Charged Particle Tracking as a QUBO Problem Solved with Quantum Annealing-inspired Optimization

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Outline

- Forewords on charged particle tracking and dataset
- Introduction to D-Wave and quantum annealing
- Hopfield Network and segment classification as a QUBO problem
- Results and outlooks
The Challenge of Charged Particle Tracking at the HL-LHC
Tracking in a Nutshell

- Particle trajectory bended in a solenoid magnetic field
- Curvature is a proxy to momentum
- Particle ionize silicon pixel and strip throughout several concentric layers
- **Thousands of sparse hits**
- Lots of hit pollution from low momentum, secondary particles

- **Explosion of hit combinatorics** in both seeding and stepping pattern recognition
- **Highly time consuming task** in extracting physics content from LHC data
Cost of Tracking

• CPU time consumption in HL-LHC era **surpasses computing budget**
  → Need for **faster algorithms**
• Charged particle track reconstruction is one of the most **CPU consuming task** in event reconstruction
  → Optimizations **mostly saturated**
• Large fraction of CPU required in the HLT. **Cannot perform tracking inclusively**
  → **Approximation** allowed in the trigger

![Graph showing time/event vs. luminosity for CMS simulation](image1)

![Graph showing <μ> vs. job count for ATLAS](image2)

@HL-LHC <μ> >200
Fast Hardware Tracking

- Track trigger implementation for Trigger upgrades development on-going
- Several approaches investigated
- **Dedicated hardware is the key** to fast computation.
- **Not applicable for offline** processing unless through adopting heterogeneous computing.

![Kalman Filter in MaxJ](image1)

![Tracklets](image2)

**Firmware Implementation - Bin**
- Each bin represents a $\sqrt{x}$ column in the HT array

**Hough Transform**
- Stubs $\phi_{st}$ at left boundary
- Sorts $\phi_{st}$ at right boundary
- Duplicates stubs if it belongs to two cells.
- Track Builder:
  - Sorts stubs in $\phi_{st}$ cells.
  - Marks $\phi_{st}$ cells with stubs in at least 4/5 layers.
- Hand Shake:
  - Controls read-out of candidates
Deep Learning Approaches

https://heptrkx.github.io/
https://indico.cern.ch/event/587955/contributions/2937540/

https://tinyurl.com/yb3v93y9
https://indico.cern.ch/event/587955/contributions/2937570/
Charged Particle Tracking Dataset

- This work uses the public dataset of the TrackML Particle Tracking Challenge (Kaggle, codalab).
- Simulating the dense environment expected for HL-HLC. Average of 200 proton-proton interaction per bunch crossing.

https://www.kaggle.com/c/trackml-particle-identification
https://competitions.codalab.org/competitions/20112
Motivation

• Classical charged particle tracking algorithms suffer from combinatorial explosion

• Embrace the combinatorics considering all possible branches of track candidates, and solve the complex optimization problem with quantum annealing
The D-Wave Computing System
D-Wave 2X™

1098 qubits
Operates at 15mK
Anneals in 5-20 μs
qubit and qubit

Quantum Circuits
Series of quantum gates operating on a set of quantum states.

Quantum Annealing
Evolution of a quantum system to a low T Gibbs state
That's D-Wave!
Quantum Annealing
Adiabatic Quantum Annealing

➢ System setup with trivial hamiltonian $H(0)$ and ground state
➢ Evolve adiabatically the hamiltonian towards the desired Hamiltonian $H_p$
➢ Adiabatic theorem: with a slow evolution of the system, the state stays in the ground state.

$$H(t) = A(t)H(0) + B(t)H_p$$

Space of Hamiltonian

\[ H_{\text{Ising}} = \sum_i h_i \sigma_i^z + \sum_{i,j} J_{ij} \sigma_i^z \sigma_j^z \]

- \( H_{\text{Ising}} \) represents the Ising Hamiltonian.
- \( h_i \) and \( J_{ij} \) are external magnetic fields and interaction terms, respectively.
- \( \sigma_i^z \) and \( \sigma_j^z \) are Pauli Z operators for quubits.

**Chimera graph embedding**

- Runs over **all** quBit pairs
- Runs over **adjacent** quBits

- \( \sim 1000 \) qubits on chimera graph can only encode \( \sim 40 \) qubits full Ising Hamiltonian
- Quadratic Unconstrained Binary Optimization (QUBO) can be mapped to an Ising Hamiltonian with change of variable \( \{0,1\} \leftrightarrow \{-1,1\} \)
Ising Model Heuristic Solution

- Monte-Carlo based method to find ground state of energy functions
- Random walk across phase space
  - accepting descent
  - accepting ascent with probability $e^{-\Delta E/kT}$
- Decrease $T$ with time

Applied to the QUBO problem, and finds the **ground state**. SA in the legends.
Charged Particle Tracking using Adiabatic Quantum Annealing

See also H. Gray et al.
https://indico.cern.ch/event/708041/contributions/3308730/
Hopfield Network Approach

- Developed by John Hopfield in 1982
- fully-connected, single-layer NN; complete graph
- vertices: \( n \) binary units, \( \{ s_n \} \in \{0, 1\}^n \)
- edges: symmetric weight matrix, \( w \in \mathbb{R}^n \times \mathbb{R}^n \)
- energy associated with each network configuration (assignment of units):
  \[
  E = -\frac{1}{2} \sum_{i,j} w_{ij} s_i s_j \quad \text{QUBO!}
  \]

[Peterson, 1989]
Framing the Problem

- **Segment** ≡ *pair of hits* on consecutive layers of the detector
- Assign a **boolean to each segment** representing whether the segment is within a track or not

- Limits the number of hits/segments
  - Separating the hits in **16 sector in φ**
  - Pre-filtering the segments on Δφ and Δz to reduce the number of spurious bad segments

- Segment opening in r-phi-z plane in which helical segments are aligned
- Azimuthal angle in cartesian coordinate in which high pT tracks segments are straight
Segment QUBO

**Helix Term**
Segments along an helix

\[
\sum_{a,b,c} \left( \frac{\cos^\lambda \theta_{abc} + \rho \cos^\lambda \phi_{abc}}{r_{ab} + r_{bc}} \right) s_{ab} s_{bc}
\]

**High pT Term**
Aligned pair of segments

\[
+ \eta \left( \frac{z_c - r_c}{r_c - r_a} \right) s_{ab} s_{bc}
\]

**Beam spot Term**
Segment pointing at the origin

\[
+ \alpha \left( \sum_{a,b \neq c} s_{ab} s_{ac} + \sum_{a \neq b,c} s_{ac} s_{bc} \right) + \sum_{a,b} \left( \beta + \gamma P(s_{ab}) \right) s_{ab}
\]

**Bifurcation Term**
No shared hits on valid segment

**Inhibition Term**
Reduced number of segments

**GP Term**
Use the quality of segment
Resolving Sub-Group

- Full all-to-all QUBO problem cannot fit on dWave. Aim at identifying sub-groups of segments that can fit on the hardware

- Train a gaussian kernel density estimator on true single segment
- Aiming at reducing the number of false segments, retaining

- Force segment off based on $\cos\theta_{abc}$
  - $\cos\theta_{abc} = 0$ if $\theta_{abc} > \theta_0$
- 5 best neighbors
- Solvable in polynomial time
QA-Tracking Workflow

1. Resolving Sub-group \((\theta_0)\)
2. Segment QUBO
3. Resolving Sub-group \((\theta_1)\)
4. Segment QUBO
Performance

- Simulated annealing and Quantum annealing are in perfect agreement at 200 tracks.
- Simulated annealing solves the exact problem at all multiplicity.
- Limitation on number of qubits prevents from solving events beyond 200 tracks on Dwave; solving a contrive problem.
- Purity and Efficiency are measured with respect to true tracks with at least three hits.

Promising tracking efficiency for the algorithm up to 2000 tracks per event.
Conclusion

- QMLQCF Scouting for applications of quantum annealing (among others) in HEP

- Charged particle tracking interpreted as a segment classification can be expressed in a QUBO problem

- Experimentation on dWave imposes some stringent algorithmic restrictions

- Limited hardware size limits the complexity of the problem that can be solved
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Problem Parameters Optimization

- Parameters of the hamiltonian are tuned using bayesian optimization, modeling the figure of merit with gaussian processes.

- Accuracy (# of properly labeled / # of segments) use as f.o.m

- Global inhibition model: $\alpha=3.\times10^{-3}$, $\beta=2.63\times10^{-8}$, $\lambda=7$

- Threshold model: $\alpha=5.\times10^{-3}$, $\beta=1.\times10^{-6}$, $\lambda=7$
Edge Affinity

- Helical bias: tracks are straight in cylindrical coordinates
- Momentum bias: high-PT tracks are straight in rectangular coordinates
- Short-edge bias: long tracks of short edge segments

\[ \sum_{a,b,c} \cos^\lambda \theta_{ab} + \rho \cos^\lambda \phi_{ab} \]

\[ r_{ab} + r_{bc} \]

\[ s_{ab}s_{bc} \]

\[ \text{Short-edge bias} \]

\[ \text{Ising variables (1 or 0)} \]
Cross-Term Penalties

- Beam spot penalty: penalize tracks that originate further from the origin

\[
\sum_{a,b,c} \eta \left( z_c - \frac{z_c - z_a}{r_c - r_a} r_c \right)^z s_{ab} s_{bc}
\]

Z-intercept penalty

Ising variables (1 or 0)
Single-Edge Bias

• Global inhibition: limits total number of edges turned on
• Prior probability: Bayesian prior based on edge position in \( rz \)-plane
  • Computed using Gaussian kernel density estimation

\[
\sum_{a,b} \left[ \beta + \gamma P(s_{ab}) \right] s_{ab}
\]

Ising variable (1 or 0)
Extra Material
References


Kaggle.”TrackML Particle Tracking Challenge.” n.d. Web. <29 June 2018>
Welcome to the Future
Quantum Computing for the Real World Today

https://www.dwavesys.com/

1999  Founded
2011  D-Wave One : 128 qubits
2013  D-Wave Two : 512 qubits
2015  D-Wave 2X : 1000 qubits
2019? 5000 qubits ?
D-Wave Hamiltonian
And
Chimera Graph
D-Wave Hamiltonian

\[ H_{\text{Ising}} = \sum_i h_i \sigma_i^z + \sum_{i,j} J_{ij} \sigma_i^z \sigma_j^z \]

- External magnetic field
- Interactions runs over adjacent qubits
D-Wave qubit Adjacency

Active qubits in green
Coupling to 5-6 qubits
Inactive qubits in red
Not a fully connected graph
Model Embedding
Full Ising Model

- Create chains of spins through the chimera graph
- Split local fields across all qubits in the chain
- Tightly couple ($J_F=6$)
- Non-unique embedding. Heuristic approach.
- Suppressing spin flip within chain as error correction.
- Use majority vote

➔ Approximately full Ising Model with ~<40 spins

https://arxiv.org/abs/1210.8395
Ising Hamiltonian

\[ H_{\text{Ising}} = \sum_i h_i \sigma_i^z + \sum_{ij} J_{ij} \sigma_i^z \sigma_j^z \]

Runs over all quBit pairs

External magnetic field

Interactions
High Luminosity LHC
The Challenge
HL-LHC Challenge

- CPU time extrapolation into HL-LHC era far surpasses growth in computing budget
- Need for faster algorithms
- Approximation allowed in the trigger
Complexity and Ambiguity

Shown trajectories are reconstructed objects

The future holds much more hits
HEP.TrkX Approaches

End-to-end hit assignment

Track following with RNN

https://heptrkx.github.io/

https://tinyurl.com/y87saehf
Tracking **Not** In a Nutshell

- Hits preparation
- Seeding
- Pattern recognition
- Track fitting
- Track cleaning

Several Times
Hit Preparation

- Calculate the hit position from barycenter of charge deposits
- Use of neural net classifier to split cluster in ATLAS
- Access to trajectory local parameter from cluster shape
- Remove hits from previous tracking iterations
- HL-LHC design include double layers giving more constraints on the local trajectory parameters
Seeding

- Combinatorics of 2 or 3 hits with tight/loose constraints to the beam spot or vertex

- Seed cleaning/purity plays in an important in reducing the CPU requirements of subsequent steps
  - Consider pixel cluster shape and charge to remove incompatible seeds

- Initial track parameters from helix fit
Pattern Recognition

- Use of the Kalman filter formalism with weight matrix
- Identify possible next layers from geometrical considerations
- Combinatorics with compatibles hits, retain N best candidates
- No smoothing procedure
- Resilient to missing modules
- Hits are mostly belonging to one track and one track only
- Hit sharing can happen in dense events, in the innermost part
- Lots of hits from low momentum particles
Kalman Filter

- Trajectory state propagation done either
  - Analytical (helix, fastest)
  - Stepping helix (fast)
  - Runge-Kutta (slow)
- Material effect added to trajectory state covariance
- Projection matrix of local helix parameters onto module surface
  - Trivial expression due to local helix parametrisation
- Hits covariance matrix for pixel and stereo hits properly formed
  - Issue with strip hits and longitudinal error being non gaussian (square)

\[
K_k = C_{k|k-1} H_k \top (V_k + H_k C_{k|k-1} H_k \top)^{-1}
\]
\[
p_{k|k} = p_{k|k-1} + K_k (m_k - H_k p_{k|k-1})
\]
\[
C_{k|k-1} = (I - K_k H_k) C_{k|k-1}
\]

- $H_k$ is the projection matrix
- $V_k$ is the hit covariance matrix
- $p_{ij}$ is the trajectory state at i given j
- $C_{ij}$ is the trajectory state covariance matrix at i given j
Track Fitting

- Use of the Kalman filter formalism with weight matrix
- Use of smoothing procedure to identify outliers
- Field non uniformity are taken into account
- Detector alignment taken into account
Cleaning, Selection

- Track quality estimated using ranking or classification method

→ Use of MVA

- Hits from high quality tracks are removed for the next iterations where applicable
A Charged Particle Journey
First order effect: electromagnetic elastic interaction of the charge particle with nuclei (heavy and multiply charged) and electrons (light and single charged)

Second order effect: inelastic interaction with nuclei.
Magnetic Field

- Magnetic field $B$ acts on charged particles in motion: Lorentz Force

- The solution in uniform magnetic field is an helix along the field: 5 parameters

- Helix radius proportional to the component of momentum perpendicular to $B$

- Separate particles in dense environment

  ➔ Bending induces radiation: bremsstrahlung

  ➔ The magnetic field has to be known to a good precision for accurate tracking of particle
Multiple Scattering

- **Deflection on nuclei** (effect from electron are negligible)
- Addition of scattering processes
- Gaussian approximation valid for substantial material traversed

**Gaussian Approximation**

\[ \theta^2 = \left( \frac{13.6 \text{MeV}}{\beta c \rho} \right)^2 \times \frac{x}{X_0} \]

- \( \beta \) - particle velocity
- \( \rho \) - material density
- \( P \) - particle momenta
Bremsstrahlung

- Electromagnetic radiation of charged particles under acceleration due to nuclei charge
- Significant at low mass or high energy
- Discontinuity in energy loss spectrum due to photon emission and track curvature
  → Can be observed as kink in the trajectory or presence of collinear energetic photons
Energy Loss

- Momentum transfer to electrons when traversing material (effect of nuclei is negligible)

\[
dE / dx = k_1 \frac{Z}{A} \frac{1}{\beta^2} \rho \left( \ln \left( \frac{2m_e c^2 \beta^2}{I (1 - \beta^2)} \right) - \beta^2 - \frac{\delta}{2} \right)
\]

- Energy loss at low momentum depends on mass: can be used as mass spectrometer

\[\beta \text{ - particle velocity} \]
\[\rho \text{ - material density} \]
\[Z \text{ - atomic number of absorber} \]
\[A \text{ - mass number of absorber} \]
\[I \text{ - mean excitation energy} \]
\[\delta \text{ - density effect correction factor - material dependent and } \beta \text{ dependent} \]

ALICE Experiment
Summary on Material Effects

- Collective effects can be estimated statistically and taken into account in how they modify the trajectory

- Bremstrahlung and nuclear interactions significantly distort trajectories