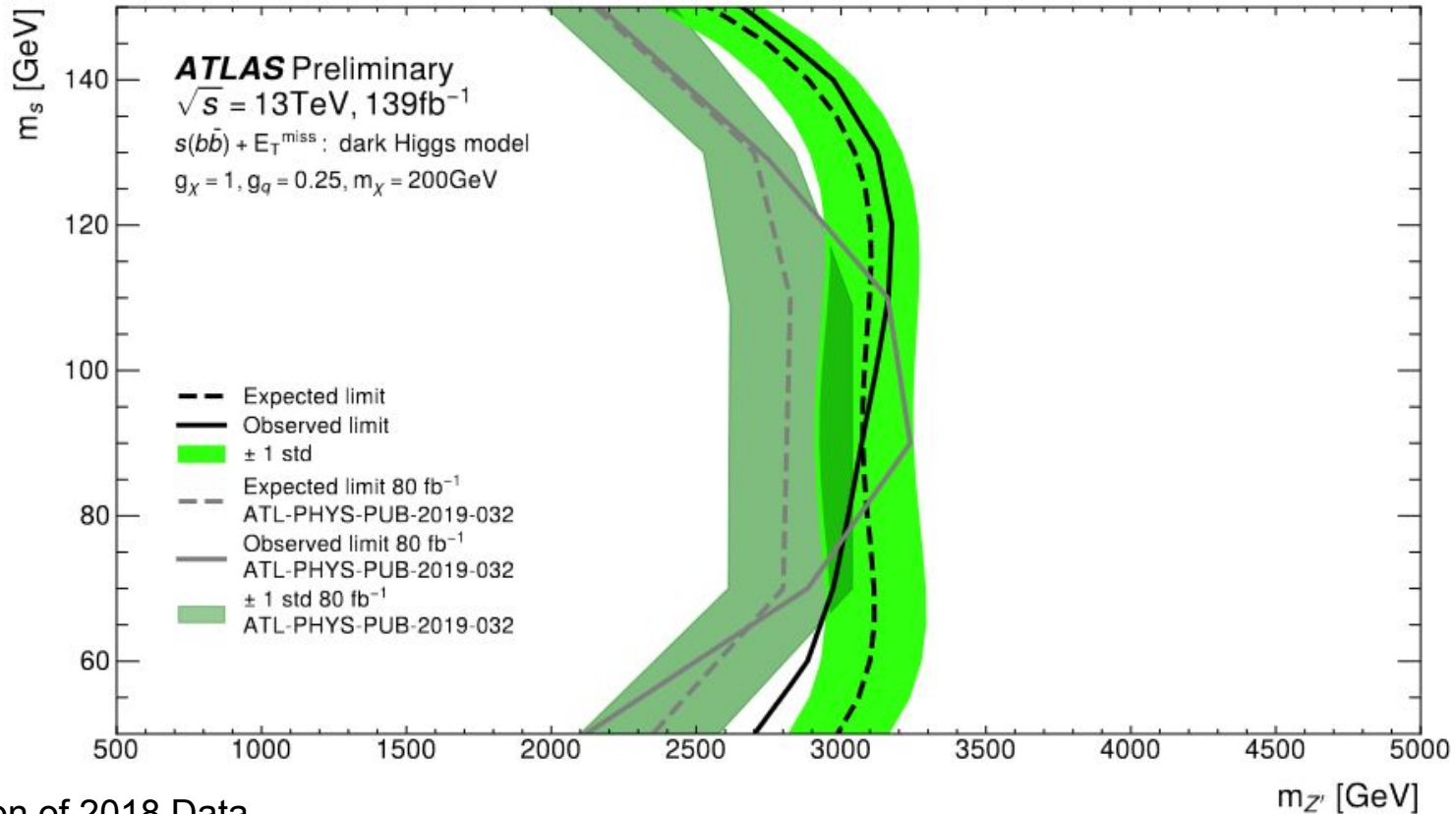
Convergence of Limits



Classification Accuracy 88%

Exclusion Limit Results

Improved Limits Over Previous Search



- Addition of 2018 Data
- Addition of m_χ and g_χ dimensions
- Gaussian Process determination of limits

Dark Higgs Mass vs Z' Mass Exclusion Limits and Entropy in 4D

ATLAS Preliminary

$\sqrt{s} = 13\text{TeV}, 139\text{fb}^{-1}$

$s(b\bar{b}) + E_T^{\text{miss}}$: dark Higgs model

$g_q = 0.25$

--- Expected Limit

— Observed Limit

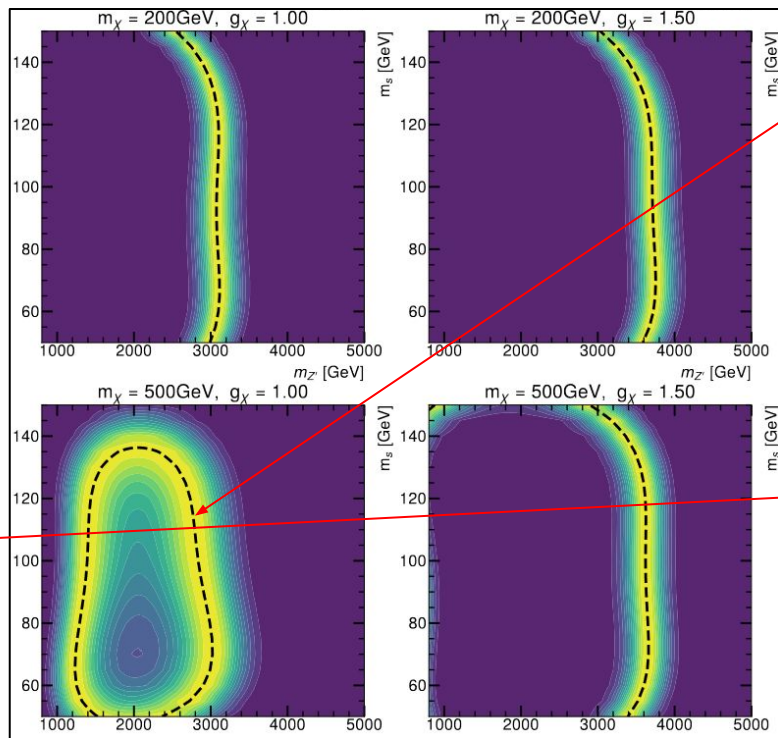
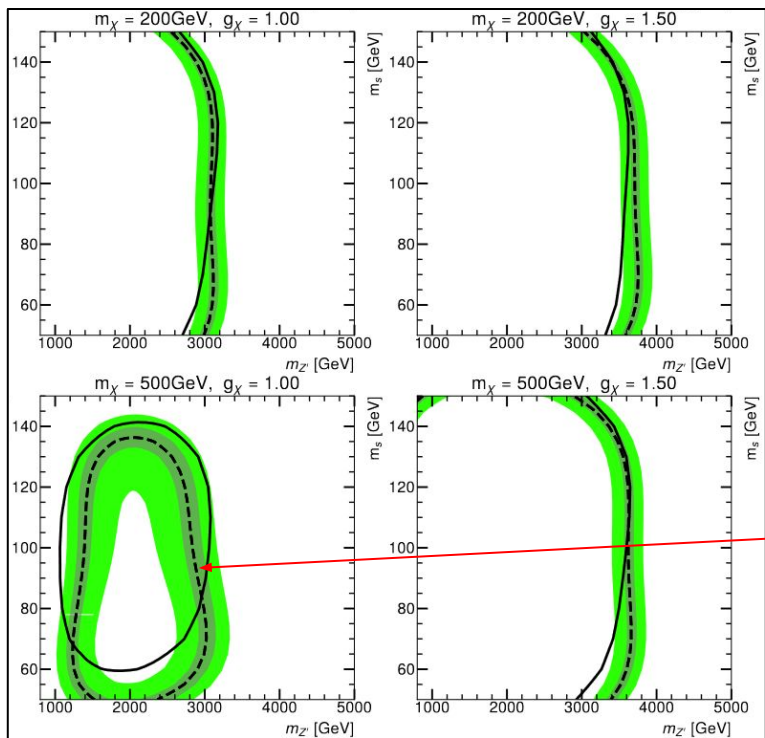
█ $\pm 1 \sigma$

█ $\pm 1 \sigma_{\text{exp}}^{\text{pred}} | D$



g_χ

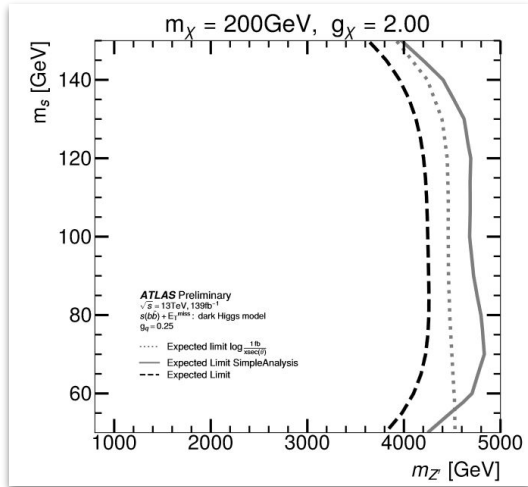
m_χ



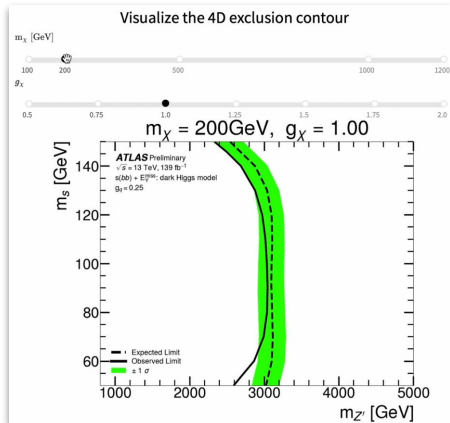
Small exclusion entropy except for exclusion contour region

Negligible intrinsic GP uncertainty

Further Consideration



- Cross-sections provide valuable approximation
 - Warm start with total cross-sections is a quick, simple and useful approximation. SimpleAnalysis may only lead to small gains
- Need for full RECAST in case of this complex physics analysis
 - This finding is true not just for a particular slice but for the whole parameter space, as determined efficiently by means of Active Learning



- [4D Exclusion Contour Visualization](#)
- Trained GP published for internal ATLAS use
- [Check out Christian's talk from earlier!](#)

Closing Remarks

- First application of Active Learning for an efficient, accurate and comprehensive interpretation of a search for new physics, using the Run 2 Mono-H(bb) Dark Matter search from ATLAS
- Gaussian Process for exclusion contour determination, making use of its uncertainty estimate in order to acquire new limits efficiently
- Improved dark Higgs boson limits
- Complexity of this analysis \Rightarrow need for full limit accuracy obtained with RECAST