Investigating the use of Quantum Annealing for Tracking, using the TrackML Dataset.

TrackML Challenge Grand Finale
CERN, July 1-2 2019

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on behalf of the **HEP.QPR**
and **QMLQCF** project teams,
with material from Heather M. Gray.

Motivation

Charged particle tracking is a computing intensive task, and mostly combinatorics.

Embrace complexity and aim to resolve combinatorics with the use of quantum computing.

Familiarize with quantum computers, and start approaching problems differently.

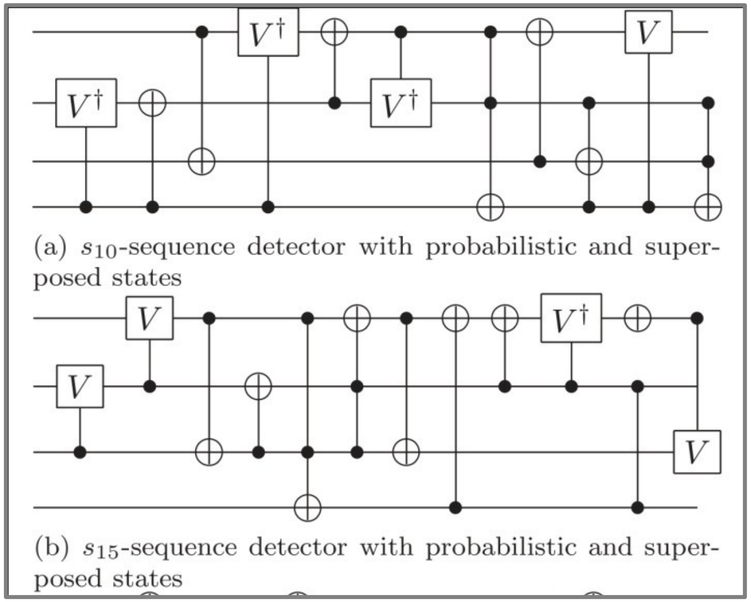
Outline

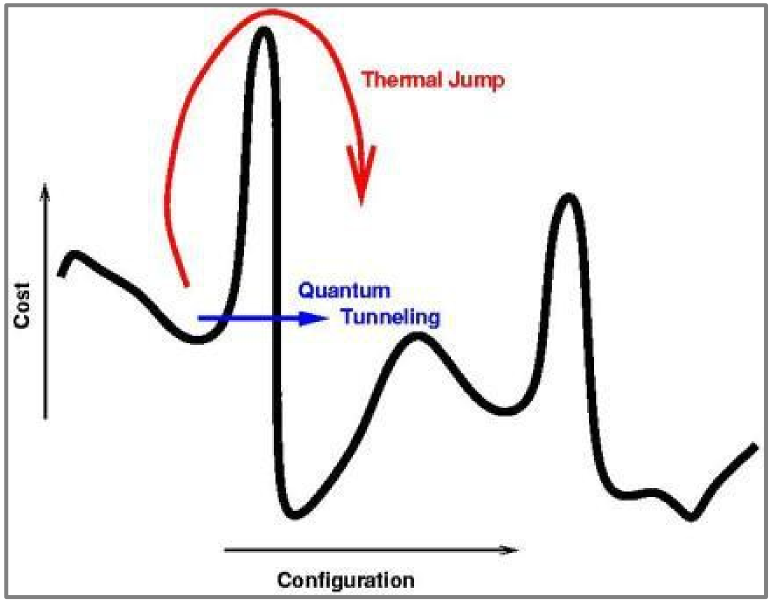
- Introduction to D-Wave and quantum annealing (QA)
- Tracking with Segment classification as a QUBO problem
- Tracking with Triplet classification as a QUBO problem
- Ambiguity resolution with QA

The D-Wave Computing System

D-Wave 2X^{TM}

qubit and qubit





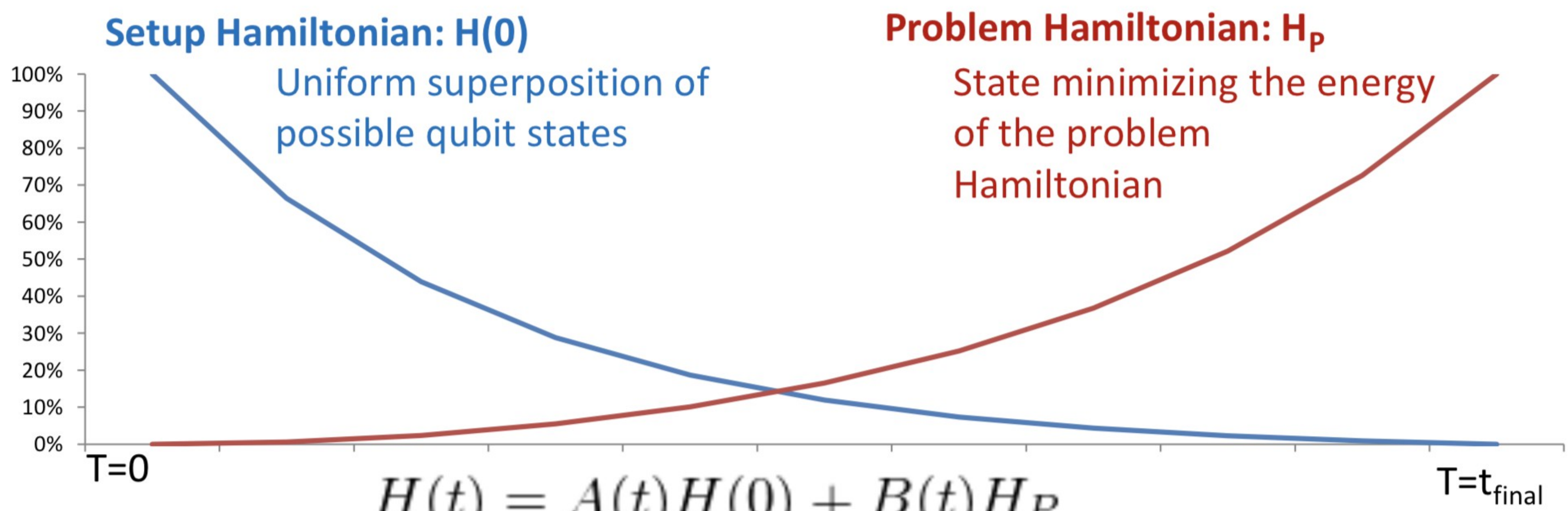
<u>Quantum Circuits</u>
Series of quantum gates operating on a set of quantum states.

<u>Quantum Annealing</u>
Evolution of a quantum system to a low T Gibbs state
That's D-Wave !

Quantum Annealing

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.



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

https://arxiv.org/abs/quant-ph/0001106
https://arxiv.org/abs/quant-ph/0104129

Space of Hamiltonian

Runs over **all** qubit pairs

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

External magnetic field

Interactions

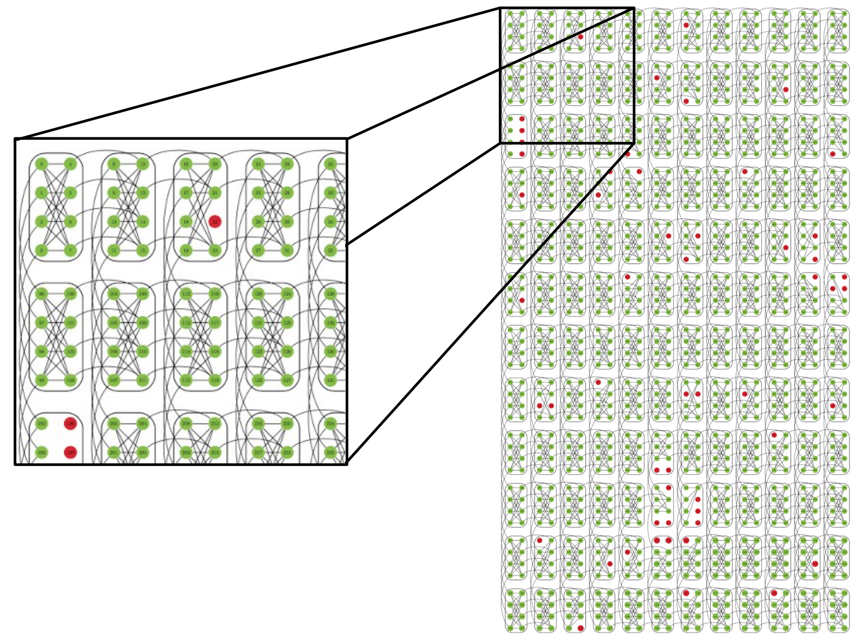
Chimera graph embedding

Runs over **adjacent** qubits

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

External magnetic field

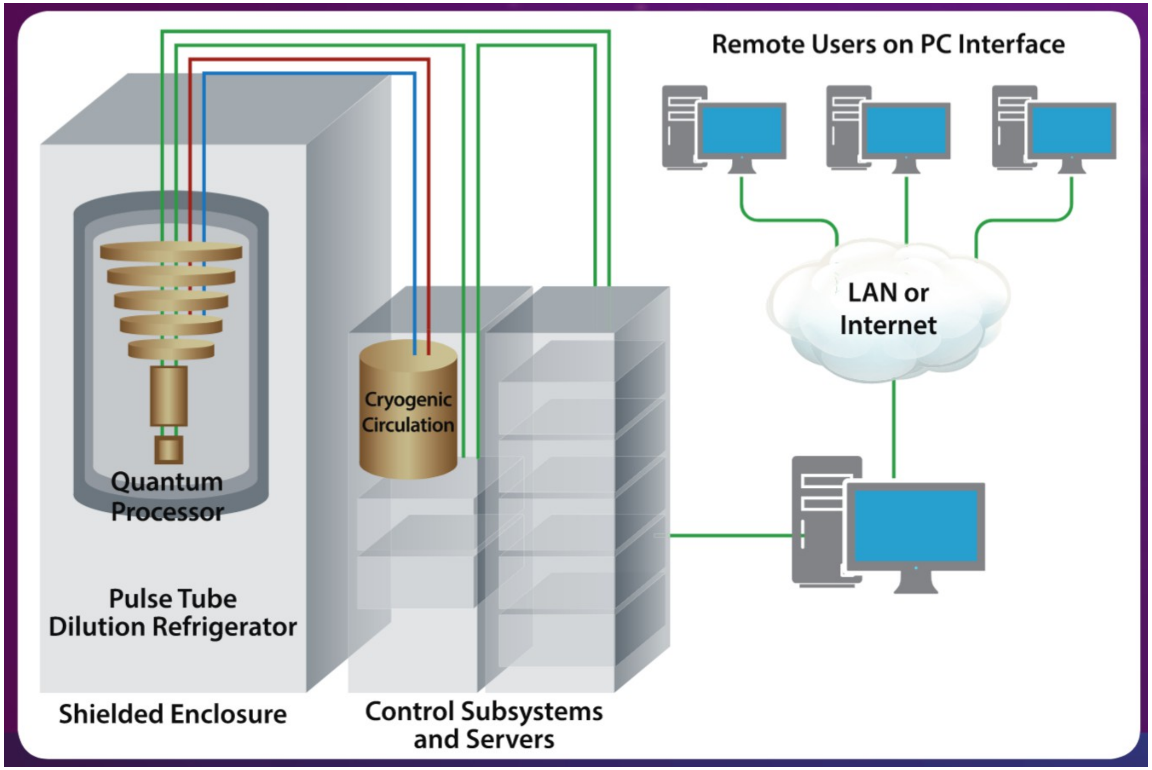
Interactions



- ~1000 qubits on chimera graph can only encode ~40 qubits full Ising Hamiltonian
- **Quadratic Unconstrained Binary Optimization** (QUBO) can be mapped to an Ising Hamiltonian with change of variable {0,1}↔{-1,1}
- Next generation (pegasus) will have better connectivity

Solving QUBO

Working on a D-Wave



- Web Interface to post the problem settings (Hp).
- A/synchronous processing.
- Distributed library for performing embedding
- Equivalent restapi to submit and retrieve solutions

➢ D-Wave processor as a service

https://www.dwavesys.com/take-leap

D-WaveSolutions

User provides

$(\mathbf{h_i} , \mathbf{J_{ij}})$

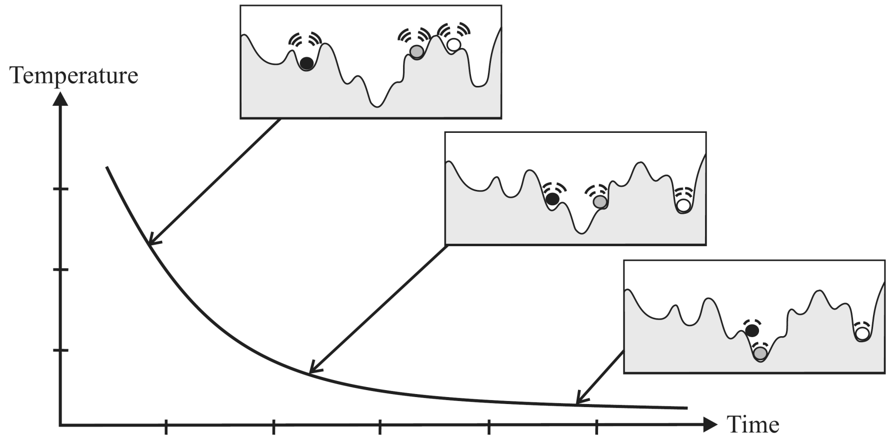
Multiple 5-20 μs
annealing cycles

D-Wave provides sampling
from lowest energy levels
(appox. Gibbs)

$(\{\boldsymbol{\sigma}_i\}_k, \mathbf{N}(\{\boldsymbol{\sigma}_i\}_k))$

Simulated Annealing

- Purely "classical" 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**.

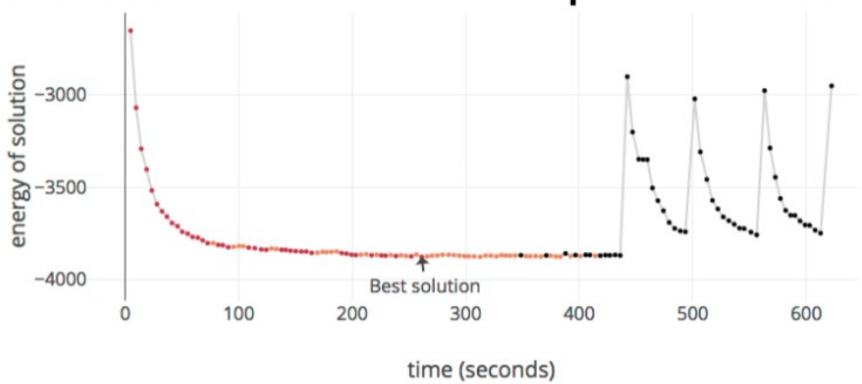
qbsolve

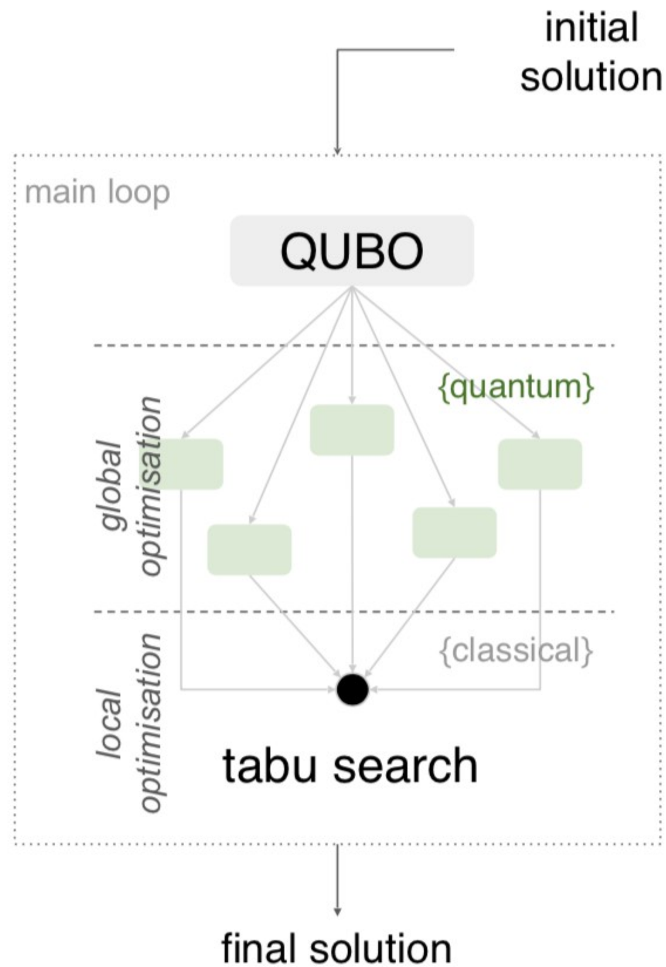
iterative hybrid classical/quantum algorithm

QBSOLV

large and/or densely connected QUBOs split into sub-QUBOs fitting the D-Wave hardware.

Tabu search on the recomposed solutions.





evolution of the solution in each qbsolv loop.
The solution is sometimes randomised to escape local minima.

Slide L. Linder

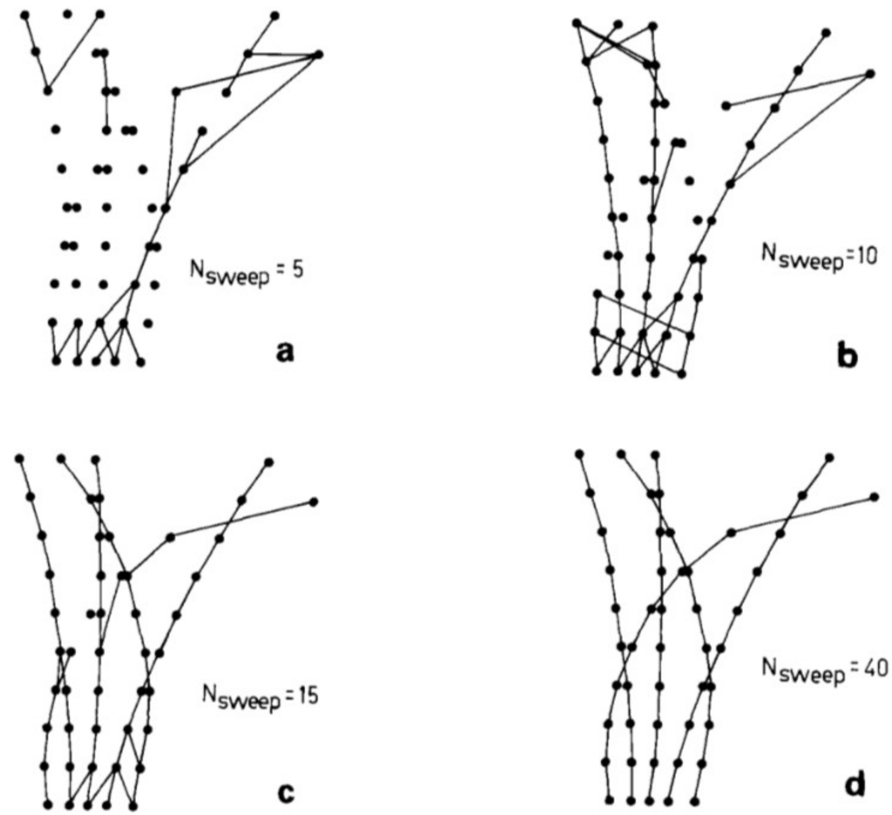
Charged Particle Tracking using Adiabatic Quantum Annealing through doublet classification

QMLQCF

Hopfield Network

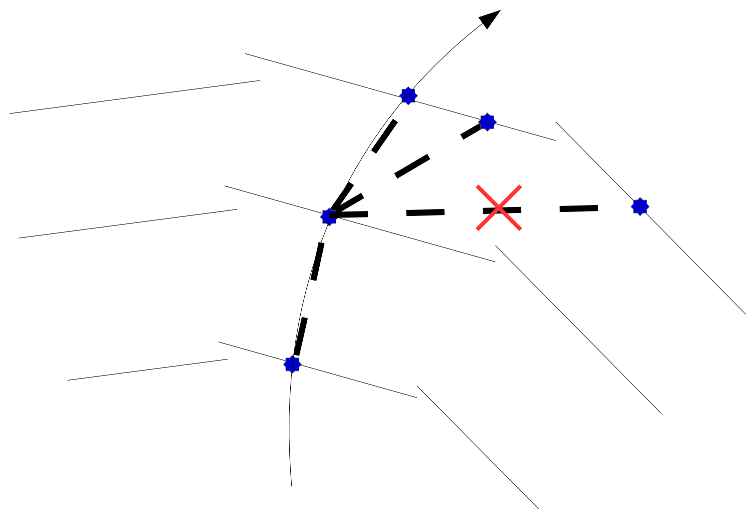
- Developed by John Hopfield in 1982
- fully-connected, single-layer NN; **complete graph**
- vertices: n binary units, $\{s_n\} \in \{0,1\}^n$
- edges: symmetric weight matrix, $w \in \mathbb{R}^n \times \mathbb{R}^n$
- energy associated with each network configuration (assignment of units):

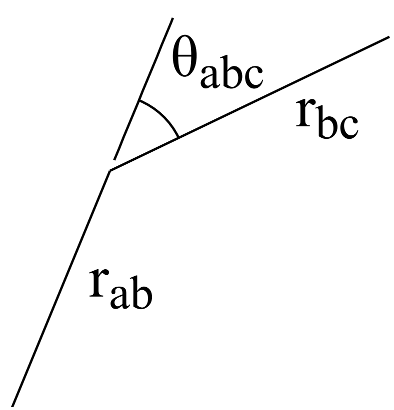
$$E = \boxed{-\frac{1}{2}\sum_{i,j} w_{ij} s_i s_j}$$ **QUBO!**



[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
  - No double hit per layer
  - 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

High pT Term
Aligned pair of segments

Beam spot Term
Segment pointing at the origin

$$\sum_{a,b,c}\left(\frac{\cos^{\lambda}\theta_{abc}+\rho\cos^{\lambda}\phi_{abc}}{r_{ab}+r_{bc}}+\eta\left(z_c-r_c\frac{z_c-z_a}{r_c-r_a}\right)^{\zeta}\right)s_{ab}s_{bc}$$

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

Bifurcation Term
No shared hits on valid segment

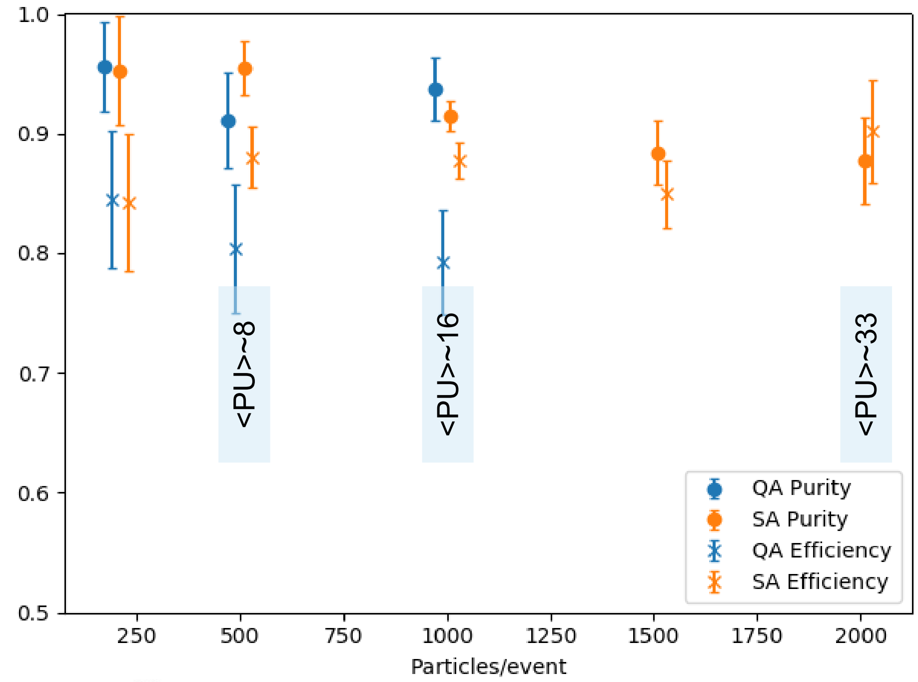
Inhibition Term
Reduced number of segments

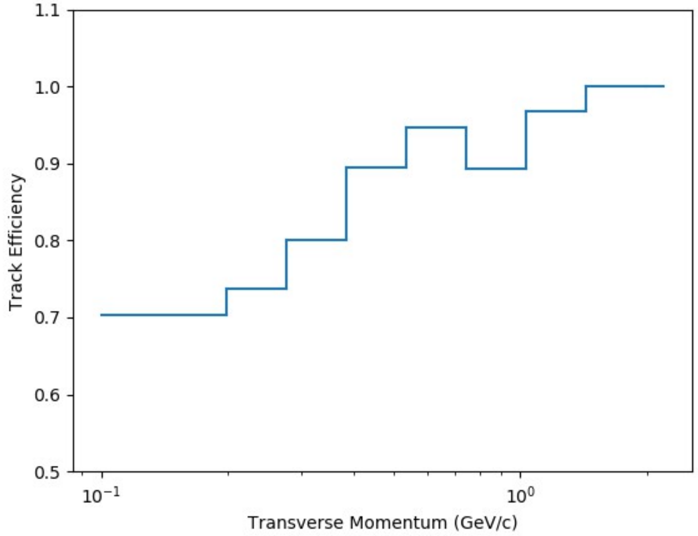
GP Term
Use the quality of segment

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





Charged Particle Tracking using Adiabatic Quantum Annealing through **triplet** classification

https://arxiv.org/abs/1902.08324

HEP.QPR

https://hep-qpr.lbl.gov/

Stimpfl-Abele & Garrido

- *"regard a track with n hits as a set of n-1 consecutive lines [doublets] with a smooth shape and without bifurcation".*
- Algorithm
  - Generate the set of potential doublets (apply cleaning cuts)
  - Binary classification task to determine which doublets should be kept in the track candidates, using Hopfield Networks

Fig. 2. Display of all generated lines for a real $Z^0 \rightarrow$ hadrons (RZ projection).

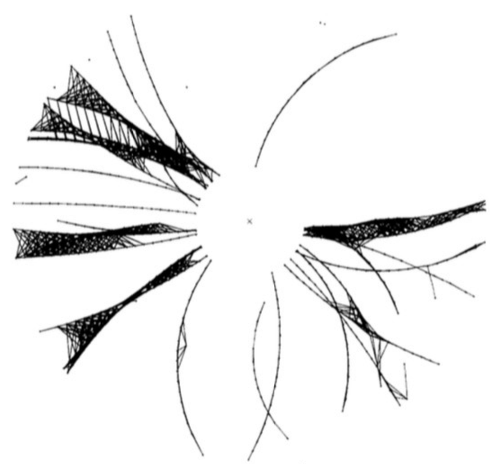


Fig. 1. Display of all generated lines for a real $Z^0 \rightarrow$ hadrons (XY projection).

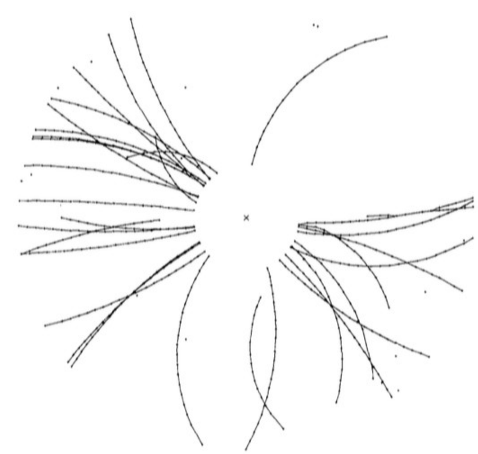
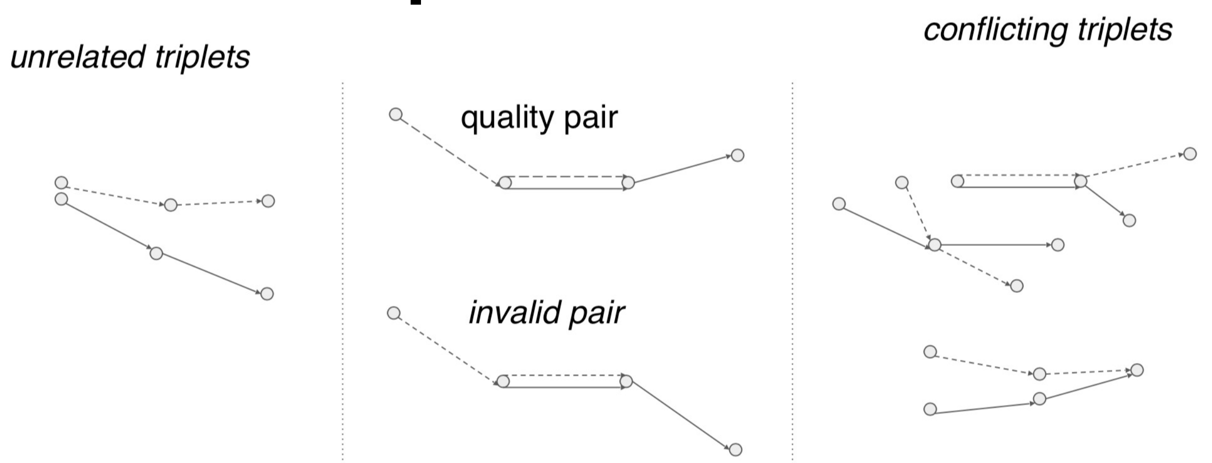


Fig. 3. Display of the activated lines after convergence for a real $Z^0 \rightarrow$ hadrons (XY projection).

https://www.sciencedirect.com/science/article/pii/001046559190048P

Triplet QUBO



$$O(a,b,T) = \sum_{i=1}^{N} a_i T_i + \sum_{i}^{N} \sum_{j<i}^{N} b_{ij} T_i T_j$$

$$b_{ij} = \begin{cases} -S(Ti, Tj), & \text{if } (T_i, T_j) \text{ form a quadruplet,} \\ \zeta & \text{if } (T_i, T_j) \text{ are in conflict,} \\ 0 & \text{otherwise.} \end{cases}$$

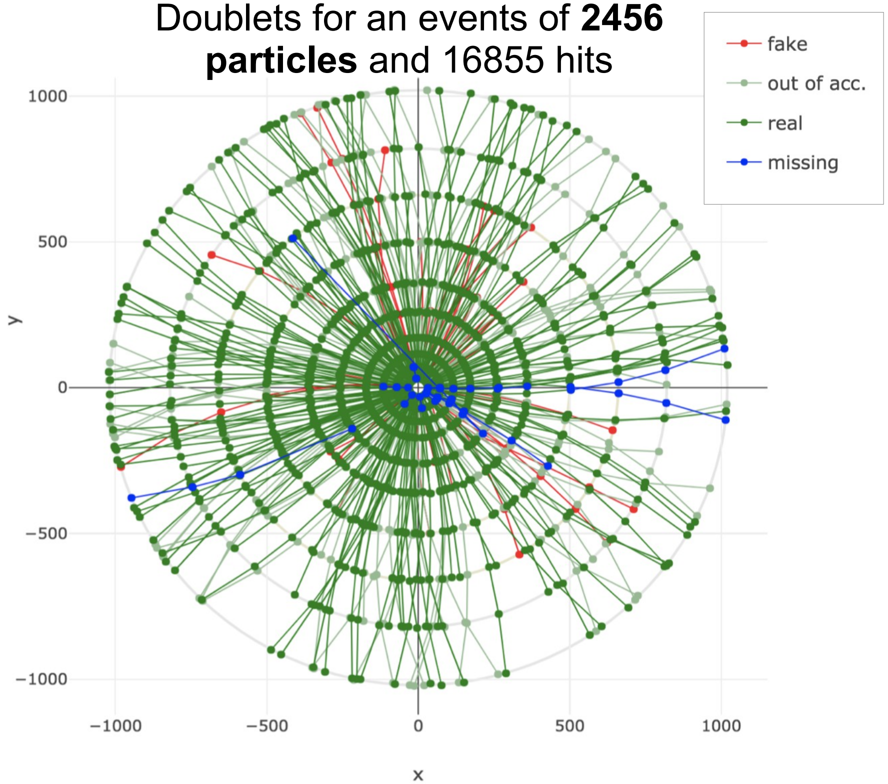
$$S(T_i, T_j) = z_1 \frac{z_2 \left(1 - |\delta(q/p_{Ti}, q/p_{Tj})|\right)^{z_3}}{(1+H_i+H_j)^{z_5}} + \frac{(1-z_2)\left(1-\max(\delta\theta_i, \delta\theta_j)\right)^{z_4}}{(1+H_i+H_j)^{z_5}}$$

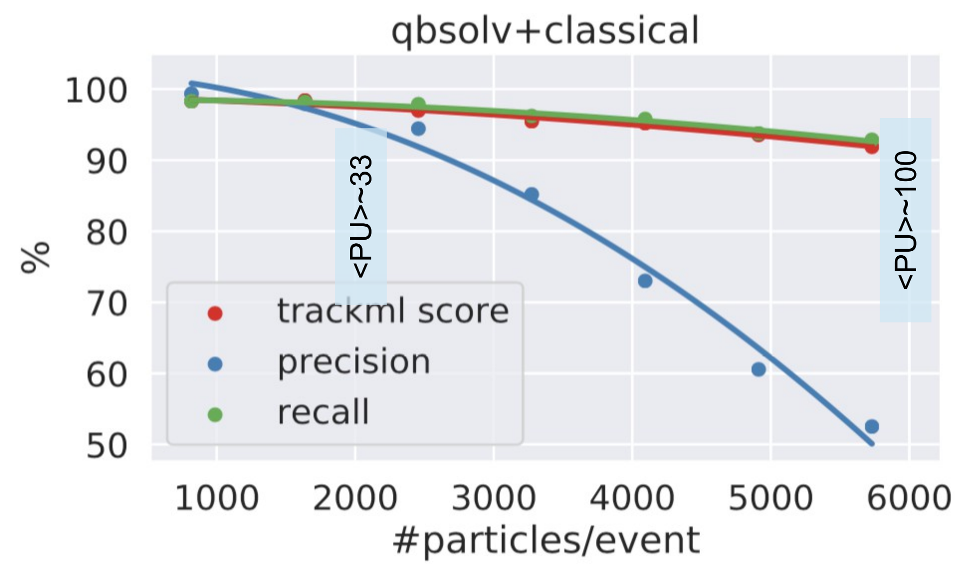
$$S(T_i, T_j) = \frac{1 - \frac{1}{2}(|\delta(q/p_{Ti}, q/p_{Tj})| + \max(\delta\theta_i, \delta\theta_j))}{(1+H_i+H_j)^2}$$

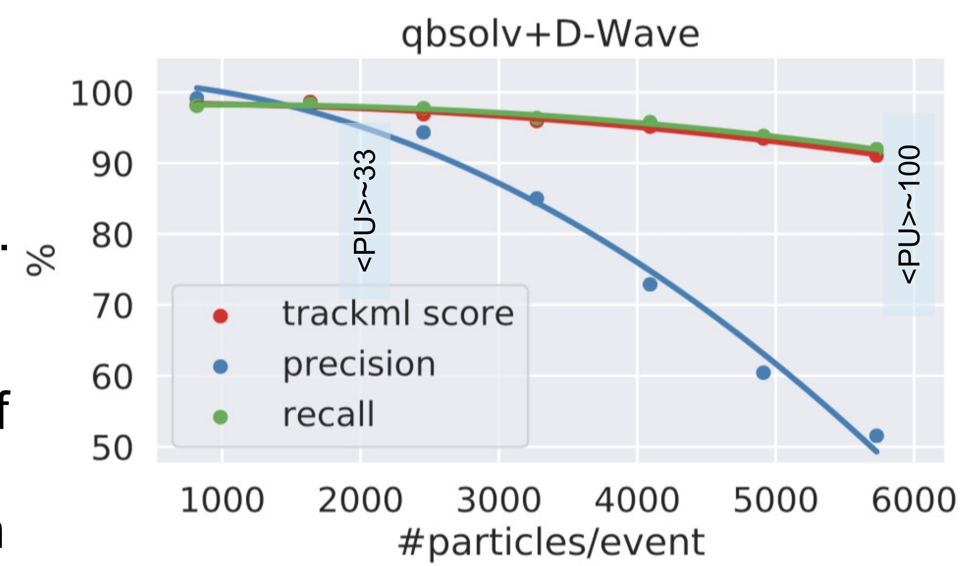
parameters tuned to favour high p_T tracks

Performance

Doublets for an events of **2456 particles** and 16855 hits







- Full problem resolution using qbsolve : classical simulator, or dwave compared.
- Hits from barrel only

- TrackML score conserved over range of event density.
- Improved performance (not shown) with more information (IP constraint, ...)

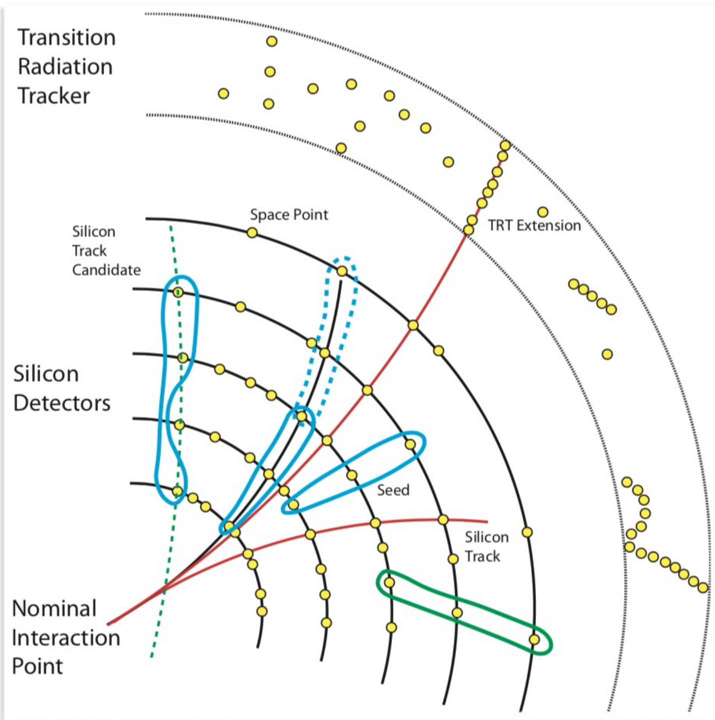
https://arxiv.org/abs/1902.08324

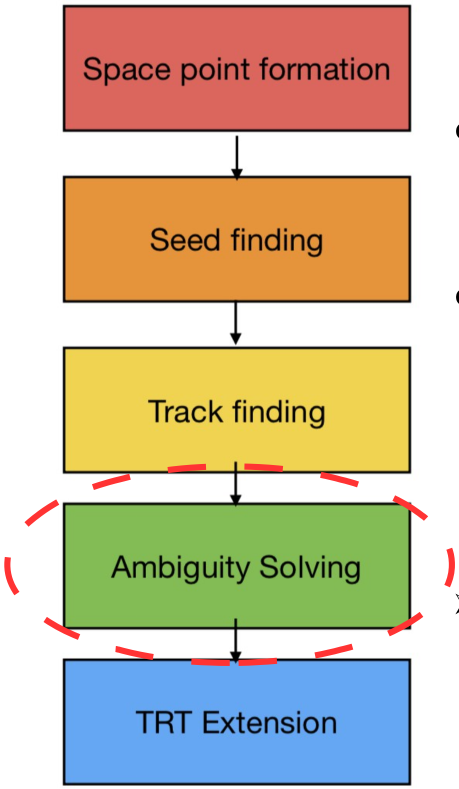
Track Ambiguity Resolution using Adiabatic Quantum Annealing

HEP.QPR

https://hep-qpr.lbl.gov/

Resolving Close-by Tracks





- Loosen constraints during pattern recognition to increase efficiency.
- Reduce fake rate by resolving ambiguities.
- Particularly relevant in dense environment like the core of a jet.

➢ Early results on resolving ambiguities from a solution of the trackML challenge : 15% purity and 70% efficiency

Conclusion

- The dataset of the TrackML Challenge is a valuable resource for the community.
- It is early for quantum computing but the exploration has begun, to prepare and think differently on algorithms.
- Promising application of Quantum annealer to charged particle tracking tasks.

QMLQCF Ackn.

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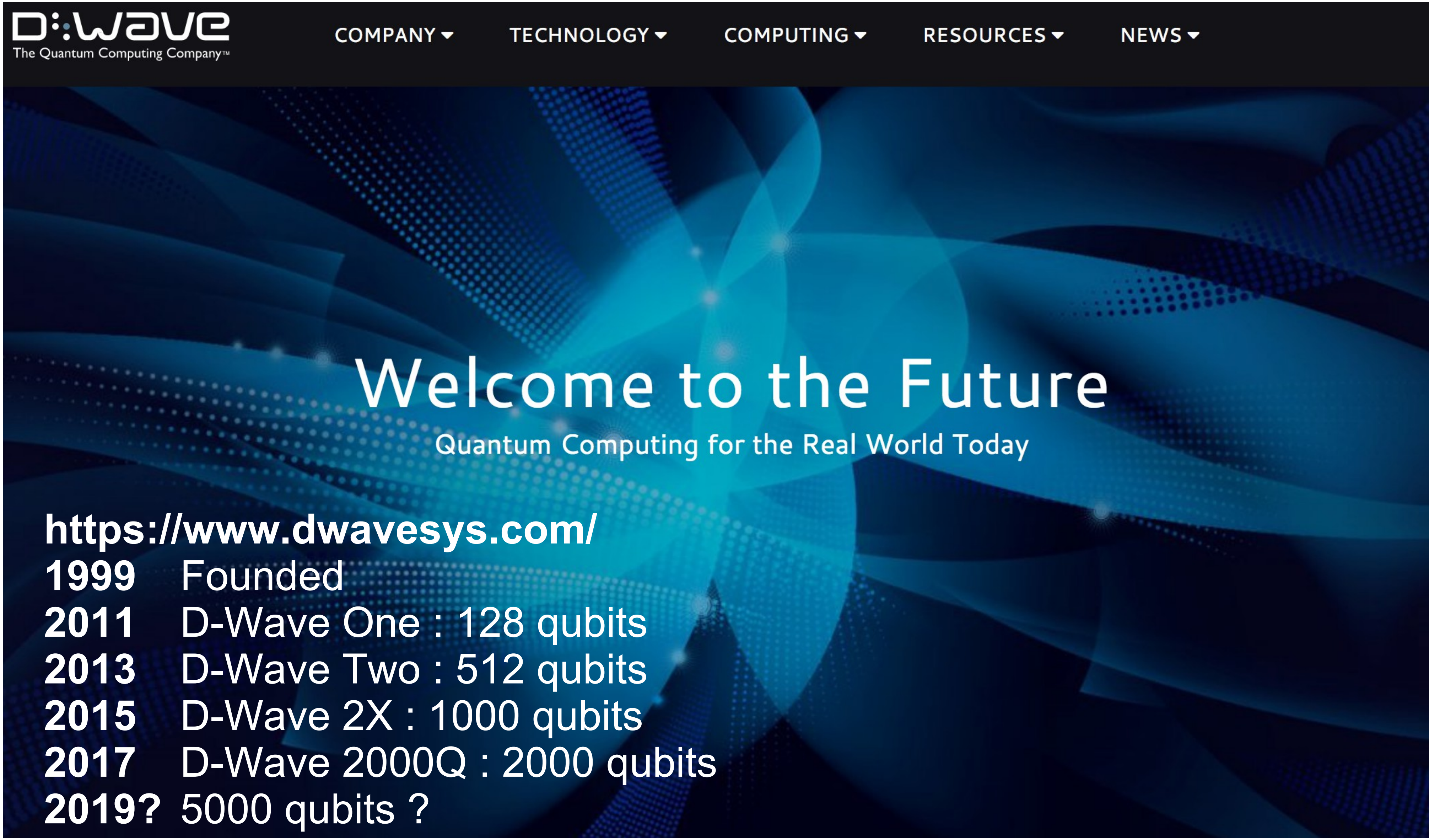
Part of this work was conducted at "iBanks", the AI GPU cluster at Caltech. We acknowledge NVIDIA, SuperMicro and the Kavli Foundation for their support of "iBanks".

Extra Material

The D-Wave Company



https://www.dwavesys.com/

1999 Founded

2011 D-Wave One : 128 qubits

2013 D-Wave Two : 512 qubits

2015 D-Wave 2X : 1000 qubits

2017 D-Wave 2000Q : 2000 qubits

2019? 5000 qubits ?

D-Wave Hamiltonian And Chimera Graph

D-Wave Hamiltonian

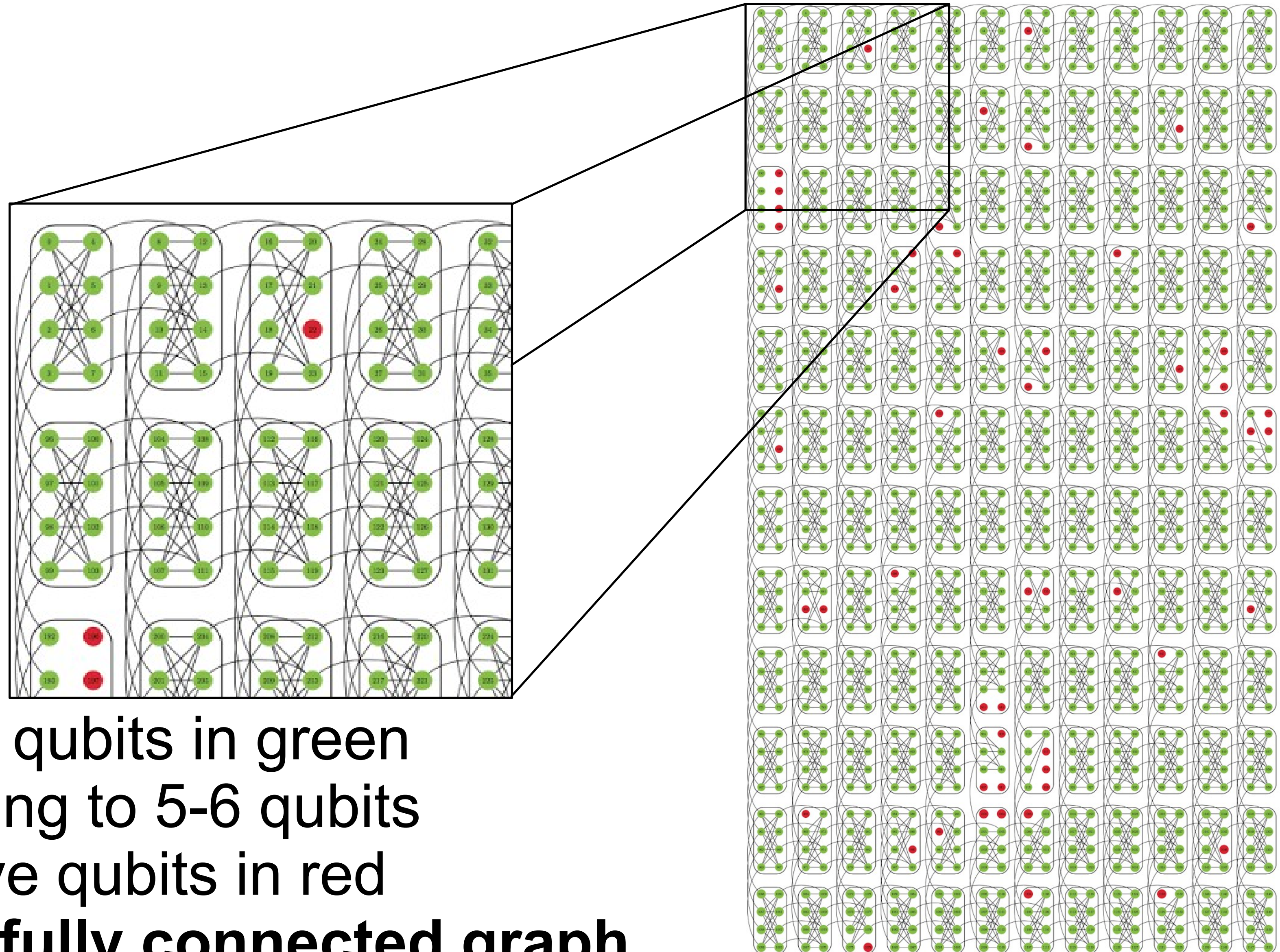
Runs over **adjacent** quBits

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

External magnetic field

Interactions

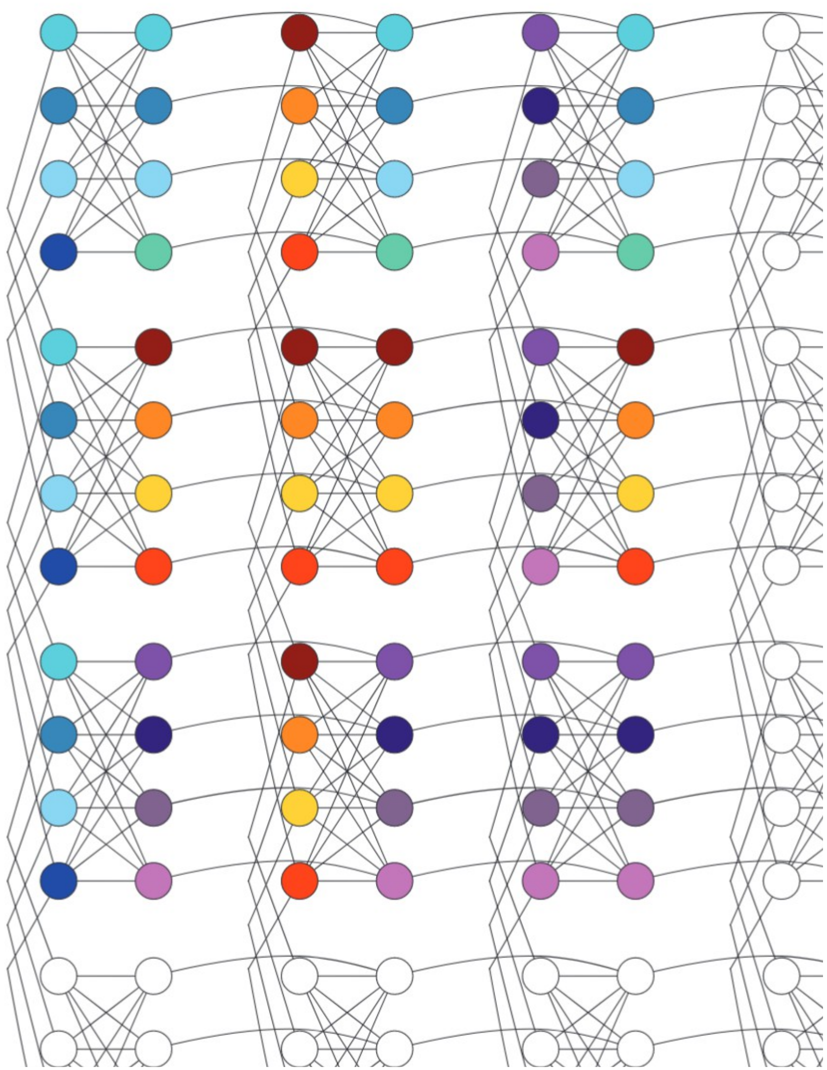
D-Wave qubit Adjacency



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

Runs over **all** quBit pairs

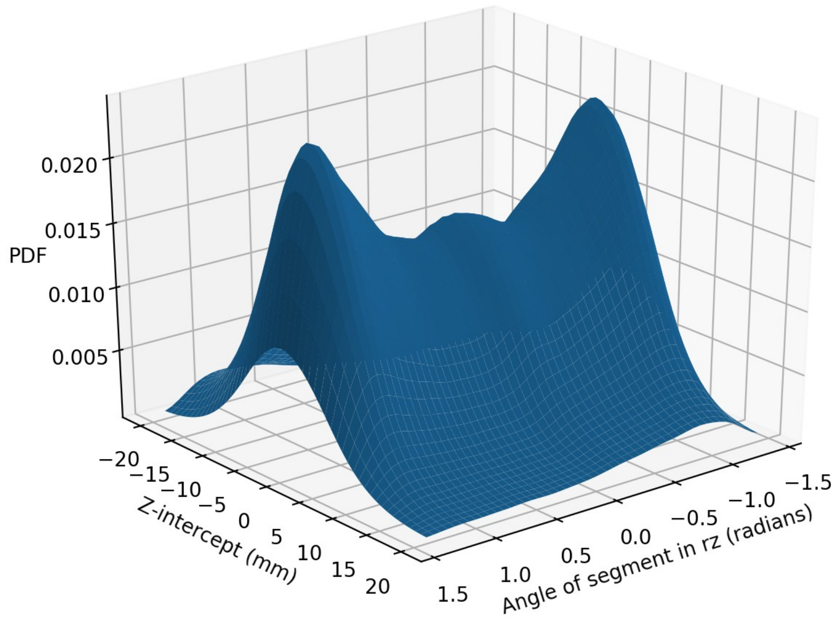
$$H_{\text{Ising}} = \sum_{i} h_i \sigma_i^z + \sum_{ij} J_{ij} \sigma_i^z \sigma_j^z$$

External magnetic field

Interactions

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

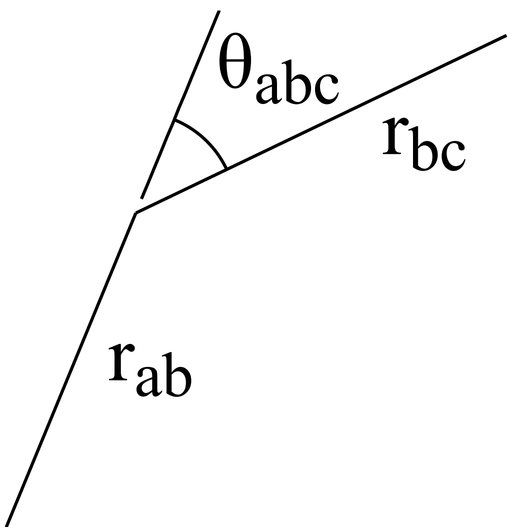
- Force segment off based on $\cos\theta_{abc}$
  - $\cos\theta_{abc} = 0$ if $\theta_{abc} > \theta_0$
- 5 best neighbors
- Solvable in polynomial time

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 : $\alpha=3.E^{-3}$, $\beta=2.63E^{-8}$, $\lambda=7$
- Threshold model : $\alpha=5.E^{-3}$, $\beta=1.E^{-6}$, $\lambda=7$

Edge Aff nity

- 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



Helical bias (cylindrical angle)

Momentum bias (rectangular angle)

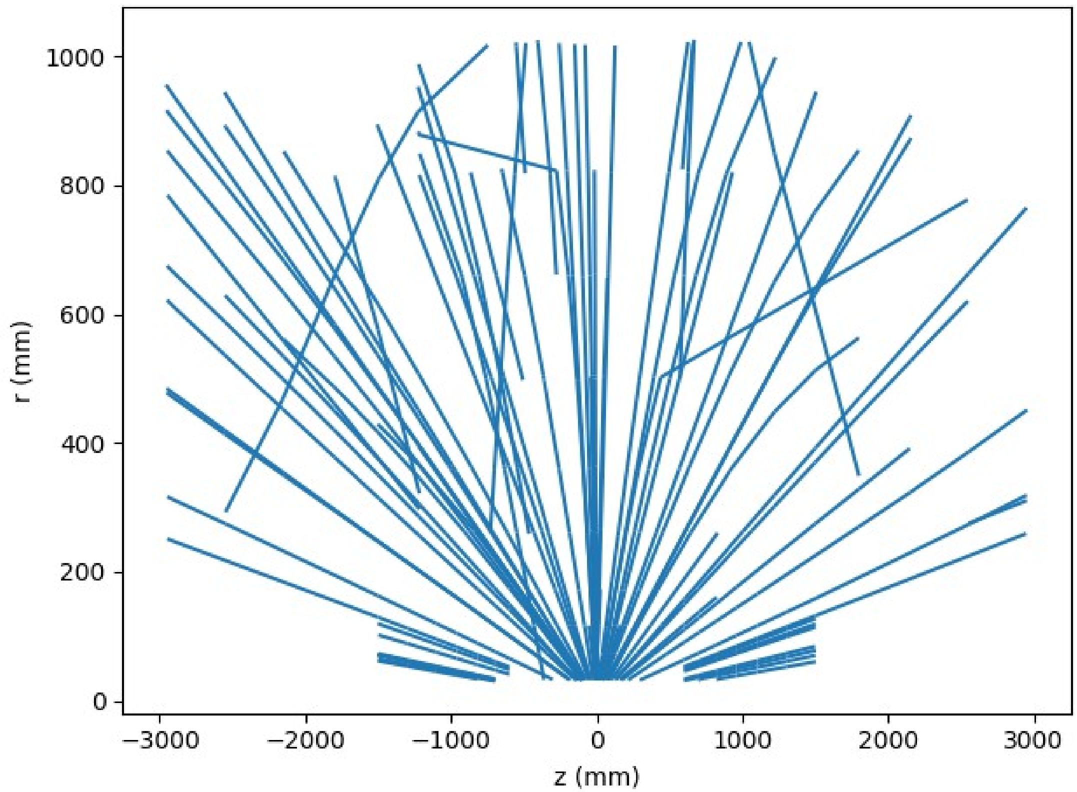
$$\sum_{a,b,c} \frac{\cos^{\lambda}\theta_{ab} + \rho\cos^{\lambda}\phi_{ab}}{r_{ab} + r_{bc}} s_{ab} s_{bc}$$

Short-edge bias

Ising variables (1 or 0)

Cross-Term Penalties

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



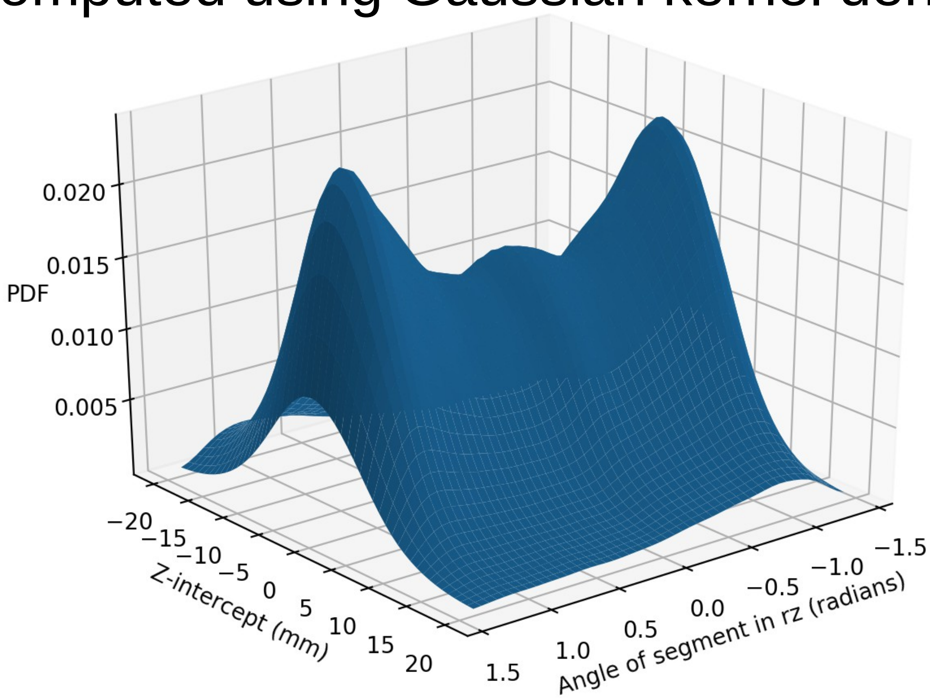
Z-intercept penalty

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

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



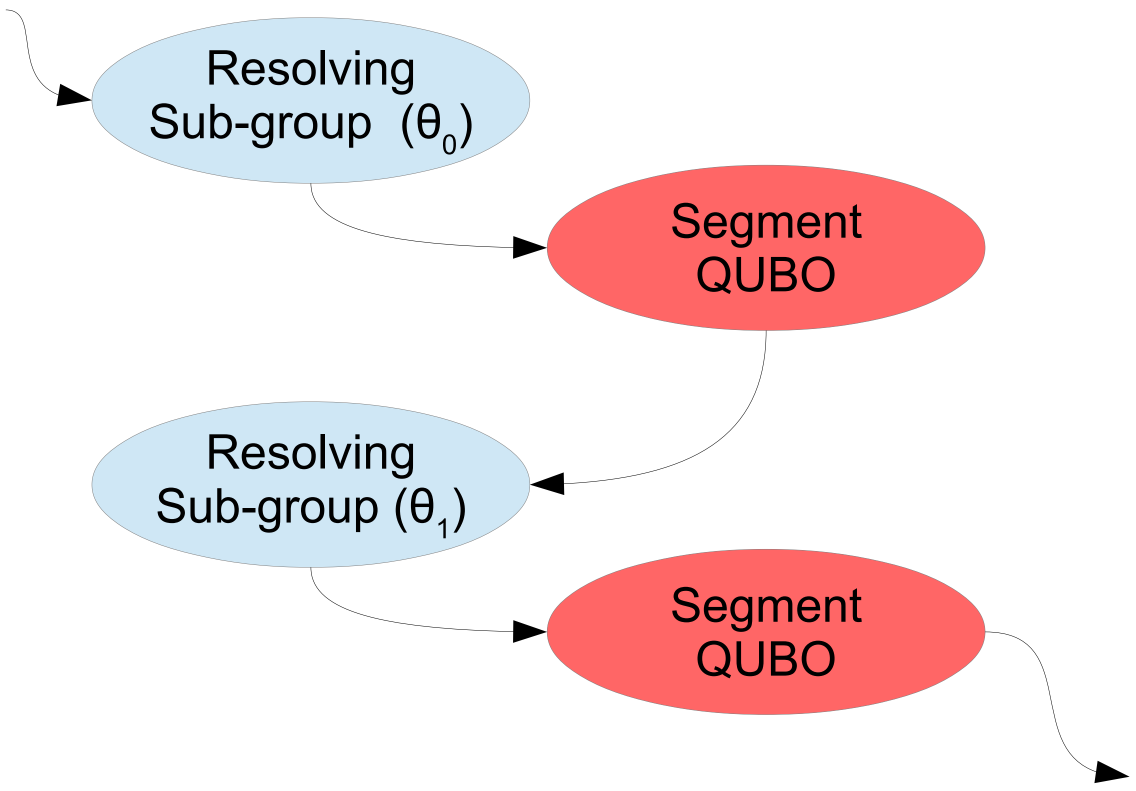
Global inhibition

Bayesian prior

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

Ising variable (1 or 0)

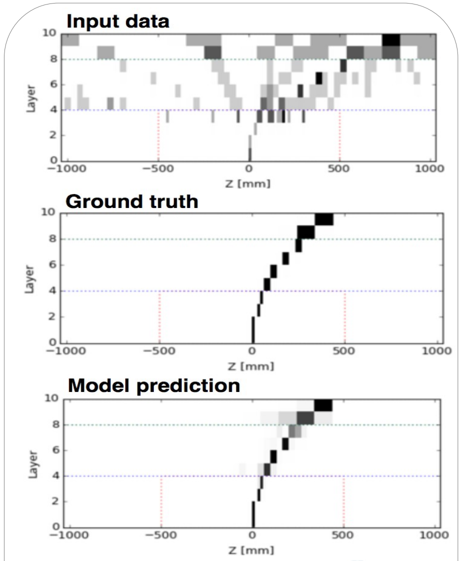
QA-Tracking Workflow



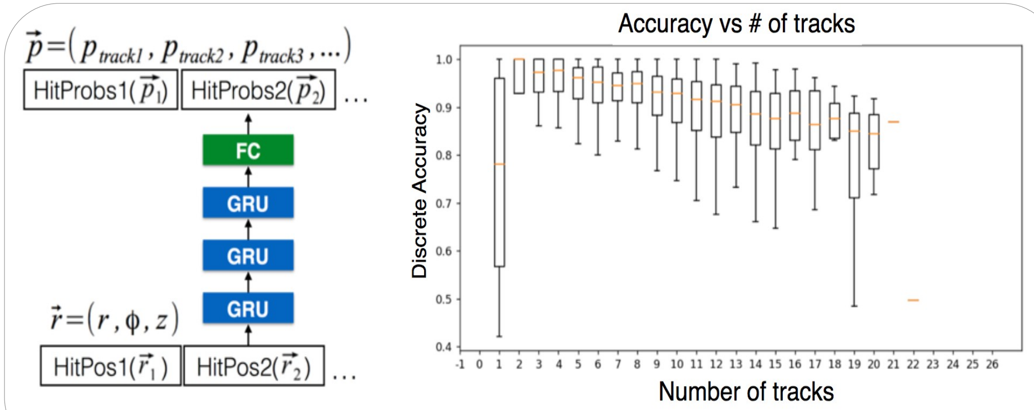
References

- Strandlie, Are, and Rudolf Frhwirth. "Track and vertex reconstruction: From classical to adaptive methods." Reviews of modern physics 82.2 (2010): 1419.
- Sirunyan, Albert M., et al. "Particle-flow reconstruction and global event description with the CMS detector." Journal of Instrumentation 12.10 (2017): 3.
- Farhi, Edward, Jeffrey Goldstone, and Sam Gutmann. "Quantum adiabatic evolution algorithms versus simulated annealing." arXiv preprint quant-ph/0201031 (2002).
- Denchev, Vasil S., et al. "What is the computational value of finite-range tunneling?." Physical Review X 6.3 (2016): 031015.
- Peterson, Carsten. "Track finding with neural networks." Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 279.3 (1989): 537-545.
- Denby, B. "Neural networks and cellular automata in experimental high energy physics." Computer Physics Communications 49.3 (1988): 429-448.
- Elkington, Joshua. Hopfield Networks. Qparticle (2014)
- Kaggle."TrackML Particle Tracking Challenge." n.d. Web. 29 June 2018

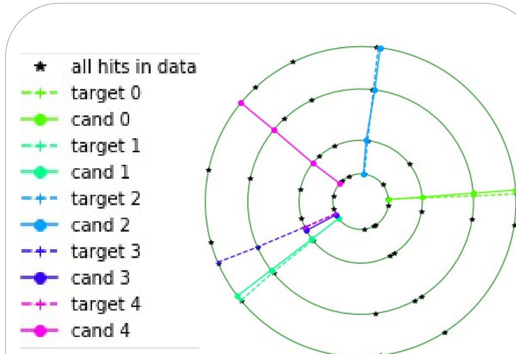
HEP.TrkX Approaches



Track following with RNN

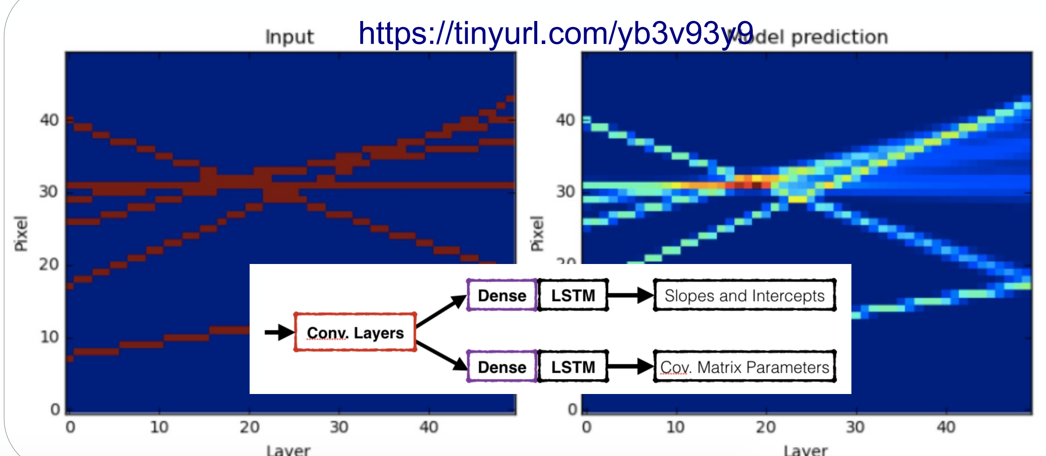


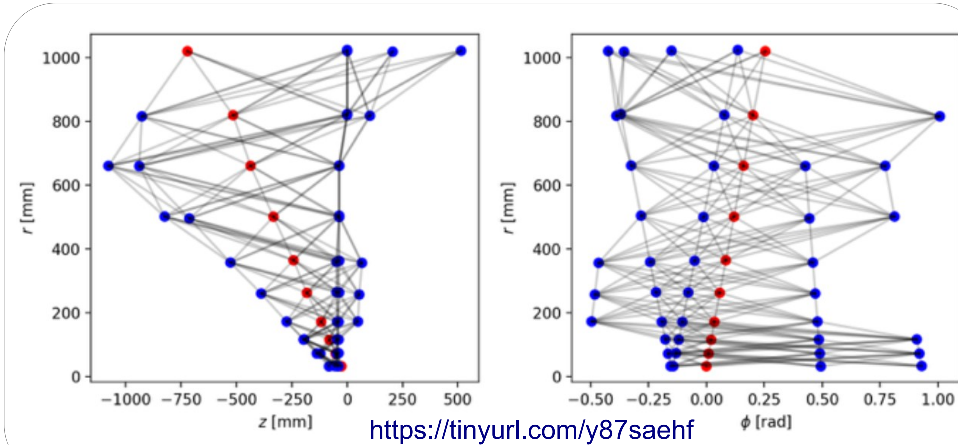
End-to-end hit assignment



Seq-to-seq track finding

https://heptrkx.github.io/





HEP.QPR Workflow

Hits in the barrel region, track with a least 5 hits, and 1 GeV or pT, no double hit per layer.