QUnfold: Quantum Annealing for Distributions Unfolding in High-Energy Physics

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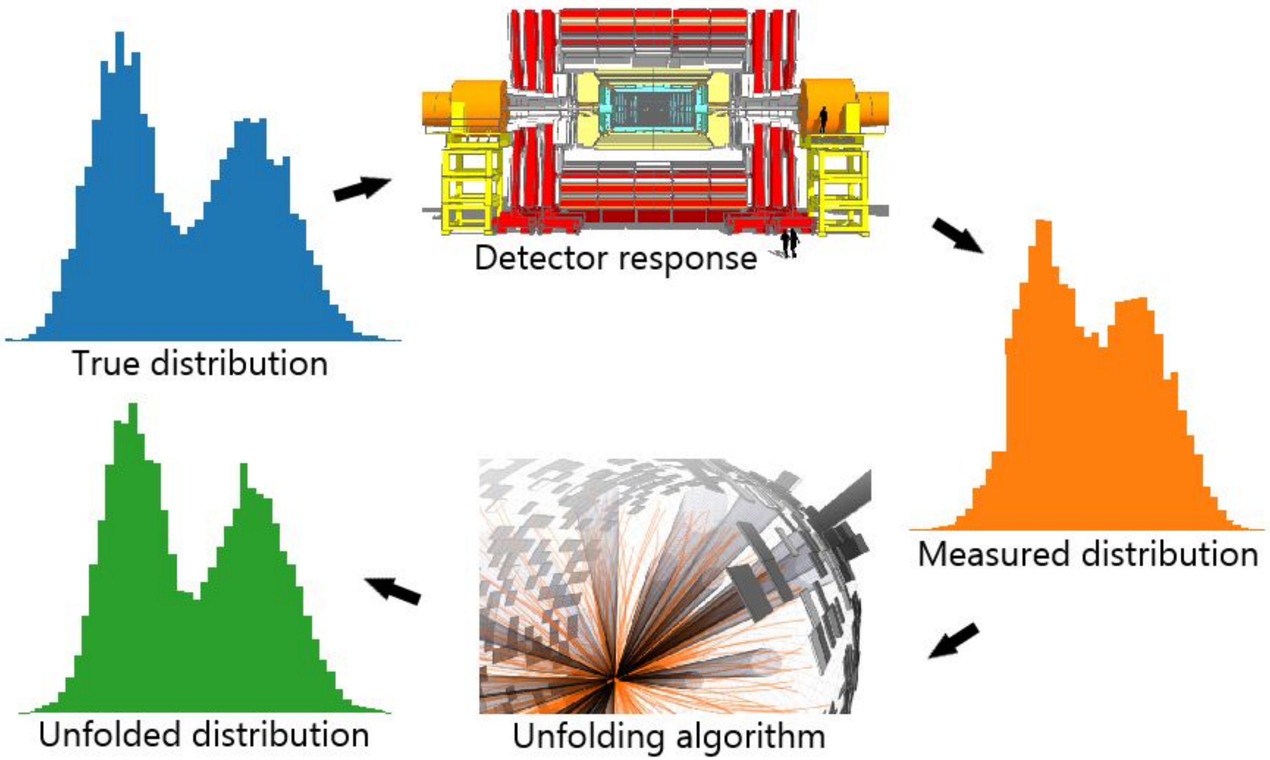
Unfolding problem

- In **High-Energy Physics** (HEP) experiments each measurement apparatus has a unique signature in terms of *detection efficiency*, *resolution,* and *geometric acceptance*
- The overall effect is that the distribution of some measured observable in a physical process is *biased* and *distorted*
- **Unfolding** is the mathematical technique to correct for this distortion and recover the original distribution



$$\vec{\mu} = R\vec{x}$$

reconstructed histogram (≈ measured histogram)

response matrix

unfolded histogram (≈ true histogram)

Unfolding techniques

Classical methods used in HEP:

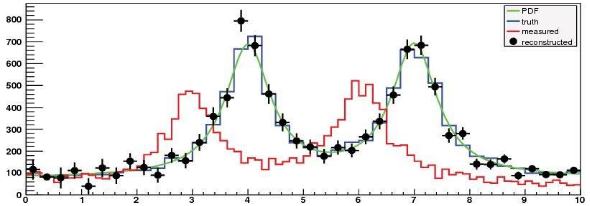
- Standard matrix inversion (never used in practice) ➡ $\vec{x} = R^{-1}\vec{d}$ with $\vec{d} \sim \vec{\mu}$
  - ill-conditioned problem
  - large statistical fluctuations
- Bin-by-bin unfolding (never used in practice)

- Likelihood-based unfolding (SVD)
- Iterative Bayesian unfolding (IBU)

} approximate solution

RooUnfold

The ROOT Unfolding Framework



Quantum-based methods:

- First proof-of-concept attempt in 2019: the model worked only for small-size problems instances and the previous generation of D-Wave quantum annealing devices was used
- QUnfold: our open-source implementation ready to be used by HEP scientists

Quantum Annealing

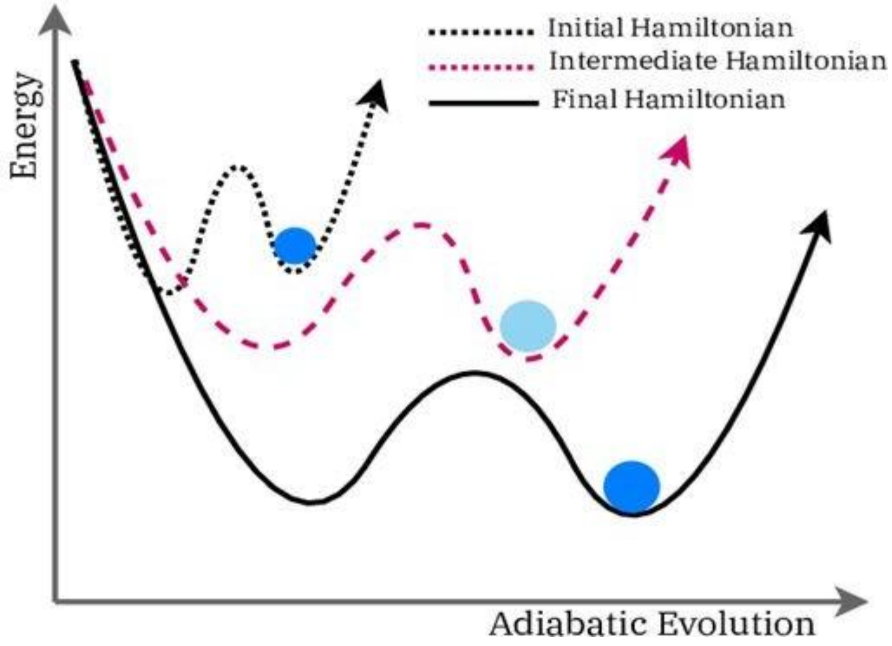
QA is a quantum optimization process to find the global minimum of an objective function $O(\vec{x})$ over a set of candidates states

1. The quantum-mechanical system is prepared in the known ground-state of an **initial Hamiltonian**

2. The problem solution is encoded in the ground-state of a **final Hamiltonian**

3. The quantum system evolution is controlled by the following time-dependent Hamiltonian:

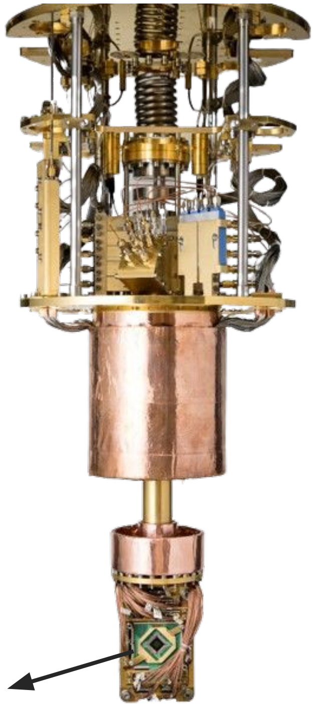
$$H(t) = A(t)H_{init} + B(t)H_{fin} \qquad A(t)\downarrow \quad B(t)\uparrow$$



Quantum Adiabatic theorem
"If the evolution is slow enough, the quantum-mechanical system stays close the ground-state of the instantaneous Hamiltonian"

D-Wave QA system

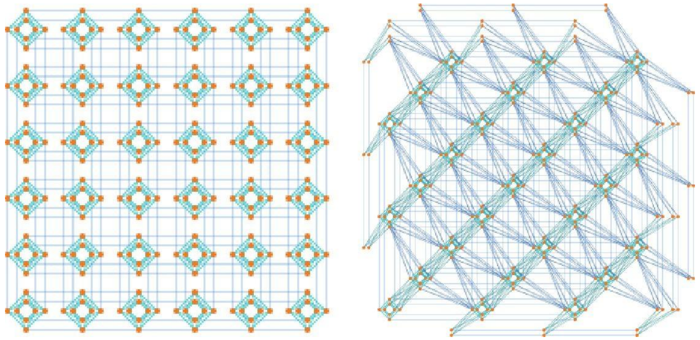
- Shielded from external electric, magnetic, and thermal effects
- Isolated from floor vibrations
- Controlled by a specialized wiring and read-out electronics



QPU

Quantum Processing Unit (QPU)

- Lattice of superconducting qubits
- Cooled down to ~15 mK by liquid Helium refrigeration system
- < 25 kW total power consumption
- <u>Physical interaction between qubits limited by a fixed topology</u>



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QUnfold QM formulation

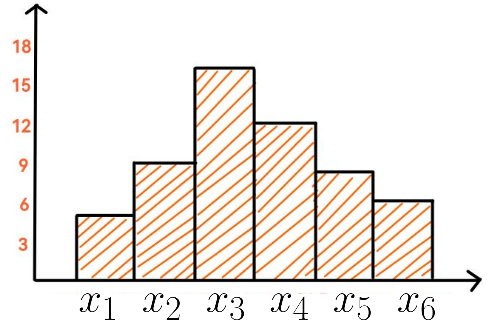
Log-likelihood maximization unfolding: $\max_{\vec{x}} \left(\log \mathcal{L}(\vec{\mu}|\vec{d}) + \lambda \mathcal{S}(\vec{\mu}) \right)$

- $\vec{\mu}$: reconstructed histogram
- $\vec{d}$: measured histogram
- $\mathcal{S}(\vec{\mu})$: regularization term (avoid overfitting statistical noise)

Quadratic Model minimization: $\min_{\vec{x}} \left(||R\vec{x} - \vec{d}||^2 + \lambda ||G\vec{x}||^2 \right)$

Tikhonov regularization: discrete 2nd order derivative (Laplacian operator G)

- Classical optimization of quadratic function, nothing quantum yet!
- $\vec{x}$ is the vector of integer numbers representing the unfolded histogram



QUnfold QUBO formulation

To get the QUBO model from the integer-variables QM, a “binarization” process based on the standard **logarithmic encoding** of the integer numbers to bit-strings is performed

$$\vec{a} = -2R^T\vec{d}$$
$$B = R^T R + \lambda G^T G$$

$$H(\vec{x}) = \sum_i a_i x_i + \sum_{i,j} b_{ij} x_i x_j = \vec{a}\cdot\vec{x} + \vec{x}^T B \vec{x}$$

The scaling of the number of binary variables (= required logical qubits) is:

- $O(N_{\text{bins}})$: linear with the number of bins in the histogram
- $O(\log(N_{\text{entries}}))$: logarithmic with the number of entries in the histogram

Example:
- Gaussian distribution
- 20 bins
- 5M entries
- $N_{qubits} \approx 350$

QUnfold software

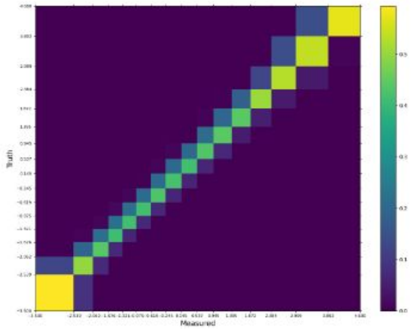
Features:

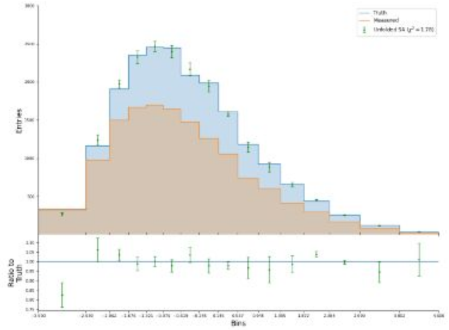
- Package implemented entirely in **Python**
- Designed to work also on real LHC data
- Based on **NumPy**, but compatible with **ROOT**
- Open-source repository on GitHub
- Available on PyPI (`pip install QUnfold`)

```python
from qunfold import QUnfolder

# Define your input response matrix and measured histogram as numpy arrays
response = ...
measured = ...
binning = ...

# Create the QUnfolder object and initialize the QUBO model
unfolder = QUnfolder(response, measured, binning, lam=0.1)
unfolder.initialize_qubo_model()

# Run one of the available solvers to get the unfolding result
sol, cov = unfolder.solve_simulated_annealing(num_reads=100)
```

Solvers:

- D-Wave Simulated Annealing
- D-Wave Quantum Annealing
- D-Wave Hybrid solver
- Gurobi integer/binary solver





QUnfold for HEP data

Dataset:

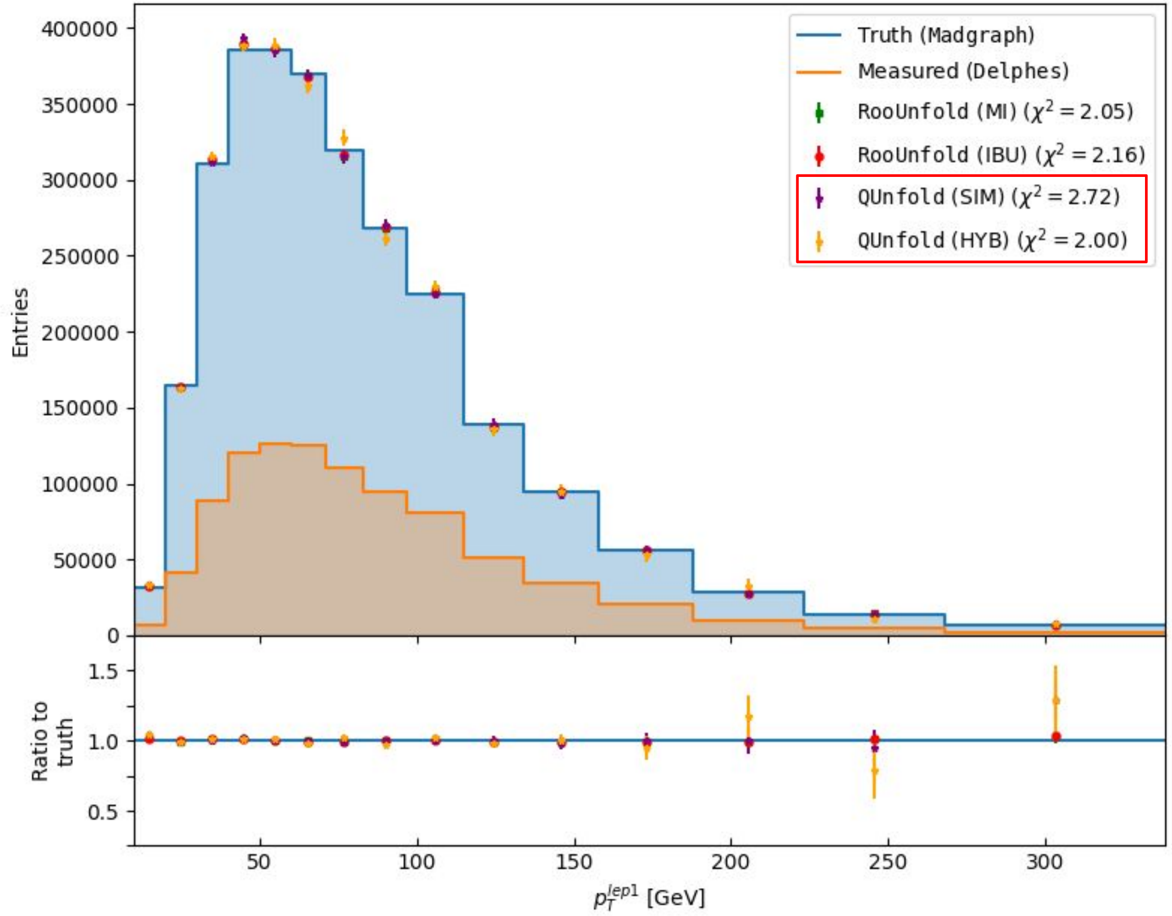
- Simulate $t\bar{t}$ **process** in the *dileptonic channel* (**2 leptons** and at least **2 *b*-jets** required in the final state)
- Generete detector-level ATLAS data (***Delphes*** sim.) and truth-level samples (***MadGraph*** gen.)
- $\approx$ 2.5M entries data are used to generate reco/truth level

Technique:

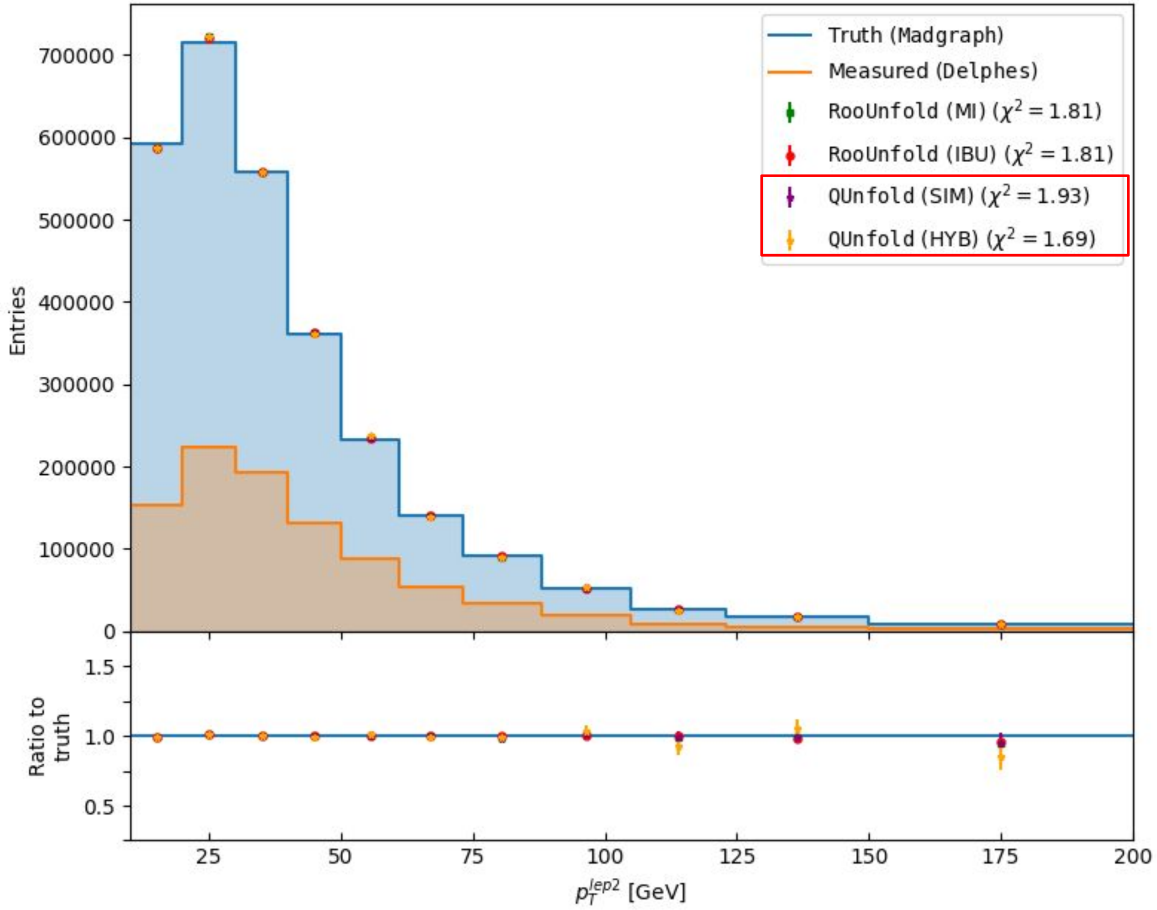
- The simulated annealing and hybrid solvers are used (quantum annealer solver is work in progress)
- The results are compared to classical HEP unfolding methods: *MI* and *IBU*, using the RooUnfold framework
- Toy Monte Carlo experiments are run to compute the covariance matrix for evaluating the quality of the result (X^2 test) and the statistical errors associated to the unfolding method

Unfolding results (1)

Leading lepton p_T

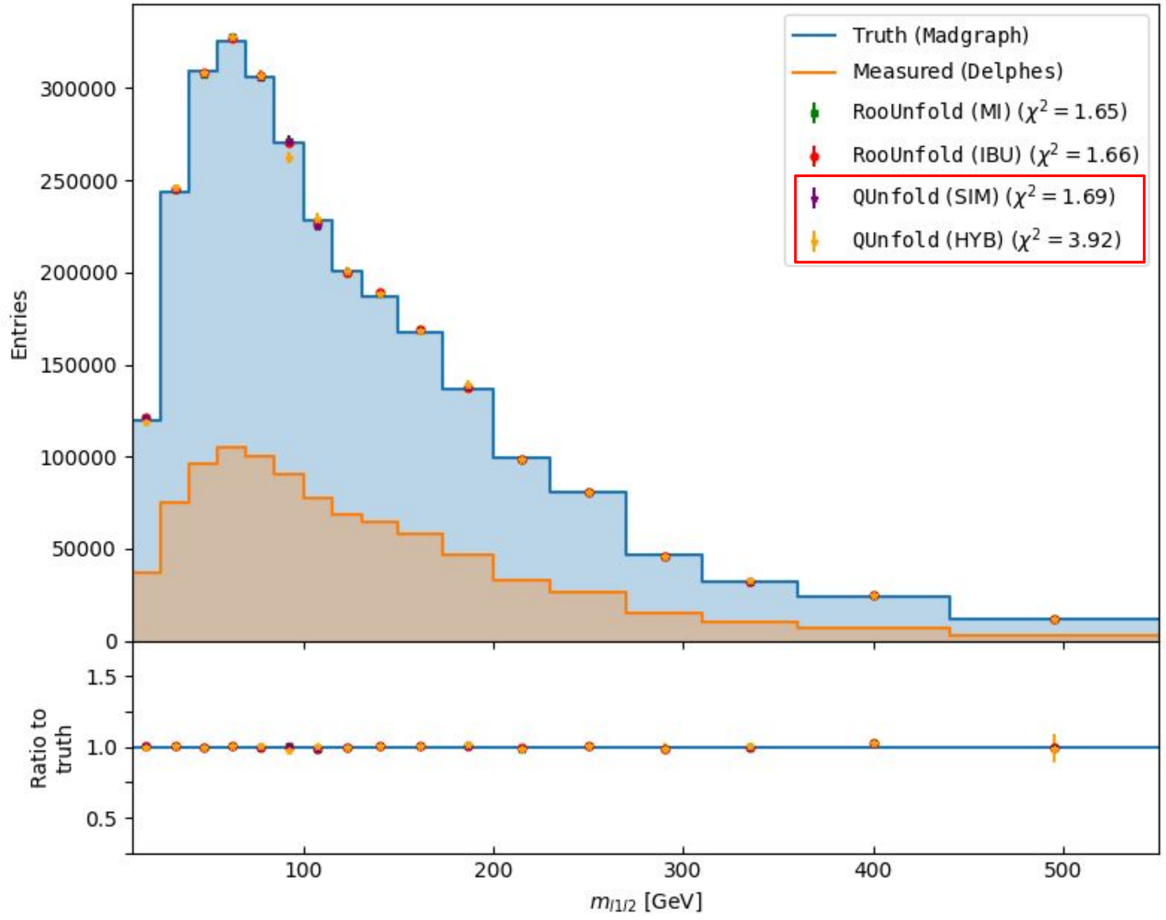


Subleading lepton p_T

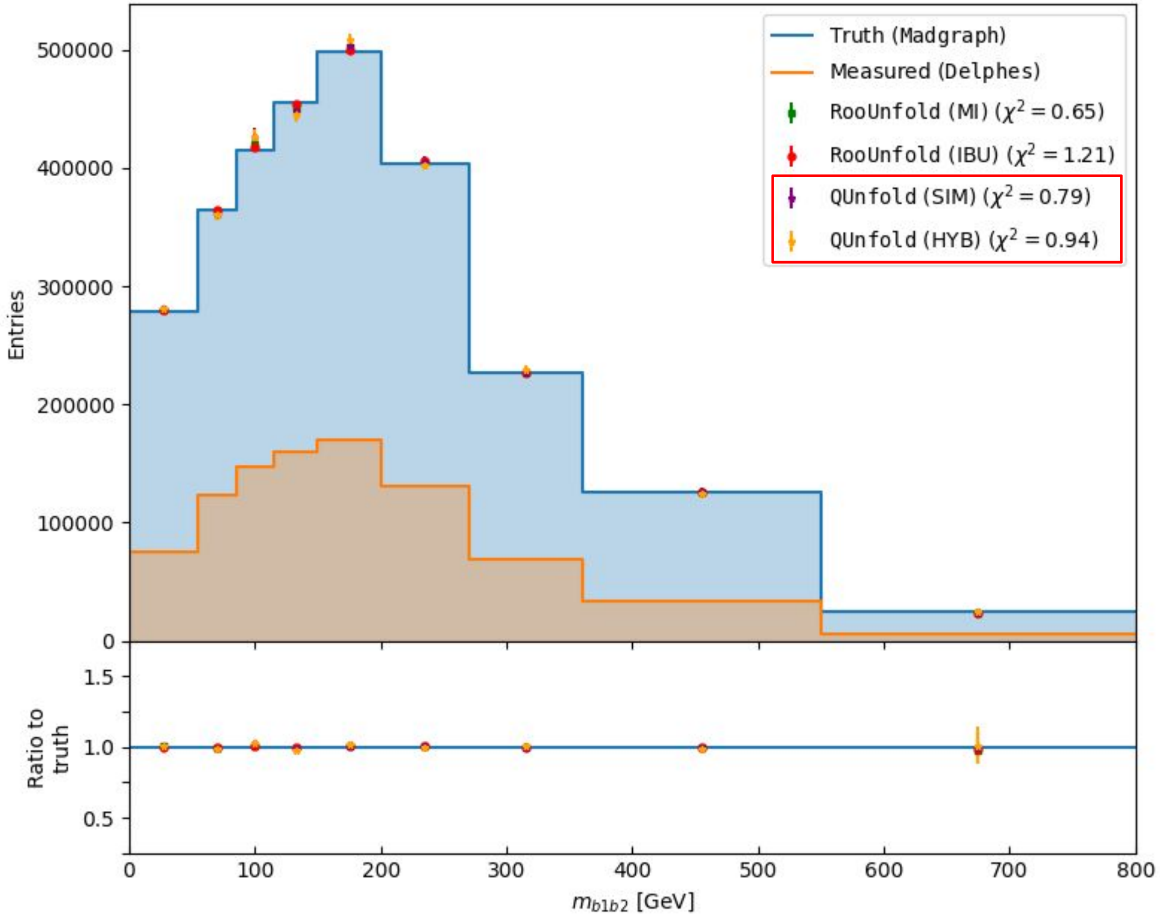


Unfolding results (2)

Leptons invariant mass



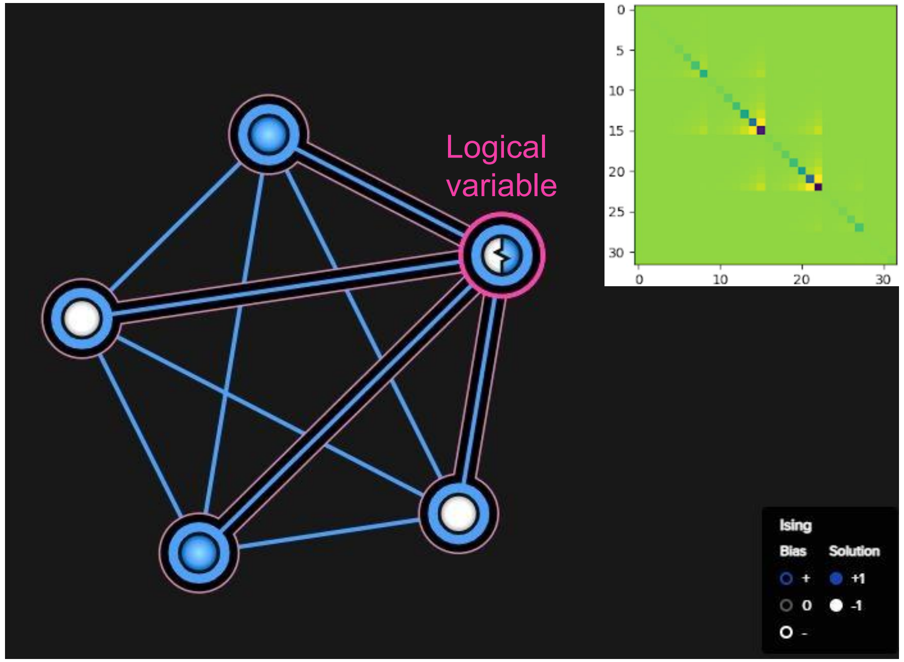
b-jets invariant mass



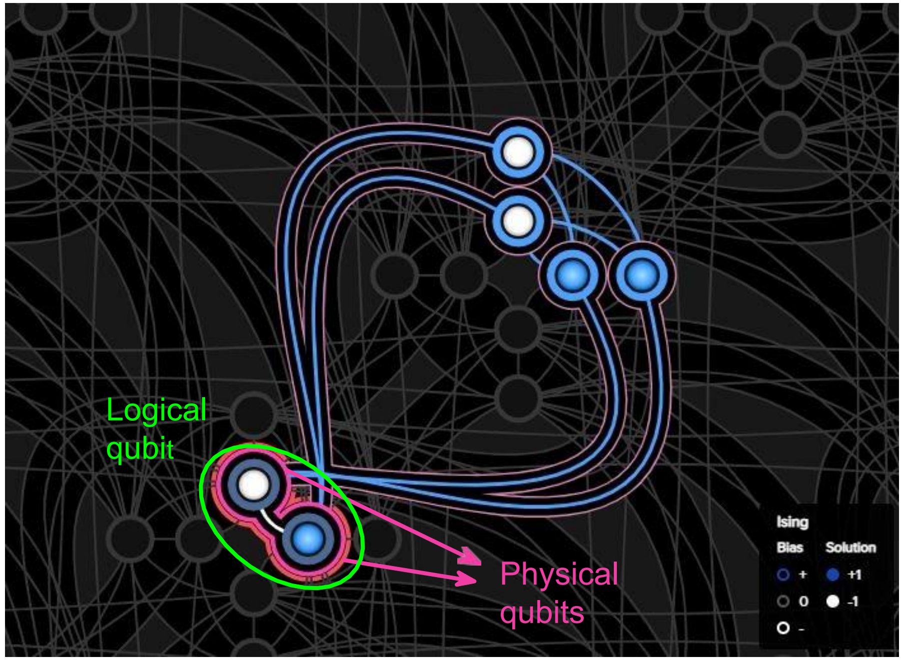
Challenge: graph embedding

Logical qubit ≠ Physical qubit

“Embedding” is the process of mapping a **source graph** (problem topology) to a **target graph** (QPU topology): <u>a cluster of physical qubits may represent a single logical qubit/variable</u>

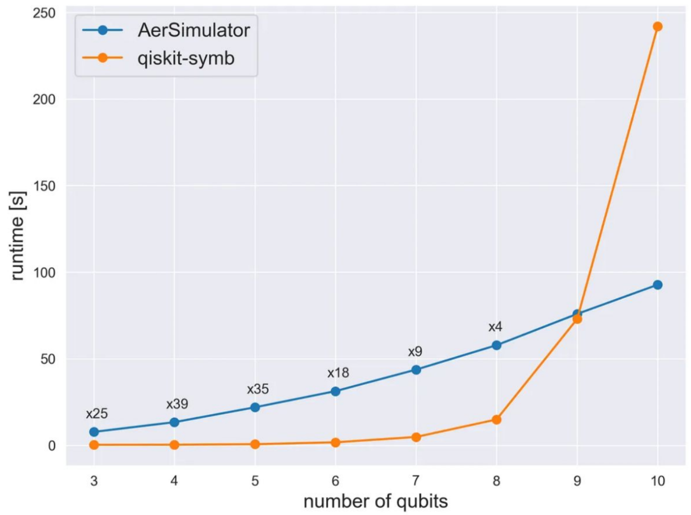


Problem graph topology



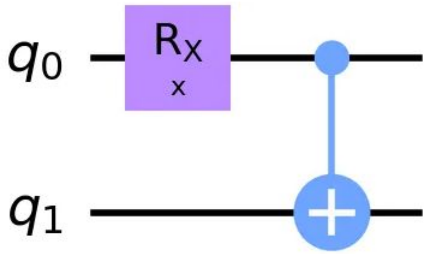
Embedding on QPU Pegasus graph topology

Off topic: “qiskit-symb”



Open-source Python package for symbolic evaluation of parametric quantum states and operators in Qiskit

- **Core functionality**: symbolic representation (state vectors, density matrices, unitary operators) of Parameterized Quantum Circuits (PQCs) using *Sympy*
- **Advanced features**: PQC objects conversion into Python functions, simplifying simulations for Quantum ML algorithms



$$\begin{bmatrix} \cos\left(\frac{x}{2}\right) & -i\sin\left(\frac{x}{2}\right) & 0 & 0 \\ 0 & 0 & -i\sin\left(\frac{x}{2}\right) & \cos\left(\frac{x}{2}\right) \\ 0 & 0 & \cos\left(\frac{x}{2}\right) & -i\sin\left(\frac{x}{2}\right) \\ -i\sin\left(\frac{x}{2}\right) & \cos\left(\frac{x}{2}\right) & 0 & 0 \end{bmatrix}$$

Conclusion

- New histogram unfolding approach based on **QUBO formulation** and **Quantum Annealing**
- **QUnfold** software ready to be tested on more HEP data analysis use-cases

Next steps:

- Further optimizations in the model definition (e.g. QUBO matrix preconditioning)
- Further studies to implement a “custom” embedding algorithm (e.g. taking into account the prior knowledge about the blocks structure of the QUBO matrix)

Thanks to CINECA for providing D-Wave resources to run quantum and hybrid solvers!

bitly

https://github.com/Quantum4HEP/QUnfold

Thanks for the attention!