# Tools, MC, ML and all that

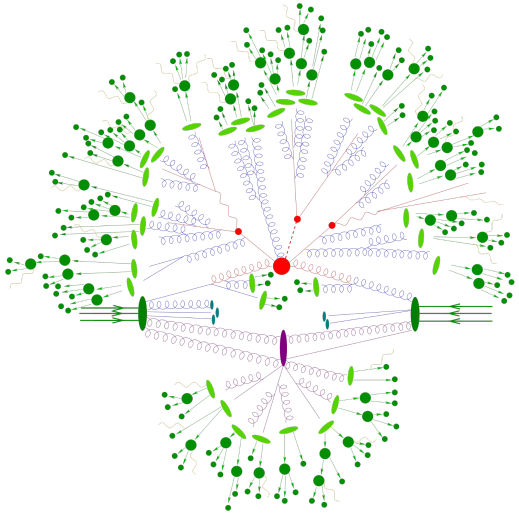
Stefan Höche, Josh McFayden, Simon Plätzer, Vinnie Mikuni

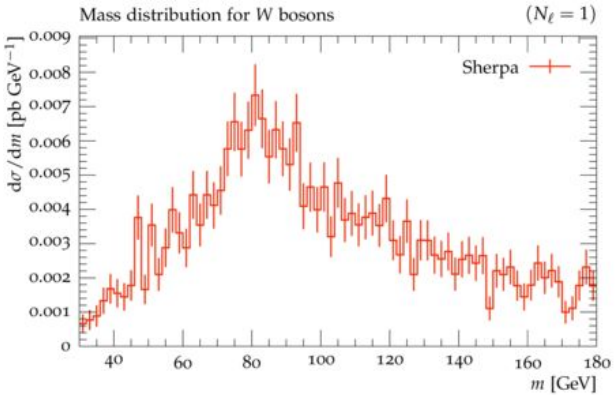
# Main topics

- Shower accuracy and uncertainties
  - New NLL showers
  - Role of hadronization
  - Extrapolation into new observables:
    - Significant collaboration with JSS and heavy flavour initiatives
- Taking stock of EW algorithms
- Interfaces and accords
- Computing and MC algorithms, reweighting

# Making collaboration easier

- Containerisation and reproducibility
  - Docker images, run cards, Rivet routines, Yoda files → HepData
  - Use these tools to make LH studies reproducible
  - Can at Docker-based workflow on e.g. lxplus be documented to lower barrier to entry for MC studies ← In progress
  - Make sure cards actually used by EXP are uploaded with TH prediction Yoda files.
  - Make available for benchmarking (c.f. point 2.), including full chain in EXP
- MC generation generic tool / interface
  - Can we revive MCPlots?



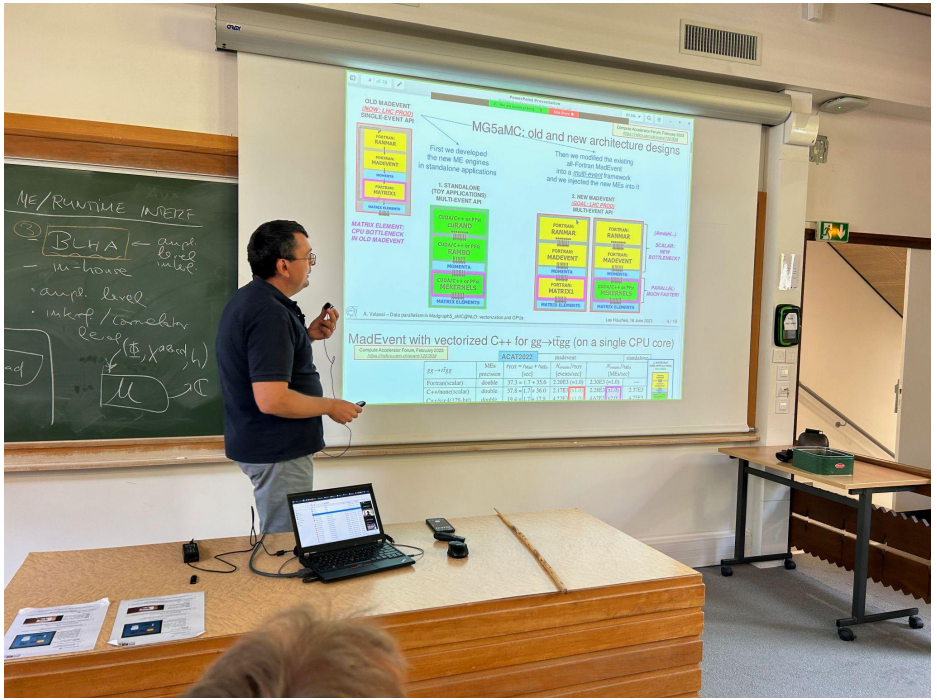



🚧 https://gitlab.cern.ch/lh23/easygen

# Attacking the computing bottlenecks: Parallelization

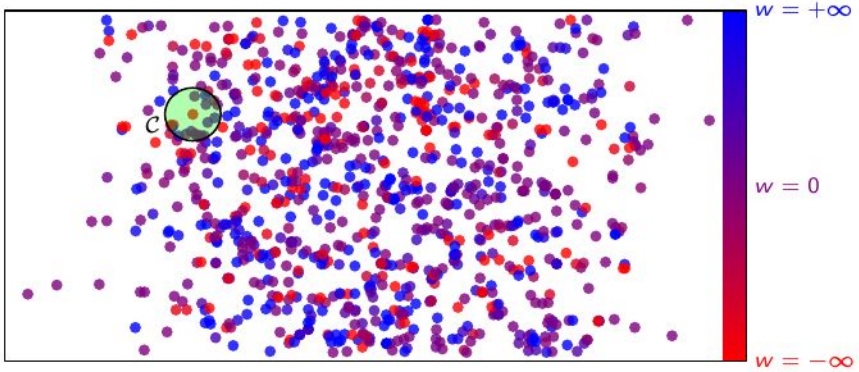
- GPU/Vectorisation/HPC
  - Experience porting codes
  - Workflows in experiments
    - How would code be run in practise
    - How to get/confirm allocations
    - Sharing of resources between EXP and TH
  - Plan for benchmarking MG4GPU and Chili/Pepper

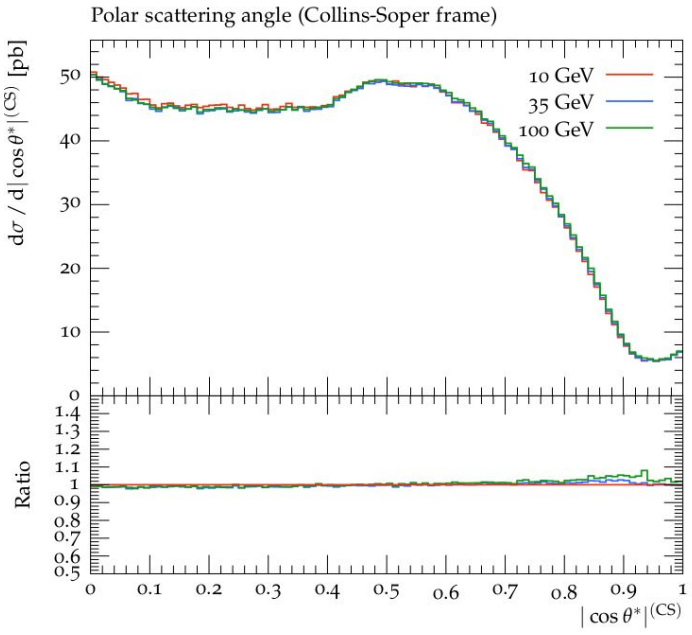
- Computing performance
  - Benchmarking current code
    - Also with examples from EXP
  - Accounting in experiments
  - Projections for future N(2,3)LO calculations
- Updates to interfaces
  - Interoperability of models
  - Modular framework
  - Multi-event API in MC generators
    - Would help for e.g. Reweighting tools



# Attacking the computing bottleneck: Reweighting

- Reweighting and derivative-based optimisation
- Reweighting to eliminate negative weights
  - NN and cell-based tools
  - Stress tests of these tools?
    - Problem areas from TH PoV
    - Validation at scale in EXP
- Usage of resampled events in particle-level simulation
- Recommendation:: Don't unweight before reweighting



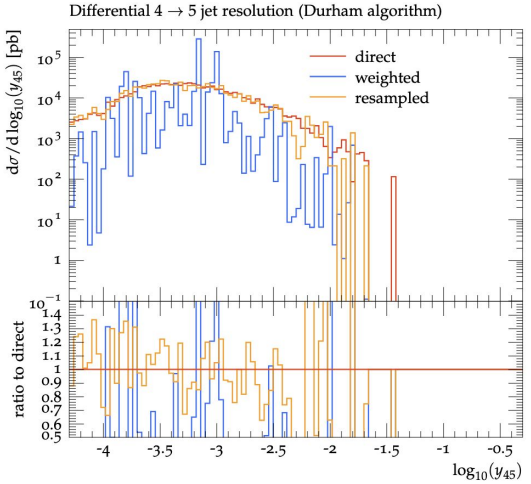



# ML for SM: Weights

*Use for resampling?*

*Olsson, Plätzer, Sjödahl – Eur.Phys.J.C 80 (2020) 10, 934*

- **2 sessions** on event weights and related topics:
  - **Andrea Valassi**: Regressing the **weight derivatives**
  - **Jeppe**: Mitigating **negative weights**
  - **Mathieu**: Regressing **ME ratios** for polarization studies
- **Questions raised**:
  - What can we reweight **reliably** and when do we need other methods?
  - How to ensure the **correct statistical properties**: physics **observables are unchanged, statistical uncertainty** is estimated correctly.

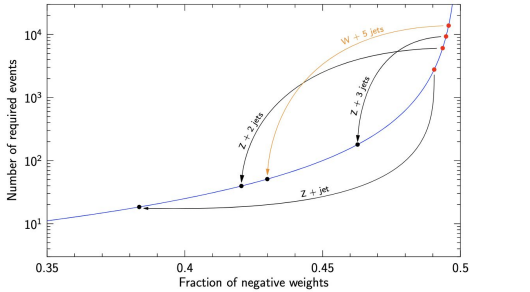



For every MC event: compute and store the *derivative with respect to θ of the MC weight $w_i$*

$$\gamma_i|_\theta = \left(\frac{1}{w_i}\frac{\partial w_i}{\partial \theta}\right)_\theta \rightarrow \gamma_i = \gamma_i|_{\theta=\theta_{\rm ref}} = \left(\frac{\partial w_i}{\partial \theta}\right)_{\theta=\theta_{\rm ref}}$$

Here assume unweighted sample at $\theta=\theta_{\rm ref}$ hence $w_i(\theta_{\rm ref})=1$

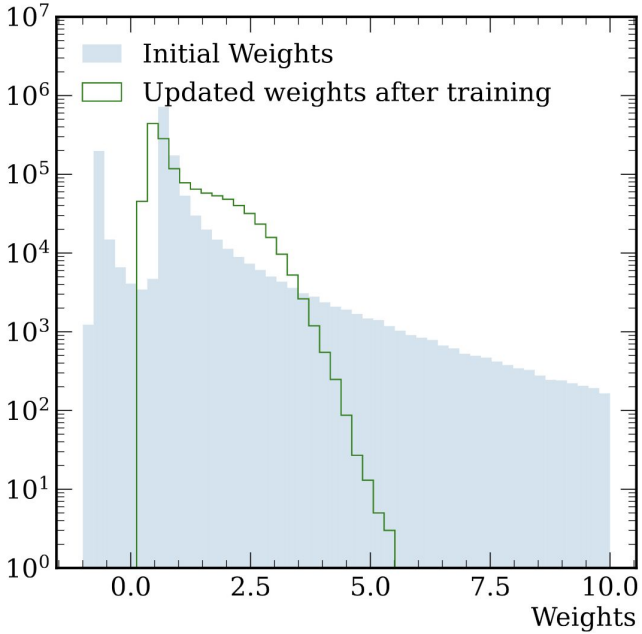
I argue that this is
***the most important MC-truth property of an event***
in a fit for θ

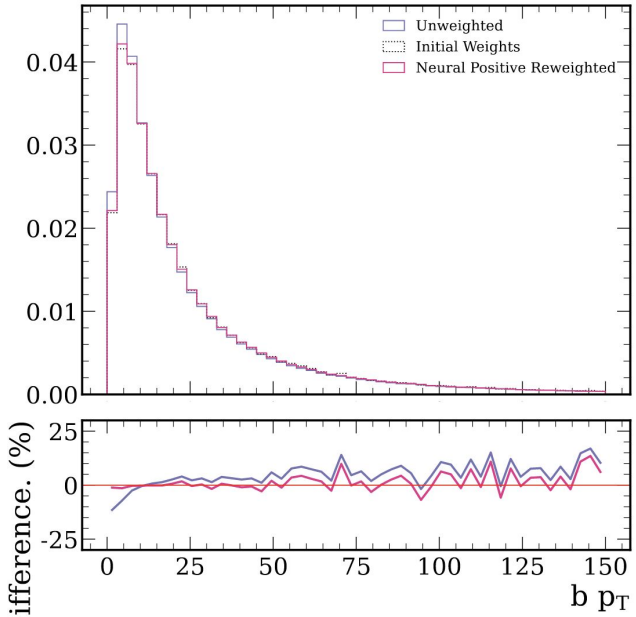



Cell resampling drastically reduces the number of required events

# ML for SM: Weights

- Working with **Jeppe** to compare different methods for **negative weight reduction**
  - Preliminary results using **ttbb** + first emission at **parton level** sample produced by **Maria**
  - Identify distributions that are **difficult to reweight**, expand to other reweighting studies
  - Ensure the **statistical uncertainty** is correctly estimated after modifying the weights

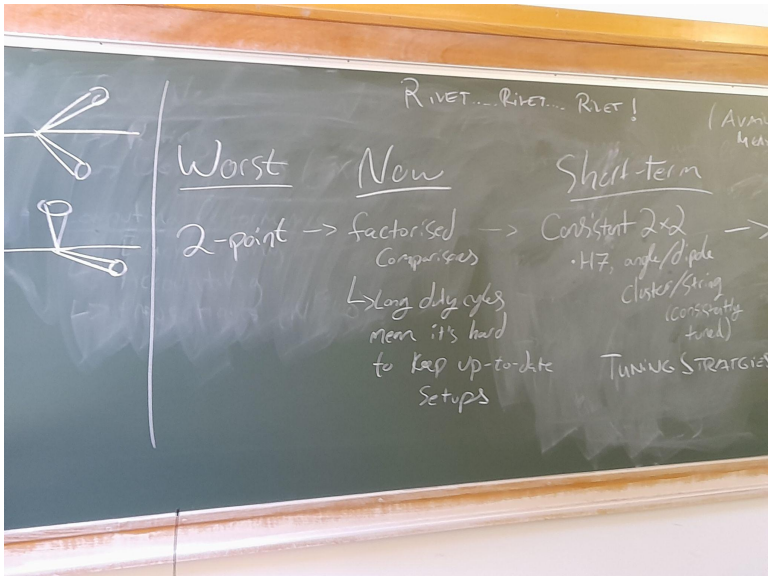


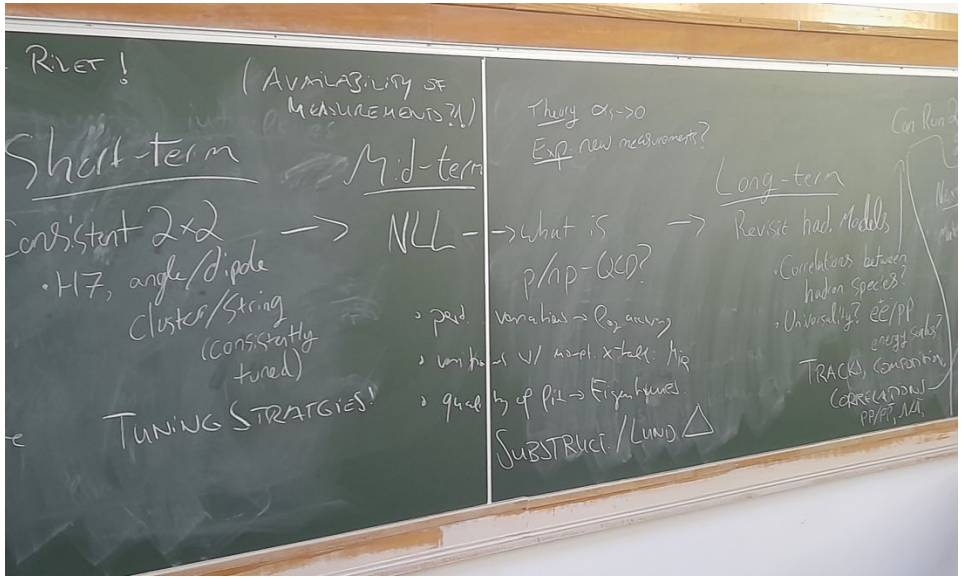




**Preliminary plots from the ML side**

# More systematic parton shower uncertainties

- Short term / Mid term / Long term goals
- Summary and recommendation document for jets (overleaf), but conclusions valid for a wider set of processes



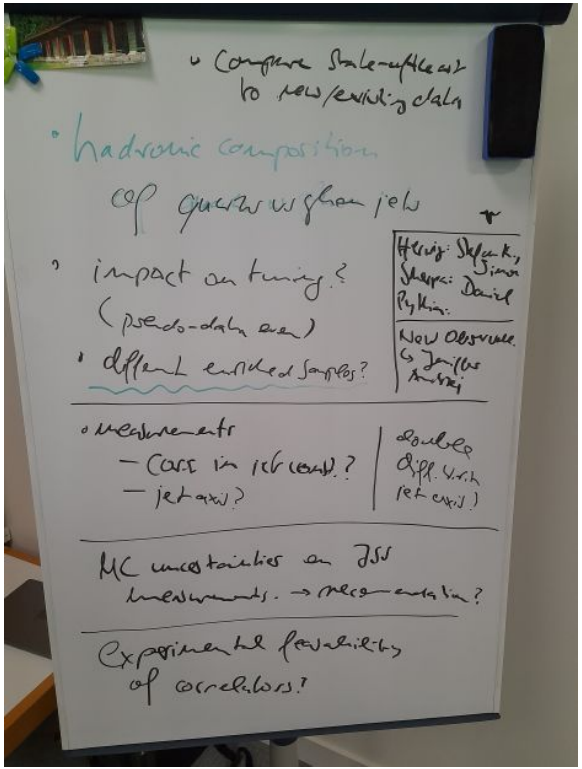
# Shower variations and hadronization

- Retuning, IR cutoff and all that
  - Theoretically more sound update of LH'17 study in planning
- Cluster and string like settings, global tune benchmark?
- A consensus that the right way to build an uncertainty model is to:
  - Change parton shower and hadronisation models
  - Take all combinations available
  - Tune consistently
  - In one generator
    - Shower A + Hadronisation X
    - Shower A + Hadronisation Y
    - Shower B + Hadronisation X
    - Shower B + Hadronisation Y

} Tune

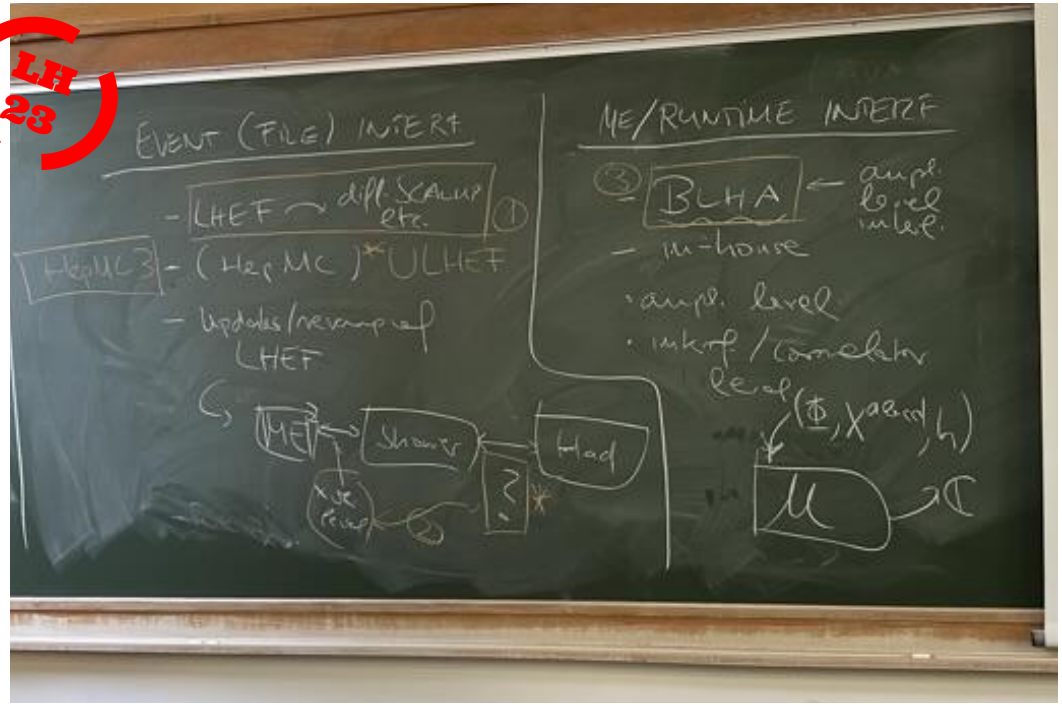
# Jet substructure, correlations and all that

- Better understanding of shower accuracy and hadronization models call for new observables
- JSS particularly interesting, as well as correlations
- Comparison to existing and exploration of new studies
- Questions to be addressed:
  - Sensitivity to hadronization
  - Impact of MPI
  - Impact of new showers
- Big study in preparation



# Accords & interfaces: Event formats

- New HDF5 standard ← LHEF/HepMC
  - Easier event sharing, smaller disk footprint
- Need for more information in intermediate stages of generation?
- Sample sharing between experiments
  - Joint/cross validation
- Publicly available theory calculations
- Amplitude-level interfaces
  - New shower paradigms
  - Higher orders beyond NLO QCD

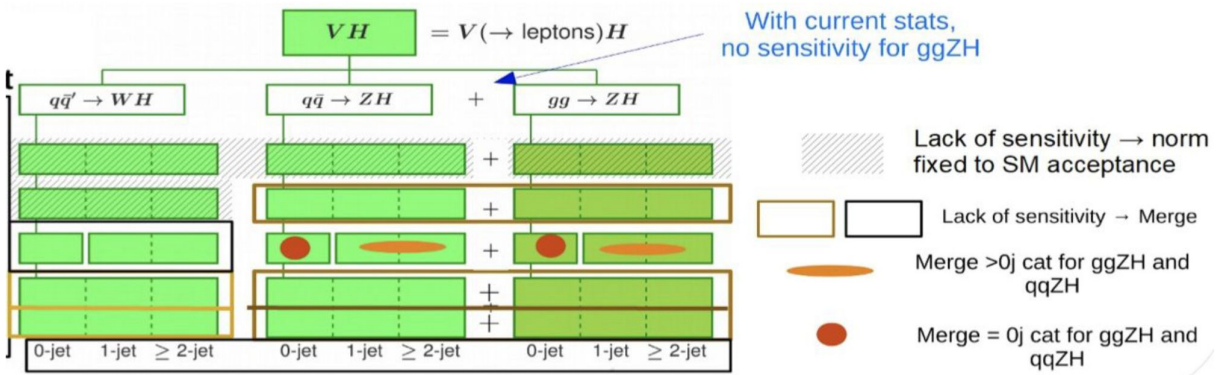


# ML for SM: Unfolding

- **Dedicated unfolding session** on Thursday
- Discussions to identify new use cases and opportunities
- **Higgs applications**: Unfolding of processes where the current STXS binning is too aggressive. Possible to define categories after unfolding or even create new categories based on unfolded variables
  - **Challenges**: Negative weights, non-negligible backgrounds, low signal yield
  - More studies to come with **Mauro**, **Philippe**, and **Karsten**

## STXS for Run3

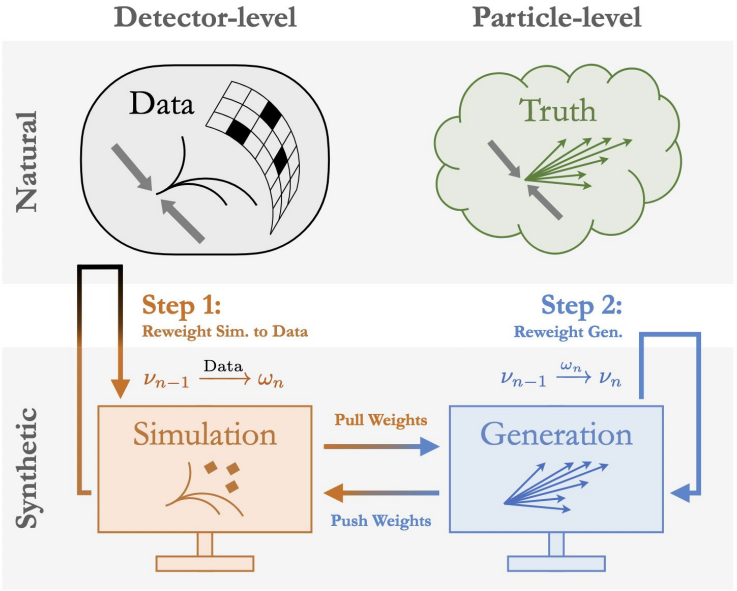
v1.2 too aggressive binning (required merging bins for lack of sensitivity)




**More in the Higgs summary**

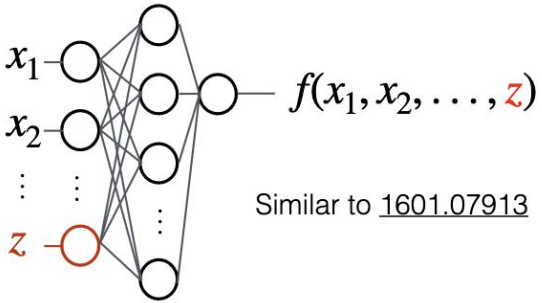
# ML for SM: Unfolding

- Discussion of feasibility of **unfolding energy correlators**
  - **Constituent level unfolding** needed to preserve the information necessary to calculate the **EECs**
  - Similar strategy **partially developed** in the context of **H1 data** to unfold generalized jet angularities
  - Interesting to think more about the **feasibility** and comparison with **standard unfolding methods**




**More in the Jet-substructure techniques summary**

# ML for SM: Experimental Uncertainties

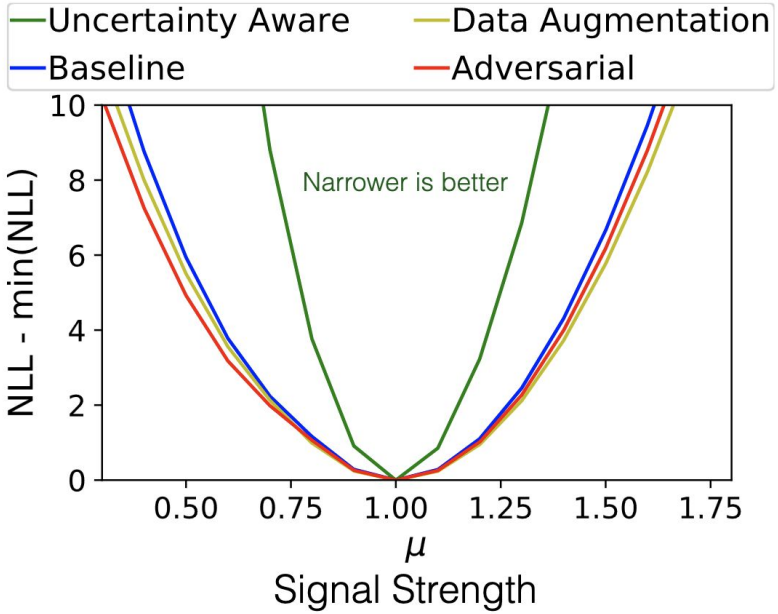



Similar to 1601.07913

Repeat for each hypothesis $z$

Data with Z = ?

- Talk from **Aishik** on including experimental uncertainties in the machine learning training
- Requires continuous **parametrization** of the observables as a function of the uncertainty source
- How much do we **trust our uncertainties**?



# How to cooperate after Les Houches

- Work has only begun!

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