Accelerating simulation-based inference in RooFit at LHCb with Clad

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Compiler Research Project Meeting

Johannes Albrecht, Marco Colonna, Jamie Gooding,
Abhijit Mathad, Biljana Mitreska, Jonas Rembser, Danilo Piparo

CERN ROOT Data Analysis Framework technische universität dortmund SMARTHEP REAL-TIME ANALYSIS FOR SCIENCE AND INDUSTRY MARIE CURIE ACTIONS

A little about me

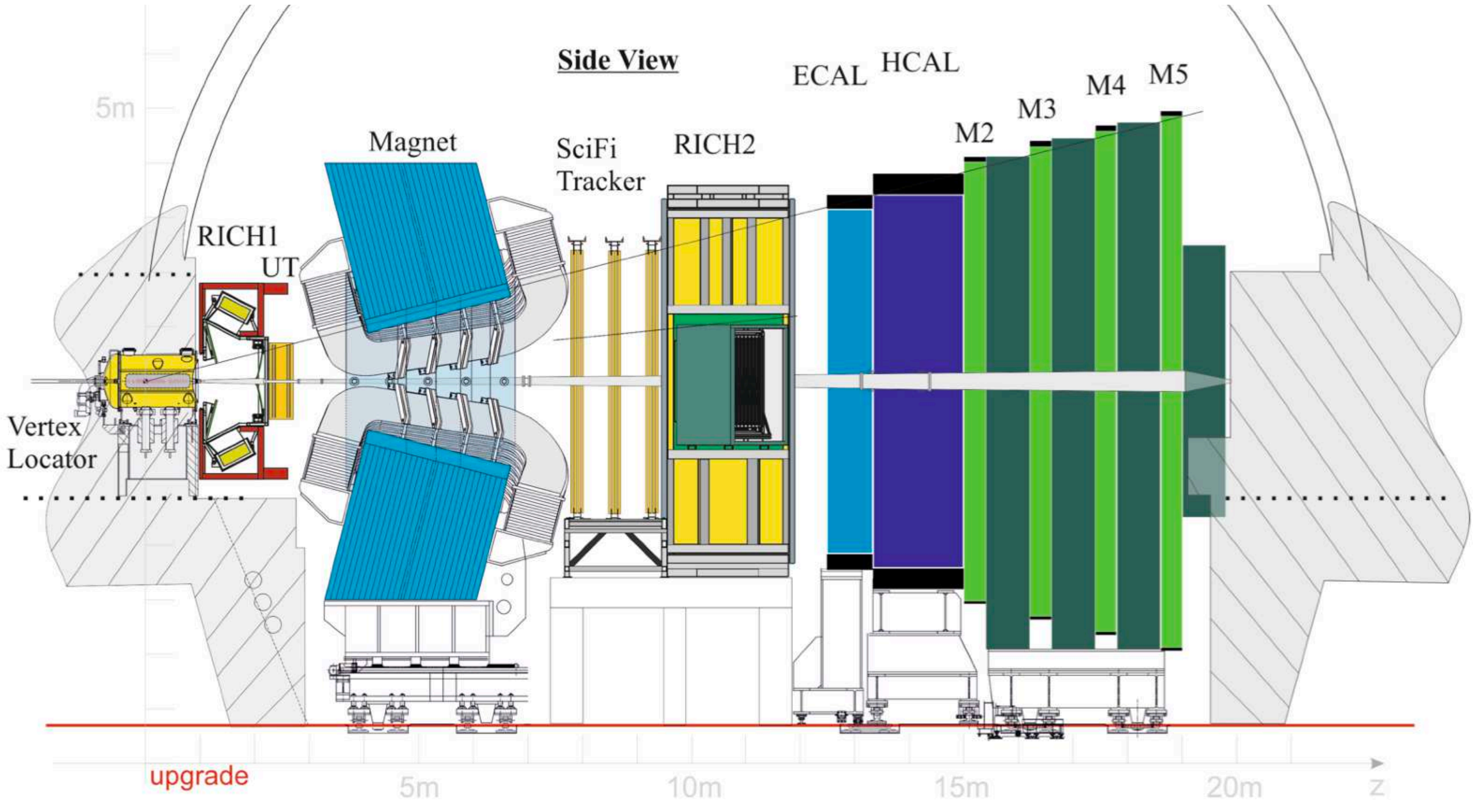
- 3rd Year Doctoral Student and SMARTHEP Early Stage Researcher at TU Dortmund in Dortmund, Germany
  - Member of LHCb since 2021 (Manchester + Dortmund)
  - Research focuses include:
    - Real-time analysis for trigger systems
    - Studies of CP-symmetry and lepton flavour universality violation in neutral b-meson decays
    - Novel tools and techniques for analysis (convener of [HEP Software Foundation](#) [Data Analysis Working Group](#))
- Currently working with Jonas Rembser and the ROOT team on a demonstrator for simulation-based inference (SBI) in an LHCb physics use case
  - Aim to produce example workflow for an LHCb physics application, whilst furthering ROOT SBI support

First of all, some physics*

This isn’t a prerequisite for understanding the rest of the talk, but adds some useful context!

The LHCb experiment at the LHC

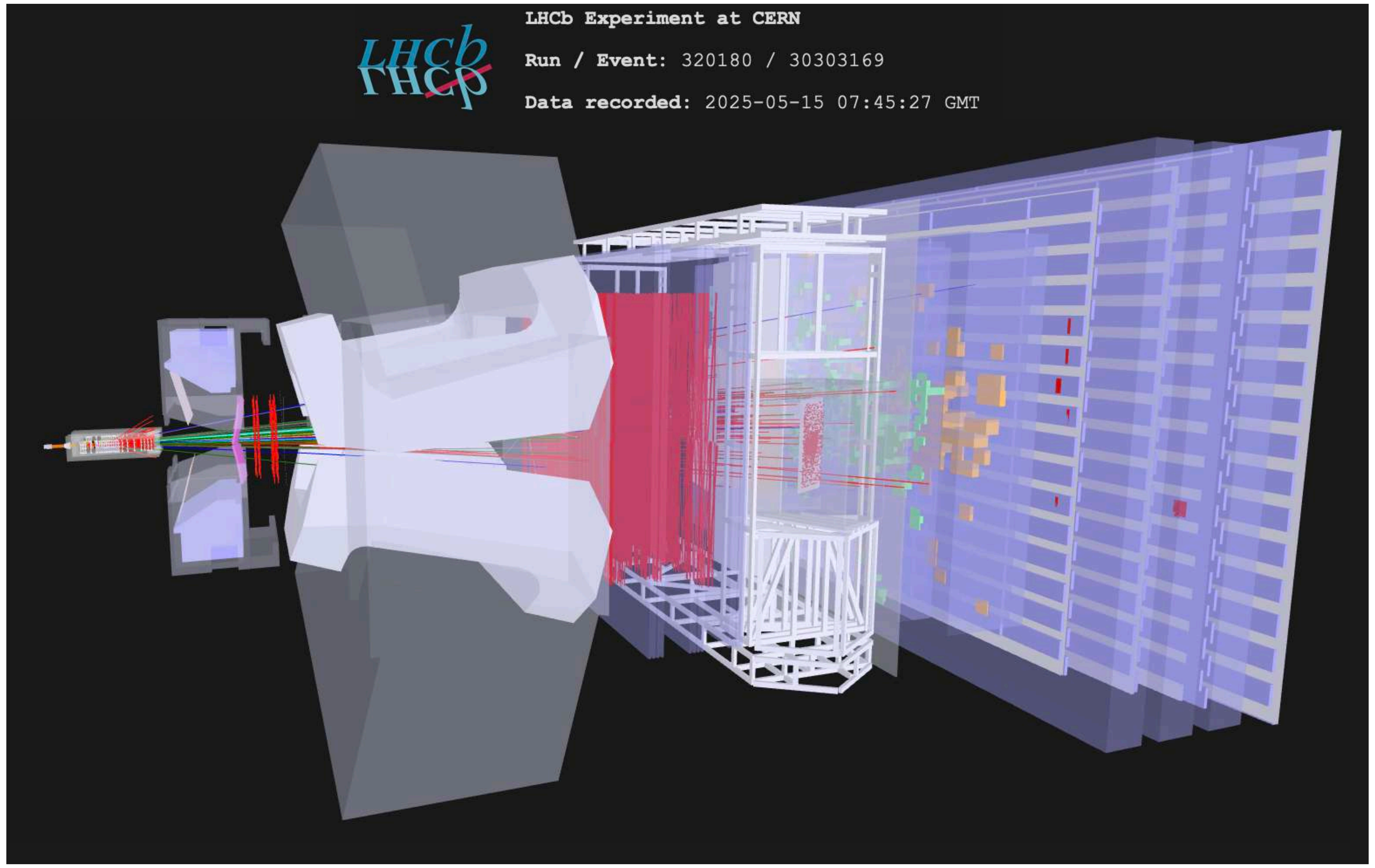
- The LHCb (Large Hadron Collider beauty) experiment is a dedicated flavour physics experiment at the LHC
  - Built to study the properties and decays of particles containing the heavy b and c quarks
  - By comparing against predictions from the Standard Model (SM, our best-understanding of particle physics) we look for signs of something out of place
  - We know something must be out there, as the SM doesn't describe gravity, dark matter, etc.
- As enormous a computing challenge as a physics/engineering challenge:
  - Processing $5\,\mathrm{TB/s}$ of data, store around $10\,\mathrm{GB/s}$
  - Statistical analyses regularly take place across datasets with millions of entries

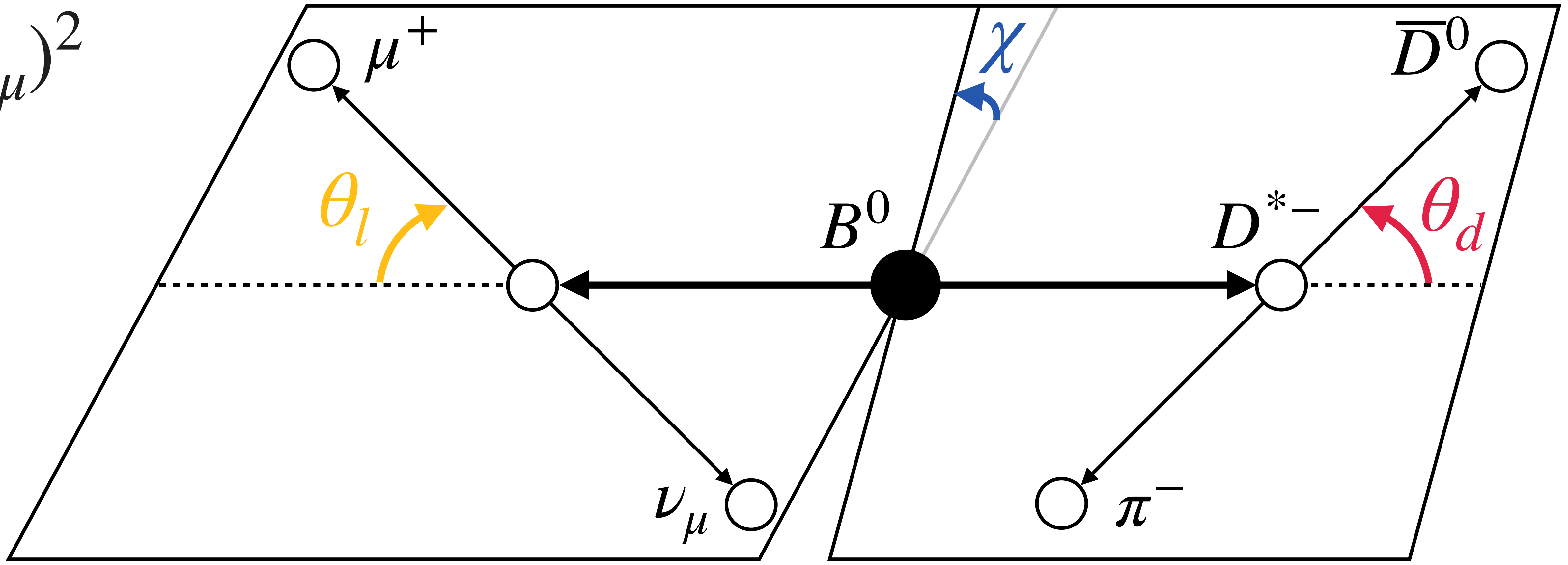


R. Aaij et al. JINST 19 (2024) P05065

Semi-leptonic $B^0 \to D^{*-}\mu^+\nu_\mu$ decays

- $B^0 \to D^{*-}\mu^+\nu_\mu$ decays readily observed at LHCb in pp collisions (e.g., *right from <u>this morning</u>*):
  - $D^{*-}(\to \overline{D}^0 \left(\to K^-\pi^+\right) \pi^-)$ and μ^+ fully reconstructed, but ν_μ <u>missing</u>
  - Angles of final state particles can be parameterised in three angles θ_d, θ_l, χ
  - We will also be interested in:
    - Momentum transfer, $q^2 = p_B^2 - p_{D*}^2$
    - Square missing mass, $M_{\text{miss}}^2 = (p_B - p_{D*} - p_\mu)^2$
- Can use the RapidSim fast MC package to generate pseudodata samples of these decays
- Angular observables may be affected by new physics (NP) contributions…





Parameterising new physics

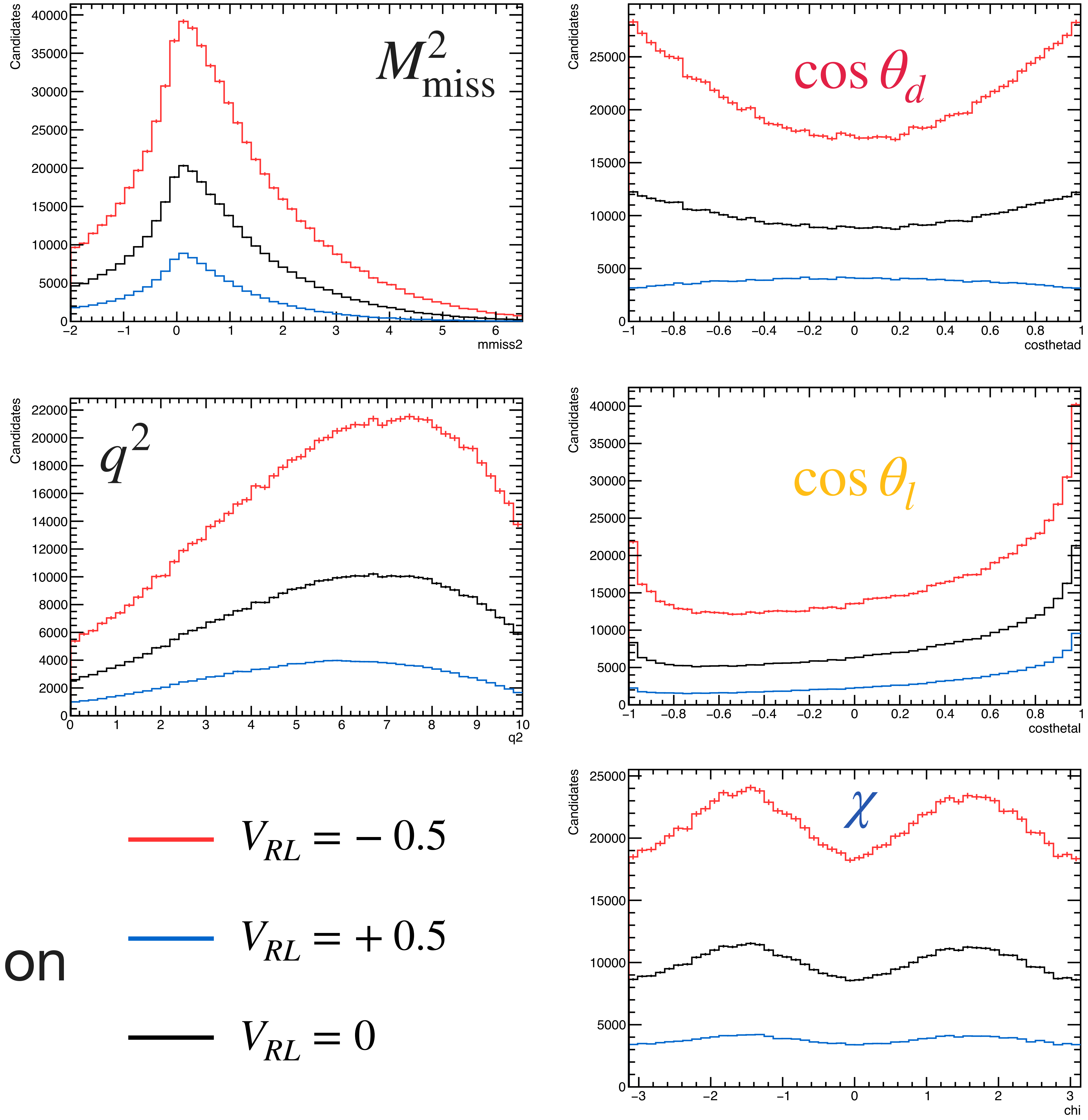
- Take an effective field theory (EFT) approach to considering decay processes
- Contributions to effective Hamiltonian expressed as Wilson operators, O_i, with coefficients, C_i:

$$H_{\text{eff}} \propto \Sigma_i \, C_i O_i \quad \text{with} \quad C_i = C_i^{\text{SM}} + C_i^{\text{NP}}$$

- These modify the decay rate with dependence on momentum scale and angular observables
- The NP (Wilson) coefficients (WCs), are complex and constructed to be 0 in the SM
- We consider contributions (with WCs) which are:
  - V_{RL}: vector coupling of right-handed Fermion to left-handed ν,
  - S_{LL}: scalar coupling of left-handed Fermion to left-handed ν
  - T_{LL}: tensor coupling of left-handed Fermion to left-handed ν
- The key takeaway from this: <u>we look at our kinematic and angular observables and fit for WCs</u>
- Note: for simplicity, we will only consider the real part of V_{RL} as our NP parameter

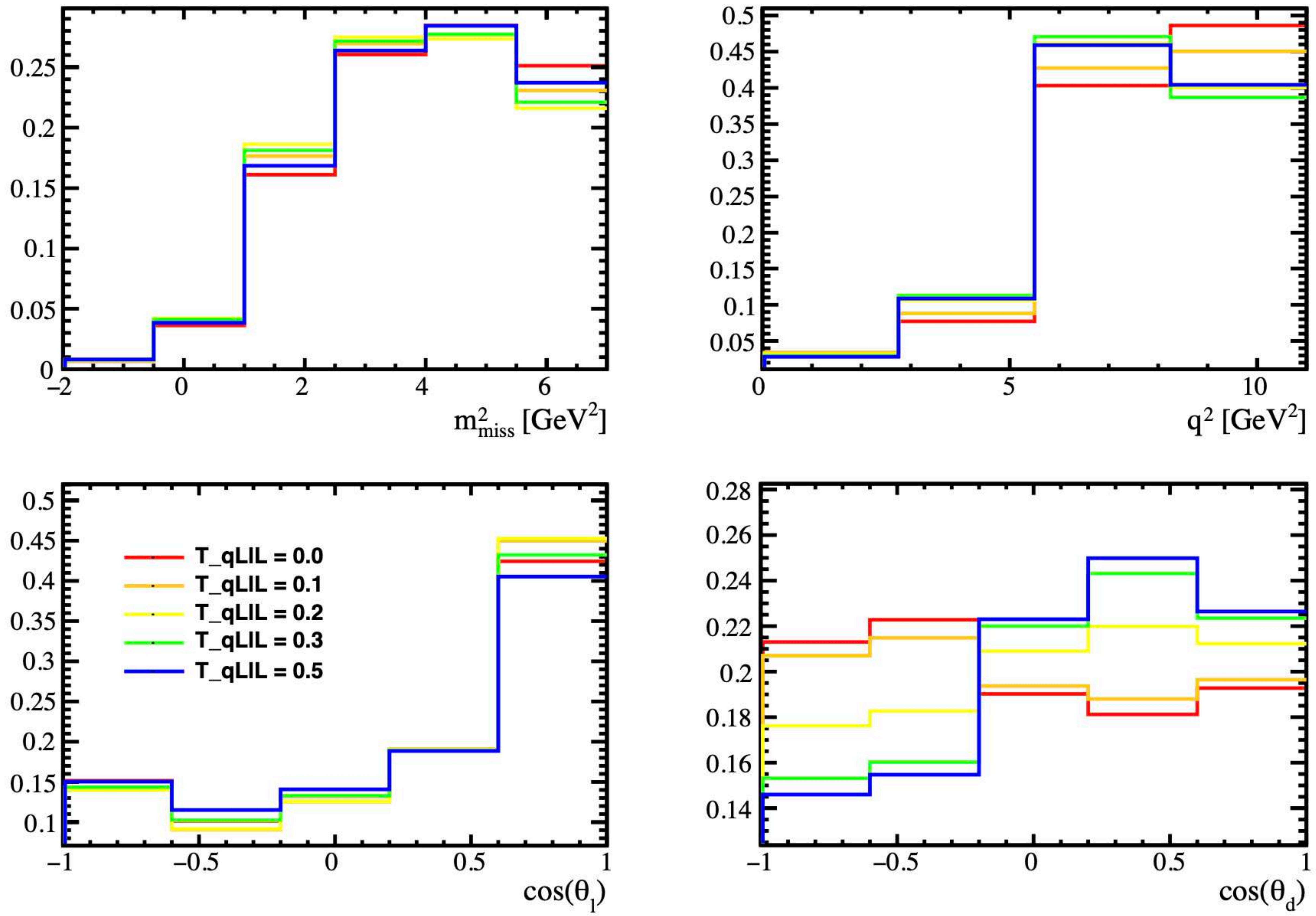
Injecting new physics

- Many tools exist to reweight samples for given NP scenarios, e.g., [HAMMER](), [EOS](), etc.
  - These compute relative rates based on specified WCs (and form factors, describing the strong interaction, excluded here for simplicity)
  - For our workflow, we use HAMMER
- We pass in our unweighted pseudodata sample and attach weights for our WC values of interest, *e.g.*, *right,* showing effect of $\mathrm{Re}\{V_{\mathrm{RL}}\}$
- In our workflow, compute weights in 4 scenarios:
  - $V_{\mathrm{RL}} = 0$, i.e., SM case
  - $V_{\mathrm{RL}} = \theta_{\mathrm{gen}}$, for θ_{gen} drawn from a uniform distribution
  - $V_{\mathrm{RL}} = \pm 0.5$, used for normalisation (*see later*)



Classical fitting of $B^0 \to D^{*-}\mu^+\nu_\mu$

- Classical approach is to bin each of the 5 dimensions and fit template histograms
  - Generate template histograms from MC simulation
  - Modify histograms with HAMMER rates
  - For each modification, compute likelihood (and gradient)
  - Repeat modification to maximise likelihood
- Often fit with [HistFactory](#)/[pyhf](#), integrated with tools like HAMMER (*e.g.*, [RooHammerModel](#) for HistFactory/[redist](#) for pyhf)
- This approach is well-established and optimised, though requires large MC sample and significant computing power



[B. Mitreska, talk in Challenges in SL B decays, September 2024](#)

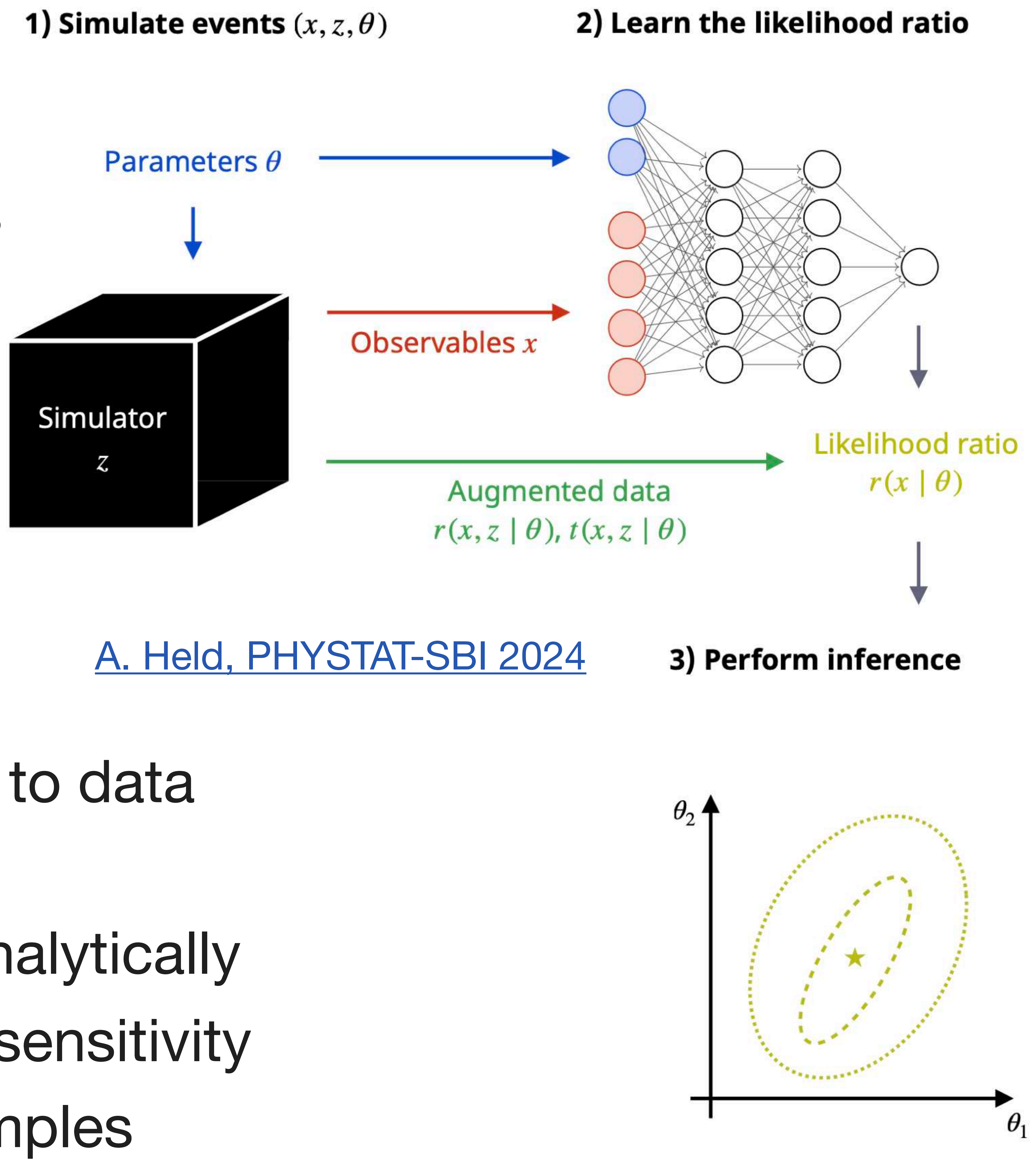
Simulation based inference

Simulation-based inference

- In lieu of analytic models for probability distributions, can learn the behaviour from simulation (*see right*)
- Train classifier to distinguish between different hypotheses
- Can apply the likelihood ratio trick: construct a negative log-likelihood ratio of hypothesis H and a reference hypothesis from the classifier score:

$$r(\theta) = -\sum_i \log\left(\frac{p_H\left(\vec{x}_i | \theta\right)}{p_{\text{ref}}\left(\vec{x}_i | \theta\right)}\right)$$

- Can compute ratio above from trained classifier and apply to data
- In our case this brings a few benefits:
  - Partially reconstructed backgrounds difficult to model analytically
  - No longer necessary to bin the data → potential gain in sensitivity
  - In principle, could reduce required size of simulation samples



A. Held, PHYSTAT-SBI 2024

Constructing a classifier to learn NP

- We construct a binary classifier NN to distinguish between samples with SM weights ($V_{\mathrm{RL}} = 0$) and NP weighted-samples ($V_{\mathrm{RL}} = \theta_{\mathrm{gen}}$ for unique θ_{gen} per event)
  - Neural network constructed as a theory-aware NN for physical features, $\vec{x}$, and theory parameters, $\vec{\theta}$, *i.e.*,
    - Base model, a dense NN (2 hidden layers with 100 nodes each) in $\vec{x}$: $s_{\mathrm{base}}\left(\vec{x}\right)$
    - Additional layer $\vec{v}\left(\vec{\theta}\right)$ of dimension $\left(n_{\theta}, n_{\vec{x}}\right)$ introduces NP modification of features:

$$\vec{x} \rightarrow \vec{x} + \vec{v}\left(\vec{\theta}\right)$$

    - This modification gives a NN with

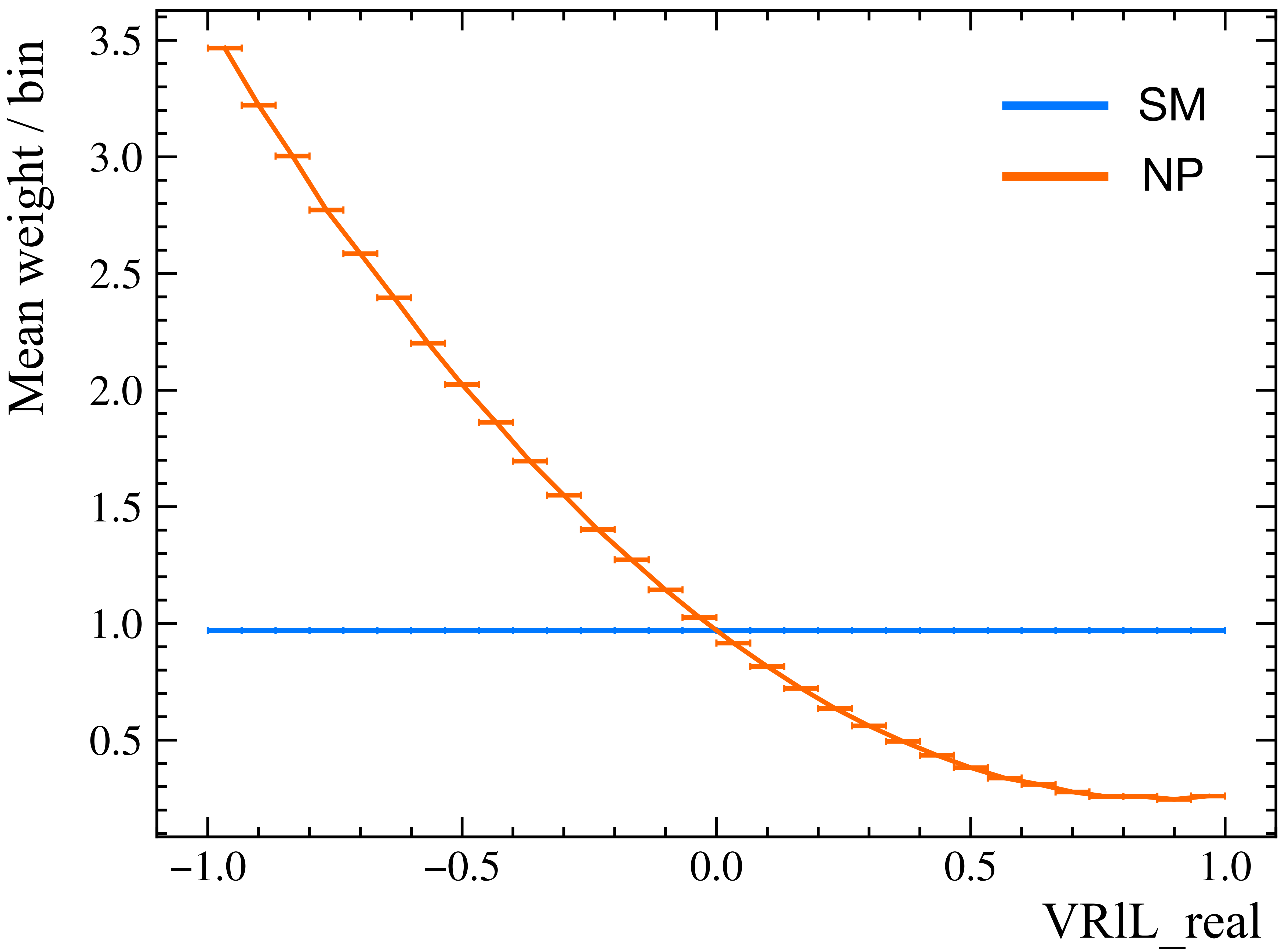
$$s_{\mathrm{base}}\left(\vec{x}\right) \rightarrow s\left(\vec{x}, \vec{\theta}\right) = s_{\mathrm{base}}\left(\vec{x} + \vec{v}(\vec{\theta})\right)$$

- At the moment, consider $\vec{\theta} = \{\theta\} = \{\mathrm{Re}\{V_{\mathrm{RL}}\}\}$ for demonstration
  - Plan to include multiple WCs and their terms in a single network

Generation of per-event weights

- We wish to generate a SM and NP weight (w^i_{SM} and w^i_{NP}) for every event
- Notice that the sum of weights has parabolic dependence on θ (*see right*)
  - Can define this normalisation as $I(\theta)$
  - Obtain this analytically by generating $\theta \in \{-0.5,\ 0,\ +0.5\}$; sum of weights for each gives 3 fixed points
- Then normalise the per-event weights as

$$w'^i_{\mathrm{SM}} = \frac{w^i_{\mathrm{SM}}}{I(0)} \qquad w'^i_{\mathrm{NP}} = \frac{w^i_{\mathrm{NP}}}{I(\theta)}$$



Training of the theory-aware NN

- Every event has weights w'^{i}_{SM} and w'^{i}_{NP}, with uniformly distributed random value of $\theta \in [-1,1]$ used for w'^{i}_{NP} per event
- Dataset constructed by concatenatenating data with w'^{i}_{SM} weights (label 0) and with w'^{i}_{NP} weights (label 1), train/test split in data of 80/20
- Using `BCEWithLogitsLoss` from PyTorch, loss is

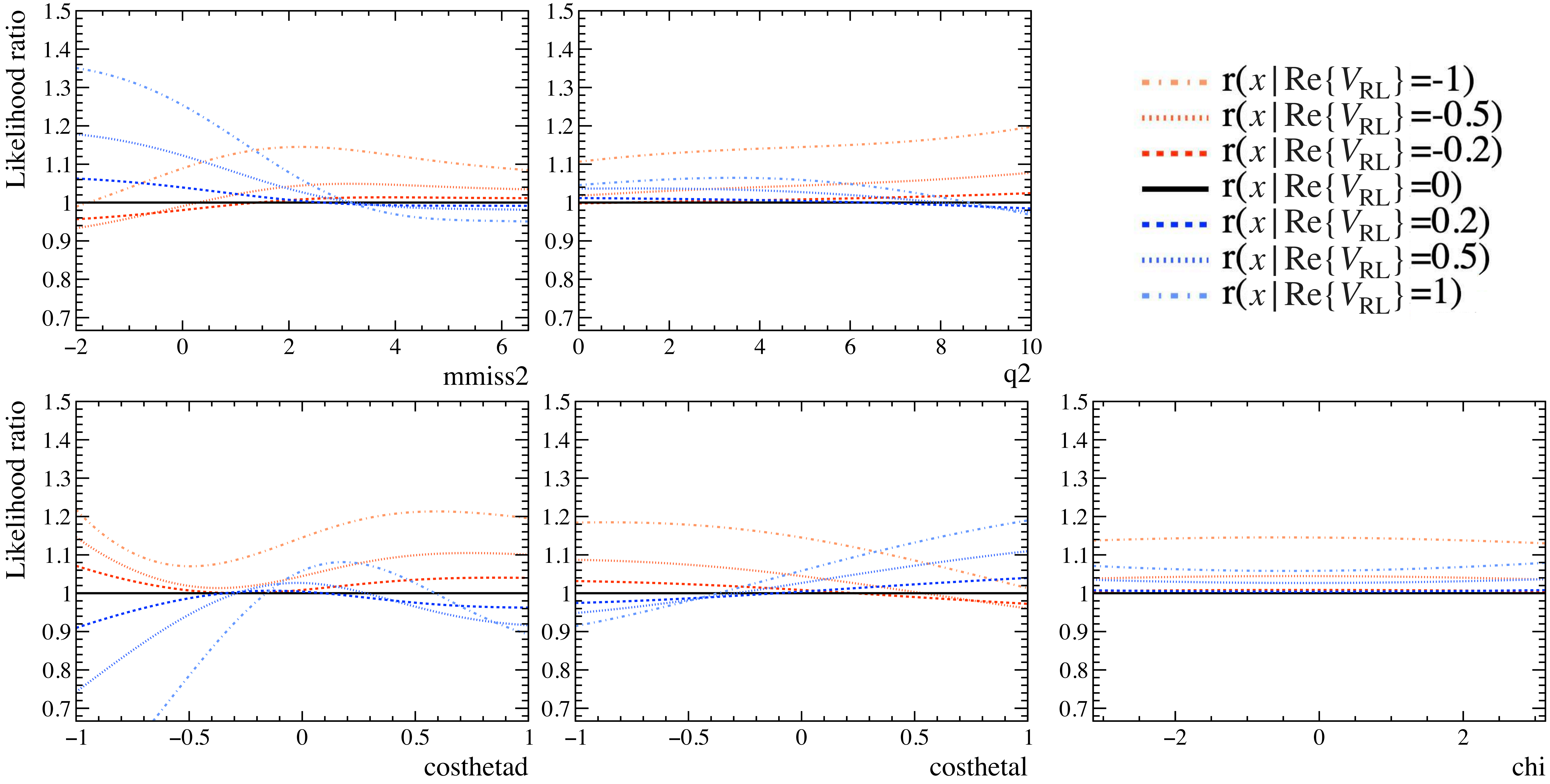
$$\mathscr{L}\left(\vec{x}\,|\,\theta\right) = \frac{-1}{S_w}\sum_i w'^{i}_{\mathrm{NP}} \log s\left(\vec{x}_i\,|\,\theta\right) + w'^{i}_{\mathrm{SM}} \log\left(1 - s\left(\vec{x}_i\,|\,\theta\right)\right) \quad \text{where} \quad S_w = \sum_i w'^{i}_{\mathrm{NP}} + w'^{i}_{\mathrm{SM}}$$

- Optimise with Adam, hyperparameters not formally tuned but are in a good ballpark:
  - Run for $1\mathrm{k}$ epochs with a learning rate of 0.005, include small L2 regularisation ($\lambda = 0.0001$)
- The likelihood ratio can be constructed from the NN score

$$r(\theta) = -\sum_i \log\left(\frac{p_{\mathrm{NP}}\left(\vec{x_i}\,|\,\theta\right)}{p_{\mathrm{SM}}\left(\vec{x_i}\right)}\right) = -\sum_i \log\left(\frac{s\left(\vec{x_i}\,|\,\theta\right)}{s\left(\vec{x_i}\,|\,0\right)}\right)$$

Probing the learned likelihood ratio

- Computing likelihood ratio in each feature for given values of θ gives insight into learned ratio:



Applying the learned likelihood ratio

- From trained models to likelihood (*see right*):
  1. Obtain likelihood ratio from NN output, *e.g.*, binding function calling the NN
  2. Convert likelihood ratio to PDF with `RooWrapperPDF`
     - Since we know sum of weights for given θ, $I(\theta)$, we can extend PDF with $I(\theta)$ as yield
  3. Create negative log-likelihood from PDF and dataset with `createNLL` method

```python
# Compute the learned likelihood ratio
llhr_learned = ROOT.RooFit.bindFunction(
    "MyBinFunc", learned_likelihood_ratio, x_var, mu_var)

# Create the learned pdf and NLL sum based on the learned likelihood ratio
pdf_learned = ROOT.RooWrapperPdf(
    "learned_pdf", "learned_pdf", llhr_learned, True)

nllr_learned = pdf_learned.createNLL(obs_data)
```

RooFit tutorial [rf615_simulation_based_inference.py]()

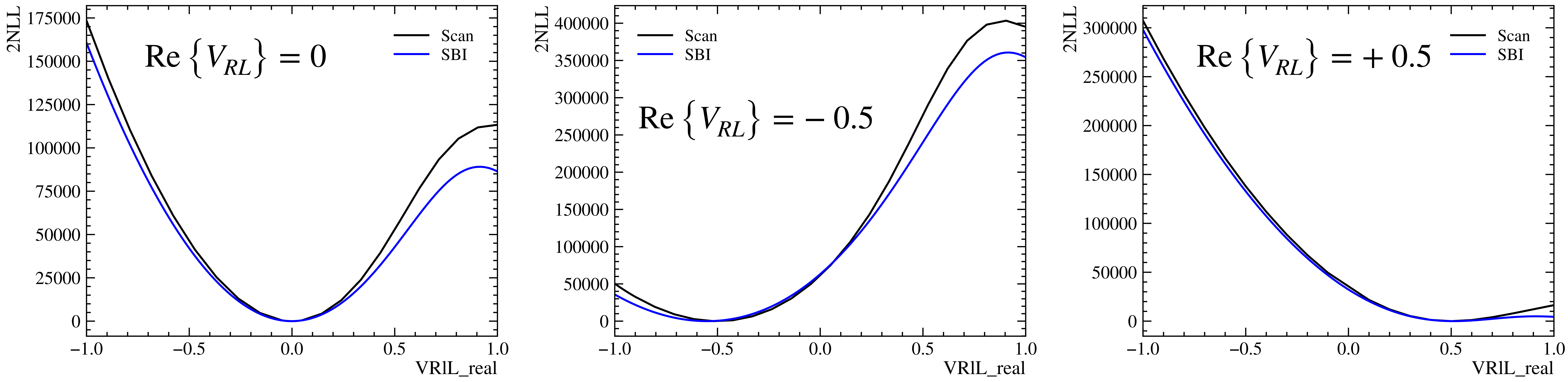
- This can then be manipulated as any RooFit likelihood object, *e.g.*, applying minimiser
- Perform Asimov test to check that NLL is sensible:
  1. Generate per-event weights for all events at a given fixed value of $\theta = \theta_{\text{gen}}$
  2. Create NLL for dataset with these weights applied
  3. Minimise and check that retrieved value θ_{min} consistent with θ_{gen}

Incorporating a “classical” comparison

- We can go one further than checking the minimised value of θ likelihood and perform a similar test for a “classical” fit setup
- Take a fitter built on pyhf, HAMMER and redist-Hammer, in use for $b \to c\tau^{-}\overline{\nu}_{\tau}$ WC global fits
  - Fit takes HAMMER histogram of 5 bins in each of M^2_{miss}, $\cos\theta_d$, $\cos\theta_l$ and χ^2, and 4 bins in q^2
  - Uses HAMMER to provide modifications of histogram passed to pyhf
  - Many thanks also to Marco for providing the setup for this project
- As in Asimov scan for SBI likelihood, apply fitter to sample with weights for a given θ_{gen}
- Aim to check that likelihood curves for SBI and classical fit are consistent

Asimov studies for SBI and classical fits

- Performing the Asimov scans for both fits:
  - Training dataset used to construct template for fit
  - Both likelihood curves computed using fits to test dataset

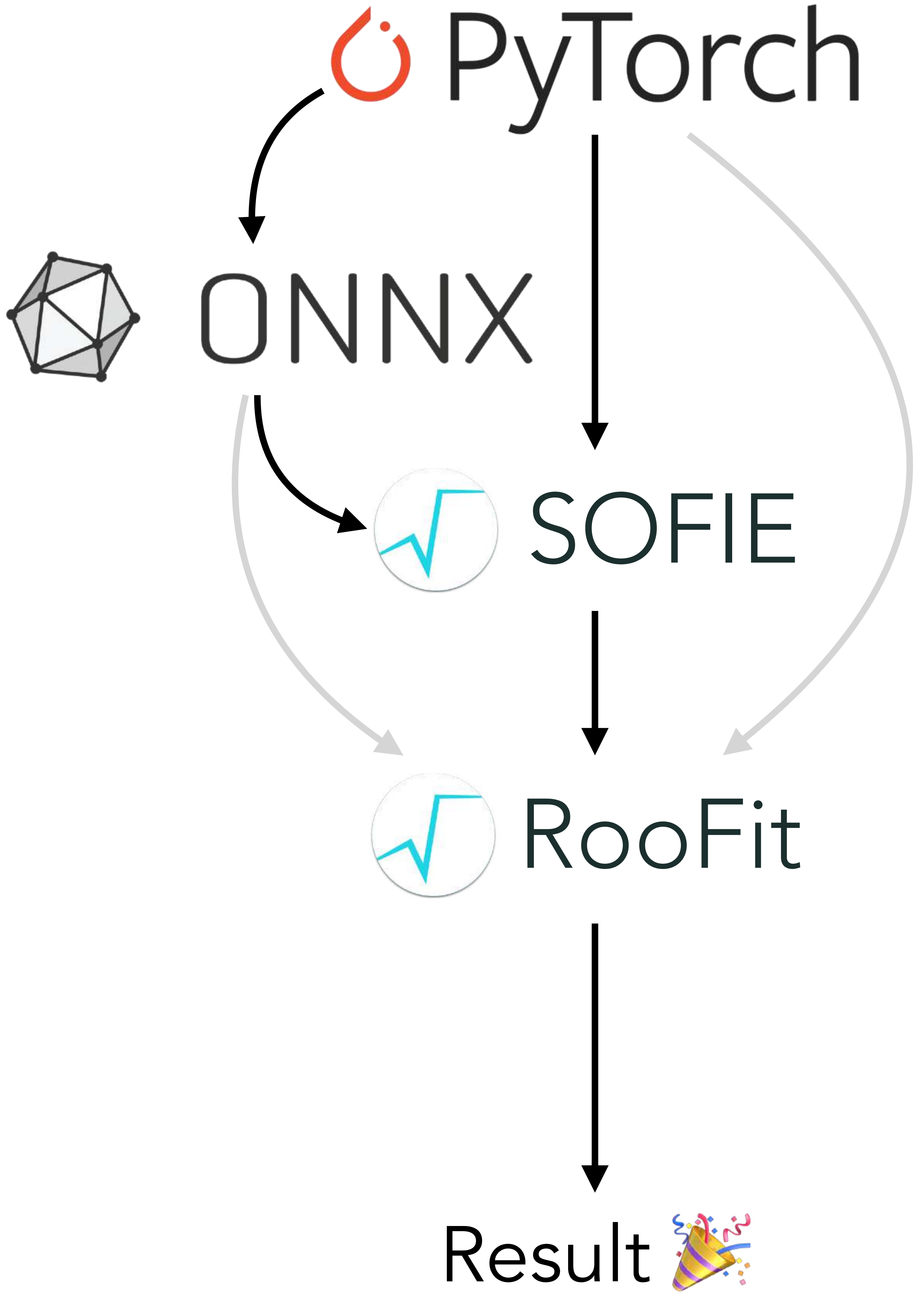


- Generally good agreement between the two fits
- Statistical power of SBI fit strongly dependent on quality of NN training

Automatic differentiation in this workflow

Converting models to code with SOFIE

- Previous RooFit examples involve directly wrapping the call of some Python function
  - Can use PyTorch or ONNXRuntime for this, depending on saved format of model
- Alternative is to use the TMVA SOFIE framework to convert a saved model (ONNX or PyTorch format) into a C++ header
- Can load these headers with ROOT and use `TFormula`/`RooFormulaVar` to manipulate NN in RooFit
- This implementation is at least as performant as wrapped calls to a PyTorch model



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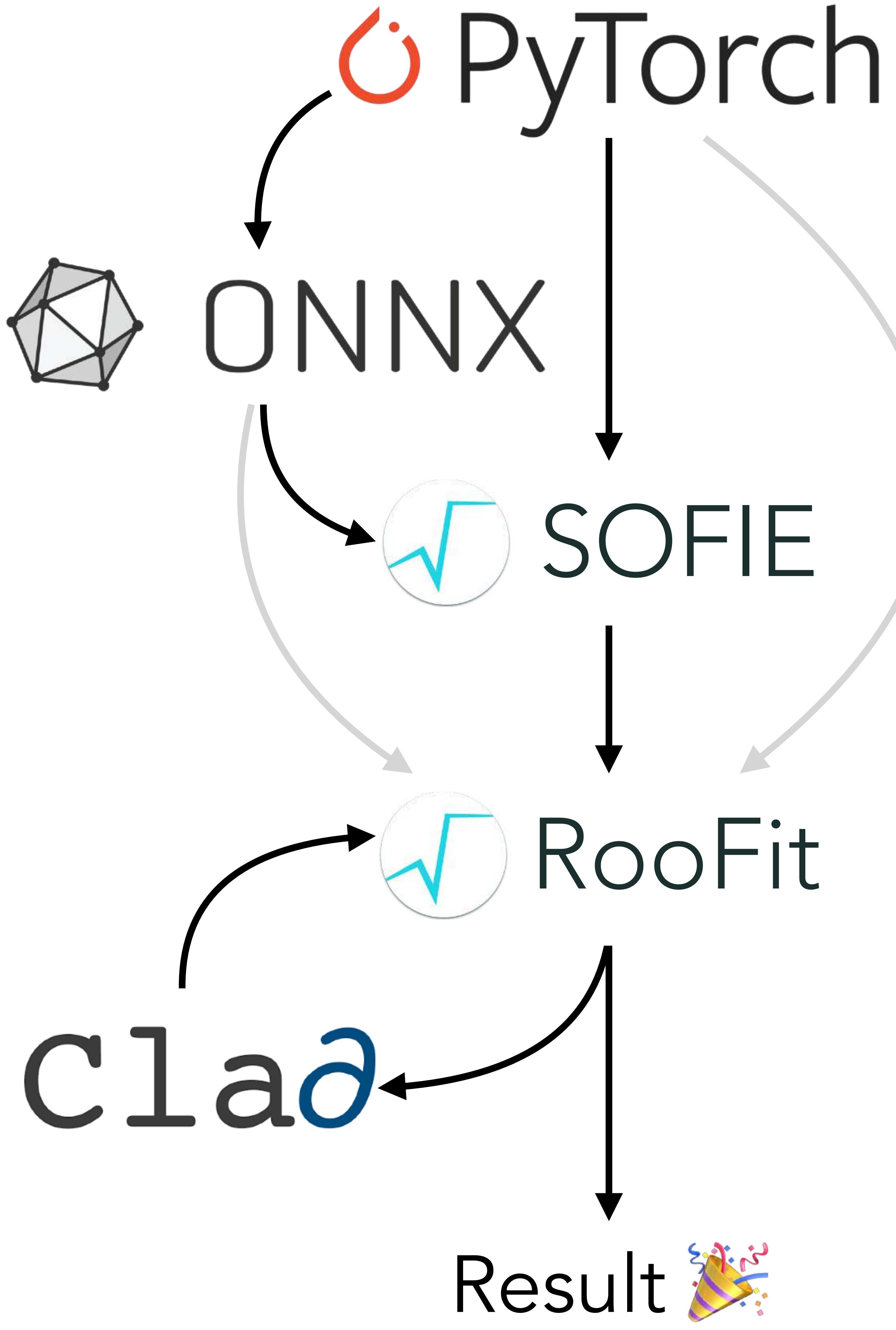
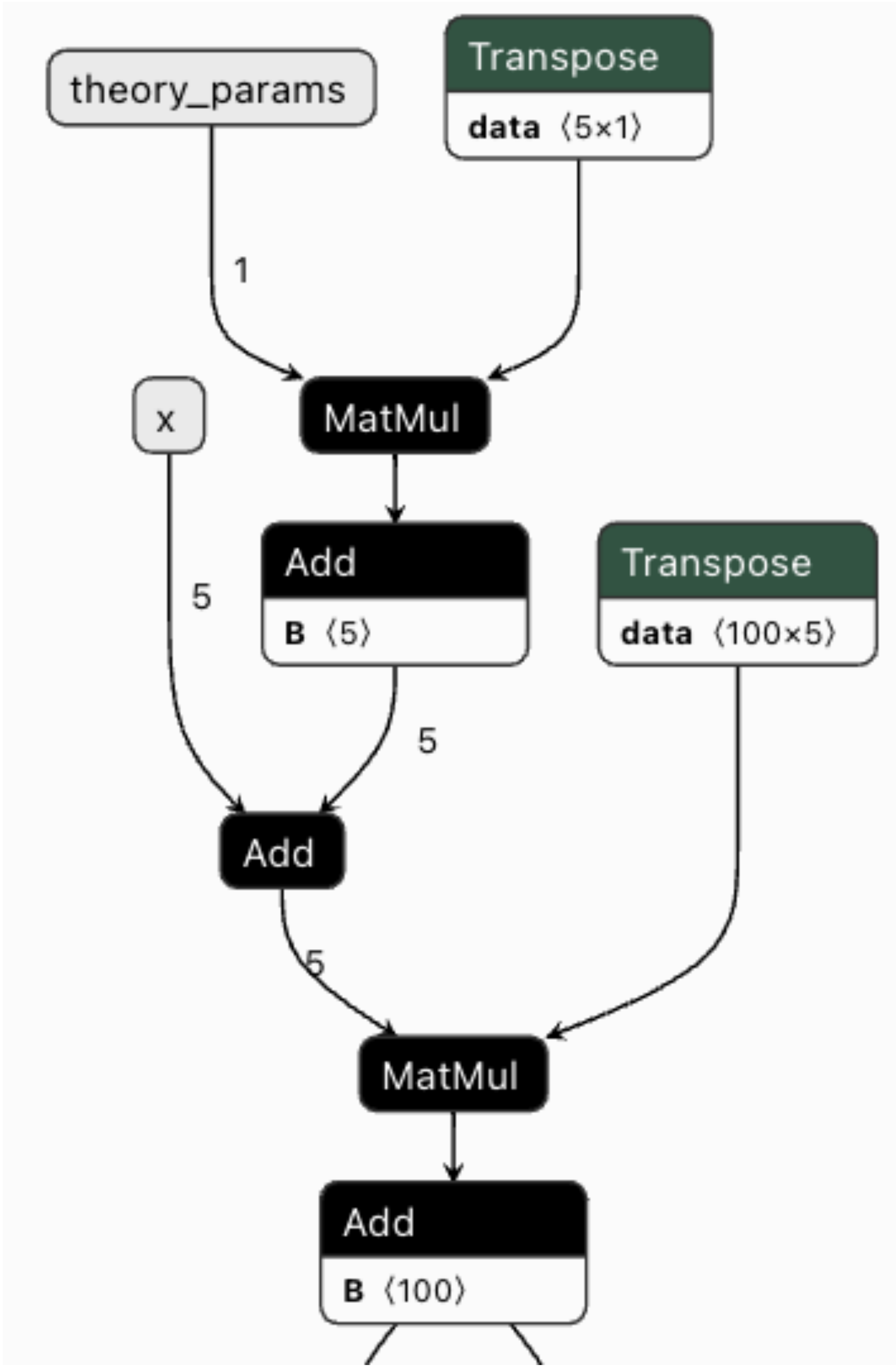
- This implementation is at least as performant as wrapped calls to a PyTorch model
- But we should be able to make this even faster…



Automatic differentiation for fast inference

- Would like to use Clad to perform automatic differentiation (AD) of code generated by SOFIE

model.pth/model.onxx



...

SOFIE

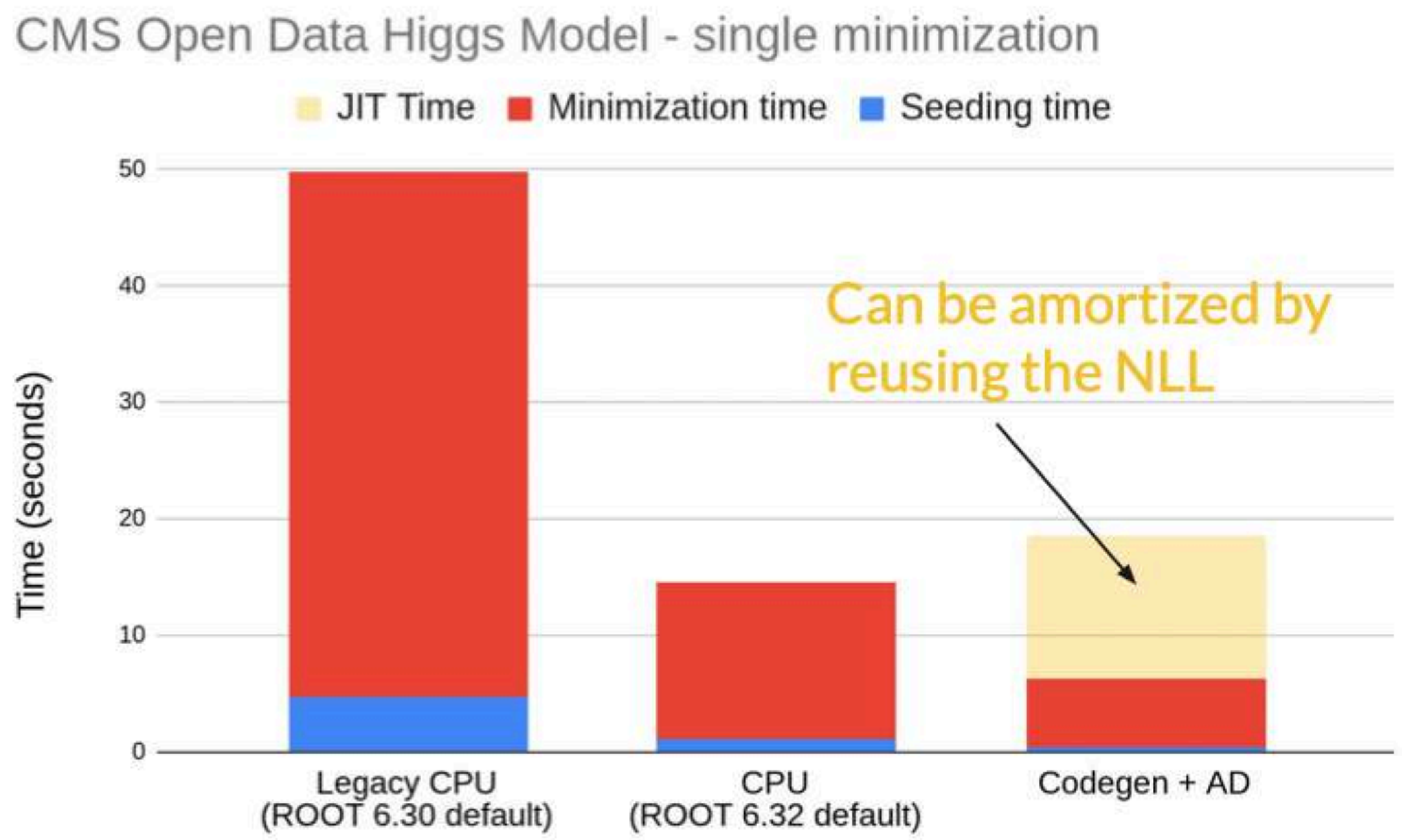
model.hxx

```
std::vector<float> infer(float* tensor_x,float* tensor_theory_params){

//--------- Gemm
   TMVA::Experimental::SOFIE::Gemm_Call(tensor_linear, false, false, 5,
   1, 1, 1,tensor_val_0, tensor_theory_params, 1,
   tensor_theory_projectorbias);

//------- Add
   for (size_t id = 0; id < 5 ; id++){
      tensor_add[id] = tensor_x[id] + tensor_linear[id] ;
   }

//--------- Gemm
   TMVA::Experimental::SOFIE::Gemm_Call(tensor_linear_1, false, false,
   100, 1, 5, 1,tensor_val_2, tensor_add, 1,tensor_base_model0bias);

//------- Sigmoid -- 5
   for (int id = 0; id < 100 ; id++){
      tensor_val_4[id] = 1 / (1 + std::exp( - tensor_linear_1[id]));
   }

//------- Mul
   for (size_t id = 0; id < 100 ; id++){
      tensor_silu[id] = tensor_linear_1[id] * tensor_val_4[id] ;
   }

//--------- Gemm
   TMVA::Experimental::SOFIE::Gemm_Call(tensor_linear_2, false, false,
   100, 1, 100, 1,tensor_val_5, tensor_silu, 1,tensor_base_model4bias);

//------- Sigmoid -- 9
   for (int id = 0; id < 100 ; id++){
      tensor_val_7[id] = 1 / (1 + std::exp( - tensor_linear_2[id]));
   }
```

...

Clad

Generated C++ code for gradients of model (included in likelihood gradients)



[J. Rembser, ICHEP 2024]

Potential analysis speedups?

Status of AD in the workflow

- The aim is to have support in RooFit/Clad so that AD can be handled by RooFit `codegen`
  - Should allow users to simply construct their likelihoods and specify the `codegen` backend
  - AD should take place all the way down from likelihood to ML inference
- Where do we stand on this? There has been quite some action on this within ROOT (thanks to Jonas for the significant work on this!):

Implement coverage of GeMM

[TMVA][SOFIE] Implement wrapper for `BLAS::sgemm_` call #18349
Merged

[TMVA][SOFIE] Implement custom pullback for Gemm operator and corresponding test #18364 Merged

[math] Forward declare `sgemm_` in custom derivatives header #18476
Merged

Refactoring of code emitted by SOFIE

[TMVA][SOFIE] Small improvements necessary for AD support #18341
Merged

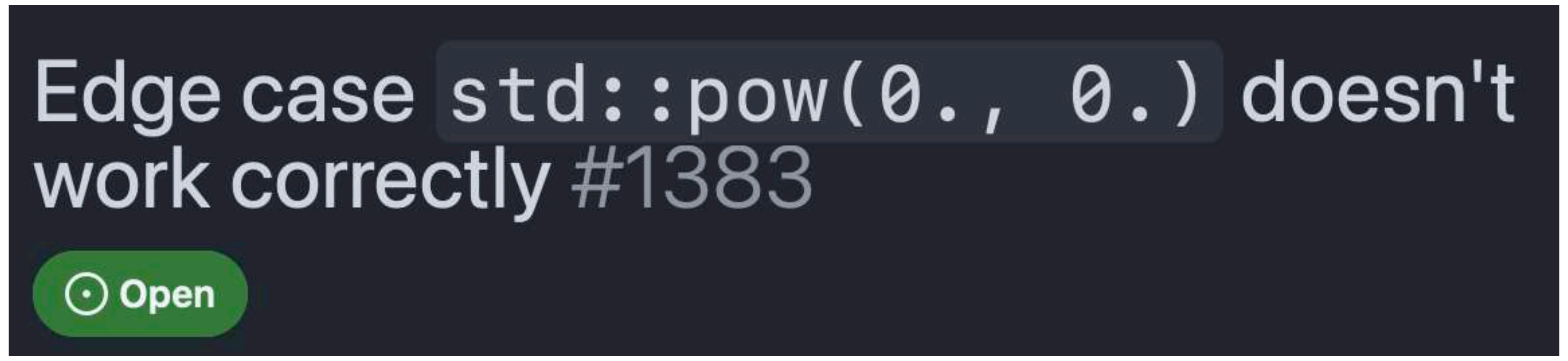
[tmva][sofie] Add overload for inference code that takes output params #18399
Merged

Implement coverage for RooWrapperPDF

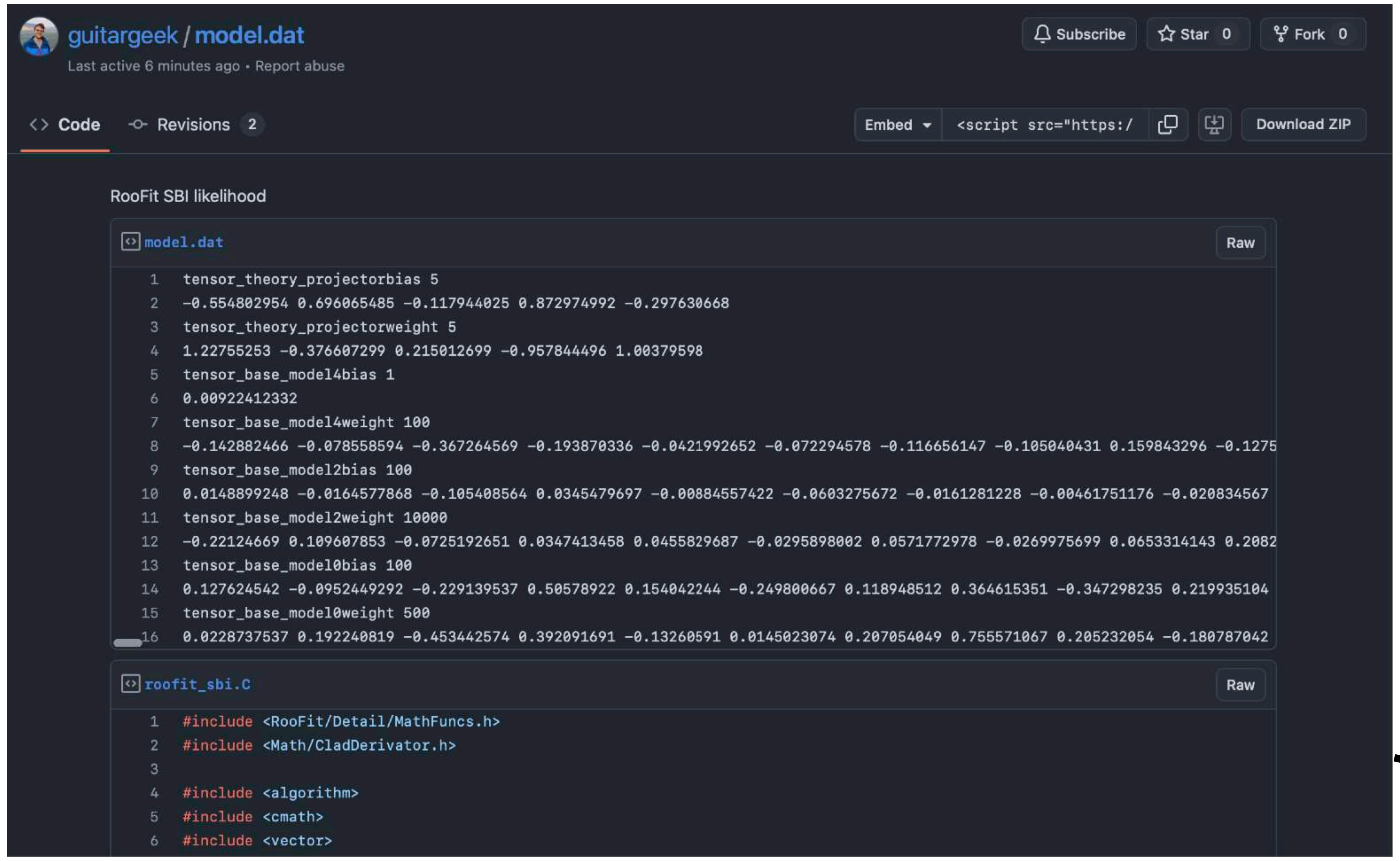
[RF] Implement codegen support for the RooWrapperPdf #18699
Merged

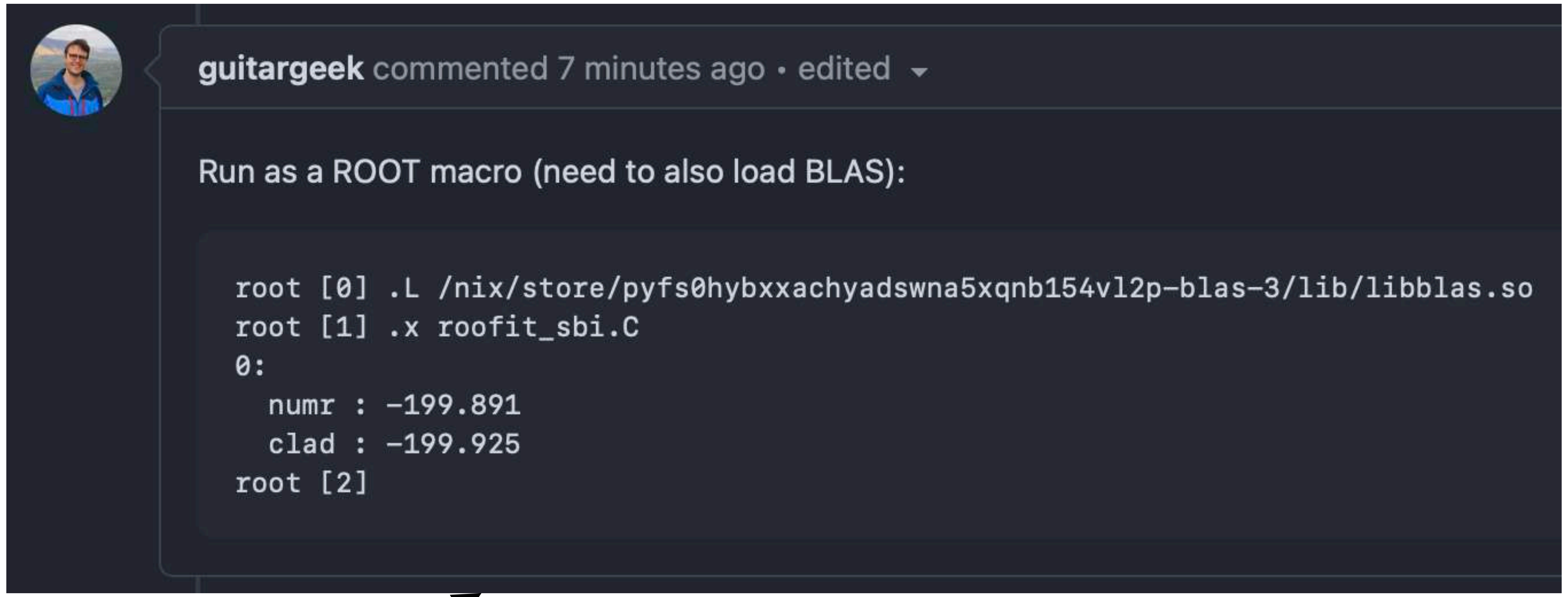
What still needs to happen?

- With some final tweaks, we can integrate fully with `codegen` functionality
- Issues opened in Clad covering the final items required for this to work



- For a full reproducer of the RooFit SBI likelihood, see the following gist:





What next?

- With this in place, should be able to simply enable AD with `codegen`
- Would like to do a comparison of performance (timing) in the statistical analysis:
    1. With a bound Python call to PyTorch
    2. With SOFIE code and AD disabled
    3. With SOFIE code and AD enabled
- Preliminary checks show that 1. and 2. are roughly consistent
- Expectation is that, for analysis size datasets, *i.e.*, upwards of $\mathcal{O}(10^6)$, JIT time becomes a small fraction of total timing in 3., and that this therefore quickly surpasses 1. and 2.
    - This is only a fair comparison if TBR optimisation is enabled

Conclusion

Conclusion

- Project well underway, with most of our goals now complete:
  - LHCb SBI fitting demonstrator workflow constructed
  - Comparisons to the current state-of-the-art established
  - AD of ML inference calls almost enabled
- Still work to be done in the final week of the project:
  - Incorporate efficiency effects in the train/test samples and start to train NNs with combinations of WC terms
  - Training and statistical inference with larger samples sizes (GPU training set up this week should enable this)
  - Consolidate the work of the last few months into a battery of statistical/performance comparisons against the current state-of-the-art

Thank you for your attention

Any questions?

Backup

The LHCb experiment

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