QUBO formulations of particle tracking algorithms

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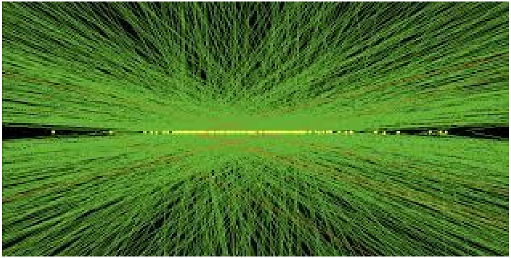
Polynomial Computer Algebra 2024
April 15-20, 2024
Euler International Mathematical Institute, St. Petersburg, Russia

Tracking crisis

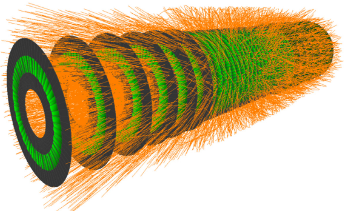


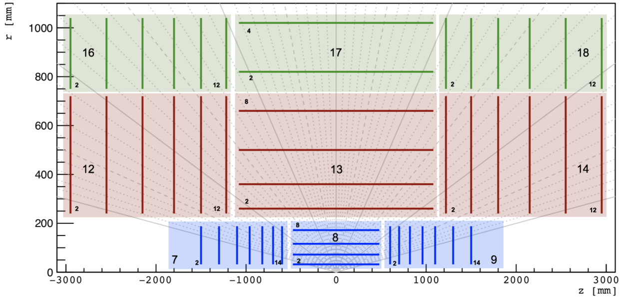
A model event on HL-LHC.

- Main problem of tracking – high luminosity of near-future particle colliders.
- High Luminosity Large Hadron Collider (HL-LHC) upgrade:
  higher luminosity = more data
  price to pay - extreme number of simultaneous interactions (pileup)
- Faster algorithms needed.

TrackML particle tracking challenge[1]

- Simulation of dense environments expected at HL-LHC.
- **Competition goal** – build an algorithm that quickly reconstructs particle tracks from 3D points left in the silicon detectors.
- **TrackML score** - "intersection between the reconstructed tracks and the ground truth particles, normalized to one for each event, and averaged on the events of the test set"





TML detector - simulation of a typical full Silicon LHC detector with high luminosity.

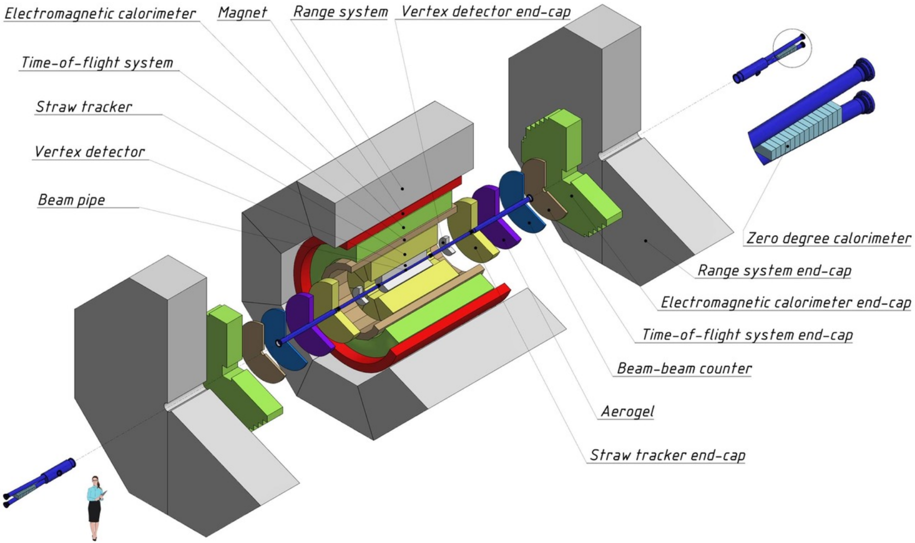
[1] *TrackML Particle Tracking Challenge. Kaggle.* 2018. URL: https://kaggle.com/competitions/trackml-particle-identification.

NICA Complex

NICA (Nuclotron-based Ion Collider fAcility) - new accelerator complex designed at the Joint Institute for Nuclear Research (Dubna, Russia) to study properties of dense baryonic matter.

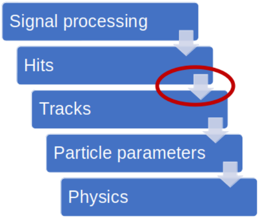
Scheme of the NICA complex with MPD, SPD, BM@N experiments.

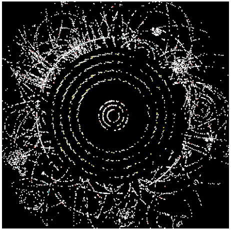
SPD setup


Electromagnetic calorimeter
Magnet
Range system
Vertex detector end-cap
Time-of-flight system
Straw tracker
Vertex detector
Beam pipe
Zero degree calorimeter
Range system end-cap
Electromagnetic calorimeter end-cap
Time-of-flight system end-cap
Beam-beam counter
Aerogel
Straw tracker end-cap

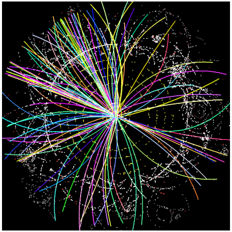
What is tracking? . . . “connect the dots”

- **tracking** - process of reconstructing the trajectory (or track) of electrically charged particles in a particle detector
- **hit** – 3d coordinates reconstructed from detector signals
- **track** - subgroup of hits left by one particle





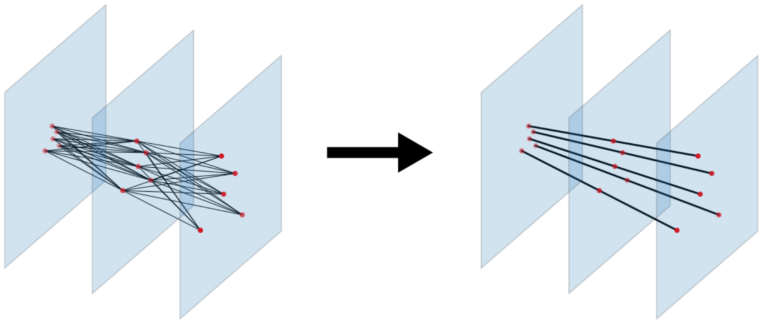
xy-projection of an event on LHC



The same event after tracking.

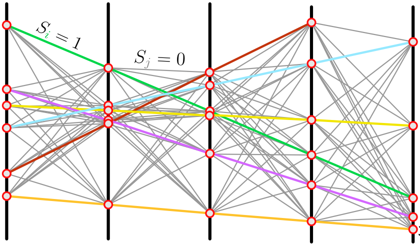
Tracking - method of segments.

“We can regard a track with n coordinates as a set of $n - 1$ consecutive lines (“ track segments”) with a smooth shape and without bifurcation.“[2]



[2] Georg Stimpfl-Abele и Lluís Garrido. “Fast track finding with neural networks”. В: *Computer Physics Communications* 64.1 (апр. 1991), с. 46—56.

Tracking - method of segments.



[3]

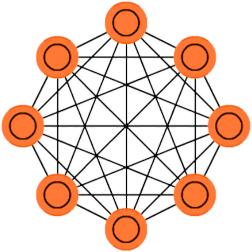
- Fist step - constructing all the possible segmets-doublets of hits in consecutive modules of the detector. Each doublet is associated with a binary variable:

$$S_i = \begin{cases} 1 & \text{if the doublet is part of a track} \\ 0 & \text{otherwise} \end{cases}$$

- Track reconstruction consists of **determining the vector $\boldsymbol{S}$** $= (S_1, S_2, \ldots S_n)$, containing the correct activation state of every doublet-neuron.

[3] Davide Nicotra и др. *A quantum algorithm for track reconstruction in the LHCb vertex detector*. 2023.

Tracking via Hopfield neural network[4]

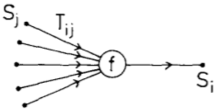


- segments = neurons of the **Hopfield network**
- **Hopfield network** – fully-connected, single-layer neural network with binary units-neurons;

  complete undirected graph:
  vertices: n binary neurons $\{s_i\} \in \{0,1\}^n$
  edges: symmetric weight matrix $w_{ij} = w_{ji}, w_{ii} = 0$
- network energy function (Lyapunov function):

$$E(\boldsymbol{s}) = -\frac{1}{2}\sum_{i,j} s_i w_{ij} s_j \ ,$$

  s_i - state of unit i
  w_{ij} - strength of the connection weight from unit j to unit i



- network updating rule:

$$s_i = \begin{cases} 1 & \text{if } \sum_j w_{ij} s_j \geq \theta_i \\ 0 & \text{otherwise} \end{cases}$$

- the network will eventually converge to a state which is a **local minimum** in the energy function (Lyapunov function)

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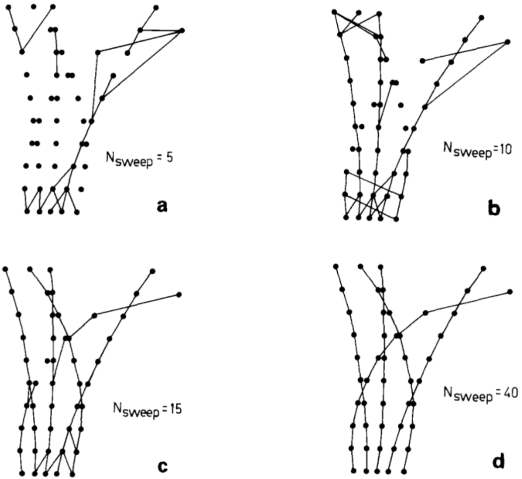
[4] JJ Hopfield. "Neural networks and physical systems with emergent collective computational abilities". B: *Proceedings of the National Academy of Sciences of the United States of America* 79.8 (апр. 1982), с. 2554—2558.

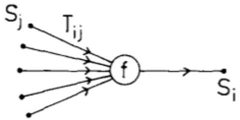
Mapping the track finding problem onto a neural network[5]



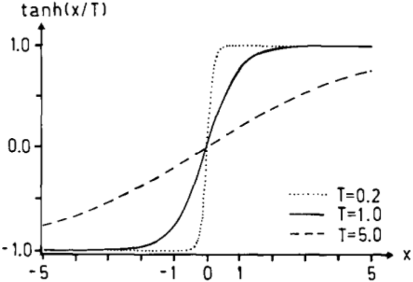
Segments with $V_{ij} > 0.1$ at different evolution stages of the mean field theory equations.

[5] Carsten Peterson. "Track finding with neural networks". B: *Nuclear Instruments and Methods in Physics Research Section A* 279.3 (1989), c. 537—545.

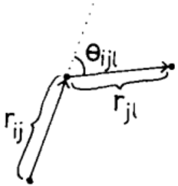
Mapping the track finding problem onto a neural network[6]



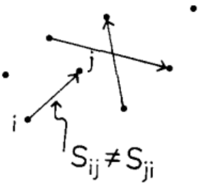
A generic neural network updating.



Sigmoid gain functions
for different temperatures T.



Definition of segment lengths r_{ij}
and angles Θ_{ijl} between segments.



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[6] Carsten Peterson. "Track finding with neural networks". B: *Nuclear Instruments and Methods in Physics Research Section A* 279.3 (1989), c. 537—545.

Tracking - method of segments.

The algorithm acts as a **doublet classifier**:[7]

input - large collection of potential doublets
output - a subset of those doublets that are believed to form true track candidates

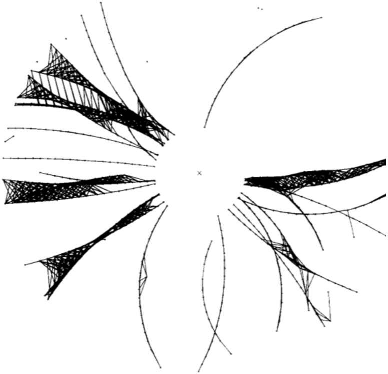


Fig. 1. Display of all generated lines for a real $Z^0 \to$ hadrons (XY projection).

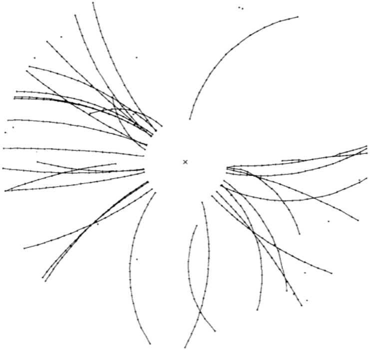


Fig. 3. Display of the activated lines after convergence for a real $Z^0 \to$ hadrons (XY projection).

[7] Georg Stimpfl-Abele и Lluís Garrido. “Fast track finding with neural networks”. В: *Computer Physics Communications* 64.1 (апр. 1991), с. 46—56.

Simulated and quantum annealing

- **simulated annealing**[8] (SA) can be regarded as a random walk on the search space, whose steps are parameterized by a temperature parameter called T. At each iteration, a random step is taken, and the step is accepted if it has a lower cost. If the new step has a higher cost, then it is accepted with a probability determined by the temperature T and the difference between the existing and the new costs. At higher temperatures, the transition between the states occurs more frequently. According to a cooling schedule, at each iteration, the parameter T is decremented, and the optimal solution is found with the help of the thermal fluctuations.
- **quantum annealing** (QA) - a quantum mechanical heuristic method for solving optimization problems (quantum fluctuations are used instead of thermal fluctuations)

[8] Scott Kirkpatrick, C. Gelatt и M. Vecchi. "Optimization by Simulated Annealing". В: *Science (New York, N.Y.)* 220 (июнь 1983), с. 671—80.

Universal (gate-based) vs. adiabatic quantum computer

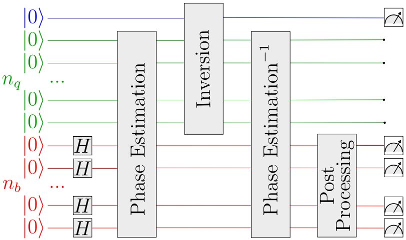
Universal quantum computer
(unitary quantum operations, measurements)
general purpose

computer	qubits
IBM Q System One (2019)	20
IBM Osprey (2022)	433

Adiabatic quantum computer
adiabatic evolution of quantum state
optimization problems

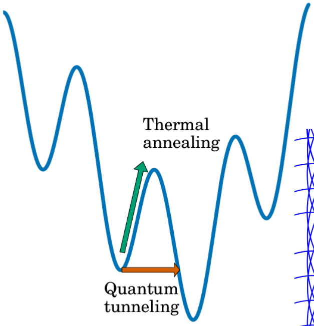
D-Wave mashine	qubits	couplers
2000Q (2017)	2000	6000
Advantage (2020)	5000	35000

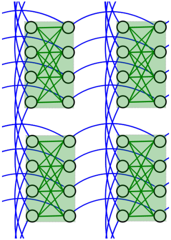
Universal (gate-based) vs. adiabatic quantum computer



Universal quantum computer
(unitary quantum operations, measurements)
general purpose
(**QUBO solution: QAOA/VQE/HHL**)

computer	qubits
IBM Q System One (2019)	20
IBM Osprey (2022)	433





Adiabatic quantum computer
adiabatic evolution of quantum state
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Quantum algorithms for tracking (QUBO)

Quantum Annealing (QA):

- Lucy Linder. *Using a Quantum Annealer for particle tracking at LHC*. 2019 - The HEPQPR.Qallse project encodes the HEP (ATLAS) pattern recognition problem into a QUBO and solves it using a D-Wave or other classical QUBO libraries (qbsolv, neal).
- Frédéric Bapst и др. "A pattern recognition algorithm for quantum annealers". В: *Comput. Softw. Big Sci.* 4.1 (2020), с. 1
- Parker S Reid. "Applied Quantum Annealing for Particle Tracking: Optimisation for the HL-LHC". Англ. Дис. ... маг. Simon Fraser University, 2021
- Alexander Zlokapa и др. "Charged particle tracking with quantum annealing optimization". В: *Quantum Machine Intelligence* 3.2 (нояб. 2021)

Variational Quantum Eigensolver (VQE):

- Tim Schwägerl и др. *Particle track reconstruction with noisy intermediate-scale quantum computers*. 2023

Quantum Approximate Optimization Algorithm (QAOA):

- Arianna Crippa и др. *Quantum algorithms for charged particle track reconstruction in the LUXE experiment*. 2023
- Lena Funcke и др. "Studying quantum algorithms for particle track reconstruction in the LUXE experiment". В: *Journal of Physics: Conference Series* 2438.1 (февр. 2023), с. 012127

Harrow–Hassidim–Lloyd (HHL):

- Davide Nicotra и др. *A quantum algorithm for track reconstruction in the LHCb vertex detector*. 2023

Quadratic unconstrained binary optimization (QUBO)

QUBO model or problem is defined as finding the binary vector $\boldsymbol{x}$ corresponding to[9]:

$$\min_{x \in \{0,1\}^n} \boldsymbol{x}^\intercal W \boldsymbol{x} + \boldsymbol{c}^\intercal \boldsymbol{x}$$

- $\boldsymbol{x} \in \mathbb{B}^n$ - set of vectors of fixed length $n > 0$
- $\mathbb{B} = \{0, 1\}$ - set of binary values (bits)
- $\boldsymbol{c} \in \mathbb{R}^n$; $W \in \mathbb{R}^{n \times n}$ - symmetric matrix whose elements $w_{\alpha\beta}$ determine the weights of each pair of indeces $\alpha, \beta \in \{1, \ldots, n\}$ of the binary vector
- Since $x_i^2 = x_i$ for $i \in \{1, \ldots, n\} \implies \boldsymbol{x}^\intercal W \boldsymbol{x} + \boldsymbol{c}^\intercal \boldsymbol{x} = \boldsymbol{x}^\intercal \left(W + \mathrm{diag}(\boldsymbol{c})\right) \boldsymbol{x}$
- Computational complexity of QUBO: the number of binary vectors-candidates rises exponentially with n ($|\mathbb{B}^n| = 2^n$).

[9] A.P. Punnen. *The Quadratic Unconstrained Binary Optimization Problem: Theory, Algorithms, and Applications*. Springer International Publishing, 2022.

Connection to Ising models

Replacing

$$x_i = \frac{1+\sigma_i}{2}, \qquad x_i \in \{0,1\},$$

QUBO is computationally equivalent to the Ising model, with the Hamiltonian:

$$H(\sigma) = -\sum_{\alpha<\beta} J_{\alpha\beta}\sigma_\alpha\sigma_\beta - \mu\sum_\beta h_\beta\sigma_\beta\,, \qquad \sigma_\alpha \in \{-1,+1\}.$$

QUBO on D-Wave: In order to solve a problem using QA, one can formulate the problem as a quadratic unconstrained binary optimization problem (QUBO) which is then easily recast into the problem Hamiltonian.

- coefficients of the quadratic model need to be set, so the **linear terms (biases)** evaluate qubits and **quadratic terms** asses the interactions between pairs of qubits (couplers).
- QUBO **cannot contain constraints** (by definition) - any constraints have to be added to the objective as penalties.
- $\mathcal{C}$ - the actual set of couplers between qubits is **restricted** in a real quantum annealer (chimera graph in D-Wave)

Note that:

1. not all couplings are available on the hardware, and therefore a process called minor embedding is needed to map the logical qubits to the physical ones.
2. Furthermore, there are specific ranges for h_i and J_{ij}, so that the coupling and the qubit bias require scaling.

Embedding constraints in QUBO

Penalty method for removing the constraints

Let us start with the penalty method for removing the constraints. Given a linear equality constraint of the form

$$\sum_{i=1}^{k} a_i y_i = b$$

where $a_i, b \in \mathbb{R}$, the transformation procedure simply transforms objective function E into

$$E(y_1, \ldots, y_k) + P\left(\sum_{i=1}^{k} a_i y_i - b\right)^2.$$

Results for SPD model data

Define the network energy s.t. its minimum corresponds to a track with smooth shape and without bifurcations.

- We formulated a QUBO based on the method of Denby (1988) and Peterson (1989) with several changes to improve the performance for SPD model data.

Our energy formula:

$$E = -\gamma \sum_{i,j,k} \left(\frac{\cos^{\lambda}(\theta_{ijk})}{(r_{ij} + r_{jk})^{\eta}} \right) s_{ij} s_{jk}$$

We favor a chain of short track segments s_{ij} and s_{jk} with a small angle θ.

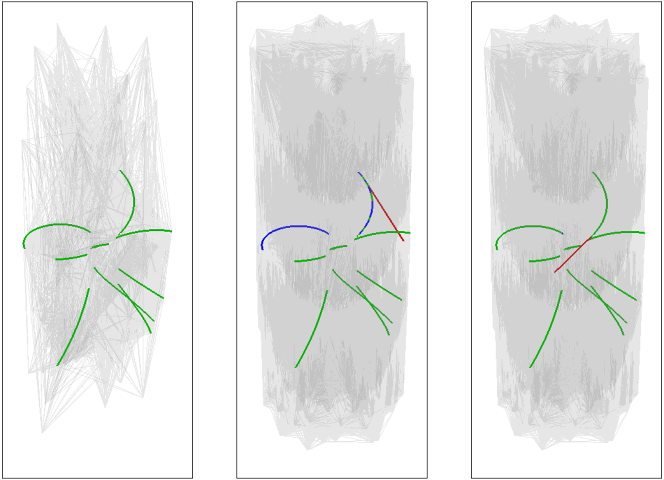
$$+ \alpha \left(\sum_{j \neq k} s_{ij} s_{ik} + \sum_{i \neq j} s_{ik} s_{jk} \right)$$

Penalty for bifurcation.

$$+ \beta \sum_{i,j} s_{ij}$$

In order to make the energy matrix sparse.

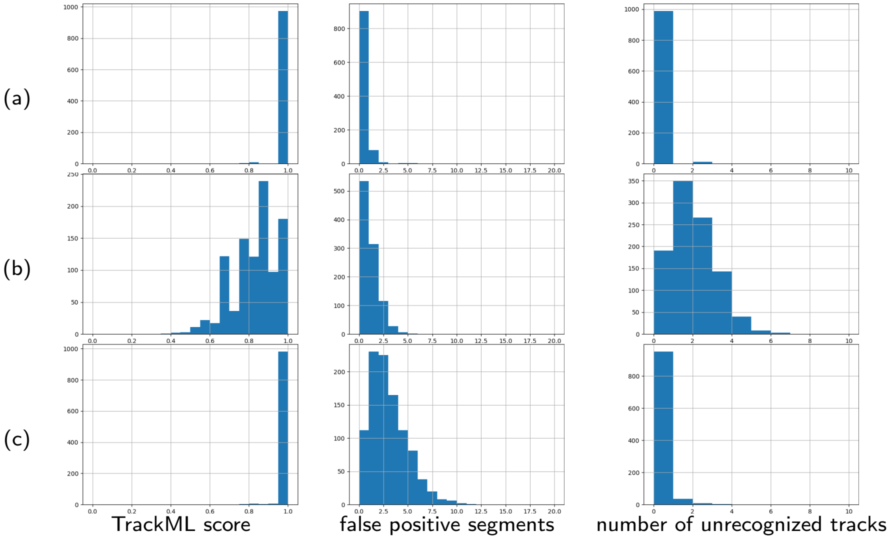
Results for SPD model data



100 noise hits | 1750 noise hits, priority to suppress false-positive segments | 1750 noise hits, priority to optimize TrackML score.

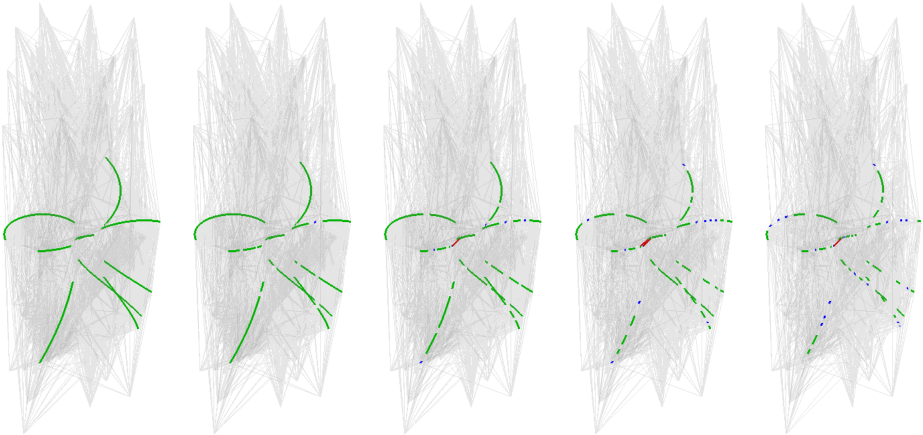
Tracking result of an event with 10 tracks.
(true positive true negative false positive false negative segments).

Results - score distributions



(a) 100 noise hits (b) 1750 noise hits, minimal number of false segments prioritized (c) 1750 noise hits, TrackML metric score prioritized

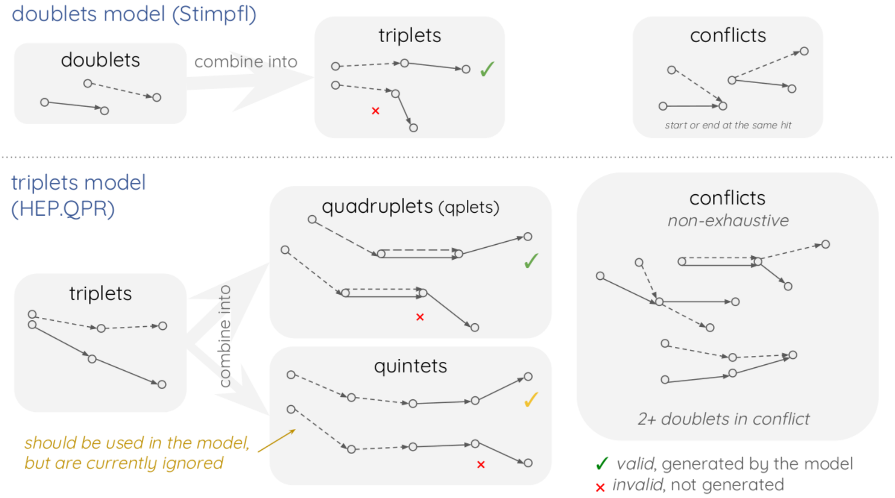
Effect of detector efficiency on tracking



Tracking result for different detector efficiencies (from left to right): 1.0,0.95,0.9,0.8,0.7.
(100 noise hits)

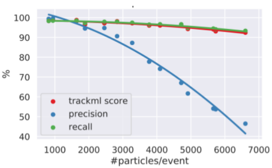
Algorithm improvements - triplet model

Using the potential of QUBO, we can use triplets instead of doublets in the model:

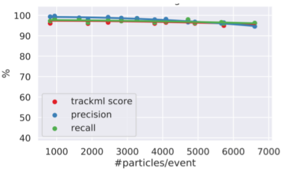


Lucy Linder. *Using a Quantum Annealer for particle tracking at LHC*. 2019

Algorithm improvements - triplet model

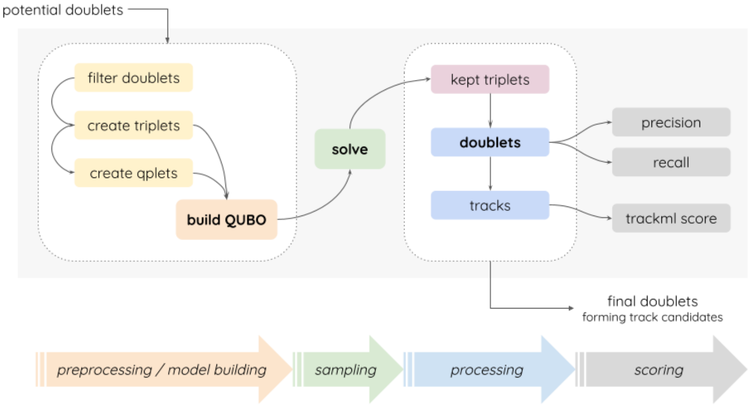


QallseMp (initial model)



QallseD0 (improved model)

Lucy Linder. *Using a Quantum Annealer for particle tracking at LHC.* 2019



Conclusions and outlook

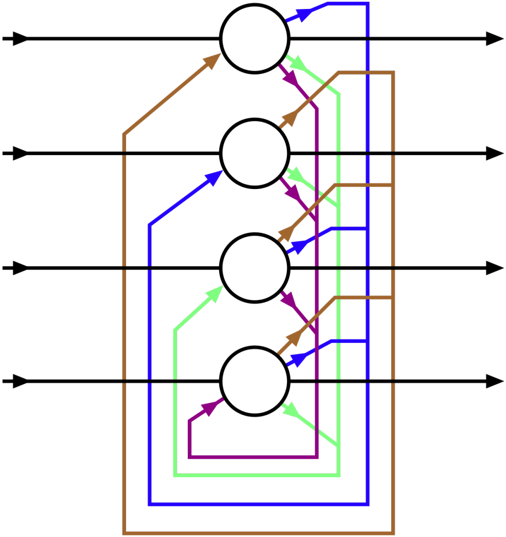
Conclusions

- An attempt to apply different modifications of the algorithm to the simulation of SPD data with noise hits (uniform distribution).
- We started to investigate the effect of detector efficiency on the tracking result.
- The method has shown good results, but under rather simple conditions. Noise hits pose notable difficulties for tracking with different methods.

Outlook

- We need to study the effect of events where fake hits are generated more correctly in terms of detector geometry (new model data soon).
- Add better segment filtering, which will possibly reduce the influence of noise hits, and also allow to test the method on TrackML competition data and compare the results.
- With the QUBO model, triplet and quadruplet (and quintet) tracking can be introduced into the Hopfield network - a dramatic reduction of false tracks is expected.
- Hyperparameter optimization.
- Other pre-/postprocessing schemes.

Thank you!



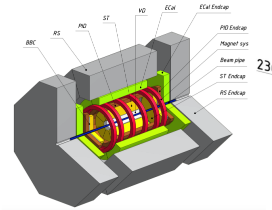
Hopfield network (with 4 neurons)

Conclusions and outlook

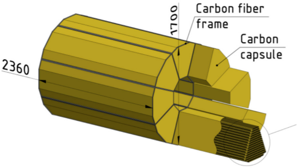
- Применение (модифицированного) подхода к данным MPD.
- Начат проект по включению триплетов, квадруплетов, квинтетов в модель QUBO (ветка проекта HEPQPR.Qallse, на HybriLIT установлены библиотеки qbsolve, neal для QUBO).
- Применение алгоритма QAOA, оценка скорости вычислений на гейтовой модели.
- Применение алгоритма HHL пока неактуально (большая глубина алгоритма для современных квантовых компьютеров).
- По мере совершенствования технологии квантового отжига (D-Wave), в будущем можно будет выработать стандардизированные тесты для сравнения с классическими алгоритмами, что позволит оценить целесообразность использования квантового оборудования в экспериментах ФВЭ.

Эксперимент SPD NICA

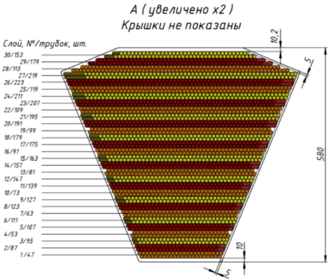
Коллаборация SPD (**S**pin **P**hysics **D**etector) планирует установить универсальный детектор во второй точке взаимодействия коллайдера NICA для изучения спиновой структуры протона, дейтрона и других явлений, связанных со спином, с помощью поляризованных пучков протонов и дейтронов при энергии столкновения до 27 ГэВ и светимости до $10^{32}\text{см}^{-2}\text{s}^{-1}$.
Данные о событиях из SPD будут поступать в виде тайм-слайсов в 10 мс, в каждом из которых будет происходить в среднем 40 событий, т. е. один тайм-слайс будет содержать 200 треков и 1100 хитов на одну станцию (причем 82,26% всех хитов являются фейками)[10].



Общая схема установки SPD.



Внешний вид SPD straw детектора (слева)



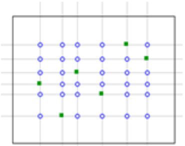
и его модуля в разрезе (справа).

Необходимо разработать алгоритм для онлайн фильтра, чтобы обрабатывать не менее 100 тайм-слайсов в секунду.

[10] D. Rusov et al, Deep Tracking for the SPD Experiment, Physics of Particles and Nuclei Letters, 2023, Vol. 20, No. 5, pp. 1180–1182.

Проблема фейковых хитов в straw-детекторе

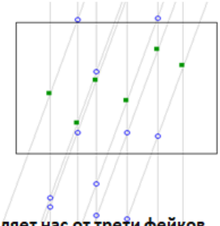
Главная трудность, вызванная спецификой **GEM детектора** – появление ложных отсчетов из-за лишних пересечений стрипов. Для **n** истинных хитов имеем **n^2 - n фейков!**

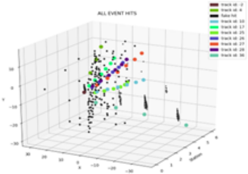


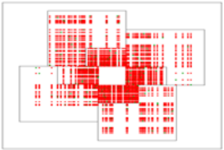
- истинный хит

- ложное пересечение

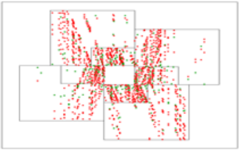
Можно уменьшить количество фейков – повернуть слой стрипов на маленький угол (5-15 градусов) по отношению к другому слою







Наклон 15° избавляет нас от трети фейков, но большая их часть остаётся.



Эти две проблемы, - наличие фейковых засорений данных и, главное, сверхвысокий темп их поступления из-за высокой светимости неизбежно требуют разработки новых методов трекинга с использованием глубоких нейронных сетей

- Механизм возникновения фейков такой же как в микростриповом GEM детекторе в BM@N.
- Трубки в straw детекторе уложены слоями 0°,5°,-5°, чтобы избавиться от значительной части из $n^2 - n$ фейков.

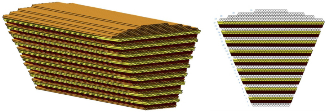
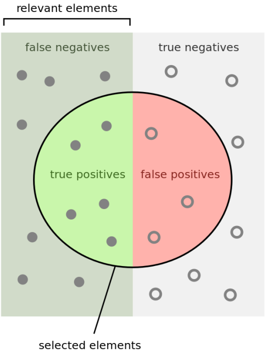


Figure 9.19: Sketch of one module (octant) of the barrel part of the straw tracker.

Схема модуля straw трекера в SPD.

Как оценивать результаты трекинга?

- TP (True Positives) - количество сегментов, верно определённых моделью как реальные;
- TN (True Negatives) - количество сегментов, верно определённых моделью как ложные;
- FP (False Positives) - количество сегментов, неверно определённых моделью как реальные;
- FN (False Negatives) количество сегментов, неверно определённых моделью как ложные;
- $D^* :=$ TP+FN - количество всех реальных сегментов (известных из симуляции Монте-Карло, или датасета, как TrackML)
- $D :=$ TP+FP - количество всех сегментов, которые модель реконструировала (множество треков, отобранных алгоритмом)



purity/precision:
Сколько отобранных элементов являются релевантными?

$$p = \frac{|D \cap D^*|}{|D|} = \frac{TP}{TP + FP}$$

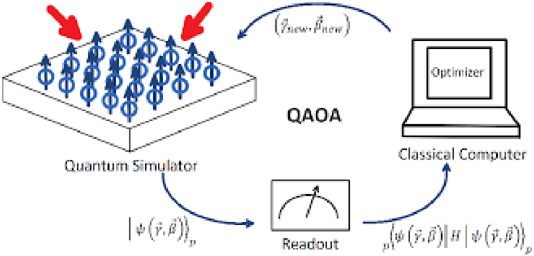
efficiency/recall:
Сколько релевантных элементов отбирается?

$$r = \frac{|D \cap D^*|}{|D^*|} = \frac{TP}{TP + FN}$$

Lucy Linder. *Using a Quantum Annealer for particle tracking at LHC*. 2019

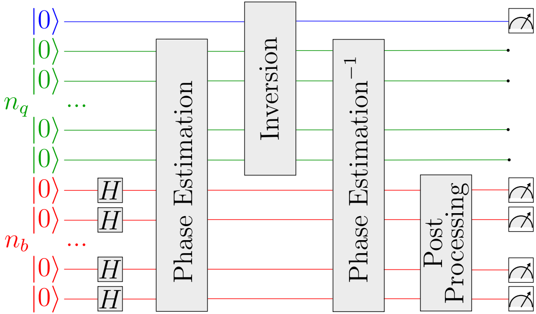
QAOA for tracking (gate-based)

- The QUBO problem can be mapped to the Ising Hamiltonian and solved using the variational quantum algorithm (VQE) or the quantum approximate optimization algorithm (QAOA) on universal (gate-based) quantum computers.
- A. Crippa et al., arXiv:2304.01690, L.Funcke et al., arXiv:2202.06874



HHL algorithm for tracking

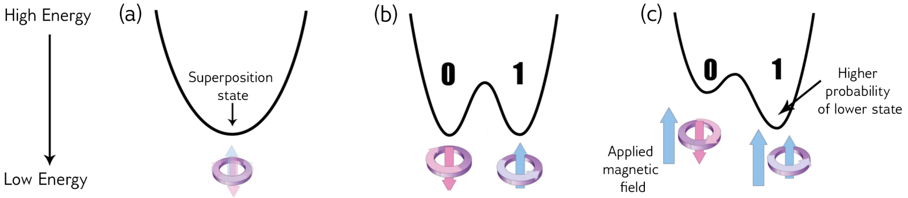
- В недавней работе[11] был представлен подход к использованию классической сети Хопфилда с добавлением алгоритма HHL, с **прямым применением к поиску треков**. Использовались данные детектора LHCb.
- Оптимизация сети Хопфилда превращается в задачу матричной инверсии и решается с помощью алгоритма HHL (Harrow-Hassidim-Lloyd - квантовый алгоритм для линейных алгебраических уравнений).

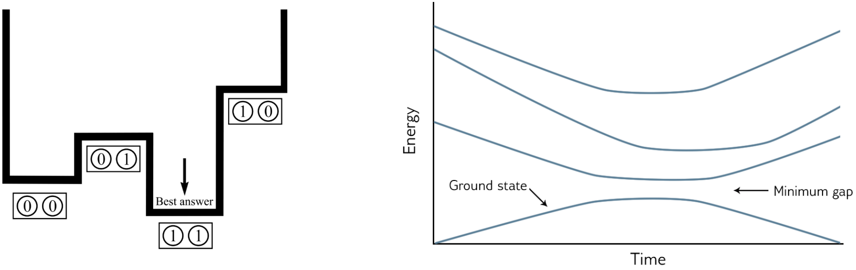


[11] Davide Nicotra и др. *A quantum algorithm for track reconstruction in the LHCb vertex detector*. 2023

Quantum annealing

A method for finding the global minimum of a given function.

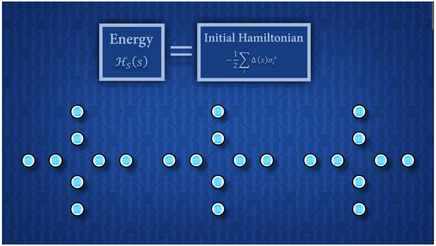




(Source: https://docs.dwavesys.com/)

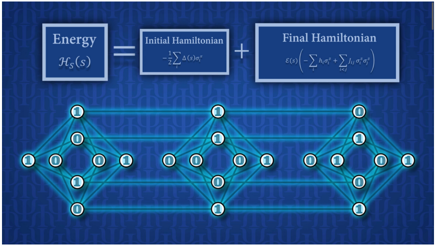
D-Wave's default anneal time is $20\mu s$ (but overhead cost, latencies, minor embedding, ...).

Quantum annealing scheme

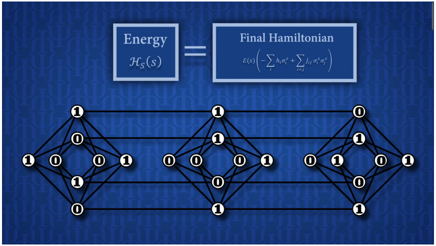


Transition from the **initial (tunneling) Hamiltonian** to the **problem Hamiltonian**.

↓

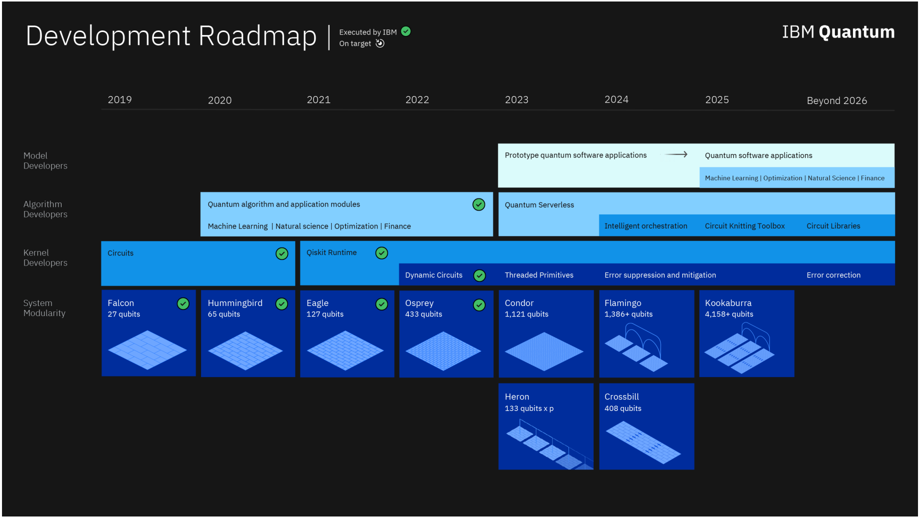


→



(Source: https://docs.dwavesys.com/)

Universal (gate-based) quantum computer



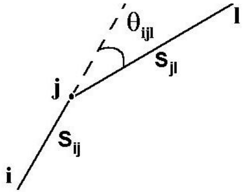
Literature

Quantum Annealing (QA) на D-Wave:

- Salvador E. Venegas-Andraca и др. "A cross-disciplinary introduction to quantum annealing-based algorithms". В: *Contemporary Physics* 59.2 (апр. 2018), с. 174—197
- https://quantum-ods.github.io/qmlcourse/book/dwave/ru/dwave.html

Tracking - method of segments

- Имеется множество N экспериментальных точек на плоскости. Требуется выбрать (распознать) среди них те, по которым проходит некоторое число непрерывных гладких кривых (треков).
- Вводится нейрон s_{ij} как направленный сегмент, соединяющий точки i, j.



- **Энергетический функционал** (Денби и Петерсон, 1988) состоит из двух частей:

$$E = E_{cost} + E_{constraint} ,$$

где

$$E_{cost} = -\frac{1}{2} \sum_{ijkl} \delta_{jk} \frac{\cos^{\lambda} \theta_{ijl}}{r_{ij} + r_{kl}} s_{ij} s_{kl} ,$$

поощряет связи нейронов соответствующим коротким смежным сегментам с малым углом между ними.

$$E_{constraint} = +a \left(\sum_{j \neq k} s_{ij} s_{ik} + \sum_{i \neq j} s_{ik} s_{jk} \right) + b \left(\sum_{i,j} s_{ij} - N \right)^2$$

запрещает как межтрековые связи (бифуркации), так и чрезмерный рост числа самих треков.

Квантовый отжиг для трекинга - общий вид QUBO

$$E = -\frac{1}{2}\left[\sum_{i,j}\left(W_{ij}^{\text{reward}} - W_{ij}^{\text{penalty}}\right) s_{ij}\right.$$

внешнее взаимодействие

$$\left. + \sum_{i,j,k}\left(U_{ijk}^{\text{reward}} - U_{ijk}^{\text{penalty}}\right) s_{ij} s_{jk}\right],$$

взаимодействие двух сегментов

$$E = -\sum_{i,j,k}\left(\frac{\cos^{\lambda}(\theta_{ijk}) + \rho\cos^{\lambda}(\phi_{ijk})}{r_{ij} + r_{jk}}\right) s_{ij} s_{jk}$$

Награждение в случае, что сегменты s_{ab} и s_{bc} короткие и изменение направления маленькое.

$$+ \eta \sum_{i,j,k}\left(z_k - \frac{z_k - z_i}{r_k - r_i} r_k\right)^{\zeta} s_{ij} s_{jk}$$

Штраф за отклонение перекрёстного члена между s_{ab} и s_{ac} от направления к центру столкновения.

$$+ \alpha\left(\sum_{j \neq k} s_{ij} s_{ik} + \sum_{i \neq k} s_{ij} s_{kj}\right)$$

Штраф за ветвление трека.

$$- \sum_{i,j}\left(\beta P(s_{ij}) - \gamma\right) s_{ij},$$

Награда сегменту в зависимости от априорной вероятности его активности $P(s_{ab})$.

Alexander Zlokapa и др. "Charged particle tracking with quantum annealing optimization". В: *Quantum Machine Intelligence* 3.2 (нояб. 2021)

Квантовый отжиг для трекинга - метод сегментов и QUBO

Alexander Zlokapa и др. “Charged particle tracking with quantum annealing optimization”. В: *Quantum Machine Intelligence* 3.2 (нояб. 2021)