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

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With increasing energy and luminosity available at the Large Hadron collider (LHC), we get a chance to take a pure bottom-up approach solely based on data. This will extend the scope of our understanding about Nature without relying on theoretical prejudices. The required computing resource, however, will increase exponentially with data size and complexities of events if one uses algorithms based on a classical computer. In this letter we propose a simple and well motivated method with a quantum annealer to identify an event-topology, a diagram to describe the history of particles produced at the classical computer. We show that a computing complexity can be reduced significantly to the order of polynomials which enables us to decode the “Big” data in a very clear and efficient way. Our method achieves significant improvements in finding a true event-topology, more than by a factor of two compared to a conventional method.

Introduction. Understanding data has been always a milestone to build the theoretical understanding of our universe. When we have a strong theoretical motivation, we design an experiment to confirm it. The recent discovery of the Higgs particle is the perfect example as we have launched high energy collider programs to identify a mechanism behind electroweak symmetry breaking [1, 2]. But when existing theories have not been supported by experiments, unbiased observations on phenomena can shed light on a way to expand our theoretical framework. With this bottom-up approach, one can take Occam’s razor. For example, the idea of dark matter emerged as a simple explanation for the observed anomaly in various galaxy rotation curves1.

The standard model of particle physics (SM) had been constructed and confirmed by various experiments, finally was proved by the Higgs discovery but its extension is required to accommodate new phenomena including dark matter. As one of robust experiments, the LHC has probed various extensions of SM so far. The most interesting result of the LHC is that it opens a new opportunity for the young generation by closing the window for the previously favorite models including weak scale supersymmetric models. To cope with the current challenge of being without any theoretical guidelines, the LHC community starts to consider model-independent and data driven methods [4].

Being independent of a theory requires huge computing power as one needs to check the whole possibilities hidden in big data. This is the very reason to adopt the art of modern computing, a machine learning (ML) to data analyses. The high energy physics (HEP) community has taken the most sophisticated ML algorithms and achieved significant progresses2. Even with these successes, there would be the fundamental gap in applying ML to the problem of HEP; (1) Current ML algorithms are optimized to extract features in commercial data. (2) The size of data from the LHC exceeds the size of commercial one by the factor of $O(10^2)$ [6]. (3) The memory bottleneck in processing big data is rooted in the current computing architecture [7, 8].

Unlike the current “classical” computer, a quantum computer has the advantage to resolve above issues by the core concepts of quantum physics; superposition principle, entanglement and quantum tunneling [9]. There have been pioneering works in applying quantum computing including [10–15]. In this letter, we would like to add our effort by proposing a simple but powerful algorithm to perform the LHC data analysis with a very minimum assumption by the help of a quantum computer.

If there is an anomaly in the LHC data, one needs to identify the structure of signals as we draw a Feynman diagram to identify an underlying signal process. An event-topology is a Feynman diagram-like drawing without the spin information. With this, we focus on a kinematic structure of how observed particles are grouped according to decays of intermediate particles some of which may be new states not present in the SM. Once we identify an event-topology, we can measure efficiently masses and spins of new particles involved in the process [16, 17]. As we will show later, identifying an event-topology in an unbiased way requires enormous computing power from combinatorics. We resolve this issue by converting the combinatorial problem into a quadratic unconstrained binary optimization (QUBO) problem. The price for this is to handle with a notorious local minimum problem, the most significant issue in current ML algorithms [18]. Here we make use of a quantum annealer thereby exploiting the quantum advantage to resolve this issue.

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1 One can find a good review about the history of dark matter [3].

2 Well maintained list of ML applications can be found in [5].
QUBO for Event-topology classification. Our only assumption on abnormal events in collider data is that observed particles are produced through 2 → 2 process. More specifically, two new particles A and B are produced and they decay into observed ones. Thus identifying an event-topology becomes a binary classification, whose computing complexity increases exponentially as $O(2^n)$ with $n$ observed particles. A schematic description is presented in Fig. 1. As we have no further assumptions, we need to set a guiding rule to assign observed particles into decay products of either A or B. Motivated by general “energy minimum principle” in various fields of physics, one attempts to minimize the total invariant mass $(P_1 + P_2)^2$. But unlike the case of signals with missing energy which have been studied extensively in the literature, we will have a trivial partonic center of energy $\sqrt{s}$ when all the final particles are visible without missing energy-momenta.

The next trial we can take is to minimize a mass difference between A and B. With the four-momentum of $i$-th particle as $p_i$, momentums of A and B are:

$$P_1 = \sum_i p_i x_i, \quad P_2 = \sum_i p_i (1 - x_i),$$

where $p_i$ is the constituent of $A$ ($P_1$) if $x_i = 1$ or $B$ ($P_2$) if $x_i = 0$ [11]. Unlike a jet clustering algorithm, we don’t require any structure or a seed in clustering particles. By focusing on the kinematics, we minimize the following function $H$, the mass difference of A and B:

$$H = (P_1^2 - P_2^2)^2$$

for all possible combinations of $\{x_i\}$. The dimension of $H$, $[H] = M^4$ is chosen to address our problem as a QUBO problem with an Ising model form:

$$H_{\text{QUBO}} = \sum_{ij} J_{ij} s_i s_j + \sum_i h_i s_i,$$

where $\{s_i\}$ is spin set with only ±1 values for spin $\uparrow$ and $\downarrow$, and $J_{ij}$, $h_i$ are the coupling strength and biases, respectively. We cast our minimization problem on $H$ into that on $H_{\text{QUBO}}$ through a change of variables $x_i = (1 + s_i)/2$ to express:

$$J_{ij} = \sum_{k\ell} P_{ik} P_{j\ell},$$

$$h_i = 2 \sum_j [\sum_{k\ell} (P_{ik} P_{j\ell} - P_{k\ell} P_{ij})],$$

with $P_{ij} = p_i \cdot p_j$. Our target function $H$ in Eq. (2) is optimized to the case of $M_A = M_B$, which is the case of most conventional new physics searches at the LHC. Thus this function $H$ can be a starting point, but we need to generalize this function to handle situations including (1) various new physics scenarios with asymmetric production of $M_A \neq M_B$, and (2) off-shell effect from the decay width of unstable particles or smearing from a detector response. We add an additional constraint term to deal with above issues:

$$H_{\text{QUBO}} \rightarrow H_{\text{QUBO}} + \lambda (P_1^2 + P_2^2)$$

$$= H_{\text{QUBO}} + \lambda \sum_{ij} P_{ij} [s_i s_j + (1 - s_i)(1 - s_j)]$$

$$= \sum_{ij} J_{ij}' s_i s_j + \sum_i h_i' s_i,$$

with $J_{ij}' = J_{ij} + 2\lambda P_{ij}$ and $h_i' = h_i - 2\lambda \sum_j P_{ij}$. Here we remove constant terms. To maintain a hierarchy between the minimum for mass difference and the minimum in total mass sum during a minimization procedure, we set $\lambda = \min(J_{ij}) / \max(P_{ij})$. This choice is based on empirical studies as in the case of choosing hyperparameters in conventional ML algorithms. Finally, we swap A and B if the number of particles assigned to A is less than the number of particles clustered into B. We maintain the ordering between numbers of constituent particles in A and B over all events.

In order to demonstrate the performance of our QUBO algorithm, we take three examples: (1) Top quark pair production, (2) Higgs and Z boson production and (3) four top-quark production via the pair of color octet $\bar{\sigma}$ scalar where each scalar decays into a top-quark pair [19]. Here we take the mass of $\bar{\sigma}$ as 600 GeV for a benchmark. All these particles decay hadronically:

$$pp \rightarrow t, \bar{t} \rightarrow \{j_1, j_2, j_3, j_4, j_5, j_6\},$$

$$pp \rightarrow H, Z \rightarrow \{j_1, j_2, j_3, j_4, j_5, j_6\},$$

$$pp \rightarrow \bar{\sigma}, \bar{\sigma} \rightarrow t, \bar{t}, t \rightarrow \{j_1, j_2, j_3, \cdots, j_{11}, j_{12}\}.$$
for a given spin state \( \{s_i\} \). In Fig. 2 we show (a) the energy spectrum of \( H_{\text{QUBO}} \) and (b) histogram of energy spectrum of \( H_{\text{QUBO}} \) with an event from a four-top-quark production process as in Eq. (7c). For the ordering of spin states in Fig. 2(a), we increase a spin state by flipping a spin in an increasing order based on a binary digit. For example with four spins, the spin order \( \uparrow \uparrow \uparrow \uparrow \rightarrow \uparrow \uparrow \uparrow \downarrow \rightarrow \uparrow \uparrow \downarrow \uparrow \rightarrow \uparrow \uparrow \downarrow \downarrow \rightarrow \cdots \) corresponds to the index as \( 0 \rightarrow 1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow \cdots \). One can try a conventional procedure called a simulated annealing to find a global minimum in \( H_{\text{QUBO}} \) distribution of Eq. (6) [24]. Simulated annealing uses a thermodynamic probability to find a global ground state. It starts with an initial temperature \( T_0 \) and gradually decreases temperature \( T \) to zero degree at each annealing step. In each step, this algorithm checks whether flipping a spin is beneficial to get a global minimum. If the energy with flipped spin is lower than the initial energy, it takes the flipped spin configuration. If not, the spin will be flipped according to the probability of Boltzmann factor, \( e^{-(E_{s+1} - E_s)/k_B T} \). But when the structure of an energy spectrum with a spin state is complicated, it will have a local minimum problem. In our case, the energy spectrum can be extremely complicated as shown in Fig. 2. In Fig. 2(a), the energy structure similar to a dense pine tree park neutralizes simulated annealing, as sudden drops and rises disable the attempt of spin flipping procedures. On top of this local minimum problem, the population near a global minimum is sparse as we observe in Fig. 2(b). Thus we choose to take a quantum advantage to find a global minimum for a complicated energy distribution.

**Quantum advantage.** Quantum annealing (QA) is optimized to handle problems in a QUBO form. It uses the adiabatic theorem to find the ground state of a complicated \( H_{\text{QUBO}} \) starting from the ground state of a trivial Hamiltonian \( H_0 \) [25];

\[
H_{\text{QA}}(t) = A(t)H_0 + B(t)H_{\text{QUBO}},
\]

where \( H_0 = \sum_i (s_{\perp})_i \) with a new spin set \( \{s_{\perp}\} \) which is transverse to the spin set \( \{s\} \) of \( H_{\text{QUBO}} \). At the beginning of \( t = 0 \), \( H_{\text{QA}}(0) = A(0)H_0 \) as \( A \neq 0 \) and \( B = 0 \). Thus the ground state of \( H_{\text{QA}}(0) \) is the same as the ground state of \( H_0 \). By adiabatically decreasing \( A \) to 0 but increasing \( B \) with a time \( t \), the ground state of \( H_0 \) can be transmitted to the ground state of \( H_{\text{QUBO}} \) via \( H_{\text{QA}} \). To realize QA process of Eq. (8), we use a commercial D-Wave Advantage™ which has 5000+ available spins (=qubits) [26].

Most of time spent by a QA procedure is dedicated to a preparation step, while required time for an annealing process is independent on the size of inputs. In our case with Eq. (3), preparation time \( T_{\text{QUBO}} \) is of \( \mathcal{O}(n^2) \). Compared to the processing time of \( \mathcal{O}(2^n) \) with the simplest but a robust brute-force scanning algorithm with a classical computer, a quantum annealer can have an enormous advantage in the computational complexity as

\[
T_{\text{QUBO}}(n) \sim \mathcal{O}(n^2) \ll \mathcal{O}(2^n),
\]

In Table I, we illustrate the performance of a quantum annealer in finding a global minimum. Monte Carlo samples for \( H_{\text{QUBO}} \) are generated as in the previous section. As we notice, current quantum annealer achieves a good performance to find a global minimum for complicated energy distributions which is not possible with simulated annealing. By assigning jets into either \( A \) or \( B \), we can re-construct the four-momenta of \( A \) and \( B \) to identify their properties as in Fig. 3. Reconstructed mass \( M_A \) and \( M_B \) with \( H_{\text{QUBO}} \) algorithm spots the true mass point (Top panel in Fig. 3). The most populated number of clustered jets in \( A \) is equal to the true number of decayed particles from \( A \) (Bottom panel in Fig. 3) for a hadronically decaying top quark in Eq. (7a), a higgs decaying into four jets via \( W^\pm \) bosons in Eq. (7b) and a color octet scalar \( \tilde{o} \) which decays into a top-quark pair, resulting in six jets as in Eq. (7c). We can apply \( H_{\text{QUBO}} \) sequentially to find the substructures of \( A \) and \( B \);

\[
H_{\text{QUBO}}^{(A)} = \sum_{ij=1}^{\ell} J_{ij}^{\alpha \beta} s_i^\alpha s_j^\beta + \sum_{i=1}^{\ell} h_i^{\alpha} s_i^\alpha,
\]

\[
H_{\text{QUBO}}^{(B)} = \sum_{ij=1}^{m} J_{ij}^{\beta \gamma} s_i^\beta s_j^\gamma + \sum_{i=1}^{m} h_i^{\beta} s_i^\beta,
\]

where \( \{s_i^\alpha\} \) is a spin set for particles clustered into \( A \) and \( \{s_i^\beta\} \) is the one for particles assigned to \( B \) after minimizing an original \( H_{\text{QUBO}} \). Here \( \ell \) and \( m \) vary in an event by event basis, only need to satisfy \( \ell + m = n \). We get additional constraints for the number of intermediate particles from the decay of each of \( A \) and \( B \) as \( A \to A_1, A_2 \) and \( B \to B_1, B_2 \). In Fig. 4, we present the result of above sequential application to the most complicated process of Eq. (7c). Sequential QA reveals the

| Process | \( pp \to Ht \) | \( pp \to HZ \) | \( pp \to \tilde{o}^+ \) |
|---------|----------------|----------------|------------------|
| Success rate | 100% | 100% | 93% |

**Table I.** Success rate in finding a global minimum of \( H_{\text{QUBO}} \) using D-Wave Advantage™.
structure of an event-topology behind 12 jets as;

\[ pp \rightarrow \hat{o} \hat{o}^*; \ (\hat{o} \rightarrow 6j), \ (\hat{o}^* \rightarrow 6j) \]  
\[ \hat{o} \rightarrow t \bar{t}, \ (t \rightarrow 3j), \ (\bar{t} \rightarrow 3j), \]  
\[ \hat{o}^* \rightarrow t \bar{t}, \ (t \rightarrow 3j), \ (\bar{t} \rightarrow 3j), \]

by measuring masses and the number of constituent jets of \( A_1 \) and \( A_2 \) as well as \( B_1 \) and \( B_2 \).

Before closing this section, we explain the effect of a constraint term \( \lambda \left( P_A^2 + P_B^2 \right) \) in Eq. (6) by showing results only with minimizing differences between \( M_A \) and \( M_B \) without the constraint term in Fig. 5. As we expect, \( H_{QUBO} \) in Eq. (3) focuses on minimizing the mass difference between \( A \) and \( B \) which is inadequate in handling situations including asymmetric processes like \( pp \rightarrow HZ \) in Eq. (7b), particles with a large decay width, and experimental defects including smearing effects mostly for multi-jet productions as in Eq. (7c).

We close this section by comparing our algorithm and an existing one. In fact, the subject of identifying event-topology has not gained much attention as the LHC studies were focused more on optimizing discovery chances of theoretically well motivated models, mostly supersymmetric ones where relevant event topologies are manifest\(^3\). If we narrow down to a clustering problem in separating decay chains, there is a hemisphere algorithm that was designed to assign visible particles correctly ac-

\[^3\] Identifying an event topology in missing energy channel was introduced in [27]
is constructed from the very minimal assumption without relying on the kinematic structure. This provides an advantage to QUBO compared to previous ones which are based on the geometry of a preassumed phase space.

**Conclusion.** In this letter, we illustrate how a bottom-up approach with data from high energy colliders can be established via a quantum algorithm. To have the full advantage of our method, a quantum computer is necessary in finding the global minimum of a complex energy distribution. The technologies of a quantum computer are on the verge of quantum supremacy [30, 31]. Thus as a theorist, it is our duty to formulate problems into a right form to have the full benefits of a quantum computer in decoding the fundamental laws of physics. As a TeV-scale high energy collider can reach the moment of $O(10^{-12})$ seconds after big-bang, the realm of “quantum universe”. Nature will reveal its secrets when we face it with quantum technologies.

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**Appendix: Quantum annealer**

We use Amazon Web Services (AWS) to access D-wave Advantage™ (Advantage), a quantum annealer by D-wave company. Advantage has 5000+ qubits, connected to each other with at least 35000 couplers which are way fewer than the number of all possible pairs $^{5000+}_2$. Thus the network among qubits is not fully connected. To

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4 The Lorentz boost factor $\gamma$ for a particle $A$ is $E_A/M_A = M_{AB}/(2M_A)$. To deal with the case of $M_A \neq M_B$, we take the approximate average of $\gamma_A$ and $\gamma_B$ as $M_{AB}/(M_A + M_B)$. 

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**FIG. 6.** Matching accuracy same as in Tab.II in terms of their boost factor $M_{AB}/(M_A + M_B)$. Here $M_{AB}$ is an invariant mass of $A$ and $B$.

**FIG. 7.** A Pegasus graph with 27 unit cells.
squeezed performance in this limited situation. Advantage has a connectivity structure among qubits, called as Pegasus graph [32]. This graph consists of unit cells each containing 8 qubits.

Fig. 7 shows a partial sample of Pegasus graph. The network structure of Pegasus is fixed with varying strength in couplers between connected qubits. To embed various QUBO problems into this fixed and non-fully connected network of qubits, Advantage uses a minor-embedding with chains of qubits [33]. For example, one needs to have a qubit which is connected to both \( q_i \) and \( q_j \), but can not find this one in a given network. In this case, it would be easier to find a chain (a set of spins, connected with each other like a chain), \( \{q_1, q_2, \cdots, q_n\} \) where \( q_1 \) is connected to \( q_i \) and \( q_n \) has a connection to \( q_j \). The connection strengths in a chain should be chosen properly so that qubits in a chain are treated as a single qubit during solving a QUBO problem. Advantage provides an automatic embedding solution with adjustable chain strength parameters [34]. Thus the required number of qubits is larger than the number of inputs in a given QUBO problem. In our case, we need 8 qubits to solve our QUBO problems with 6 visible particles for processes in eqs. (7a) to (7b) and 24 qubits for 12 particles in a process of Eq. (7c) as in Fig. 8.

As a quantum annealer has various systematic errors especially in the status of qubits during operations, a performance of Advantage will drop with increasing number of required qubits. The required number of qubits in Eq. (7c) is three times larger compared to the one in eqs. (7a) to (7b) while the number of input visible particles only increases by the factor of two. To reduce errors, a method which is called the spin reversal transform was introduced [35]. The spin reversal transform flips the sign of selected coefficients of QUBO problem which Advantage minimizes. The spin reversal transform does not change the ground state of QUBO problem, so one can average out the biases which come from systematic errors. We use default spin chain strength parameter and set the number of spin reversal transform to 10 to minimize systematic errors. A recent work suggests that one can increase the success rate in QA through a parallelization procedure which processes several events in a single QA operation [36].

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