Computational tools for the Future Colliders

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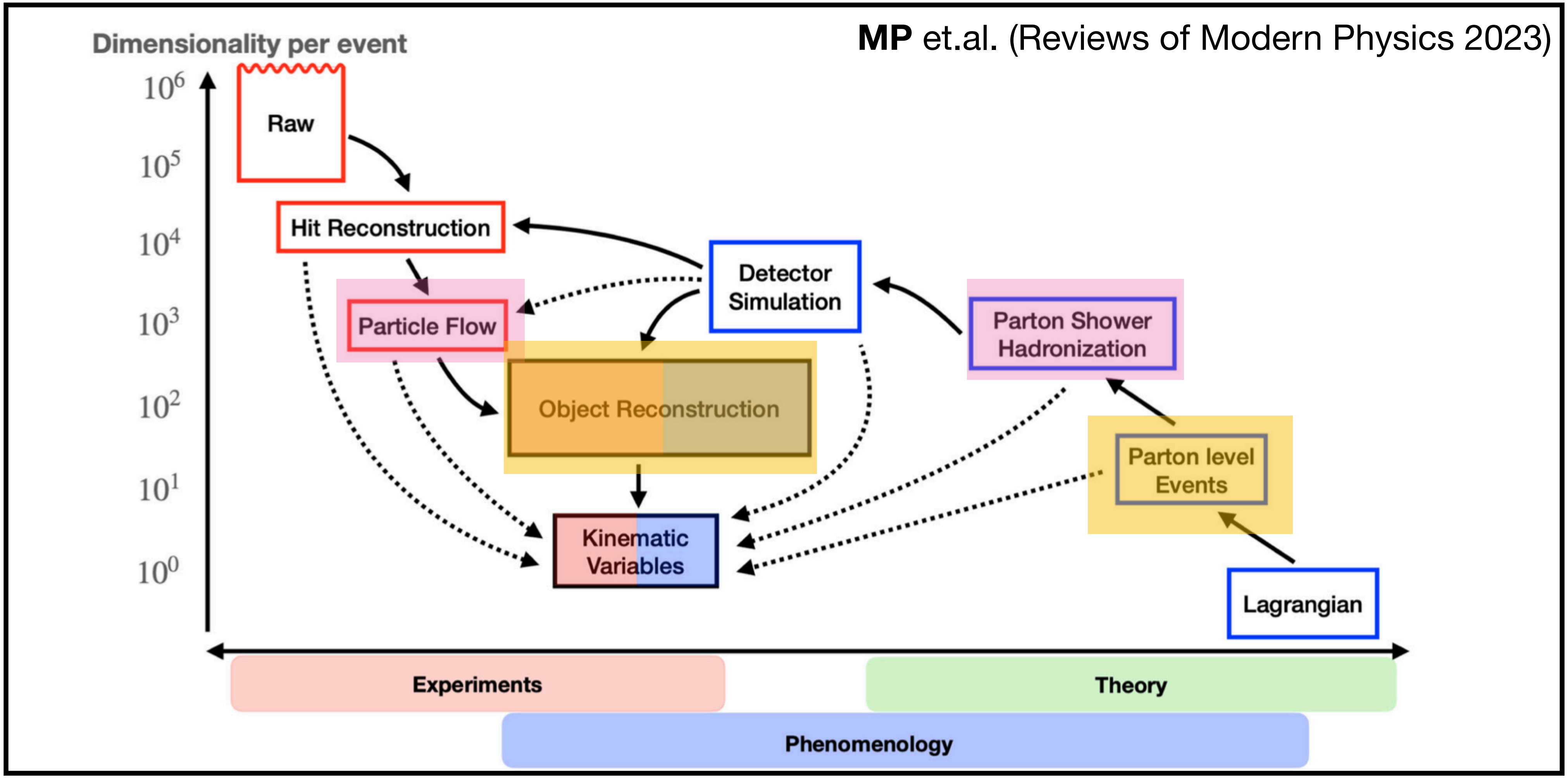
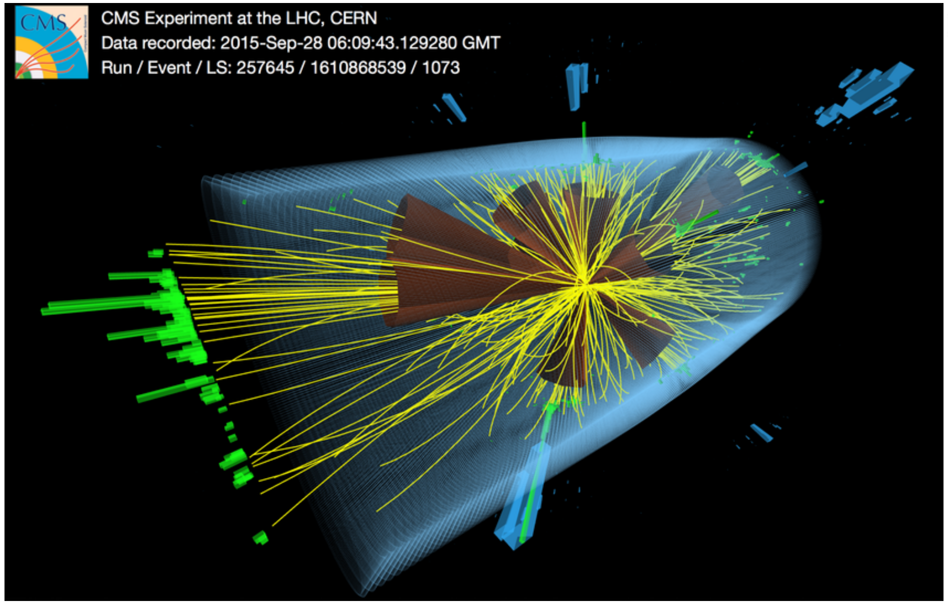
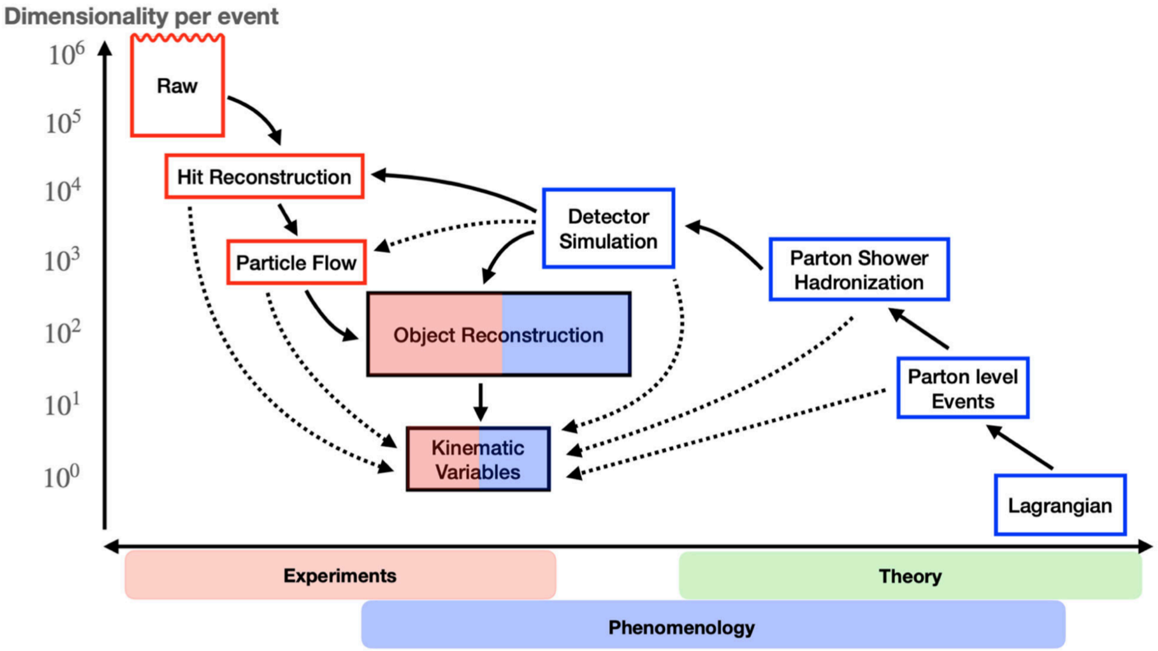
Understanding Physics using Colliders

- Recent advancements in Machine Learning (**ML**) allow us to fully exploit **all available information**, including raw-level data such as detector responses.



High multiplicity in High Energy collisions



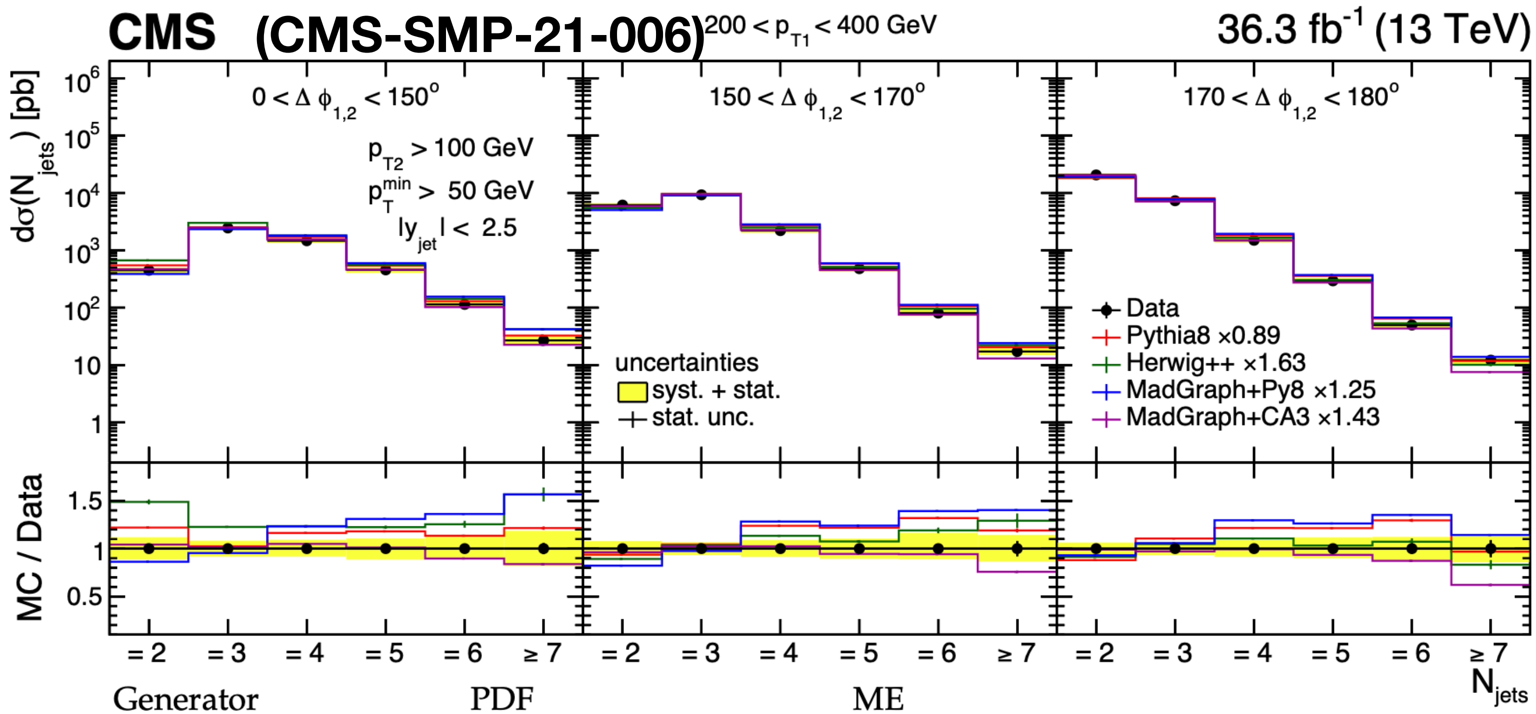


- Precise expectations from a simulation is required
  (1) Monte Carlo integration using ML

- Data-driven approaches without theoretical bias to fully exploit all possibilities.
  (2) Event reconstruction using Quantum Algorithm

Importance of Precision

- For Machine Learning which requires "**training**", **the big amount of well-understood data is necessary.**



Generator	PDF	ME
PYTHIA8 [23]	NNPDF 2.3 (LO) [25]	LO $2 \to 2$
MADGRAPH+PY8 [4]	NNPDF 2.3 (LO) [25]	LO $2 \to 2,3,4$
MADGRAPH+CA3 [4]	PB-TMD set 2 (NLO) [1]	LO $2 \to 2,3,4$
HERWIG++ [26]	CTEQ6L1 (LO) [27]	LO $2 \to 2$

- At large jet multiplicities, all generators tend to deviate from the data, indicating that our current simulations still lack sufficient precision in this complex region

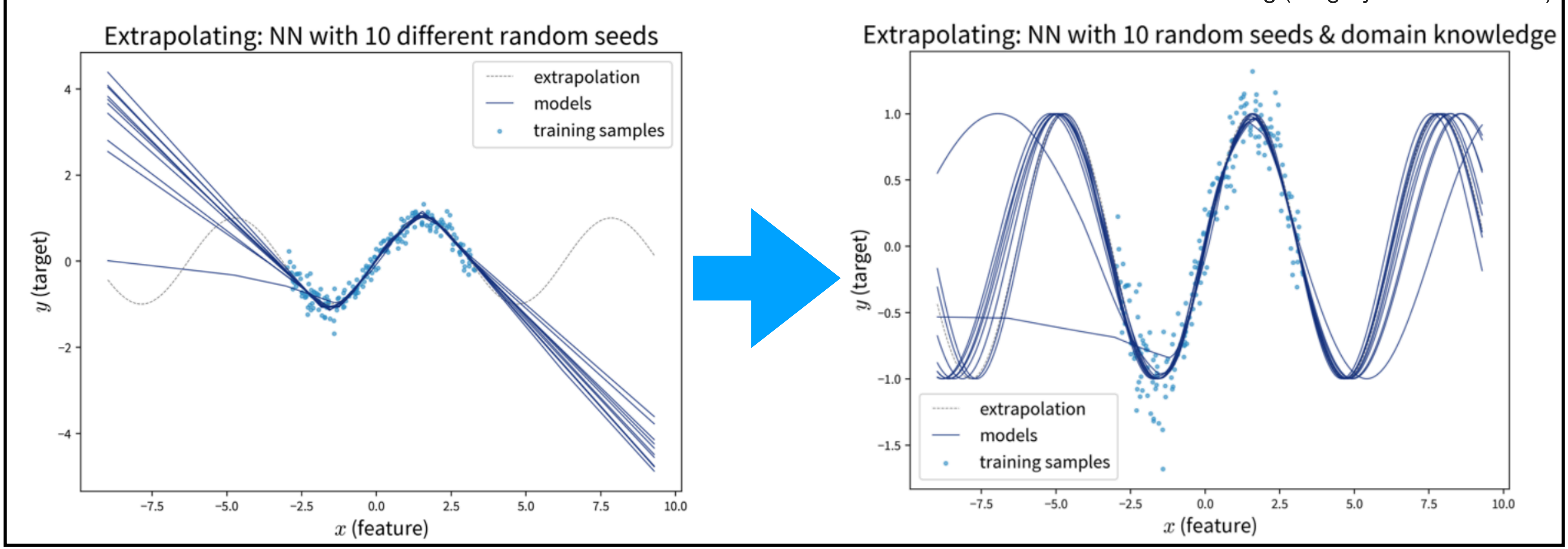
Importance of Theory

- We need **HUGE "training data"** to feed the **"data hungry" Neural Net**.

- One can dream of "data-driven" machine learning.

  - We cannot guarantee the estimation out of Controlled samples.
    : **NO magic can do "Exploration".**
    : Domain knowledge is strongly required.

A Practitioner's Guide to Machine Learning (Blog by Franziska Horn)



(1) Monte Carlo Integration

- $$\sigma = \frac{1}{2s} \int \prod_{i=1}^{n} \frac{d^3 p_i}{(2\pi)^3 2E_i} \delta\left(k_1 + k_2 - \sum_{i=1}^{n} p_i \right) |M_{fi}|^2 \theta_{\text{cut}}(p1, \cdots, p_n)$$

- For an observable $O(p_1, \cdots, p_n)$, we need to calculate the differential distribution of

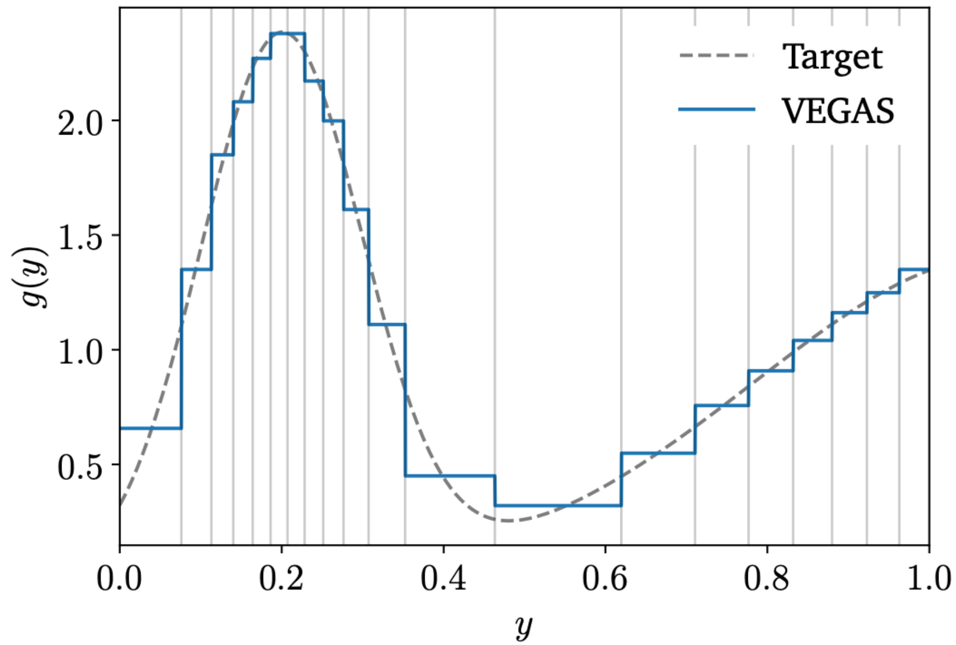
$$\frac{d\sigma}{dO} = \frac{1}{2s} \int \prod_{i=1}^{n} \frac{d^3 p_i}{(2\pi)^3 2E_i} \delta\left(k_1 + k_2 - \sum_{i=1}^{n} p_i \right) |M_{fi}|^2 \theta_{\text{cut}}(p1, \cdots, p_n) \delta(O - O(p1, \cdots, p_n))$$

- **Precise numerical Integration in high dimensional phase space that may contain nontrivial singularities**

Monte Carlo Integration: Domain vs Value Partitioning

- **Riemann-style: VEGAS**

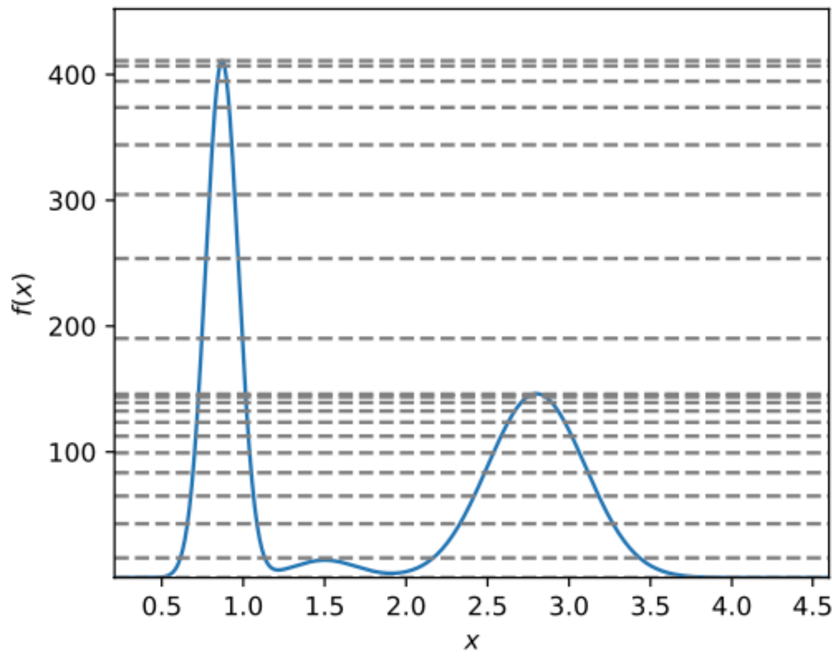
from MadNIS (Theo Heimel et.al. arXiv:2311.01548)



- **Stratified Sampling**: Divide domain **into sub-domains.**
  For example, if we divide the domain into N divisions, $\sigma \propto \frac{1}{N}$ instead of $\sigma \propto \frac{1}{\sqrt{N}}$

- **VEGAS**: Adaptive importance sampling
  - divides the domain along coordinates.

- **Lebesgue**-style

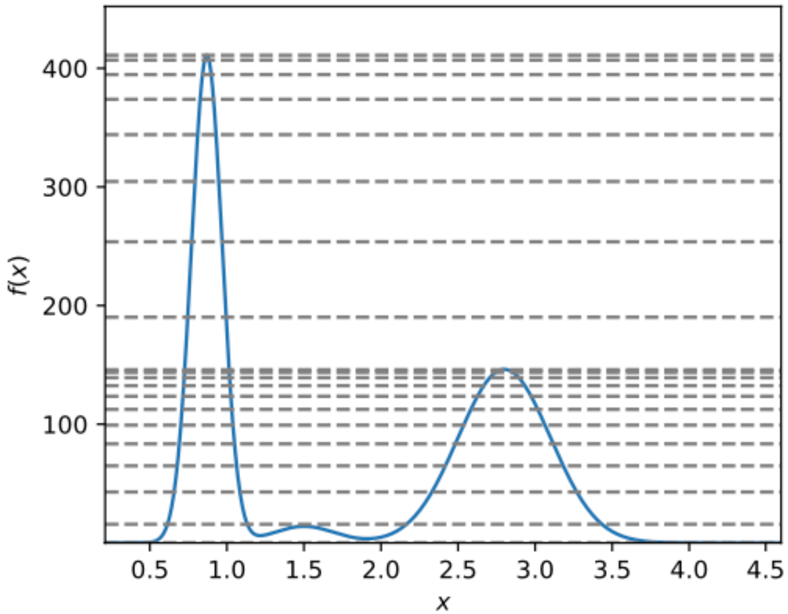


- **Alternative approach**: Integrate by function values instead of coordinates.

- **Lebesgue integration**: group by $f(x)$ rather than x.
  - More efficient when the integrand has a **singular or sharply peaked** structure.

  - A classical example: $f(x) = \begin{cases} 1 & \text{if } x \in P \\ 0 & \text{if } x \in Q \end{cases}$

Our approach: Lebesgue



- **Divide the space of integrand (classes)**

$$\Phi_j = \{\vec{x} \,|\, l_j < f(\vec{x}) \leq l_{j+1}\}$$

- The integral : $I_\Phi\left[f(\vec{x})\right] = \int_\Phi \mathrm{d}^d x\, f(\vec{x}) = \sum_{j=1}^{n} \int_{\Phi_j} \mathrm{d}^d x\, f(\vec{x}) = \sum_{j=1}^{n} V_{\Phi_j} \langle f \rangle_{\Phi_j}$

V_{Φ_j} : Volume of Φ_j .

- We recast the **problem of integration** → **classification problem**

MP. et al, Computational Physics Communication 319 (2026) 109907

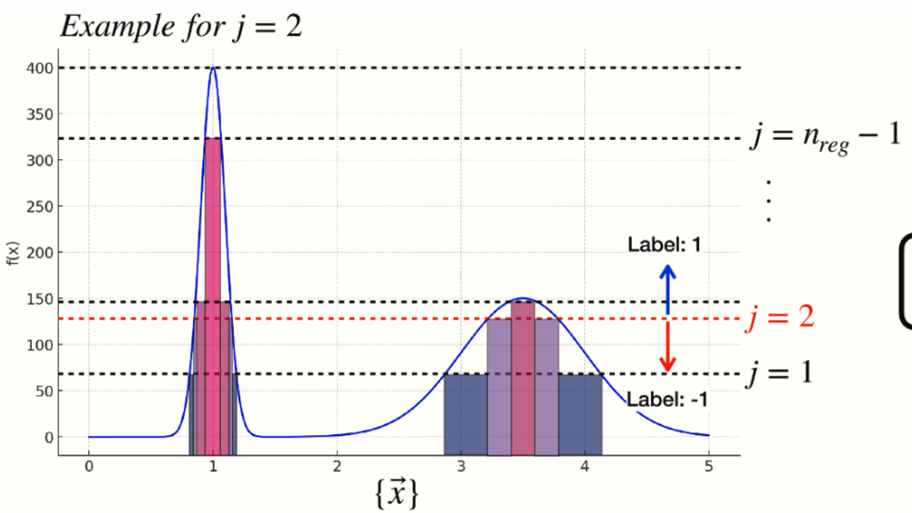
Monte Carlo with ML

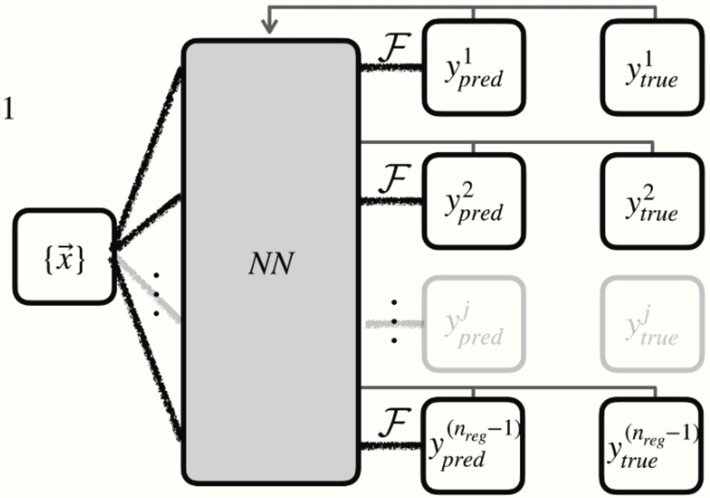
$$I_\Phi[f(x)] = \int_\Phi \mathrm{d}^d x\, f(x) = \sum_{j=1}^{n} \int_{\Phi_j} \mathrm{d}^d x\, f(x) = \sum_{j=1}^{n} V_{\Phi_j} \langle f \rangle_{\Phi_j}$$

- here, if we can "correctly" decide $x \in \Phi_j$, we can calculate

$$V_{\Phi_j} \simeq \frac{N_j}{N_{\text{total}}} V_{\text{total}}\,, \quad \langle f \rangle_{\Phi_j} \simeq \frac{1}{N_j} \sum_{i=1}^{N_j} f(x_i)$$ with large sample N_{total}

- **It is crucial to estimate V_{Φ_i}.** With iterative ML algorithm,





$[ex]: \ \{\ \vec{x}_i\,,\ y_i = (\ y^1, y^2, \cdots, y^{(n_{reg}-1)}\ ) = (\ -1,\ -1,\ 1,\ \cdots,\ 1\ )\ \}$

example

- $\infty - \infty = \text{finite}$: We are testing "fine-tuning" function of

with gaussians, $g(x;\mu,\sigma) = \dfrac{1}{\sigma\sqrt{2\pi}} \exp\left[\dfrac{(x-\mu)^2}{2\sigma^2}\right]$ and $G(\vec{x};\vec{\mu},\sigma) = \prod_{j=1}^{7} g(x_j;\mu_j,\sigma)$

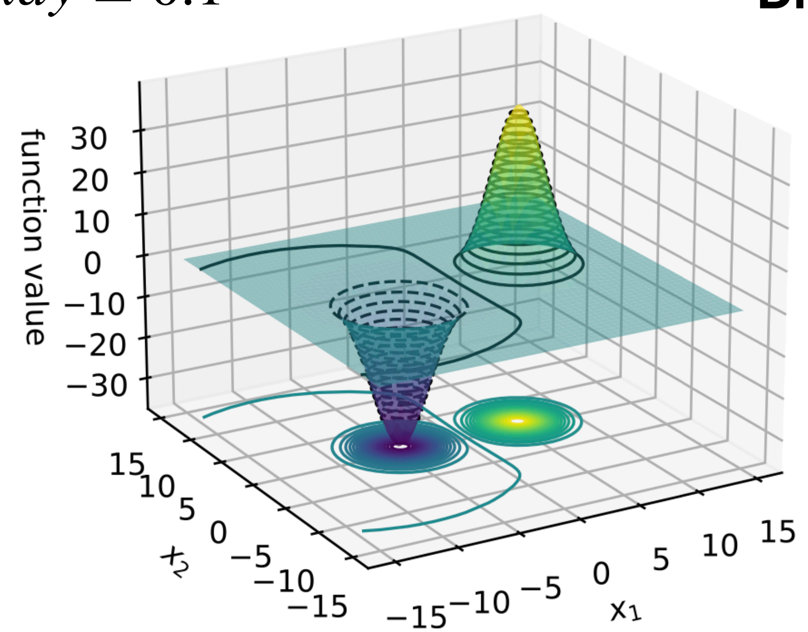
Two large peaks which are canceled each other, and one small contribution from broad distribution

$$f_{7D}(\vec{x}) = 100 \times \left[G(\vec{x};\vec{\mu}_+,\sigma_+) - G(\vec{x};\vec{\mu}_-,\sigma_-)\right] + 0.1 \times G(\vec{x};\vec{0},\sigma_0)$$

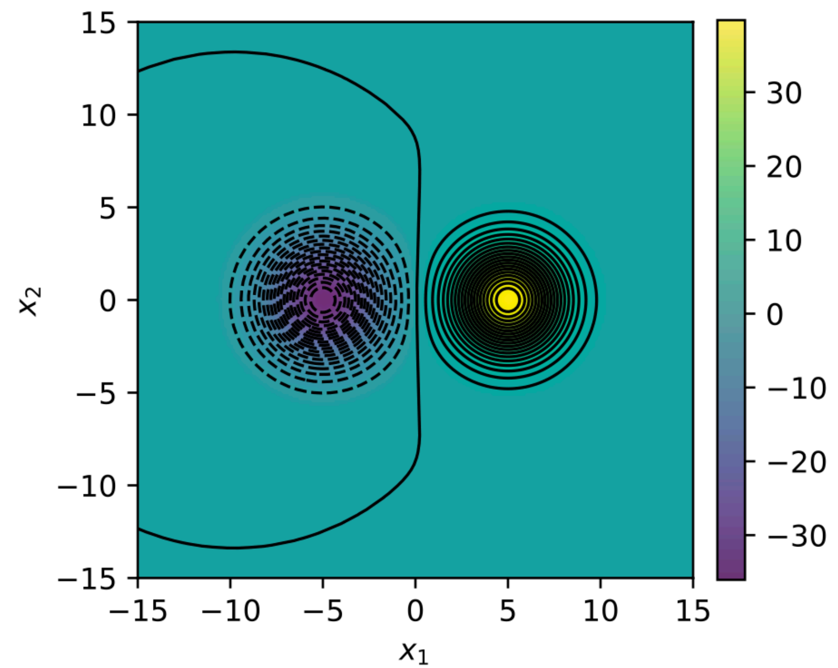
$$\sigma_+ = \sigma_- = 0.3$$

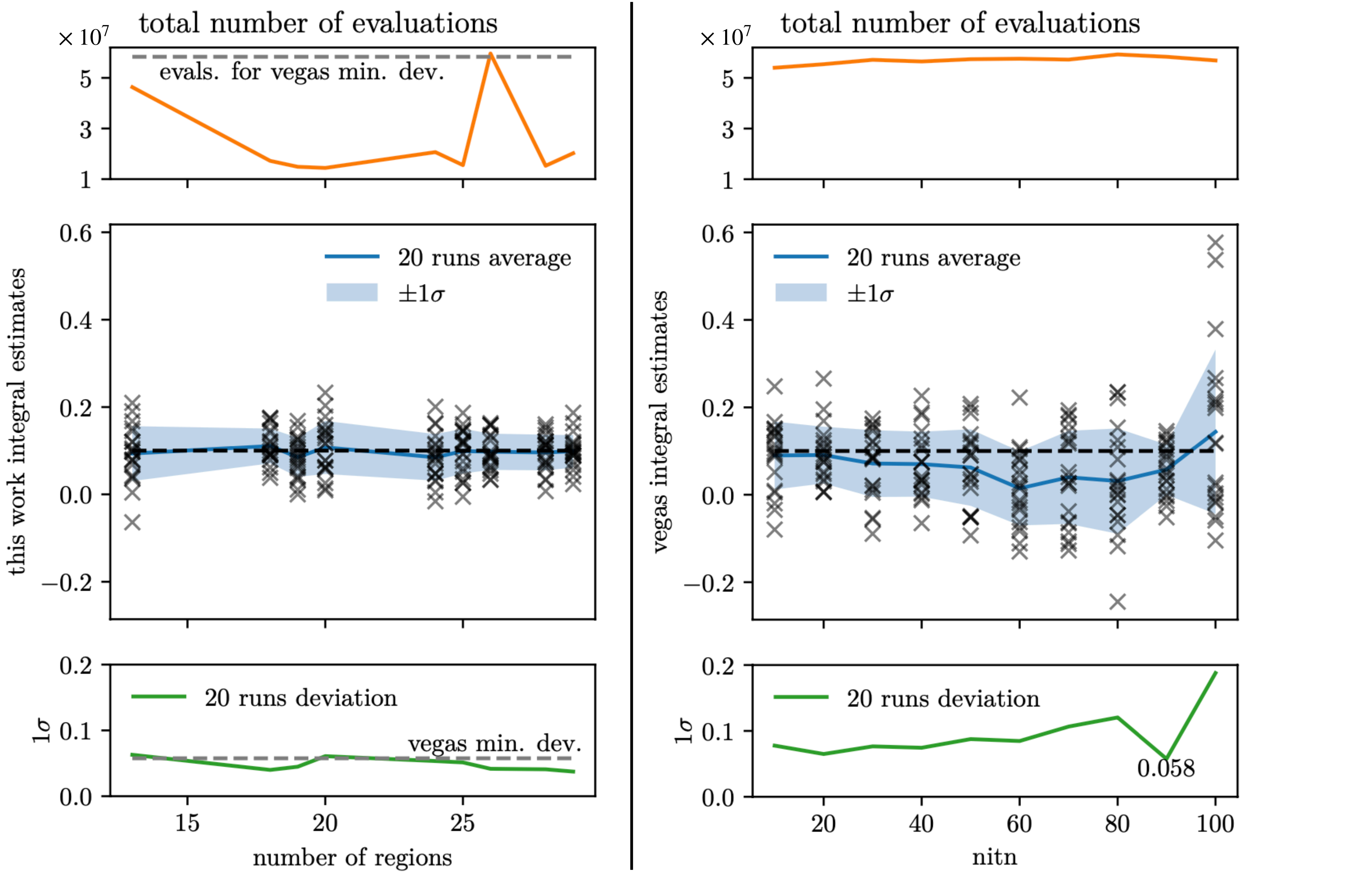
$$\sigma_0 = 1.0$$

$$\int f(\vec{x})dxdy \simeq 0.1$$



Divisions for equal "absolute" contributions

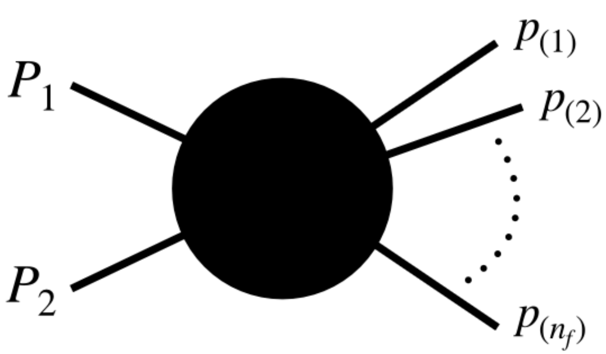


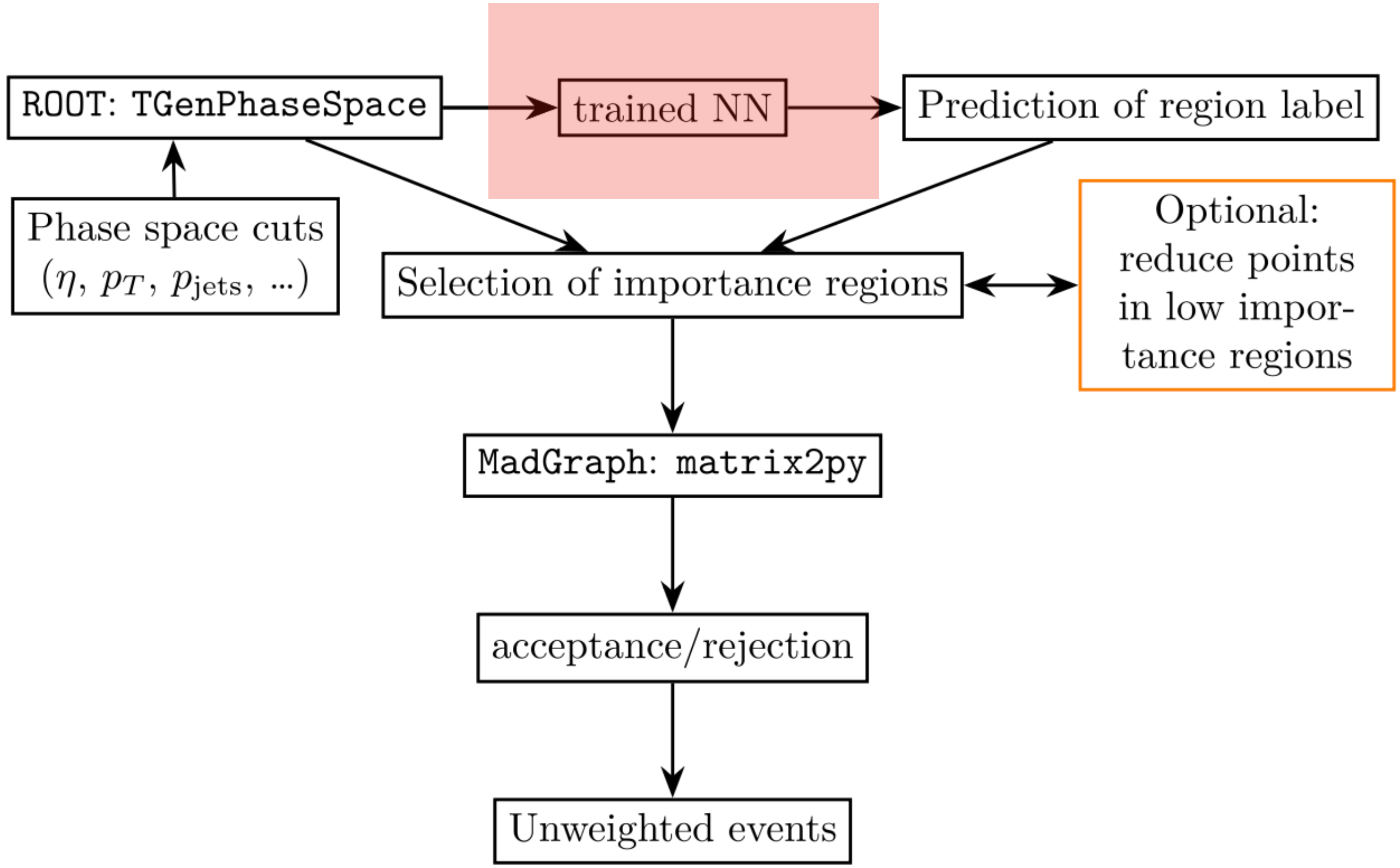


LeStrat-Net **VEGAS**

- LeStrat-Net achieves comparable precision with significantly fewer function evaluations and exhibits improved statistical stability compared to VEGAS.

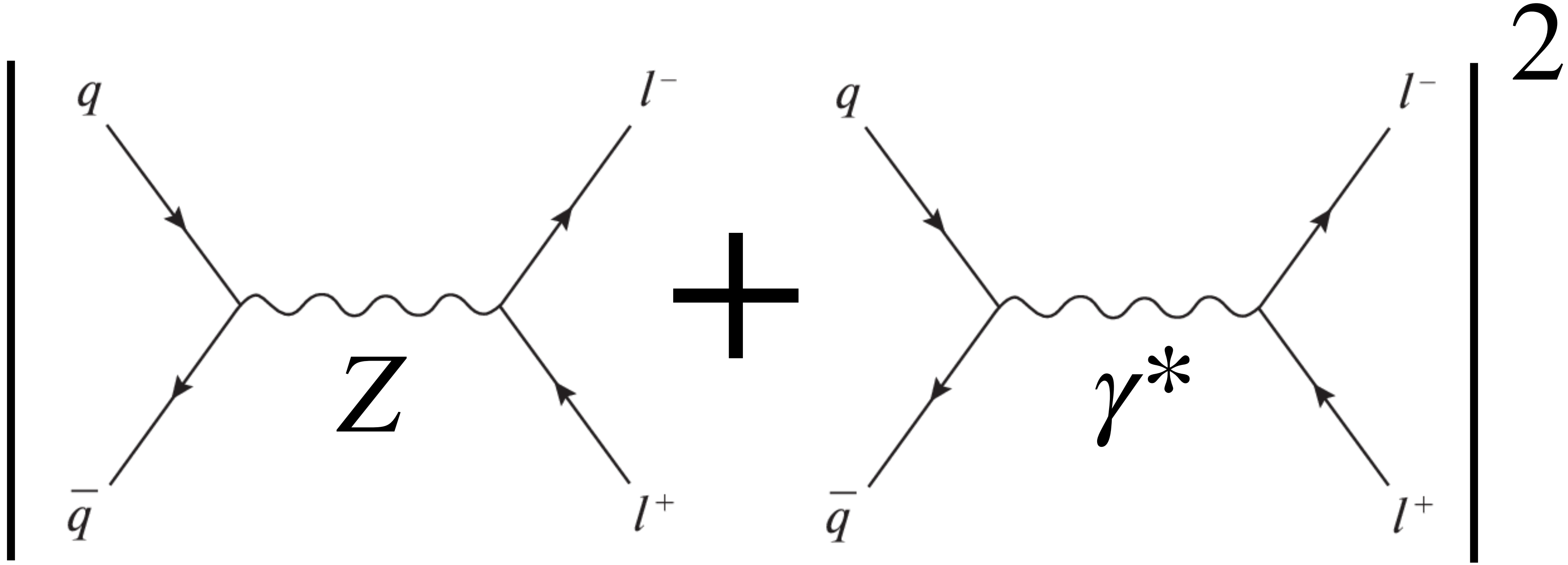
Generating MC samples with NN

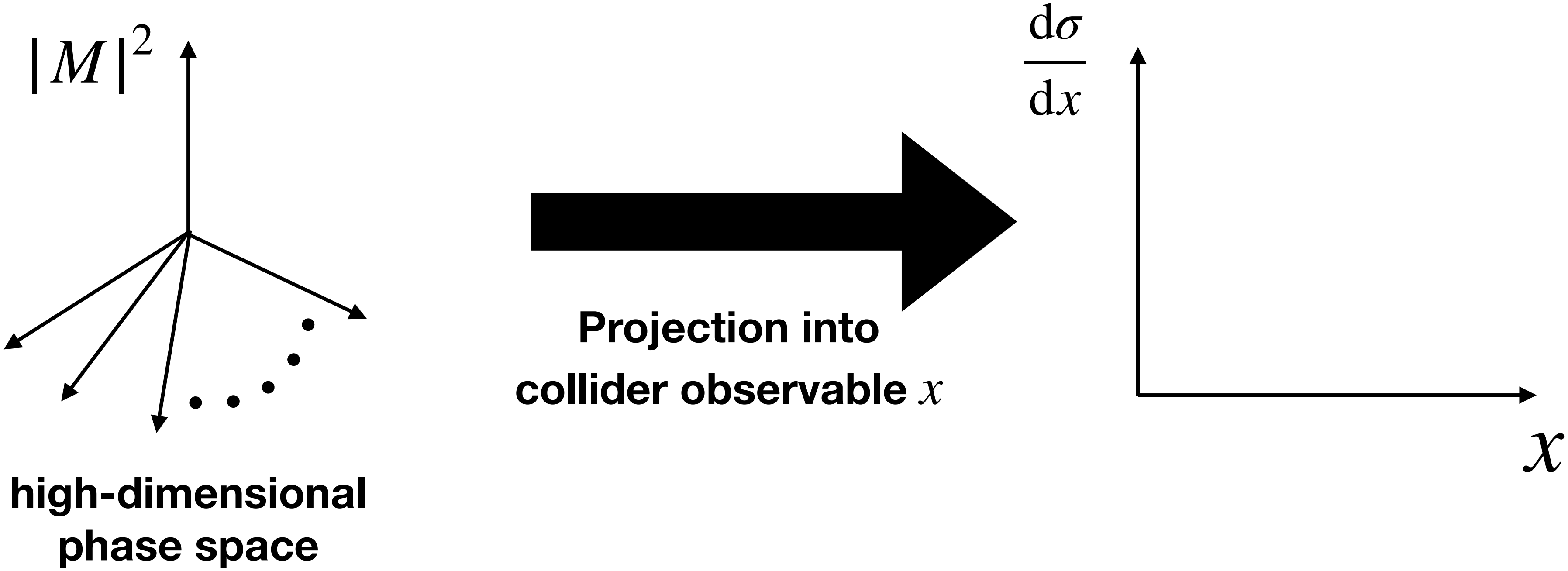




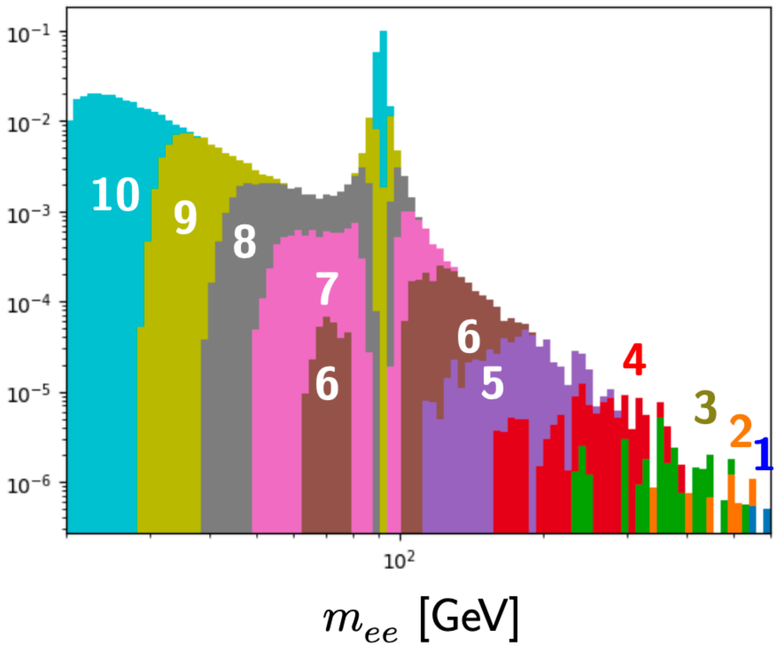
- Weight of a phase space point p is $\omega(p) = \Pi_j f(x_j, \mu) \, |M_{n_i \to n_f}(p)|^2 \, |J(p)|$
- Apply acceptance/rejection to unweight the events.

$2 \to 2$ process with interference



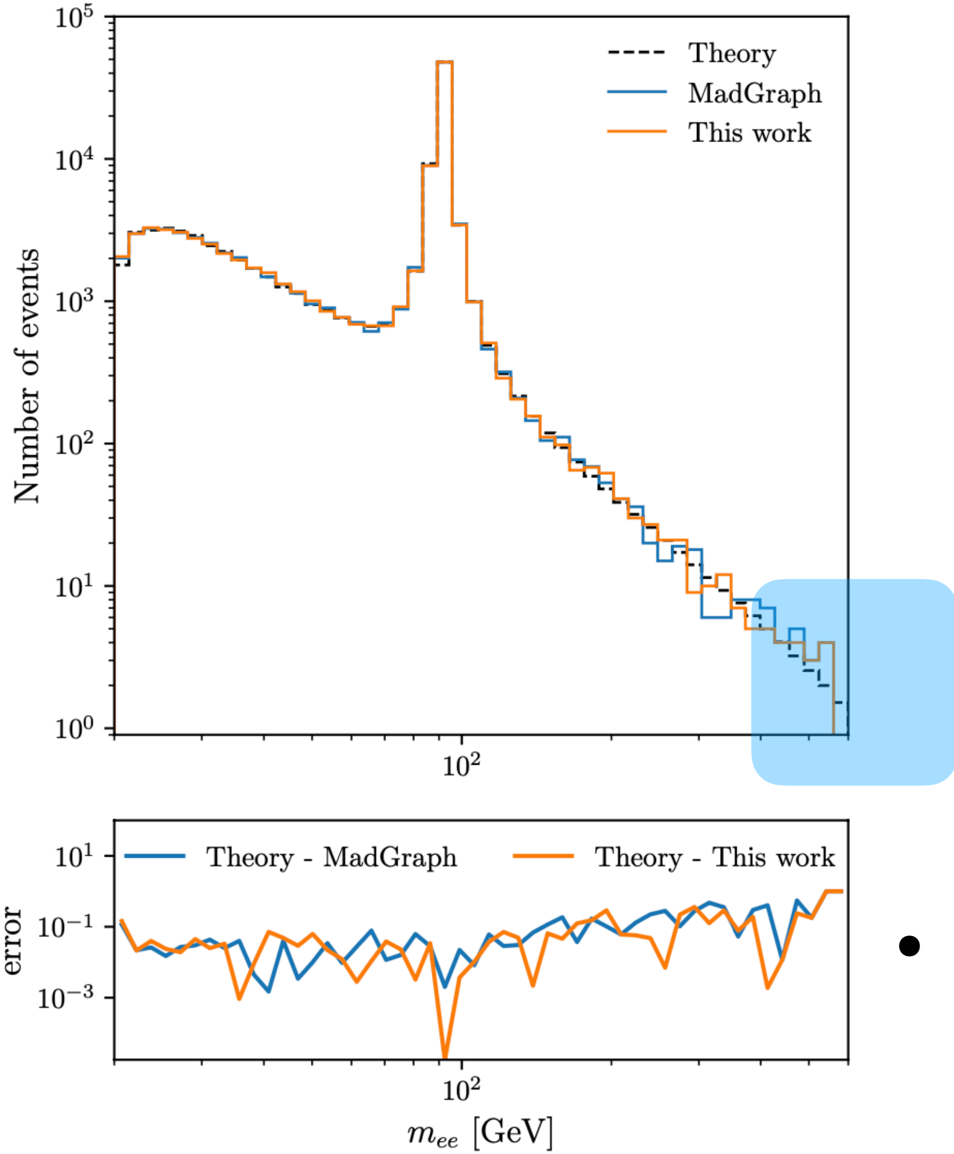


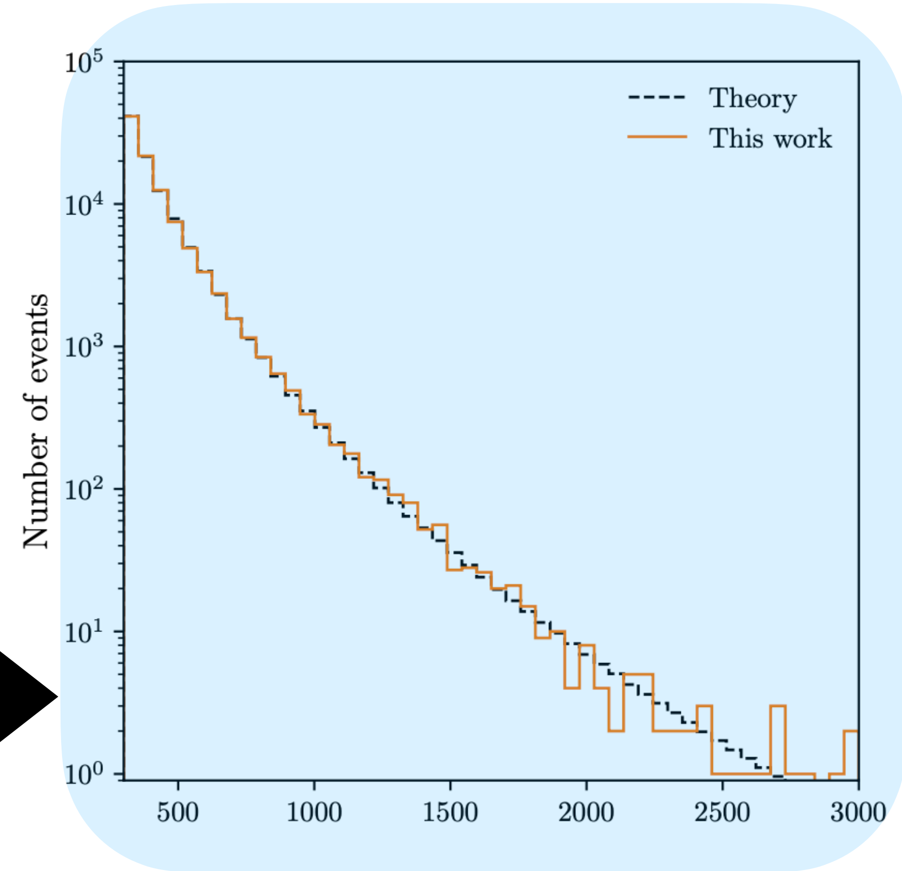
e^-e^+ invariant mass projection



- Sample each region until enough events are accumulated. **NN can tell which regions points belong to**.
- Select points using correct result.

Sample as long as we want





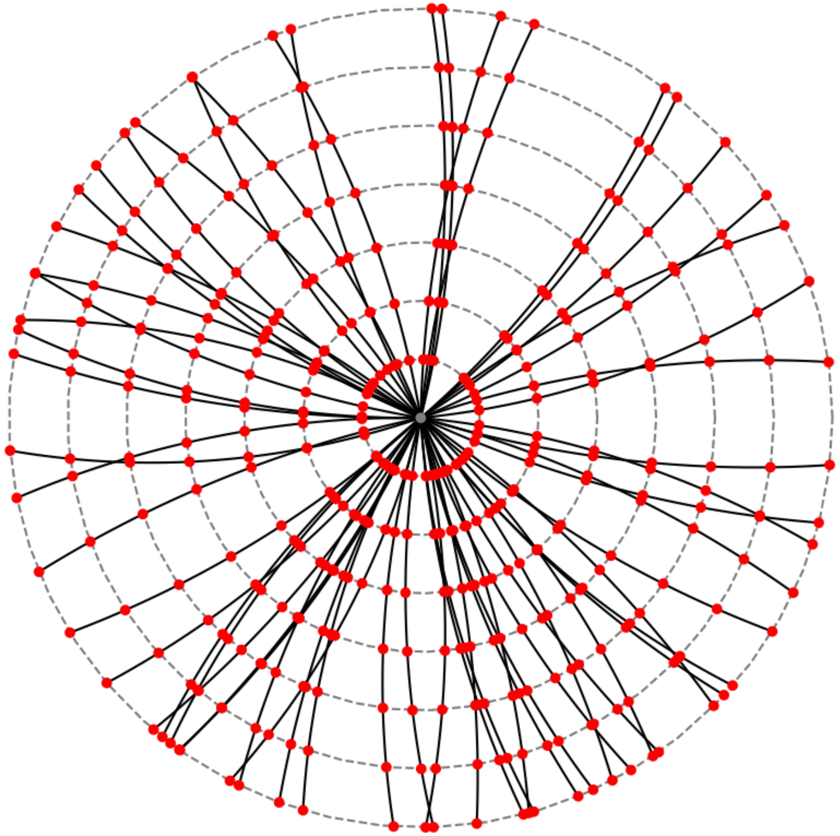
- As we divide phase-space region according to importance, we can **zoom into "rare events"**

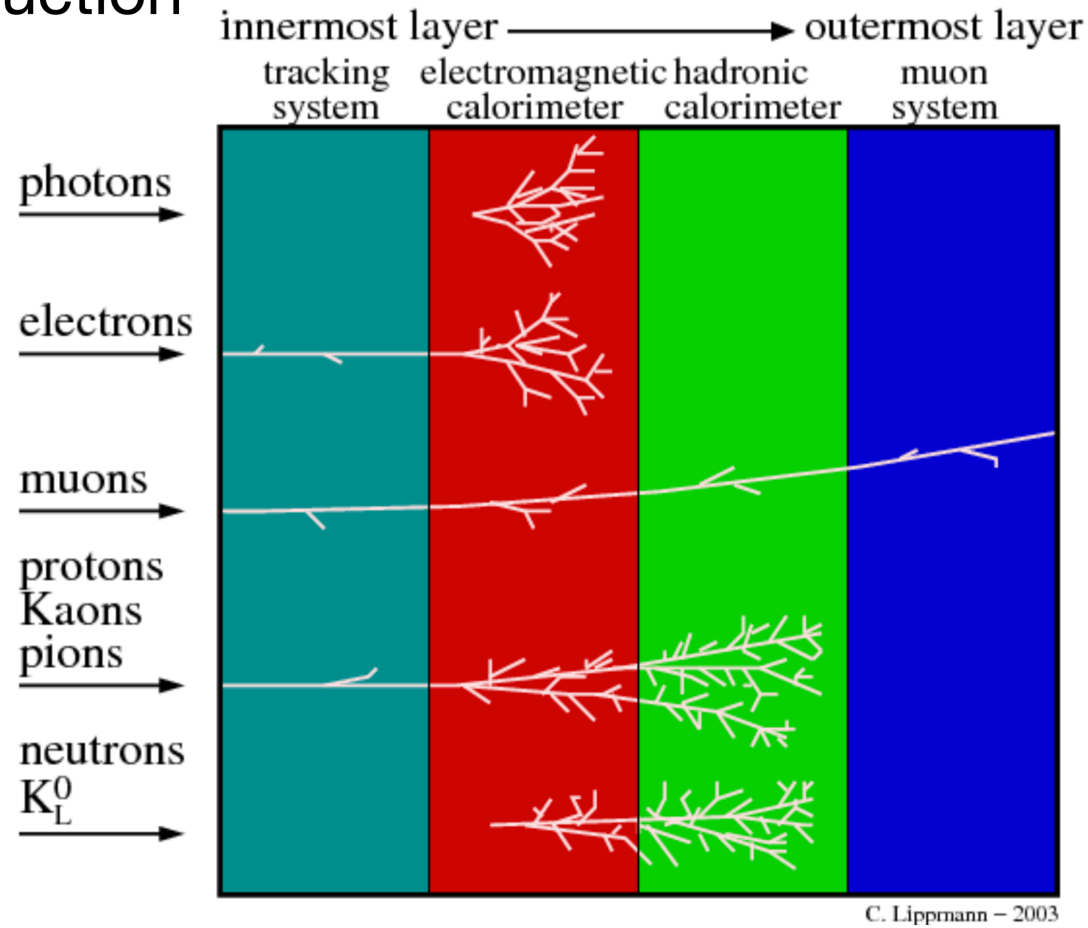
(2) **Event reconstruction on an event-by-event basis using Quantum Computations**

- to identify a physics behind complicated data

Combinatorial problem

- At the level of particle reconstruction

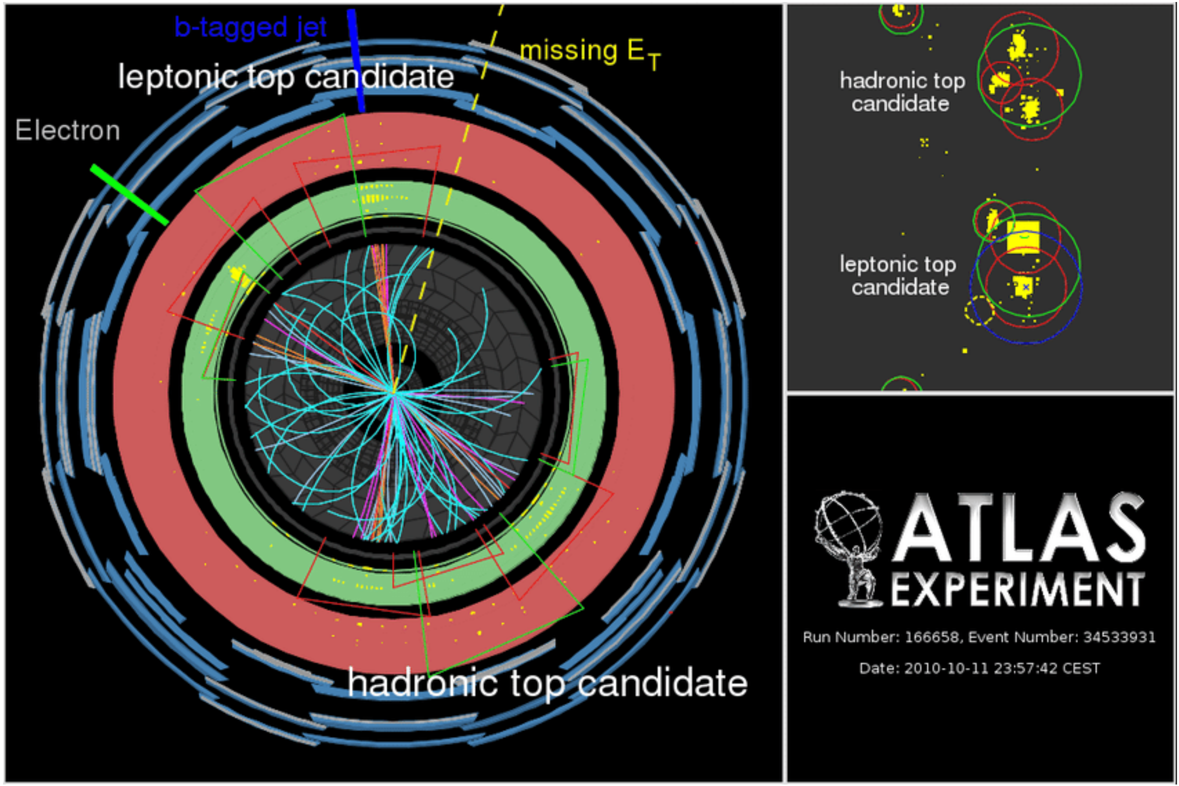


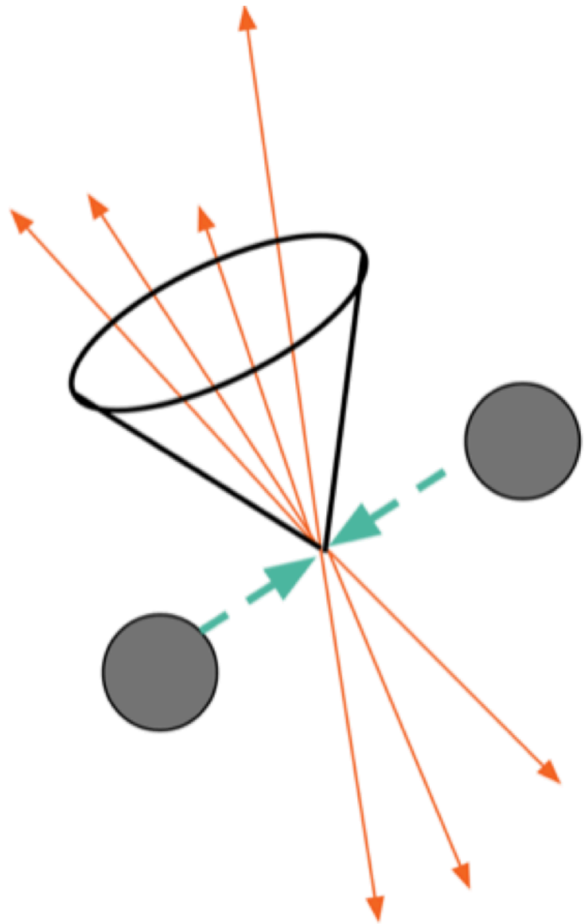


- Utilizing sub-detectors,
  Muons, electrons/photons, π , K, p ...

Combinatorial problem

- At the level of object reconstruction

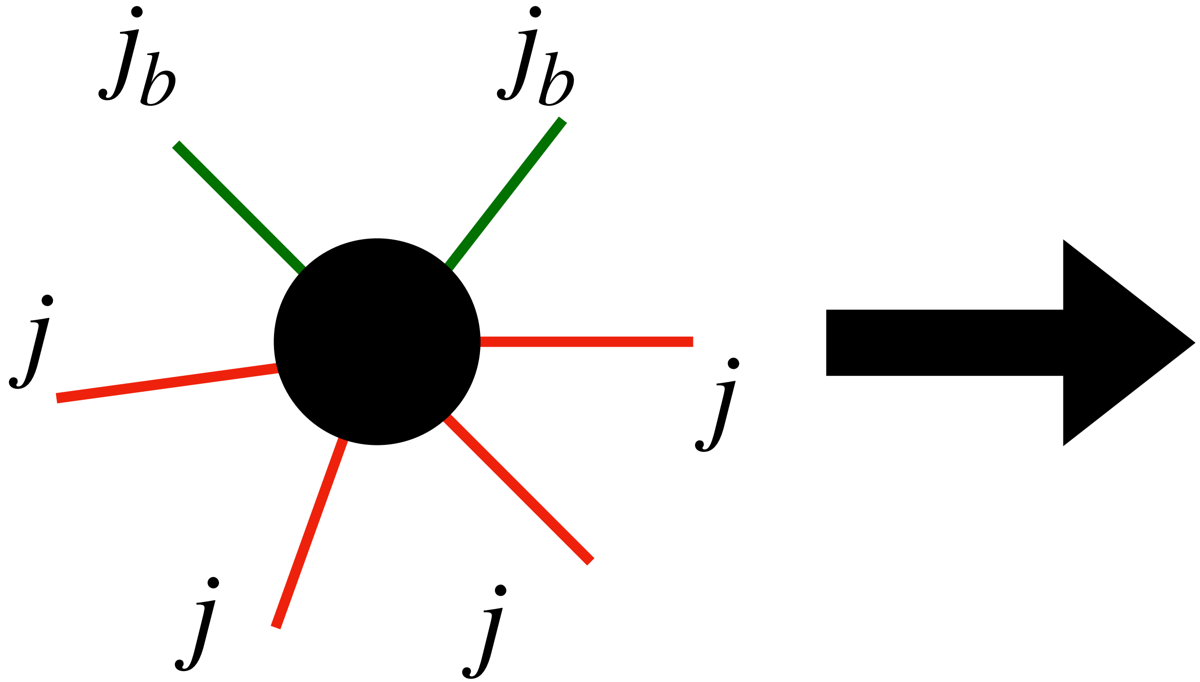


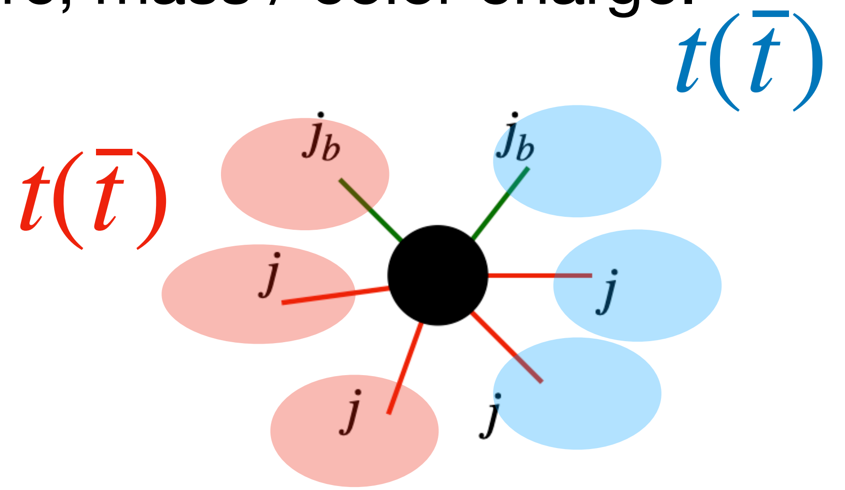


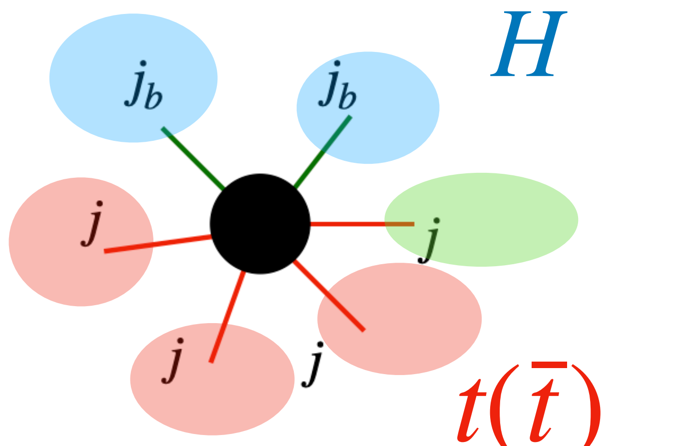
- Utilizing particle information,
  (1) isolated (good) leptons/photons,
  (2) jet objects
  (→ jet charge, particle ID can be used for jet properties)

Combinatorial problem

- At the level of "**mother particle**" reconstruction
- If **we know (assume)** the decay structure, mass / color charge.







- Guided by kinematic/QCD information,

For example, see arXiv:2311.116674
(Exploring the Synergy of Kinematics and Dynamics for Collider Physics)

But, we **need (should) not assume** anything from High Energy Collider.

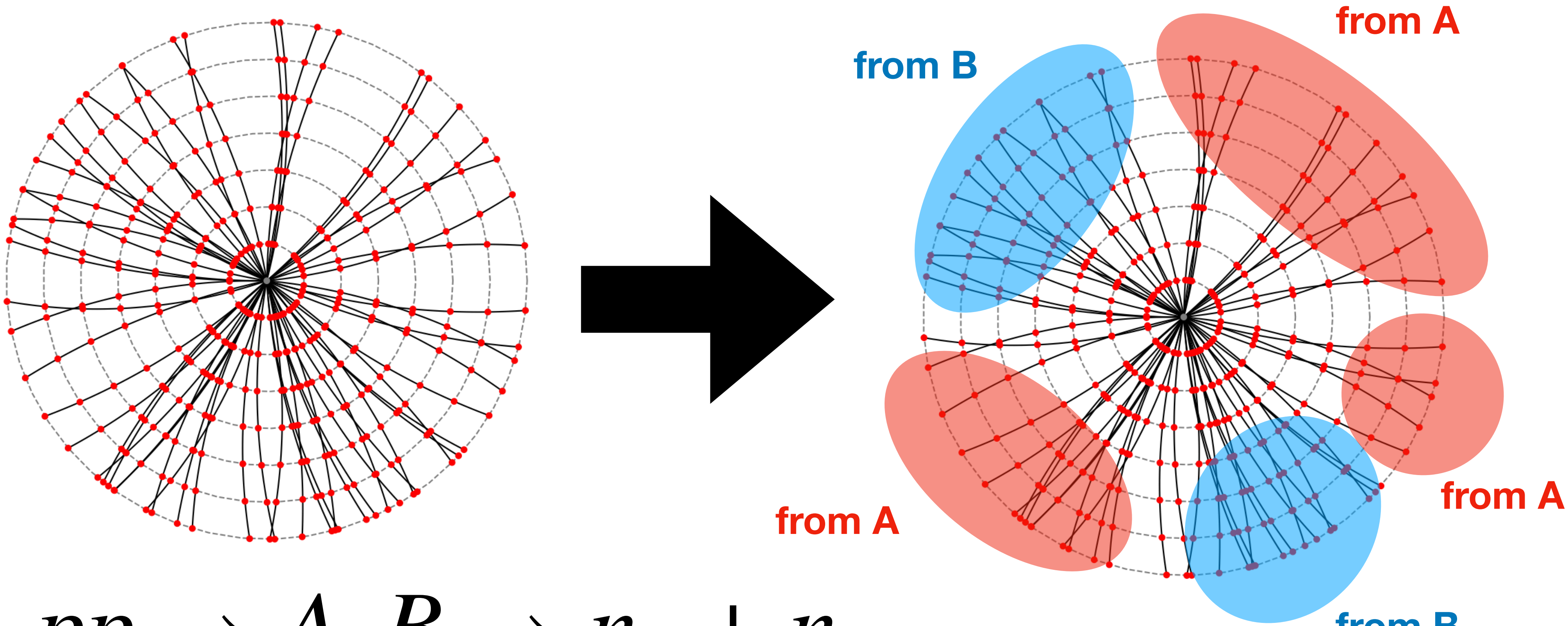
- Of course, nobody stops you to check what you want to see.

Event Reconstruction without prejudices

- As the **Colliders** (including the current LHC) **have killed various favorable new physics models**, providing us a precise details of the Standard Model (SM).

- If we see something beyond the expectation from the SM,
  - We need to reconstruct the "event-topology", to identify a physics behind the signal.
  - **To minimize assumptions, we start from unsupervised (or weakly supervised) methods**

Combinatorial problem



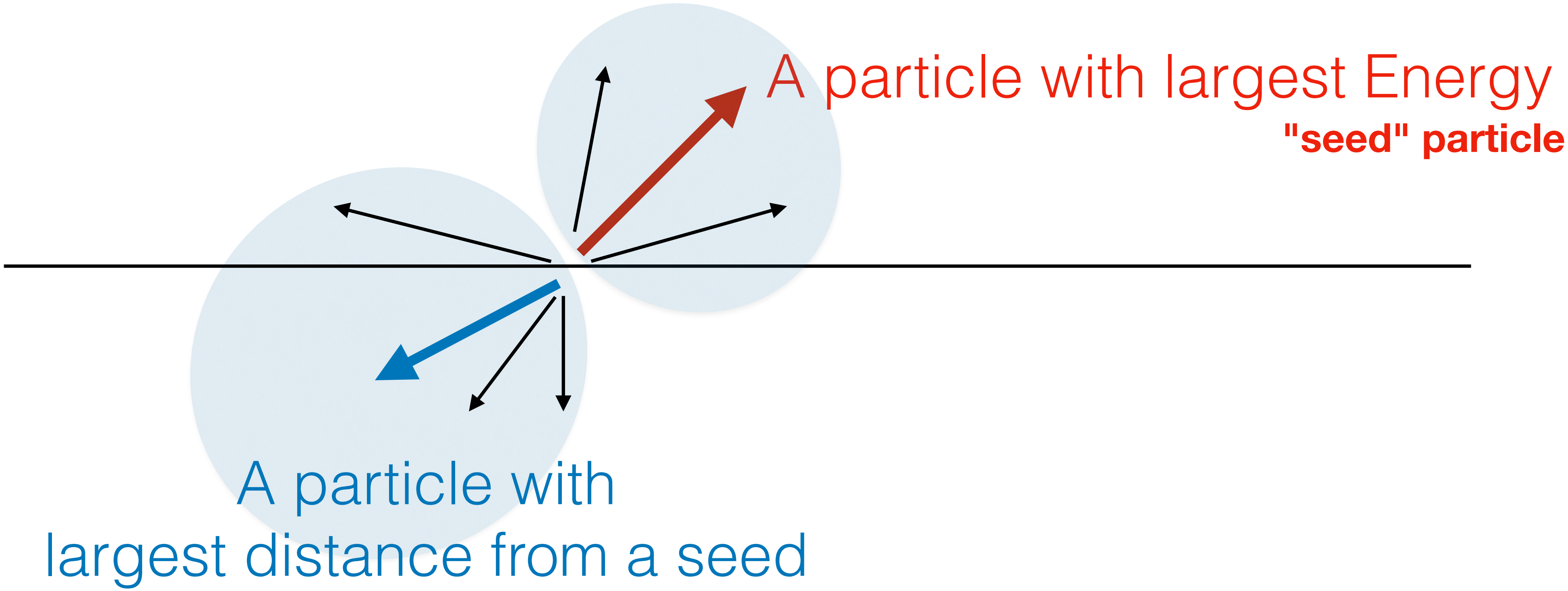
$$pp \rightarrow A, B \rightarrow n_A + n_B$$

(number of particles from the decay of A or B)

- It would be natural to start with two particles
  - Particle–antiparticle creation ensured by **CPT** and **gauge symmetries**
  - Z_2 symmetry to ensure the **stability** of (possible) dark matter

A Classic algorithm

- **Hemisphere method**: a seed-based method (iterative and converge)
  - Take two particles and clustering other particles based on these two.



With a proper metric d, one decides which hemisphere a particle belongs to.

Combinatorial problems at the LHC

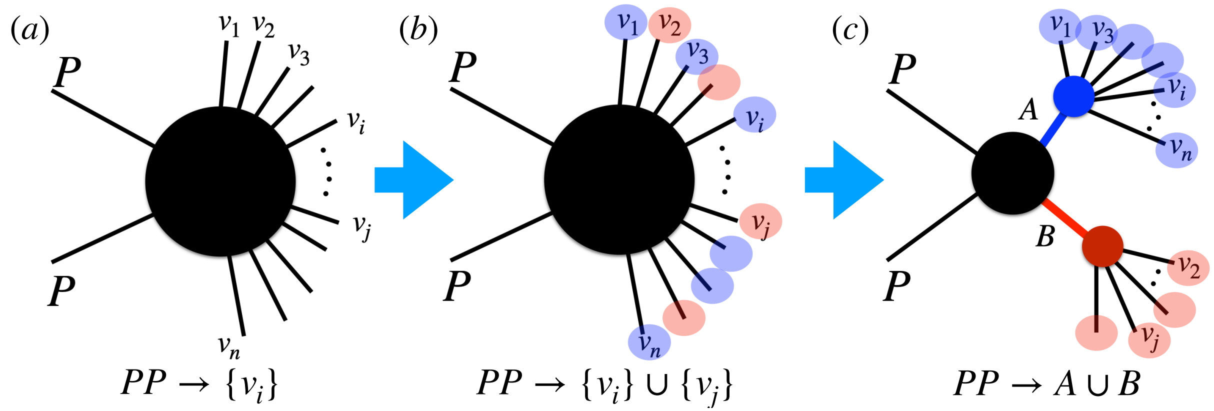


FIG. 1. (a) n-observed particles (b) Dividing n particles into two groups for $2 \to 2$ process (c) Identified event-topology with A and B.

- Assuming $2 \to 2$ production with subsequent decays, identification of an event-topology becomes a binary classification, with 2^{n-1} possibilities.
- Combinatorial problem: What would be an efficient way of assigning all observed particles in two decay chains?

p_i is the momentum of constituent of A if $x_i = 1$ $\qquad P_1 = \sum_i p_i \, x_i$

p_i is the momentum of constituent of B if $x_i = 0$ $\qquad P_2 = \sum_i p_i \, (1 - x_i)$

Minimize the mass difference: $H = \left(P_1^2 - P_2^2\right)^2$ for all possible combinations of x_i

Hybrid quantum-classical approach for combinatorial problems at hadron colliders, 2410.22417

Leveraging Quantum Annealer to identify an Event-topology at High Energy Colliders, 2111.07806

Minimization using Ising model

- If we replace $x_i \to \frac{1+s_i}{2}$ with $s_i \in \{+1, -1\}$

$$H_P = \left(P_A^2 - P_B^2\right)^2 \to H_P + \lambda\left(P_A^2 + P_B^2\right)$$

$$= \sum_{ij} J_{ij} s_i s_j + \frac{\lambda}{2} \sum_{ij} P_{ij} s_i s_j \text{ with } P_{ij} = p_i \cdot p_j \text{ and } J_{ij} = \sum_{kl} P_{ik} P_{jl}$$

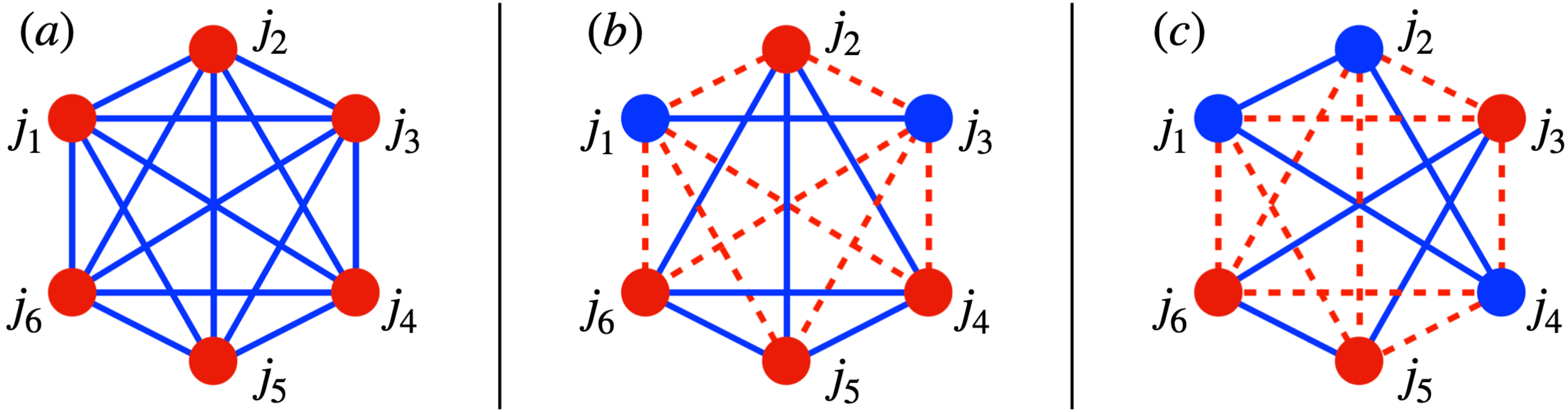
- We take $\lambda = \frac{\min(J_{ij})}{\max(P_{ij})}$

- QUBO : Quadratic Unconstrained Binary Optimization

  A generic QUBO problem: $H_{\text{QUBO}} \equiv \sum_{ij} J_{ij} s_i s_j + \sum_k h_k s_k$

- Turn into a combinatorial problem into a graph problem.

  For example, $pp \to AB \to j_1, j_2, \cdots, j_6$



(a)
- All jets are from **A**

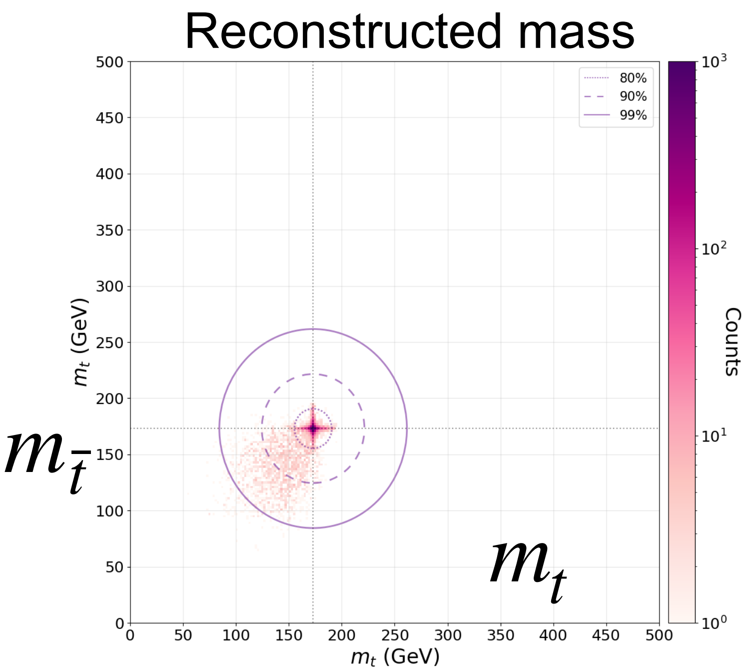
(b)
- $\{j_2, j_4, j_5, j_6\}$ from **A**
- $\{j_1, j_3\}$ from **B**

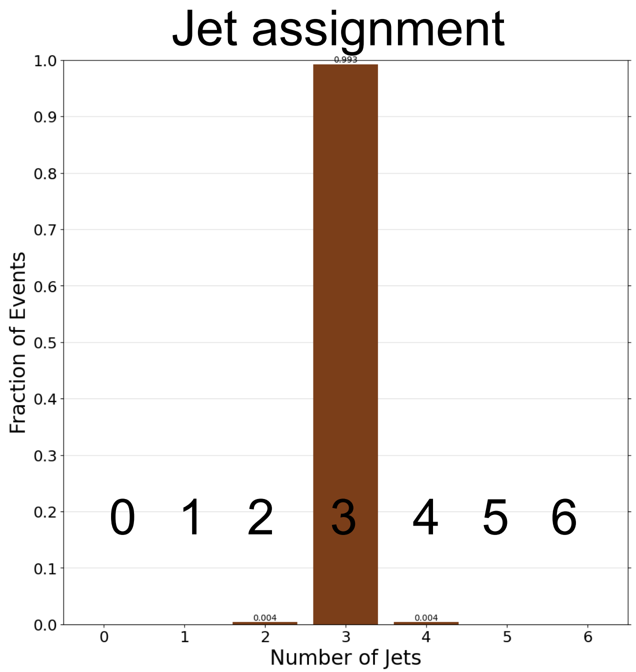
(c)
- $\{j_3, j_5, j_6\}$ from **A**
- $\{j_1, j_2, j_4\}$ from **B**

$$H_p = \sum_{ij} J_{ij} s_i s_j + \frac{\lambda}{2} \sum_{ij} P_{ij} s_i s_j$$

- **Edges connecting nodes from the same parent particle** ($s_i s_j = +1$) contribute **positively** to H_P and are shown as solid (blue) lines
- **Edges connecting nodes from different parent particles** ($s_i s_j = -1$) contribute **negatively** to H_P
- The task of finding the **correct combinatorics** is equivalent to identifying the graph configuration that **minimizes** H_P

Parton-level truth and hemisphere method



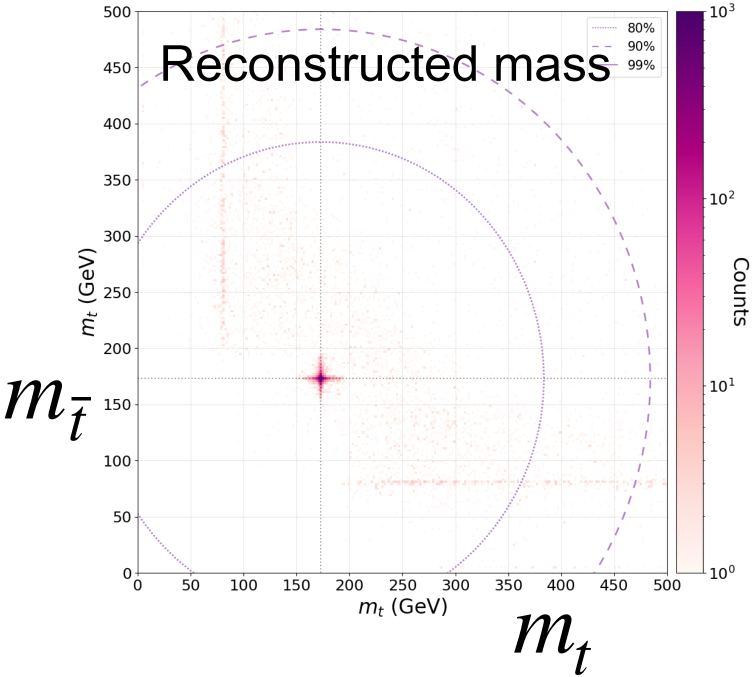


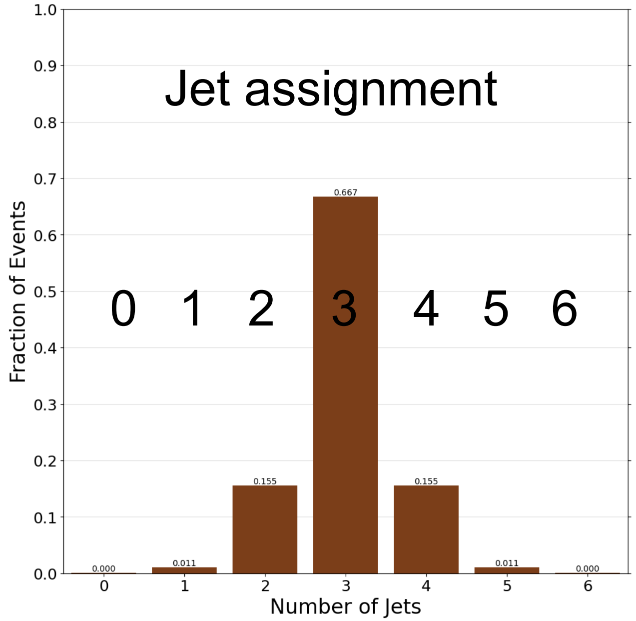
parton-level truth

79% overal efficiency

No mass information used.

Hybrid quantum-classical approach for combinatorial problems at hadron colliders: 2410.22417





Hemisphere method

50% overal efficiency

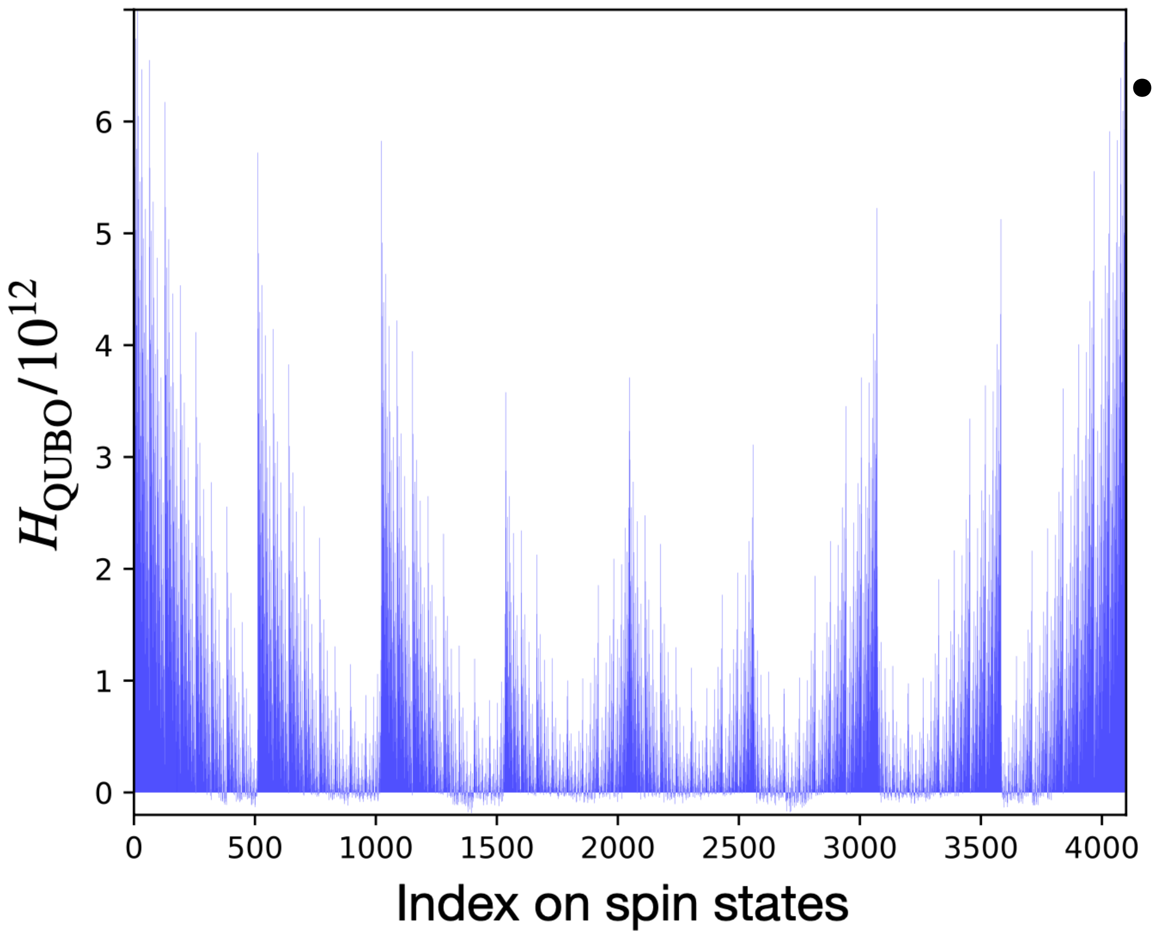
No mass information used.

Issue

Difficulty in finding the ground state of an Ising Hamiltonian

Combinatorial complexity

Landscape of energy distribution



$\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow \rightarrow \uparrow\uparrow\uparrow\uparrow\uparrow\downarrow \rightarrow \cdots \rightarrow \downarrow\downarrow\downarrow\downarrow\downarrow\downarrow$ $(n_{\mathrm{spin}} = 2^{12} = 4096)$

- Due to the rapidly changing shape of the potential, **any classical algorithm would fail.** (except the brute-force scanning)

- This example is from an event of 12 particles from a collision

Minimization with an adiabatic process

$$H(t) = \left(1 - \frac{t}{T}\right) H_0 + \left(\frac{t}{T}\right) H_P \text{ from } t = 0 \text{ to } t = T$$

- H_0 : The initial Hamiltonian whose ground state is easy to prepare.

- H_P : The problem Hamiltonian whose ground state is a solution to the optimization problem.

: Thus at $t = T$, we will have a solution for a hamiltonian $H(T) = H_P$

Utilizing Gate Quantum Circuit

- Starting from a well-known QAOA (arXiv:1411.4028) (Quantum Approximation Optimization Algorithm)

$$H(t) = (1 - a(t))\, H_M + a(t) H_P$$

- with $H_M = \sum \sigma_i^X$ and $H_P = H_{\text{QUBO}} = \sum J_{ij} \sigma_i^z \sigma_j^z + \lambda \sum P_{ij} \sigma_j^z \sigma_j^z$

- Starting from the ground state of H_M : $|\psi_0\rangle = |-\rangle$, evolve to the ground state of H_P : $|\psi\rangle = U(T,0)\,|\psi_0\rangle$

$$U(T,0) = U(T, T - \Delta t) U(T - \Delta t, T - 2\Delta t) \cdots U(\Delta t, 0)$$
$$= \prod_{j=1}^{p} U(j\Delta t, (j-1)\Delta t)$$

- Evolution operator $U(T,0)$

$$U(T,0) \approx \prod_{j=1}^{p} e^{-i\Delta t H(j\Delta t)} = \prod_{j=1}^{p} \exp\Big[-i\Delta t\big[(1-a(j\Delta t))H_M + a(j\Delta t)H_P\big]\Big]$$

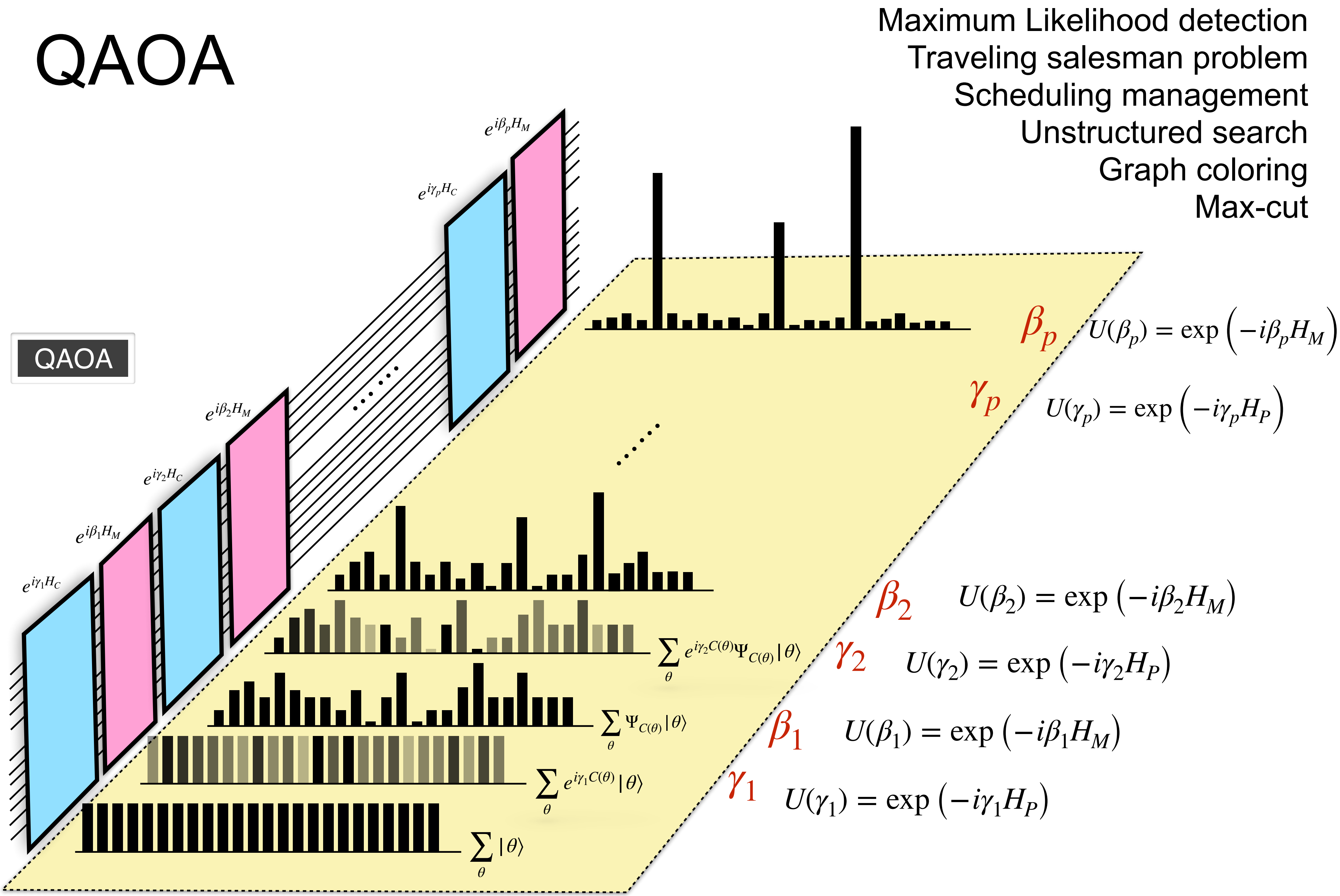
- With Suzuki-Trotter decomposition, $\lim_{p\to\infty} (e^{iAt/p}e^{iBt/p})^p = e^{i(A+B)t}$

$$U(T,0) \approx \prod_{j=1}^{p} \exp\Big[-i\Delta t(1-a(j\Delta t))H_M\Big]\exp\Big[-i\Delta t a(j\Delta t)H_P\Big]$$

$$= \prod_{j=1}^{p} \exp\Big[-i\beta_j H_M\Big]\exp\Big[-i\gamma_j H_P\Big]$$

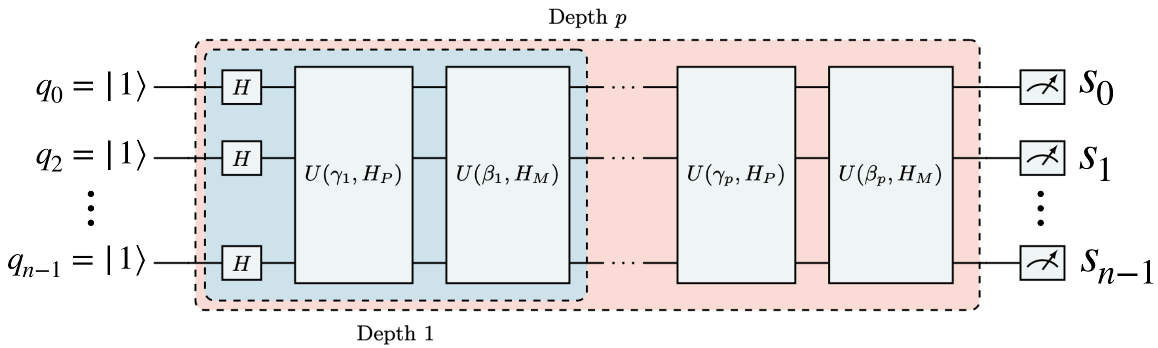
$$|\psi\rangle \equiv |\boldsymbol{\beta},\boldsymbol{\gamma}\rangle = \sum_{j=1}^{p} U(\beta_j, H_M)U(\gamma_j, H_P)|-\rangle^{\otimes n}$$

Works in the adiabatic limit or $p \to \infty$



QAOA
Maximum Likelihood detection
Traveling salesman problem
Scheduling management
Unstructured search
Graph coloring
Max-cut
QAOA
$e^{i\gamma_1 H_C}$
$e^{i\beta_1 H_M}$
$e^{i\gamma_2 H_C}$
$e^{i\beta_2 H_M}$
$e^{i\gamma_p H_C}$
$e^{i\beta_p H_M}$
$\sum_\theta |\theta\rangle$
$\sum_\theta e^{i\gamma_1 C(\theta)} |\theta\rangle$
$\sum_\theta \Psi_{C(\theta)} |\theta\rangle$
$\sum_\theta e^{i\gamma_2 C(\theta)} \Psi_{C(\theta)} |\theta\rangle$
β_p $U(\beta_p) = \exp\left(-i\beta_p H_M\right)$
γ_p $U(\gamma_p) = \exp\left(-i\gamma_p H_P\right)$
β_2 $U(\beta_2) = \exp\left(-i\beta_2 H_M\right)$
γ_2 $U(\gamma_2) = \exp\left(-i\gamma_2 H_P\right)$
β_1 $U(\beta_1) = \exp\left(-i\beta_1 H_M\right)$
γ_1 $U(\gamma_1) = \exp\left(-i\gamma_1 H_P\right)$

Machine Learning (to make QAOA more efficient)



Measurement:

$$L(\beta,\gamma) \equiv \langle \psi(\beta,\gamma) | H_P | \psi(\beta,\gamma) \rangle$$

Using "classical optimizer"

update

$$(\beta,\gamma) \to (\beta^*,\gamma^*)$$

- Find the minimum of a given hamiltonian H.

  - The state $|\psi(\beta,\gamma)\rangle = U(\beta,\gamma)|0\rangle$

  - $L(\beta,\gamma) \equiv \langle \psi(\beta,\gamma) | H_P | \psi(\beta,\gamma) \rangle \simeq \frac{1}{N_s} \sum H_P(s_0, \cdots, s_{n-1})$

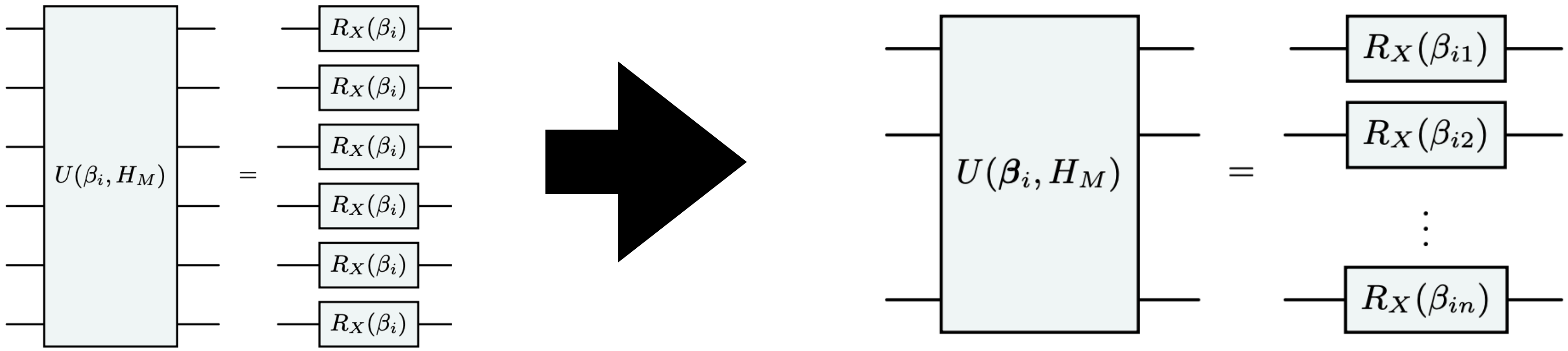
  will have a minimum when $|\psi(\beta^*,\gamma^*)\rangle = U(\beta^*,\gamma^*)|0\rangle \simeq |\psi_{\min}\rangle$

- Finding the $(\beta^*,\gamma^*) = \operatorname{argmin} L(\beta,\gamma)$ with a classical optimizer method. (For example, Gradient Descent Method)

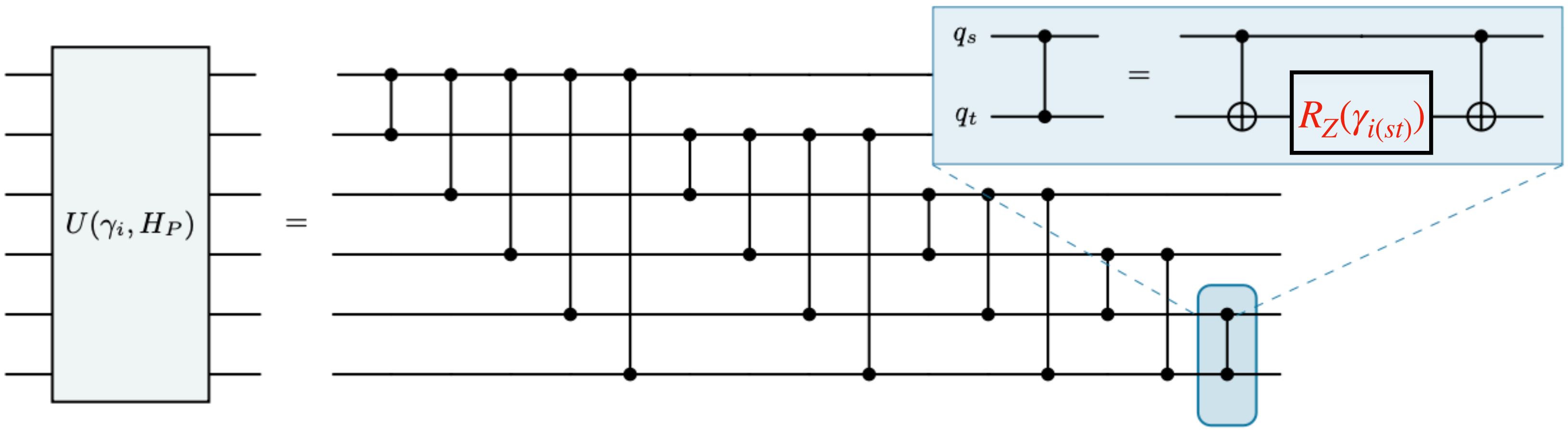
Variations of QAOA

- Multi Angle (MA)-QAOA: What if each qubit has its own free parameter? (**increase degree of freedom**, shifting burdens from QC to Optimizer)

Different parameters for each qubit in H_M

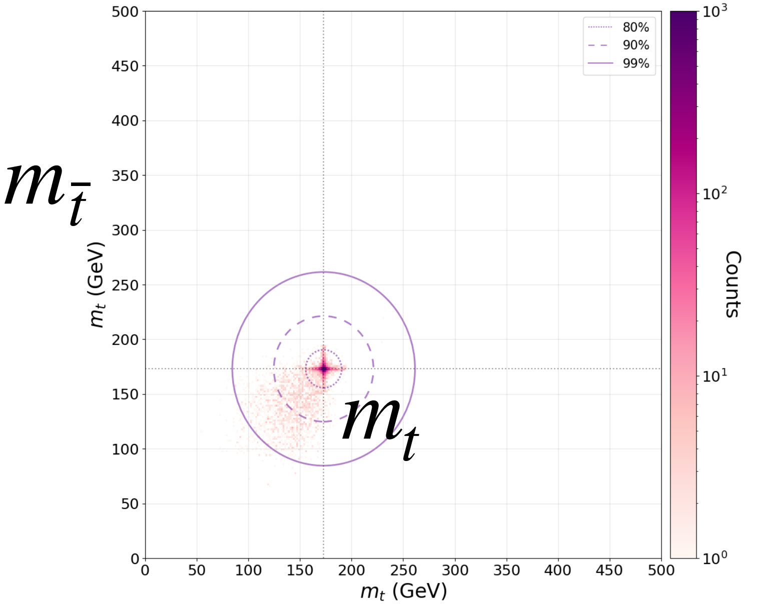


Different parameters for each pair of two qubits in H_P

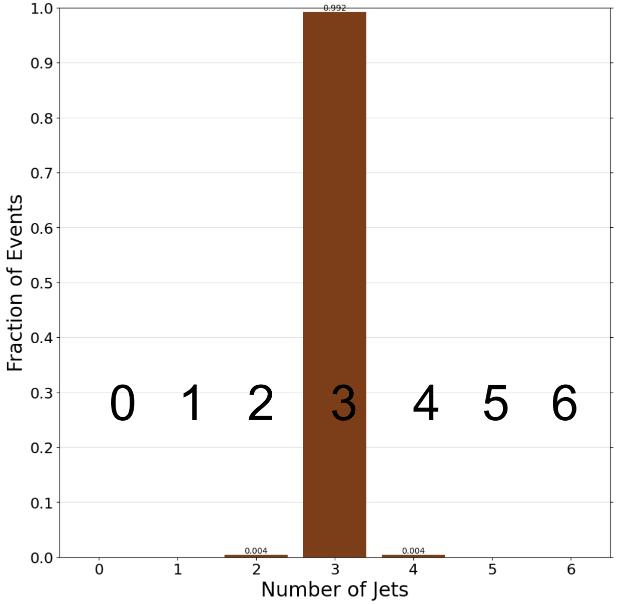


Results from Quantum Optimization Algorithm

Reconstructed mass



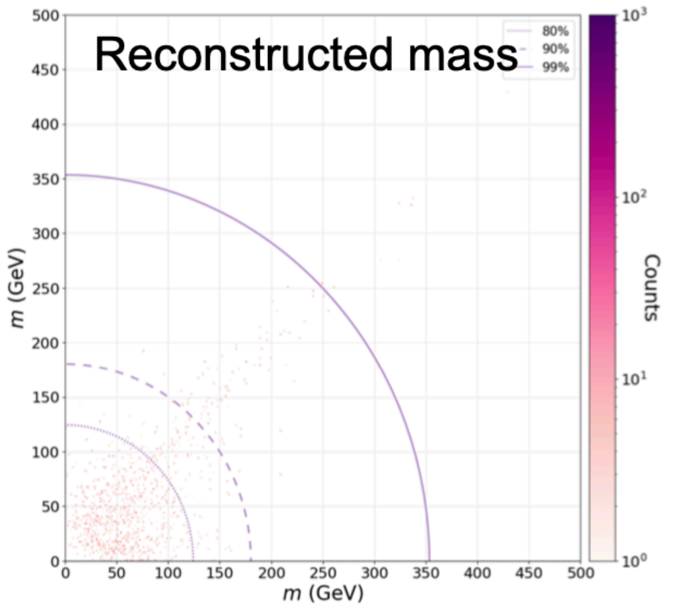
Jet assignment

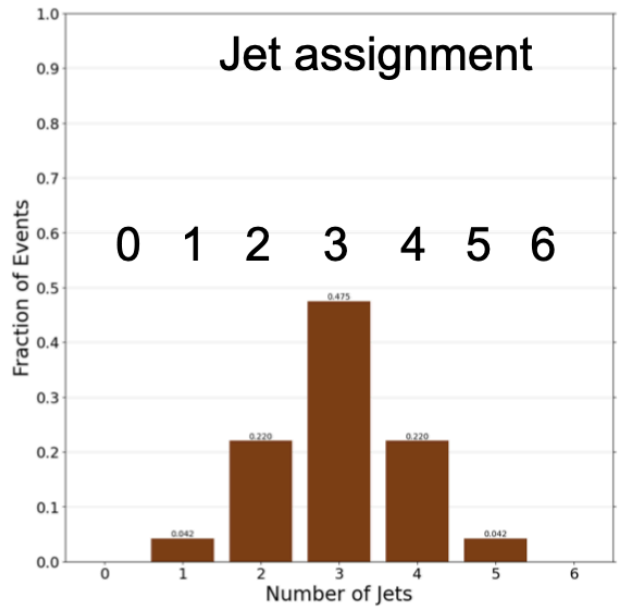


$pp \to t\bar{t} \to 6j$

79% overal efficiency

No mass information used.





$pp \to 6j$ (QCD backgrounds)

multi-jet (6 jets)

Comparison

Methods	matching accuracy (efficiency)		n_{train}	$n_{\text{parameters}}$	depth (p)	n_{CNOT}	n_{R_Z}	n_{R_X}
	parton-level	smeared events						
Hemisphere	50%	48%	N/A					
QAOA	55%	53%	N/A	16	8	240	120	48
ma-QAOA	75%	73%		168				
FALQON	72%	69%		2	250	7,500	3,750	1,500
SPANet	91%	70%	5×10^5	10^6	N/A			
	81%	62%	2×10^4	1.9×10^3				

- Hybrid Quantum Methods are strong with smearing by detector. (**SPANet is a supervised learning algorithm**, “SPANet: Generalized permutation-less set assignment for particle physics using symmetry preserving attention,” SciPost Phys. 12, 178 (2022), arXiv:2106.03898"

Conclusion

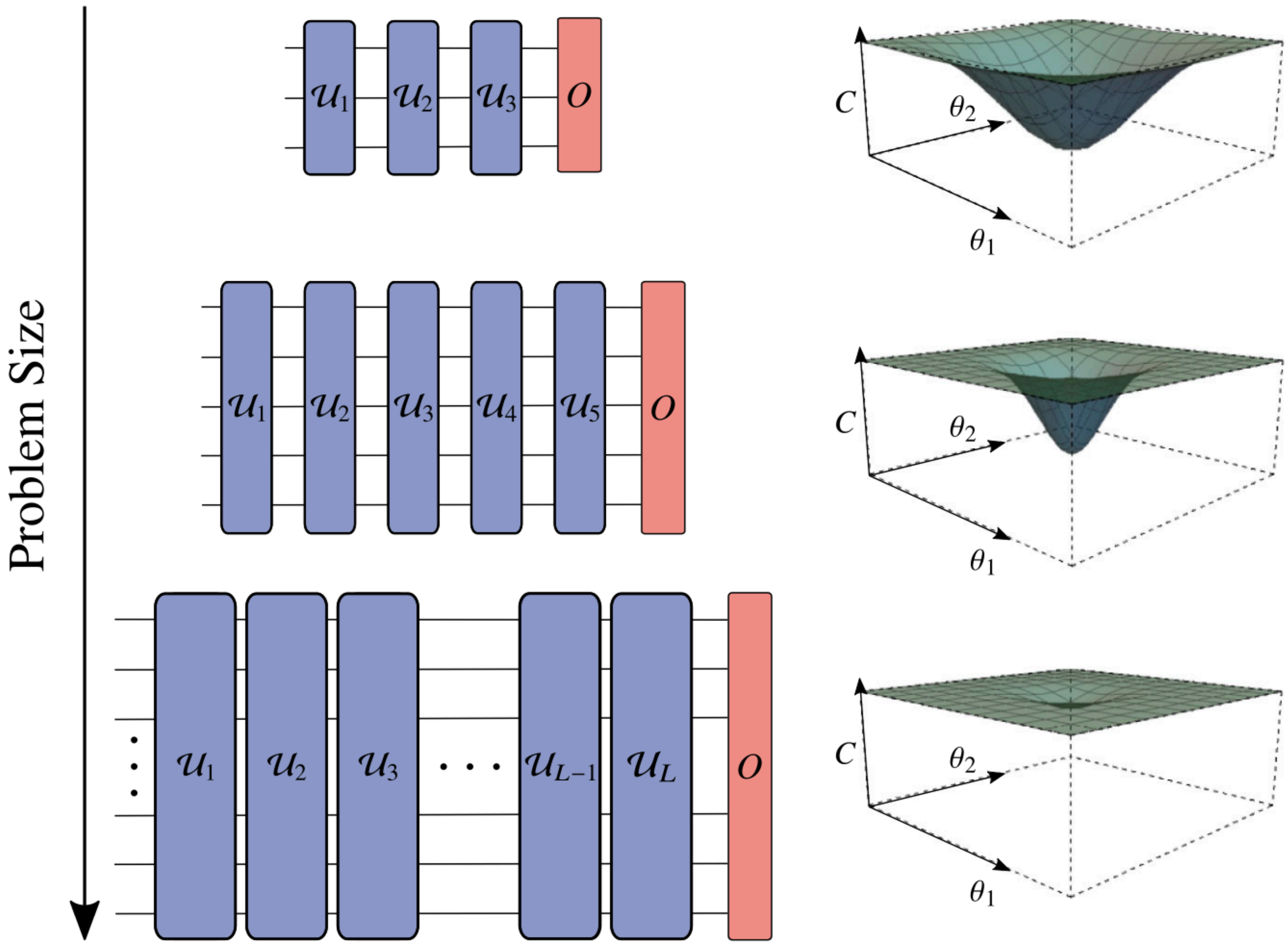
- **Lebesgue-style Monte Carlo with LeStrat-Net**:
  Comparable precision with **far fewer evaluations** and **stable uncertainties**, enabling targeted sampling of rare regions in high-dimensional phase space.

- **Model-agnostic event-topology reconstruction**:
  Formulating the combinatorial assignment as an Ising/QUBO optimization problem, solved by QAOA and its variants, enables robust, unsupervised reconstruction of event topologies **on an event-by-event basis**, without relying on model assumptions.

- **Outlook**: integrate with CEPC simulation chain (generator → detector), benchmark on CEPC-like processes ($e^+e^-\to ZH/WW/ZZ$), and explore hardware-aware quantum algorithms (FALQON/ma-QAOA) for near-term quantum devices.

Back-up

- With increasing size of a circuit, the gradient vanishes exponentially.



Nature Communications volume **12**, Article number: 6961 (2021) by Samson Wang et.al.

- FALQON (Feedback-Based Quantum Optimization): Purely QC

Alicia B. Magann et.al., PRL 129, 250502 (2022)

$$H(t) = H_P + \beta(t) H_M$$

$$i \frac{\mathrm{d}}{\mathrm{d}t} |\psi(t)\rangle = (H_P + \beta(t) H_M) |\psi(t)\rangle \longrightarrow \quad E_\mathrm{p}(|\psi(t)\rangle) = \langle \psi(t) | H_\mathrm{p} | \psi(t) \rangle$$

$$\frac{\mathrm{d}E_P}{\mathrm{d}t} = \langle \psi(t) | i \left[H_P + \beta(t) H_M, H_P \right] | \psi(t) \rangle = \beta(t) \langle \psi(t) | i \left[H_M, H_P \right] | \psi(t) \rangle$$

$$\equiv A(t)\beta(t) < 0$$ **if we take** $\beta(t) = -A(t-\tau)$