QUBO formulations of particle tracking algorithms

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Abstract. SPD (Spin Physics Detector) is a planned future experiment on the NICA megascience project developed in Dubna. Based on modeling data of the SPD experiment, this work is the first attempt to use the Hopfield network approach to formulate a QUBO problem and use simulated annealing to estimate the feasibility of the future use of quantum annealing to speed up present SPD particle tracking approaches.

Introduction

One of the key stages of data processing from particle physics experiments is the reconstruction of trajectories (tracks) of interacting particles from measurement data. In many future experiments, such as the High-Luminosity Large Hadron Collider (HL-LHC) or the SPD experiment planned at the NICA collider in Dubna, a special difficulty will be caused by the extremely high frequency of interactions.

In SPD, a very high data acquisition rate of 20 GB/sec resulting from 3 MHz collision frequency implies that tracks of several events will be overlapped and recorded in a single time-slice. Besides this, a strong contamination of data by fake measurements due to the specifics of used track detectors [2] will further raise the bar for track reconstruction (tracking) algorithms performance.

In our recent study [1], methods based on the Hopfield neural network for tracking simulated events of the SPD experiment were investigated. The minimum of the network energy function, corresponding to the solution of the problem, was obtained via simulated annealing.

However, it has been shown in recent works [7, 8] that combinatorial optimization problems can be successfully solved using quantum annealing techniques. For this purpose, the track reconstruction problem is formulated as quadratic unconstrained binary optimization (QUBO) and can be natively solved by quantum annealers, such as the commercially available D-Wave machines. Although the quantum speed-up potential is not yet clear, the anneal time of $\approx 20\mu s$, independently of the size of the problem, promises an acceleration that deserves to be explored. So far, current D-Wave hardware yields results very similar to classical solvers - the anneal needs to be run multiple times, as noise, thermal fluctuations and other external factors may interfere with the process. Further complications arise due to various overhead costs and the necessity to split large QUBOs into small instances that fit the hardware [7].

We should also point out an interesting possibility of applying algorithms for gate-based quantum computers, like the Quantum Approximate Optimization Algorithm (QAOA), the Variational Quantum Eigensolver (VQE) and the Harrow-Hassadim-Lloyd (HHL) algorithm, which, when applied to the optimization of the Hopfield network, can serve to further accelerate the search for the global minimum of the proposed matrix representing the network energy function.

The Hopfield network approach

A track with n hits (3d coordinates from detectors) can be regarded as a set of $n-1$ consecutive lines ("track segments") with a smooth shape and without bifurcation [6]. Based on methods developed in the late eighties (Denby 1988 [3]; Peterson 1989 [4]) and the beginning of nineties (Stimpfl-Abele and Garrido [6]), the Hopfield network [5] approach uses for track reconstruction a method that optimizes an energy function for which we chose the following form:

$$E = -\gamma \sum_{i,j,k} \left(\frac{\cos^{\lambda}(\theta_{ijk})}{(r_{ij} + r_{jk})^{\eta}} \right) v_{ij} v_{jk} + \alpha \left(\sum_{j \neq k} v_{ij} v_{ik} + \sum_{i \neq j} v_{ik} v_{jk} \right) + \beta \sum_{i,j} v_{ij} \,, \quad (1)$$

where θ_{ijl} is the angle between possible track segments v_{ij} and v_{jk} (equal to one when active and zero otherwise) of length r_{ij} and r_{jk}, respectively. The second term is a penalty for an undesired track bifurcation, the third one is a constant inhibition term which helped us make the energy matrix more sparse.

This way, we obtain a segment classification task, where each term of the energy function E is designed for geometric rewards and penalties weighted by parameters $\gamma, \lambda, \alpha, \beta$, such that tracks composed of short track segments (doublets) that lie on a smooth curves with no bifurcations are biased, cf. [8].

Results for SPD modeling data

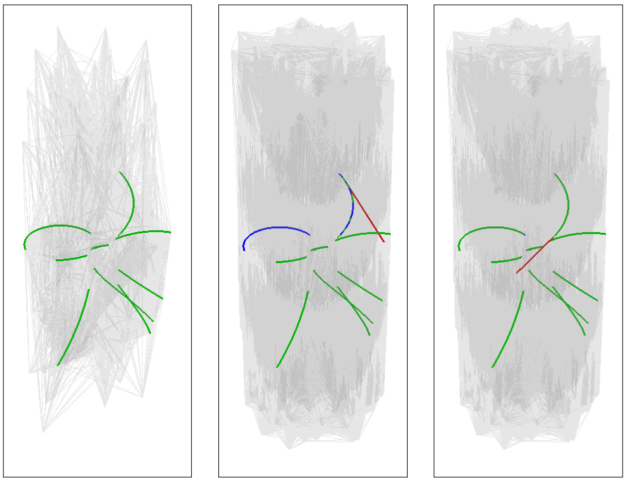
An example of the results of our method for an event with 10 tracks with different number of noise hits and sets of optimized parameters is shown in Fig. 1. Due to the large number of detector layers, tracks consist of a large number of short segments, which facilitates their reconstruction. However, it can be seen that a larger amount of noise hits decreases the tracking quality.

QUBO formulation of the particle tracking problem

Energy function (1) resembles a QUBO, which is defined as

$$\min_{\boldsymbol{x} \in \{0,1\}^n} \boldsymbol{c}^{\mathsf{T}} \boldsymbol{x} + \boldsymbol{x}^{\mathsf{T}} Q \boldsymbol{x} \,, \quad (2)$$

where the minimum is taken over the collection of binary vectors $\boldsymbol{x}$ of length n, $\boldsymbol{c} \in \mathbb{R}^n$ and $Q \in \mathbb{R}^{n \times n}$ is a symmetric matrix. QUBO does not, by definition,



(a) (b) (c)

FIGURE 1. Results of tracking of an event with 10 tracks. True positive, true negative, false positive and false negative segments are shown. (a) 100 noise hits (b) 1750 noise hits, minimization of false-positive segments prioritized (c) 1750 noise hits, TrackML [9] metric prioritized [1, 8].

contain constraints, so any potential constraints have to be incorporated to the objective function as penalties through reformulation techniques. A drawback of such an approach is that such squared penalty will result in a QUBO with $O(n^2)$ quadratic terms. However, there exist approaches to design more efficient ways to represent such constraints for optimization with quantum annealers such as D-Wave (e.g. [10]).

When QUBO is solved on a quantum annealer, each linear coefficient c_i of QUBO is mapped as a bias onto a distinct qubit i, and each quadratic coefficient q_{ij} is encoded as a weight of a link between qubits i and j, called a coupler [10].

The mapping from the QUBO problem to the graph, describing the interconnection between the qubits in the hardware ("chimera" graph structure in the current D-Wave architecture) is a limitation of this approach, and is currently dealt with through so-called minor-embedding [12]. More on QUBO/Ising formulations of NP problems can be found in [11].

To improve the performance of the algorithm, we plan to formulate QUBO to identify the best pairs of triplets, instead of doublets. A triplet T_i is a set of three hits (a, b, c) or a pair of consecutive doublets (a, b and b, c). Two triplets of hits (a, b, c) and (d, e, f), can be combined to form a quadruplet if $b = d \wedge c = e$ or a quintet if $c = d$. The objective function (2) to minimize has two components: a linear term that weighs the quality of individual triplets and a quadratic term used to express relationships between pairs of triplets:

$$\sum_{i=1}^{N} a_i T_i + \sum_{i}^{N} \sum_{j<i}^{N} b_{ij} T_i T_j \, , \tag{3}$$

where T are all potential *triplets*, a_i are the *bias weights*, and b_{ij} the *coupling strengths* computed from the relation between the triplets T_i and T_j [7].

Conclusion and outlook

We attempted to apply several modifications of the algorithm to the simulation of SPD data with the presence of fake hits. The method showed good results, but under rather simple conditions. Fake and noise hits pose notable difficulties for tracking by different methods. We need to study the impact of events where fake hits are generated more correctly in terms of the geometry of the experimental setup. An improvement of the energy function, which gives us the QUBO model, has to be worked out. More advanced segment filtering methods are needed (e.g. using triplets [7]), which would possibly reduce the impact of noise hits, and also allow the method to be tested on TrackML [9] data. Finally, a method to assess the timing performance of the algorithm needs to be developed.

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