Doublet-based QUBO

LBNL-ICEPP Quantum Computing Mini-Workshop

12 / 02 / 2019

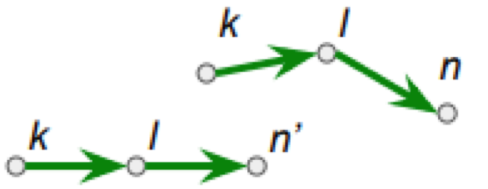
Masahiko Saito

- Use HEPQPR.Qallse (https://github.com/derlin/hepqpr-qallse)
- Thanks Lucy!

From Lucy's talk: https://indico.fnal.gov/event/18104/session/23/contribution/61/material/0/2.pdf

Stimpfl-Abele & Garrido (1990) *ref*

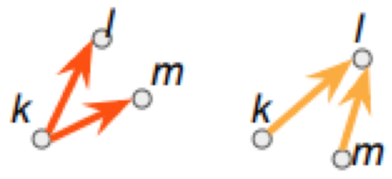
Energy function of the Hopfield Network:



"***connection strength***", interest of connecting two doublets

$$E = -\frac{1}{2}\Big[\sum_{kln} T_{kln} V_{kl} V_{ln}$$
$$-\alpha\Big(\sum_{klm(l\neq m)} V_{kl} V_{km} + \sum_{klm(k\neq m)} V_{kl} V_{ml}\Big)$$
$$-\beta\Big(\sum_{mn} V_{mn} - N_a\Big)\Big], \quad V \in \{0,1\}$$

avoid "***conflicts***", a hit belongs to at most one track



activate only the expected number of neurons (N_a)

$$T_{kln} = \frac{cos^{\lambda}\theta_{kln}}{d_{kl} + d_{ln}}$$

favour short and almost straight connections

parameters: λ α β

Stimpfl-Abele & Garrido (1990) *ref*

$$O(a;b;q) = \sum_{i=1}^{N} a_i q_i + \sum_{i}^{N}\sum_{j}^{N} b_{ij} q_i q_j \quad q_i \in \{0,1\}$$

- "easy" to adapt to a QUBO / QMI
  - set the qubit bias weights a_i to 0
  - set the coupling strength b_i to either a connection strength (T) or a conflict constant (α term)
  - drop the β term
- but…
  - efficient early selection of doublets need an *origin assumption*
  - "*favor straight connections*" …
  - no "continuity" between doublets → zigzag patterns

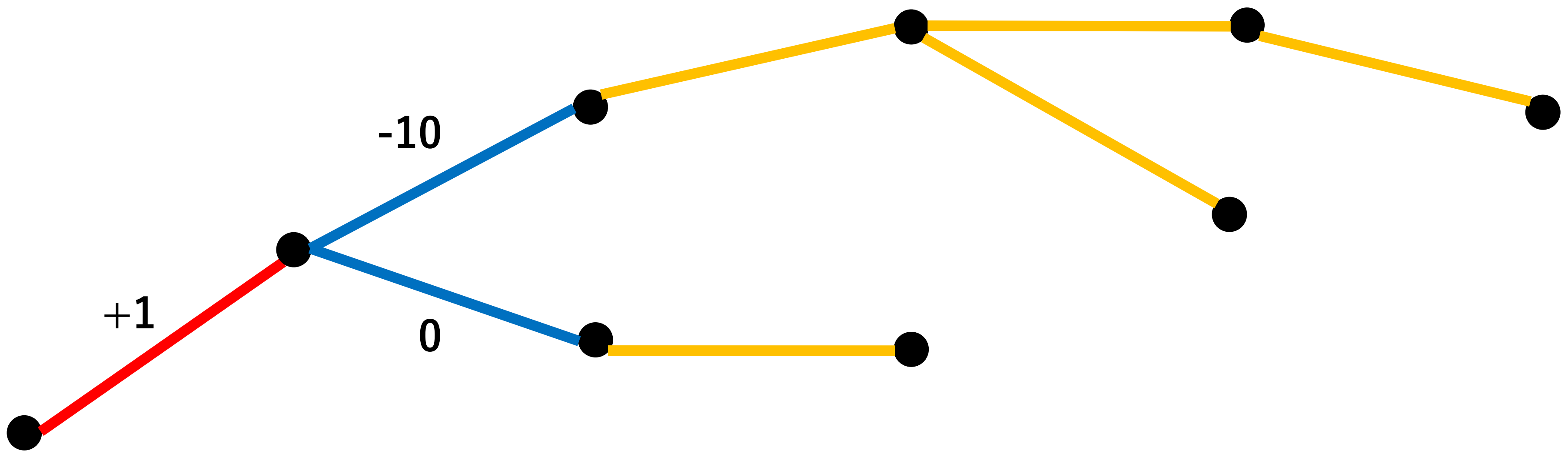
This can be solved by adding long-ranged term?

OK for high P_T tracks only,

breaks on dense datasets (> 400 particles/event)

$$E = -\frac{1}{2}\left[\sum_{kln} T_{kln} V_{kl} V_{ln} - \alpha\left(\sum_{klm(l\neq m)} V_{kl} V_{km} + \sum_{klm(k\neq m)} V_{kl} V_{ml}\right) - \beta\left(\sum_{mn} V_{mn} - N_a\right)\right]$$

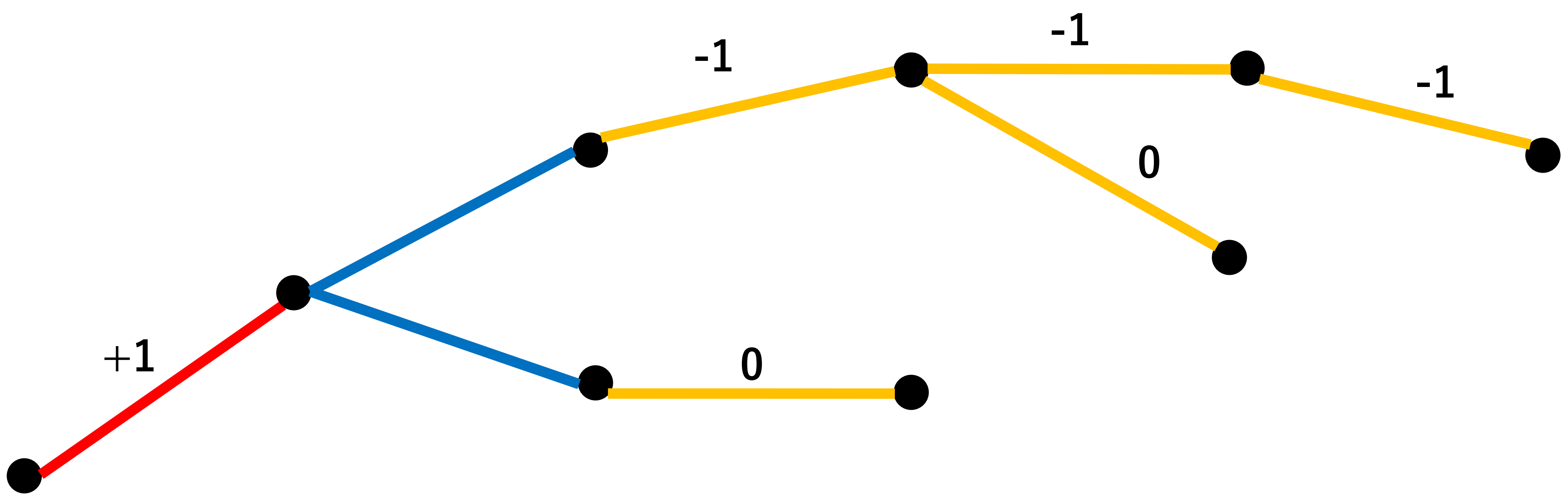
Original term :
for neighborhood nodes



$$E = -\frac{1}{2}\left[\sum_{kln} T_{kln}V_{kl}V_{ln} - \alpha\left(\sum_{klm(l\neq m)} V_{kl}V_{km} + \sum_{klm(k\neq m)} V_{kl}V_{ml}\right) - \beta\left(\sum_{mn} V_{mn} - N_a\right) + \gamma\left(\sum_{klmn(k\neq l\neq m\neq n)} V_{kl}V_{mn}\right)\right]$$

Original term : for neighborhood nodes

Additional term : for connected (or all) nodes



advantage : can check if the many associated doublets exist

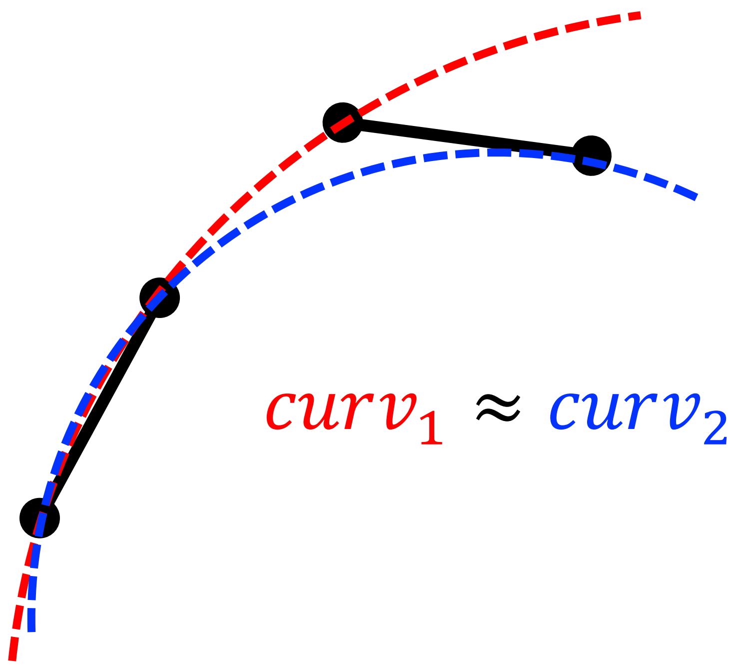
disadvantage: increase QUBO size / building time

$$E = -\frac{1}{2}\left[\sum_{kln} T_{kln}V_{kl}V_{ln} - \alpha\left(\sum_{klm(l\neq m)} V_{kl}V_{km} + \sum_{klm(k\neq m)} V_{kl}V_{ml}\right) - \beta\left(\sum_{mn} V_{mn} - N_a\right) + \gamma\left(\sum_{klmn(k\neq l\neq m\neq n)} V_{kl}V_{mn}\right)\right]$$

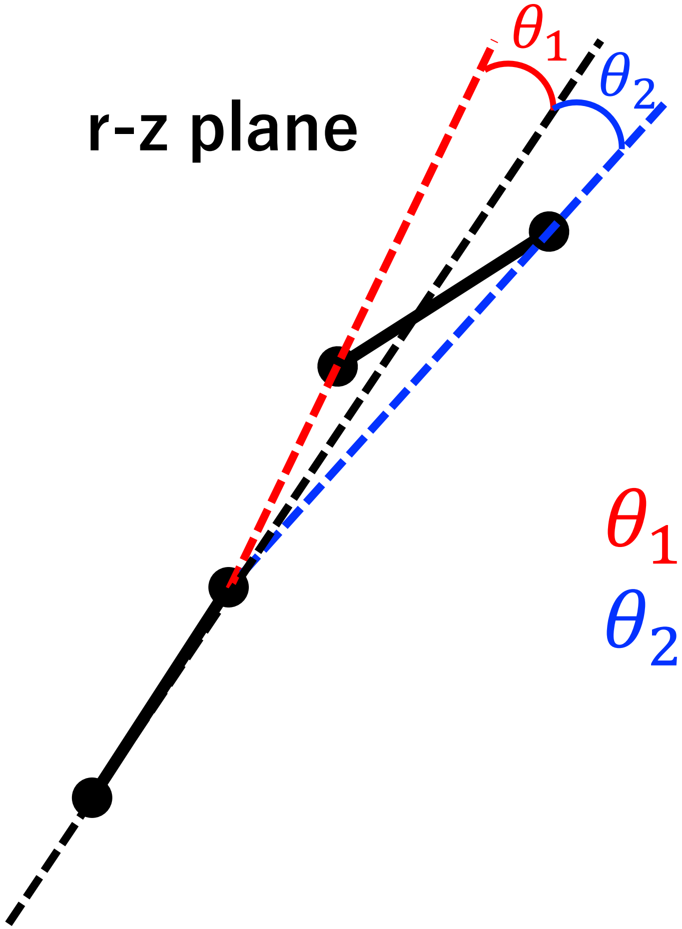
Original term :
for neighborhood nodes

Additional term :
for connected (or all) nodes

x-y plane



r-z plane



$\theta_1 \approx 0$
$\theta_2 \approx 0$

$$E = -\frac{1}{2}\left[\sum_{kln} T_{kln} V_{kl} V_{ln} - \alpha\left(\sum_{klm(l\neq m)} V_{kl} V_{km} + \sum_{klm(k\neq m)} V_{kl} V_{ml}\right) - \beta\left(\sum_{mn} V_{mn} - N_a\right) + \gamma\left(\sum_{klmn(k\neq l\neq m\neq n)} V_{kl} V_{mn}\right)\right]$$

T_{kln}: 0 (temporary)

α: +50 (constant)
not allow shared hits

β: +1 (constant)

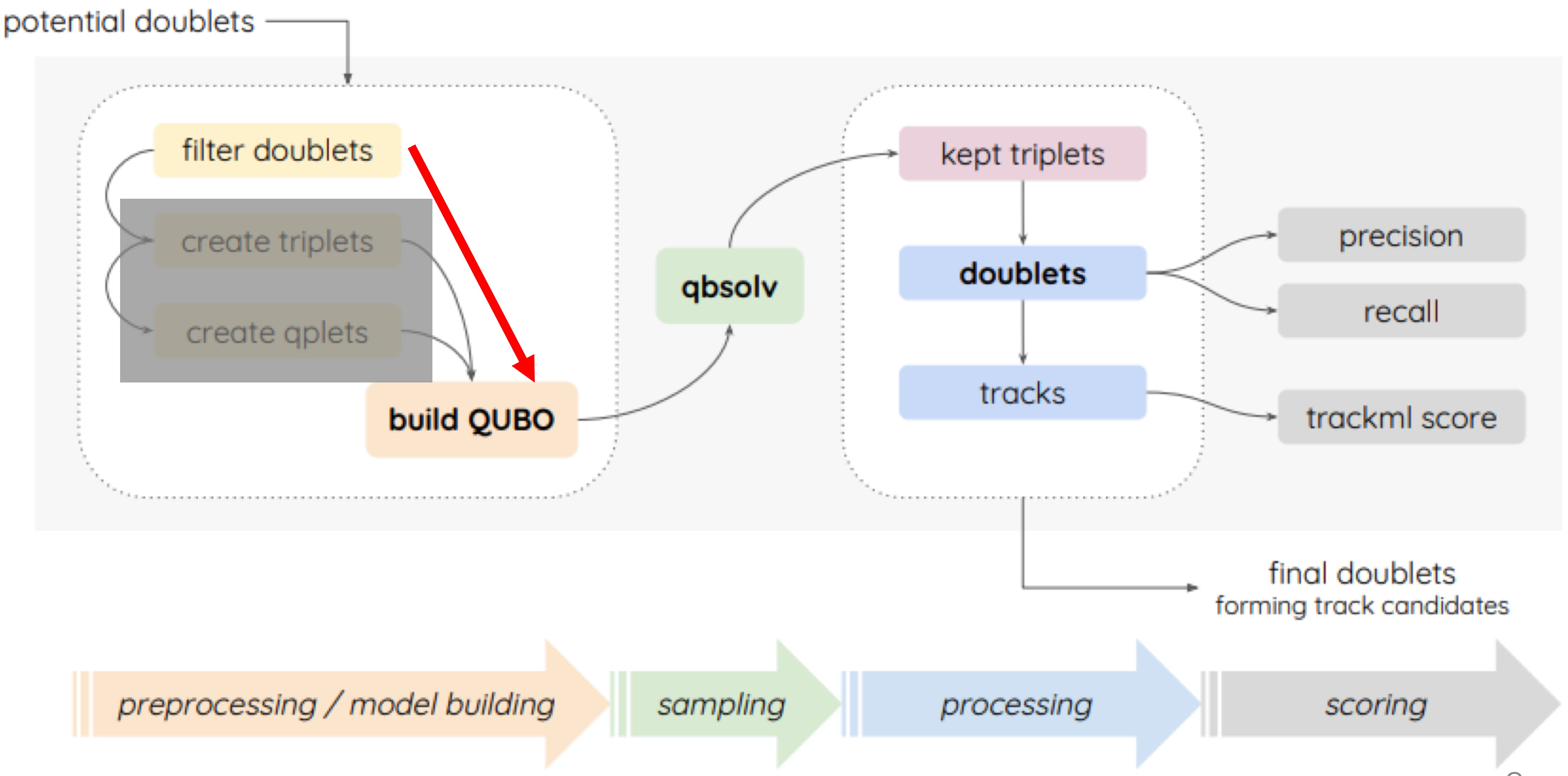
N_a: 0

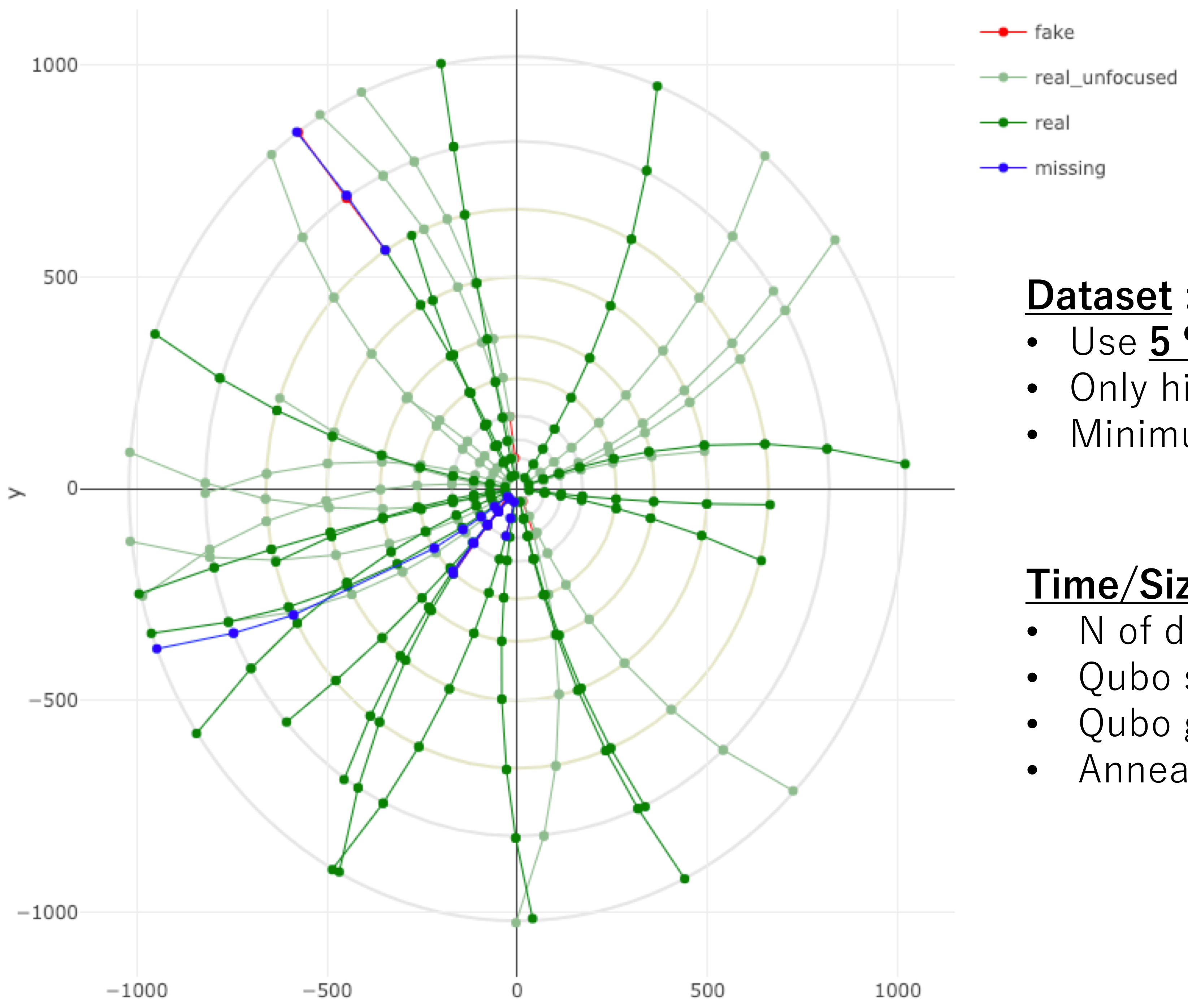
γ: +0.3 * penalty

$$\text{penalty} = \frac{1}{2}\left((1 - dcurv)^2 + \left(1 - \sqrt{drz_1^2 + drz_2^2}\right)^2\right)$$

$0 < \text{penalty} < 1$

Algorithm overview



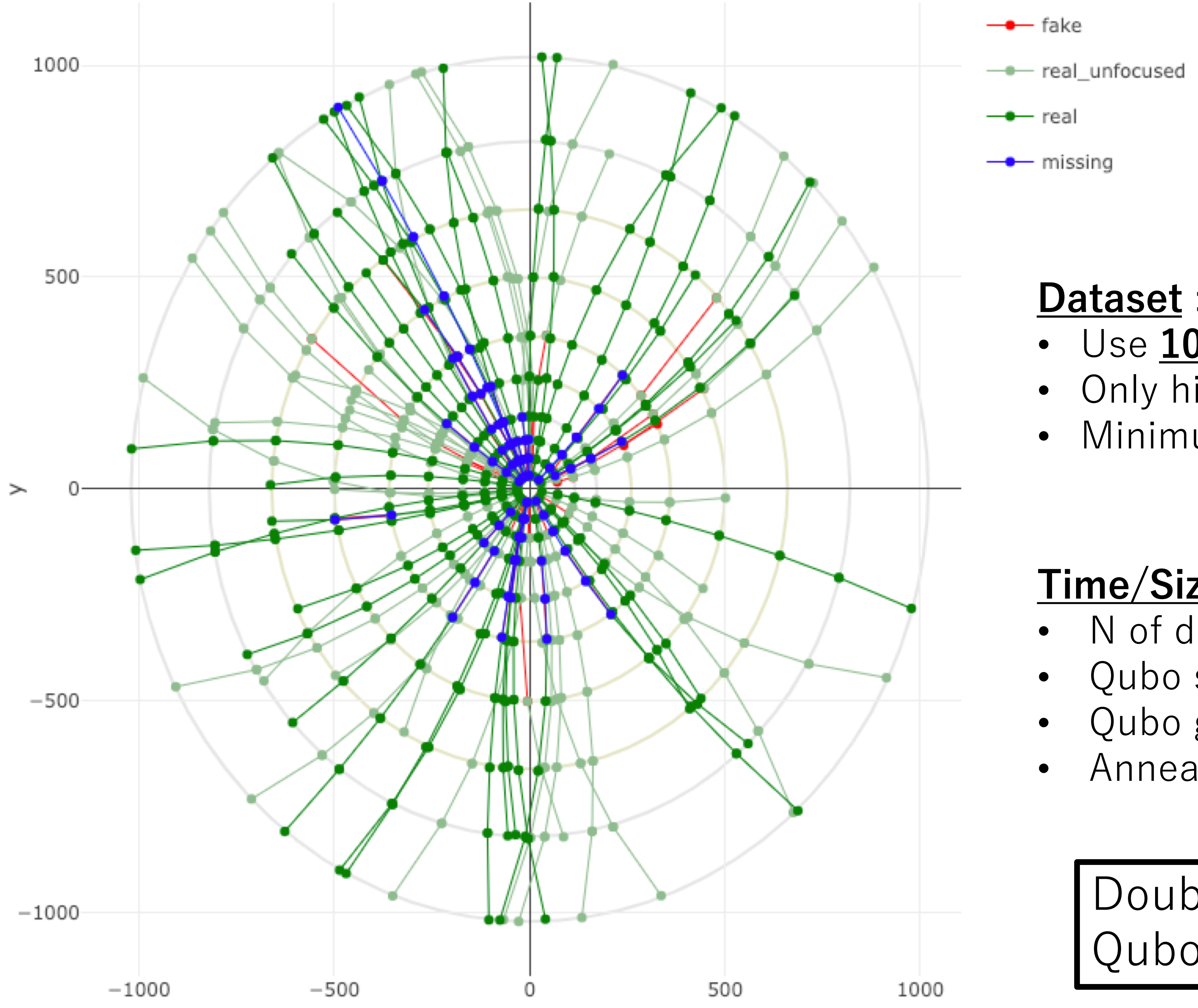


Dataset :

- Use **5 %**
- Only high pT tracks (> 1 GeV)
- Minimum N of hits >= 8

Time/Size :

- N of doublets = **13073**
- Qubo size = 233110
- Qubo generation time = 42.5 sec
- Annealing time = 8.6 sec (neal)



Dataset :

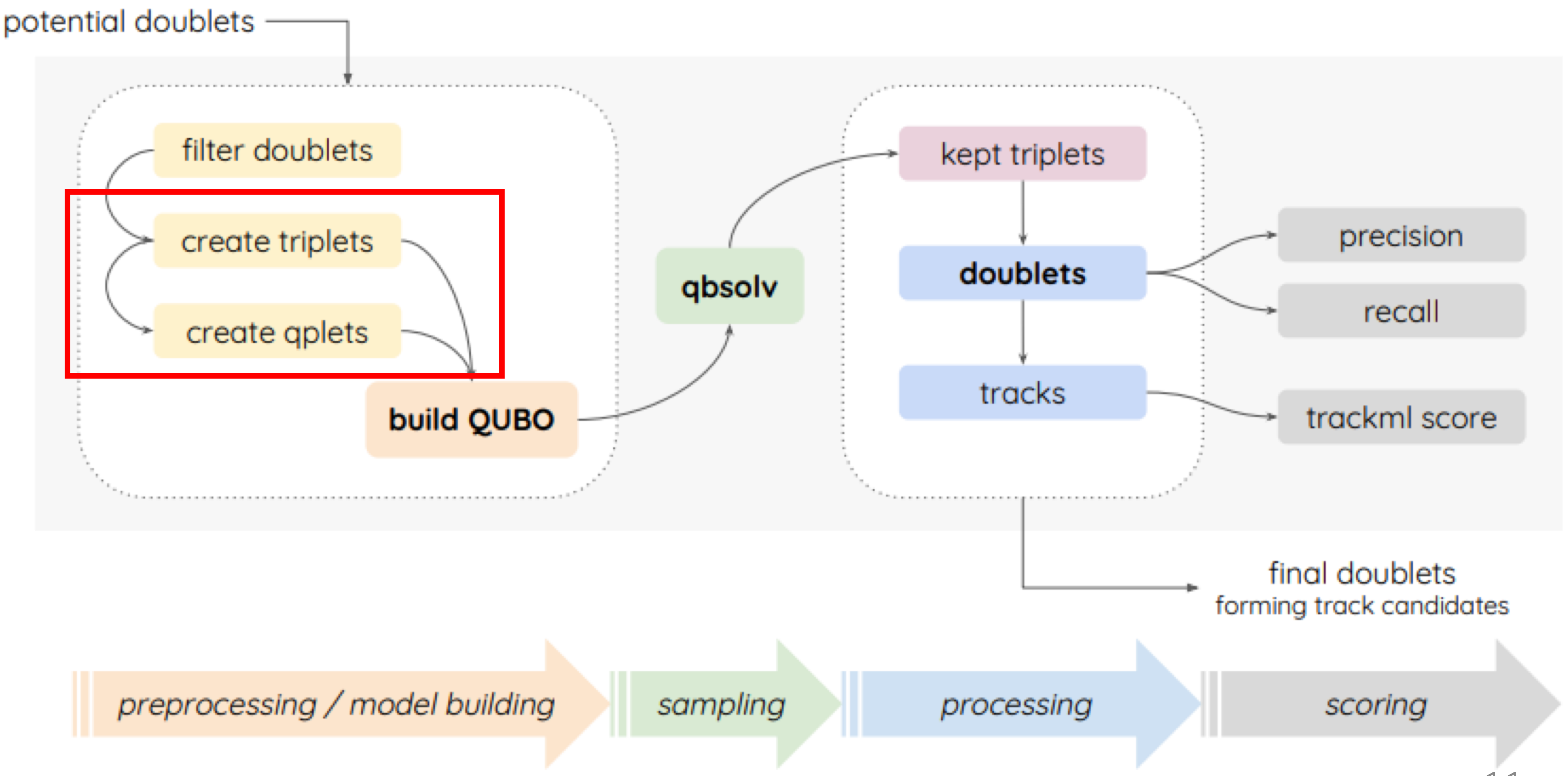
- Use **10 %**
- Only high pT tracks (> 1 GeV)
- Minimum N of hits >= 8

Time/Size :

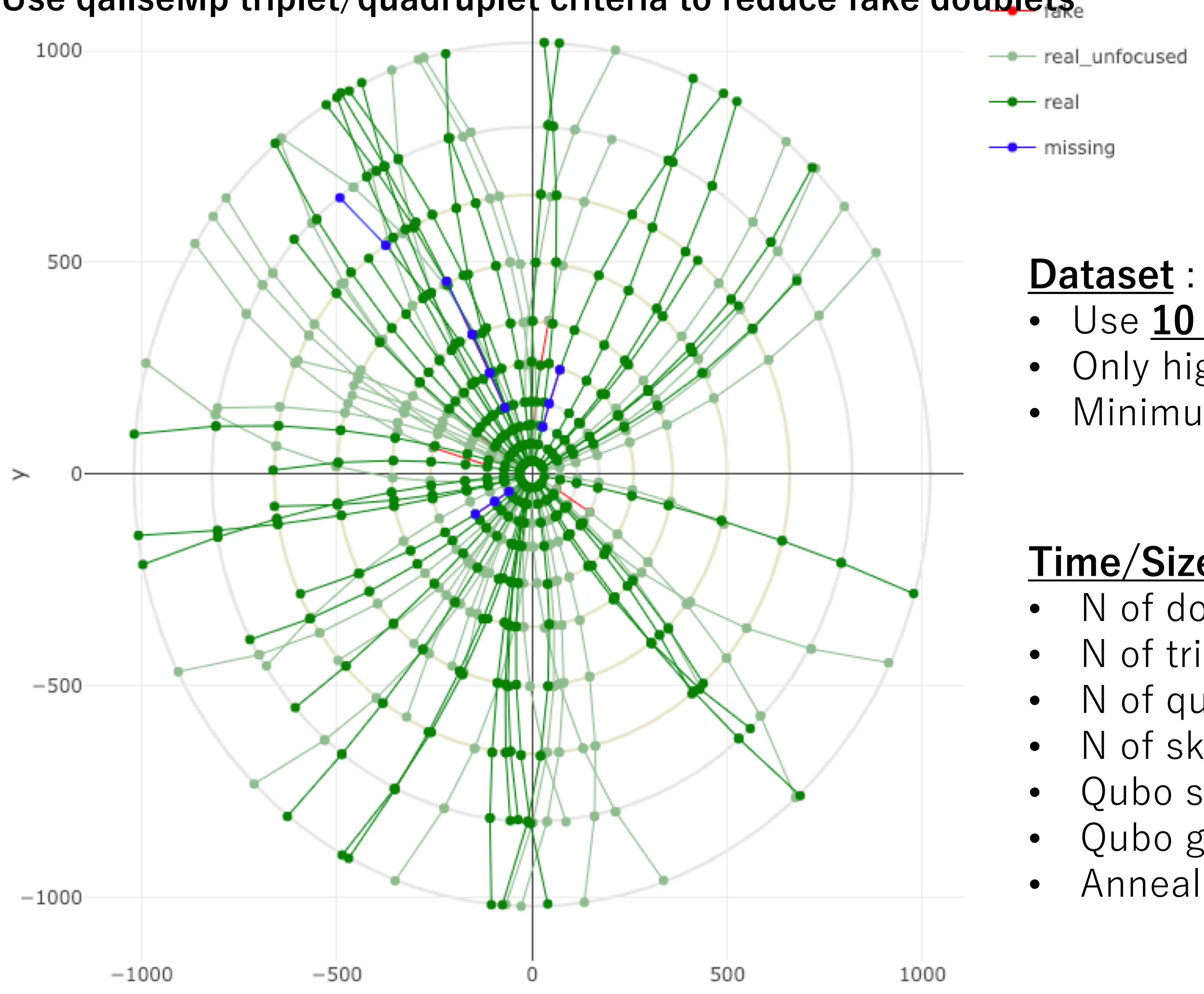
- N of doublets = **56997**
- Qubo size = 2178115
- Qubo generation time = 884.28 sec
- Annealing time = 73.29 sec (neal)

Doublet size ∝ $O(N_{hit}^2)$
Qubo size ∝ $O(N_{hit}^4)$

Algorithm overview



Use qallseMp triplet/quadruplet criteria to reduce fake doublets



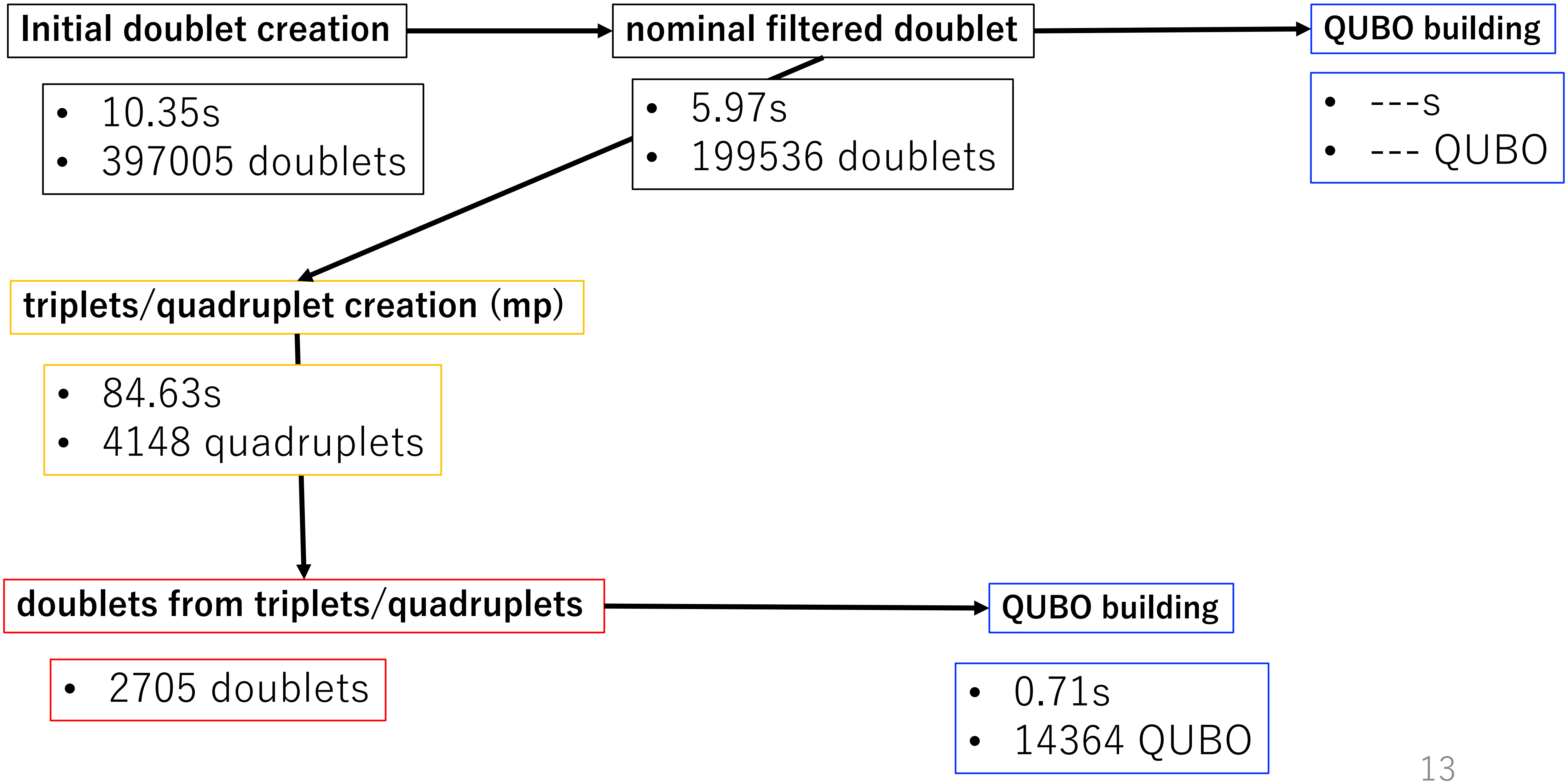
Dataset :

- Use **10 %**
- Only high pT tracks (> 1 GeV)
- Minimum N of hits >= 8

Time/Size :

- N of doublets = **56997**
- N of triplets = 17722
- N of quadruplets = 1979
- N of skimmed doublets = **1447**
- Qubo size = 7757
- Qubo generation time = 0.42 sec
- Annealing time = 0.35 sec (neal)

pT > 1 GeV, N of hits >= 8, 20%



Stimpfl-Abele & Garrido (1990) *ref*

$$O(a;b;q) = \sum_{i=1}^{N} a_i q_i + \sum_{i}^{N}\sum_{j}^{N} b_{ij} q_i q_j \quad q_i \in \{0,1\}$$

- "easy" to adapt to a QUBO / QMI
  - set the qubit bias weights a_i to 0
  - set the coupling strength b_i to either a connection strength (T) or a conflict constant (α term)
  - drop the β term
- but…

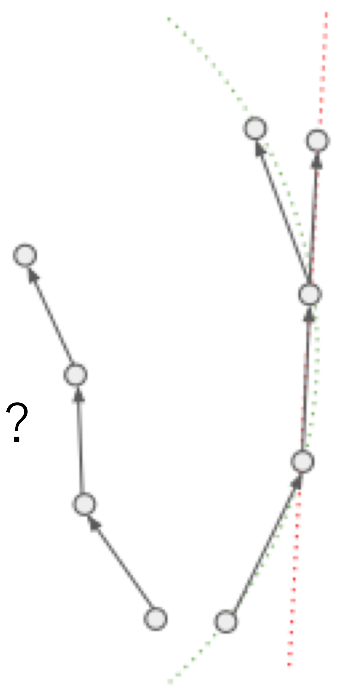
Try this

  - efficient early selection of doublets need an *origin assumption*
  - *"favor straight connections"* …
  - no "continuity" between doublets → zigzag patterns

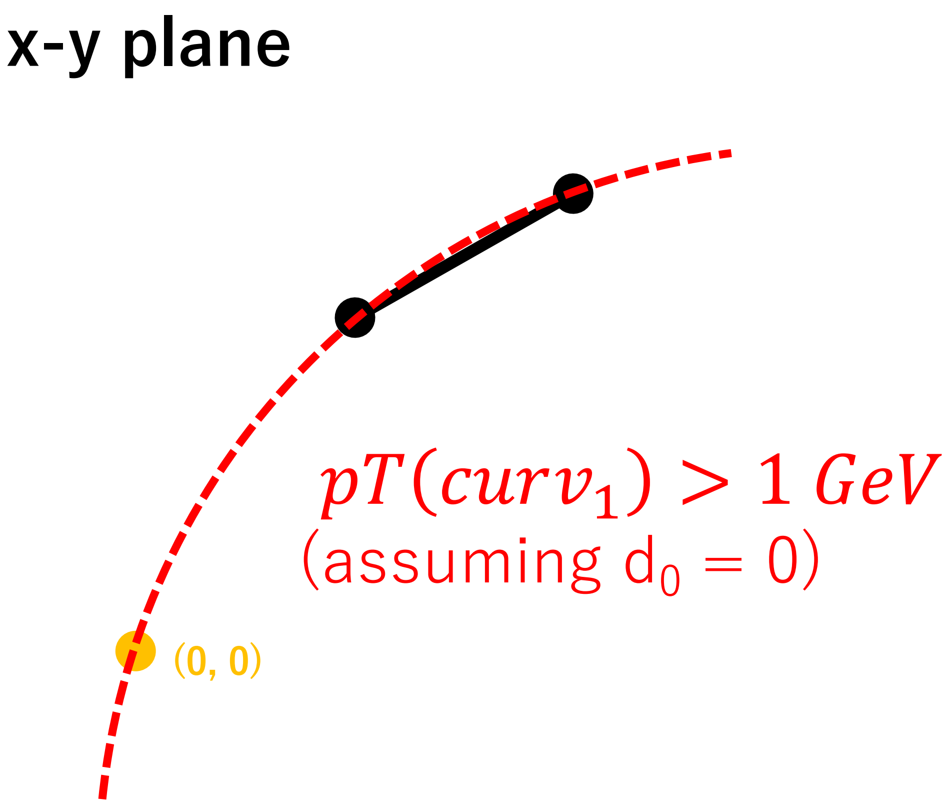
This can be solved by adding long-ranged term?

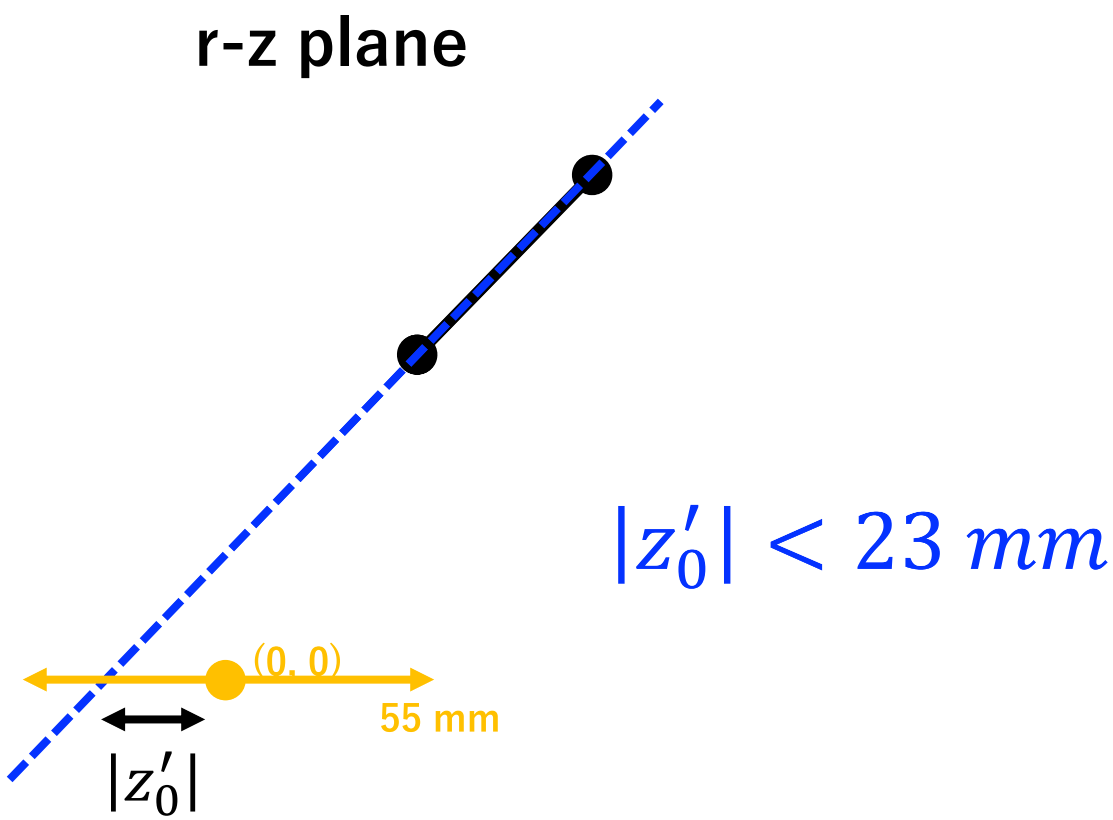
OK for high P_T tracks only,

breaks on dense datasets (> 400 particles/event)

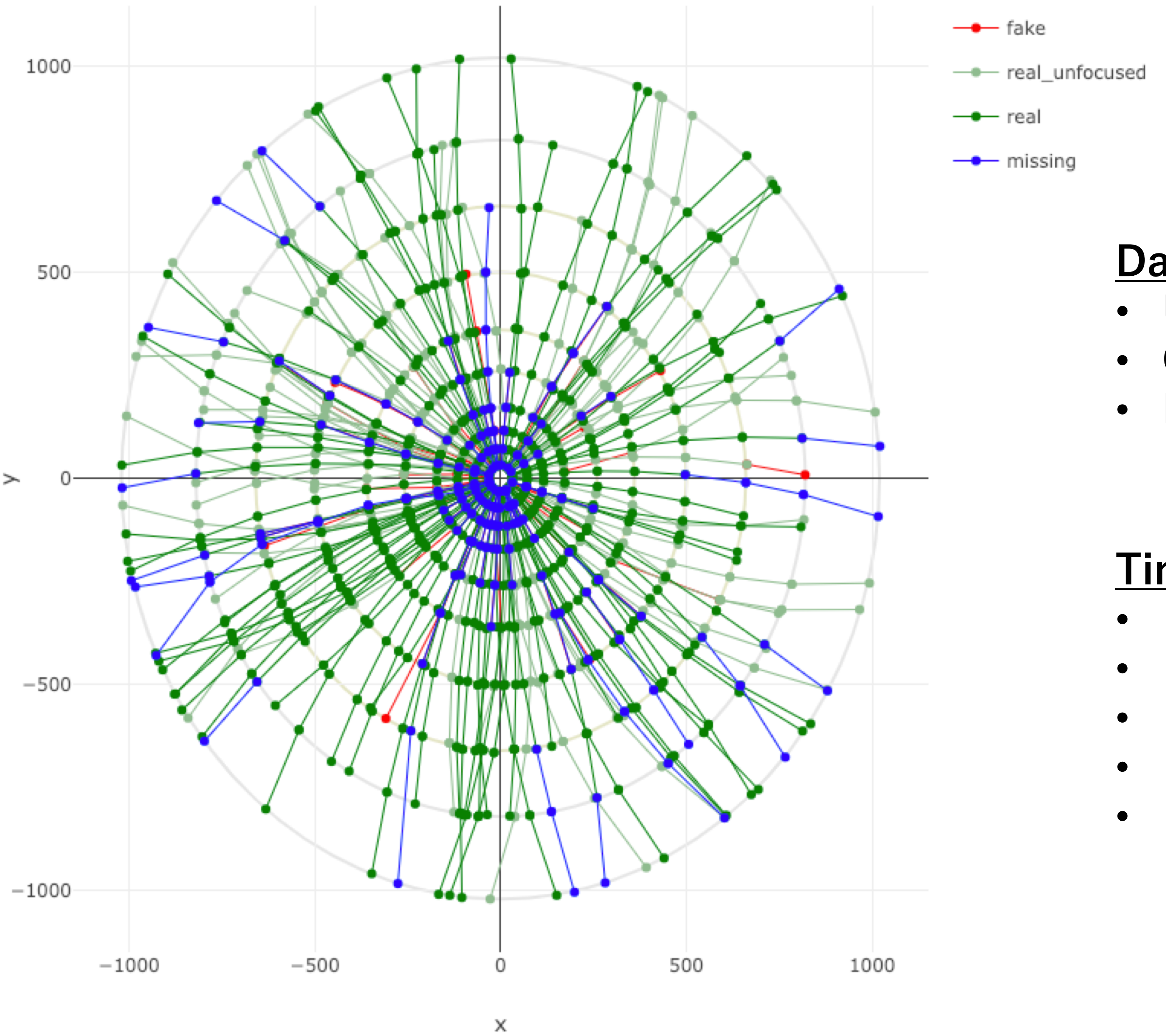


Doublet selection by “origin” constraint





Use “origin” constraint



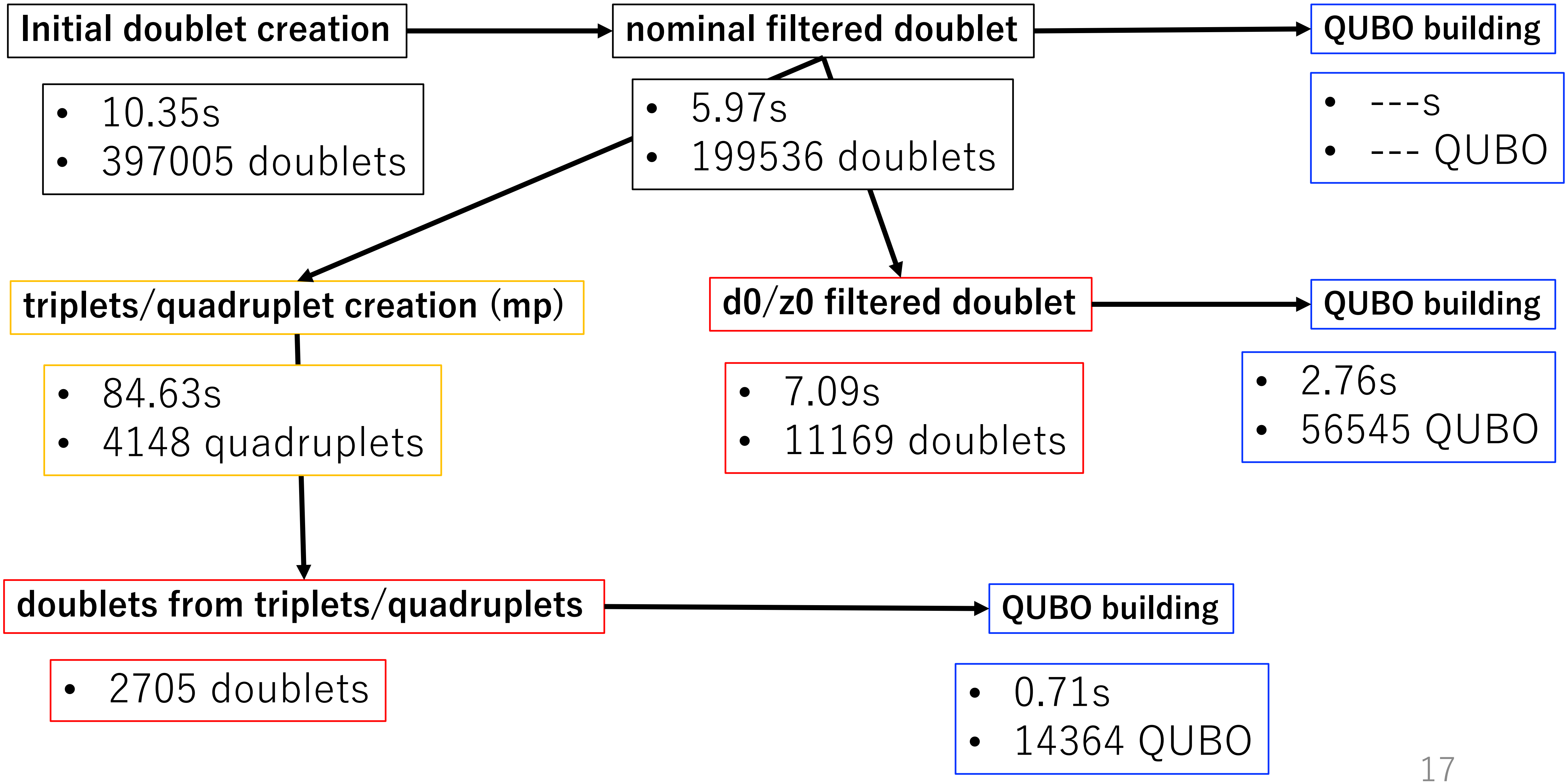
Dataset :

- Use **20 %**
- Only high pT tracks (> 1 GeV)
- Minimum N of hits >= 8

Time/Size :

- N of doublets = **195533**
- N of skimmed doublets = **11022**
- Qubo size = 55809
- Qubo generation time = 3.05 sec
- Annealing time = 2.88 sec (neal)

pT > 1 GeV, N of hits >= 8, 20%



Summary

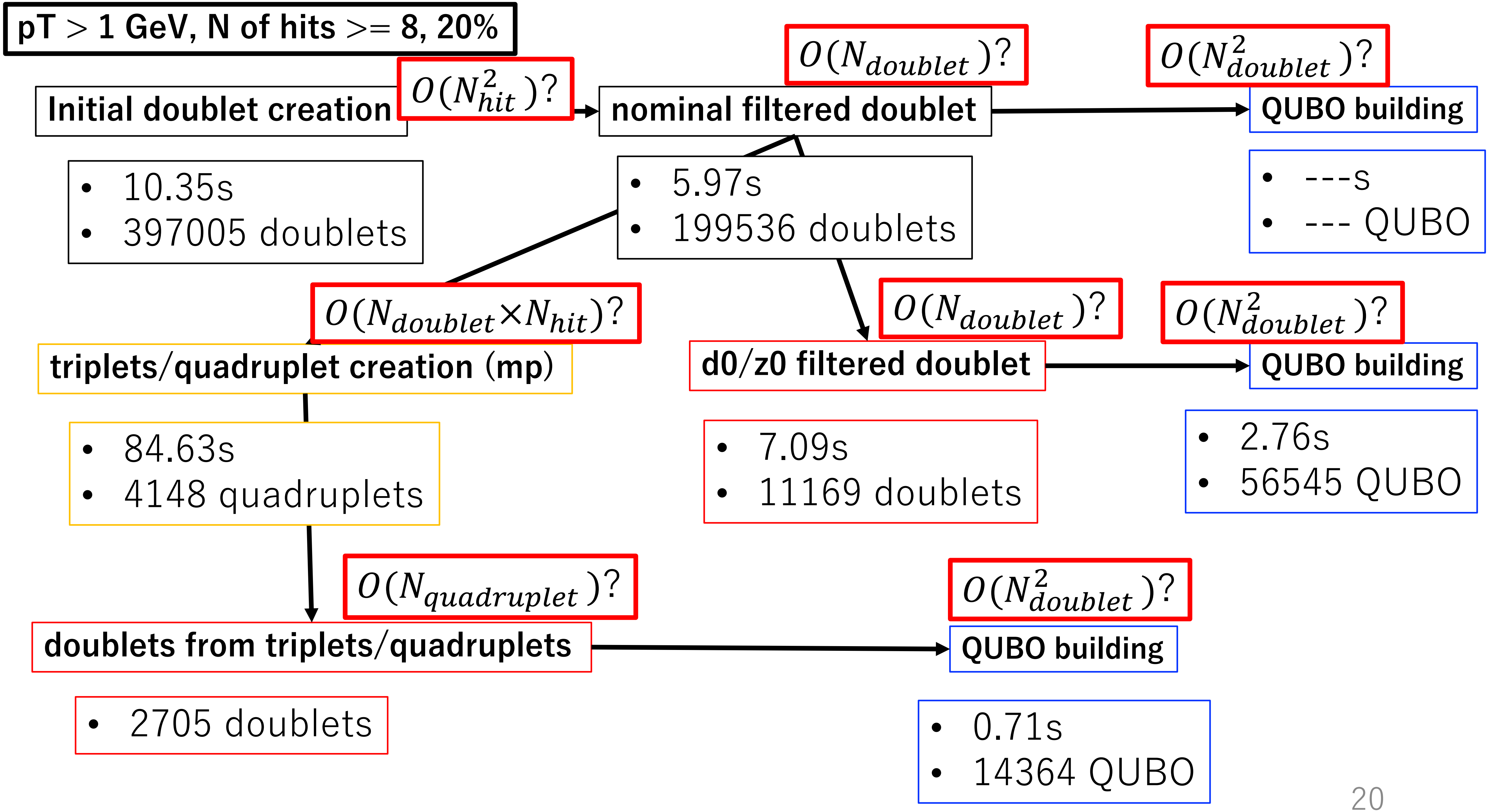
- Long-range profit term works as expected.

- Accuracy/Fake in doublet strategy is worse than triplet strategy
  - The use of xplet of more hits(information) is better?

- Reconfirmed that doublet-based QUBO needs early selection
  - $\sim O(N^2_{doublet})$
  - $\sim O(N^4_{hit})$

- Fake doublet can be reduced by
  - Triplet/Quadruplet creation : $O(N_{doublet} \times N_{hit})$
  - Tight d0/z0 constraint: $O(N_{doublet})$, but miss important signatures
    - e.g. photon conv., B-jets, some long-lived new particles
  - Other idea?

backup


pT > 1 GeV, N of hits >= 8, 20%
Initial doublet creation
$O(N_{hit}^2)$?
• 10.35s
• 397005 doublets
nominal filtered doublet
$O(N_{doublet})$?
• 5.97s
• 199536 doublets
$O(N_{doublet}^2)$?
QUBO building
• ---s
• --- QUBO
$O(N_{doublet} \times N_{hit})$?
triplets/quadruplet creation (mp)
• 84.63s
• 4148 quadruplets
$O(N_{doublet})$?
d0/z0 filtered doublet
• 7.09s
• 11169 doublets
$O(N_{doublet}^2)$?
QUBO building
• 2.76s
• 56545 QUBO
$O(N_{quadruplet})$?
doublets from triplets/quadruplets
• 2705 doublets
$O(N_{doublet}^2)$?
QUBO building
• 0.71s
• 14364 QUBO

pT > 1 GeV, N of hits >= 8

Initial doublet creation

5%: 1.24s, 24648 doublets
10%: 3.08s, 96886 doublets
20%: 10.35s, 397005 doublets

→

Nominal filtered doublet

5%: 0.47s, 13003 doublets
10%: 1.35s, 49347 doublets
20%: 5.97s, 199536 doublets

→

QUBO building

5%: 37.69s, 226422 QUBO
10%: 592.12s, 1655672 QUBO
20%: ---s, --- QUBO

Triplets/quadruplet creation

5%: 1.62s, 2756 triplets, 866 quadruplets
10%: 10.97s, 14105 triplets, 1737 quadruplets
20%: 84.63s, 99468 triplets, 4148 quadruplets

Doublets from triplets/quadruplet

5%: 667 doublets
10%: 1282 doublets
20%: 2705 doublets

→

QUBO building

5%: 0.15s, 3370 QUBO
10%: 0.30s, 6649 QUBO
20%: 0.71s, 14364 QUBO

pT > 1 GeV, N of hits >= 8

Initial doublet creation

5%: 1.24s, 24648 doublets
10%: 3.08s, 96886 doublets
20%: 10.35s, 397005 doublets

nominal filtered doublet

5%: 0.47s, 13003 doublets
10%: 1.35s, 49347 doublets
20%: 5.97s, 199536 doublets

QUBO building

5%: 37.69s, 226422 QUBO
10%: 592.12s, 1655672 QUBO
20%: ---s, --- QUBO

triplets/quadruplet creation (mp)

5%: 1.62s, 2756 triplets, 866 quadruplets
10%: 10.97s, 14105 triplets, 1737 quadruplets
20%: 84.63s, 99468 triplets, 4148 quadruplets

d0/z0 filtered doublet

5%: 0.43s, 1209 doublets
10%: 1.74s, 3496 doublets
20%: 7.09s, 11169 doublets

QUBO building

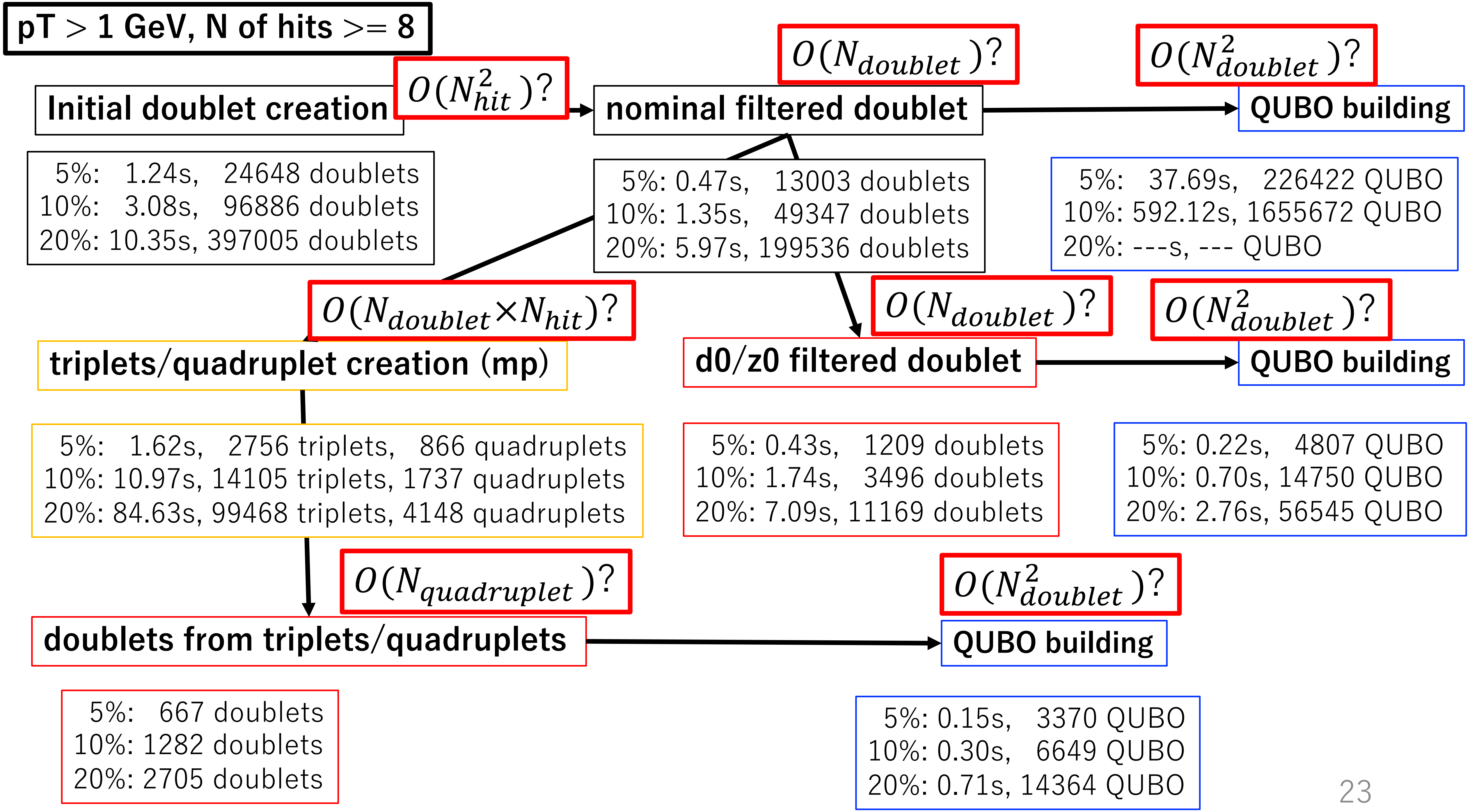
5%: 0.22s, 4807 QUBO
10%: 0.70s, 14750 QUBO
20%: 2.76s, 56545 QUBO

doublets from triplets/quadruplet

5%: 667 doublets
10%: 1282 doublets
20%: 2705 doublets

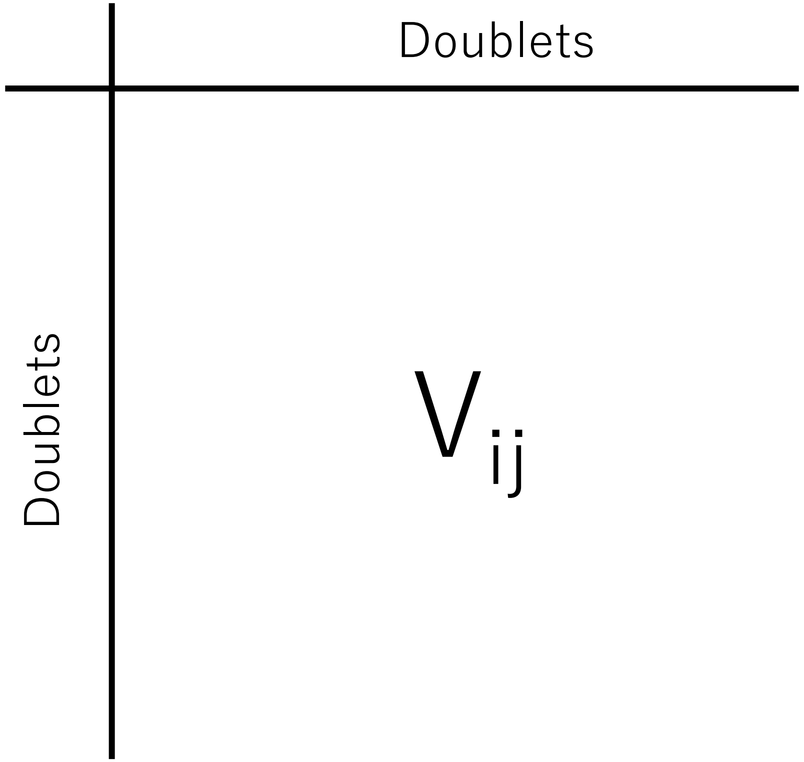
QUBO building

5%: 0.15s, 3370 QUBO
10%: 0.30s, 6649 QUBO
20%: 0.71s, 14364 QUBO


pT > 1 GeV, N of hits >= 8
Initial doublet creation
$O(N_{hit}^2)$?
5%: 1.24s, 24648 doublets
10%: 3.08s, 96886 doublets
20%: 10.35s, 397005 doublets
nominal filtered doublet
$O(N_{doublet})$?
5%: 0.47s, 13003 doublets
10%: 1.35s, 49347 doublets
20%: 5.97s, 199536 doublets
$O(N_{doublet}^2)$?
QUBO building
5%: 37.69s, 226422 QUBO
10%: 592.12s, 1655672 QUBO
20%: ---s, --- QUBO
$O(N_{doublet} \times N_{hit})$?
triplets/quadruplet creation (mp)
5%: 1.62s, 2756 triplets, 866 quadruplets
10%: 10.97s, 14105 triplets, 1737 quadruplets
20%: 84.63s, 99468 triplets, 4148 quadruplets
$O(N_{doublet})$?
d0/z0 filtered doublet
5%: 0.43s, 1209 doublets
10%: 1.74s, 3496 doublets
20%: 7.09s, 11169 doublets
$O(N_{doublet}^2)$?
QUBO building
5%: 0.22s, 4807 QUBO
10%: 0.70s, 14750 QUBO
20%: 2.76s, 56545 QUBO
$O(N_{quadruplet})$?
doublets from triplets/quadruplets
5%: 667 doublets
10%: 1282 doublets
20%: 2705 doublets
$O(N_{doublet}^2)$?
QUBO building
5%: 0.15s, 3370 QUBO
10%: 0.30s, 6649 QUBO
20%: 0.71s, 14364 QUBO

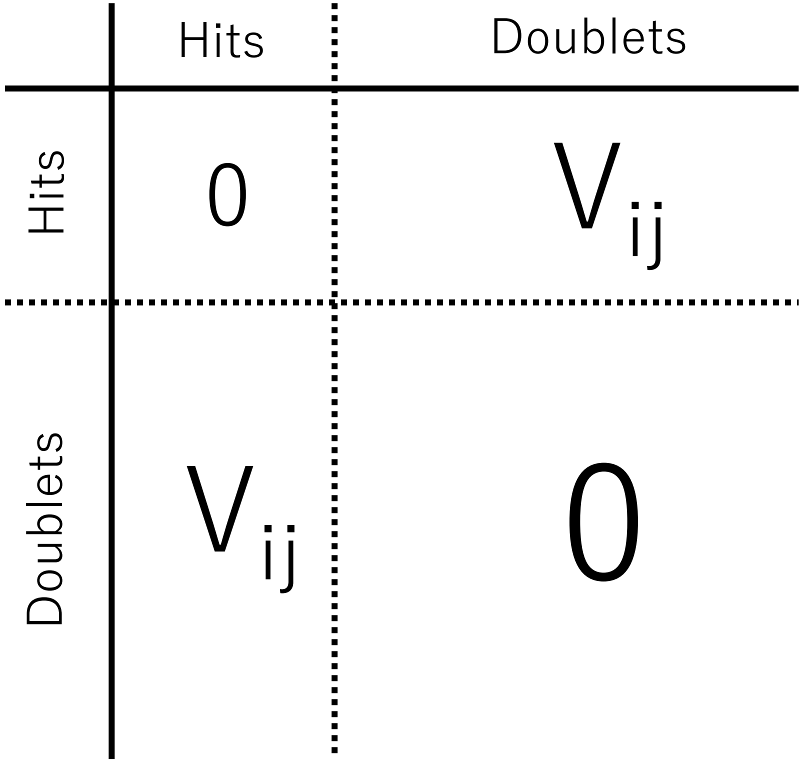
QUBO matrix

Doublet-Doublet QUBO



$$\text{N of QUBO} = N_{doublet}^2$$

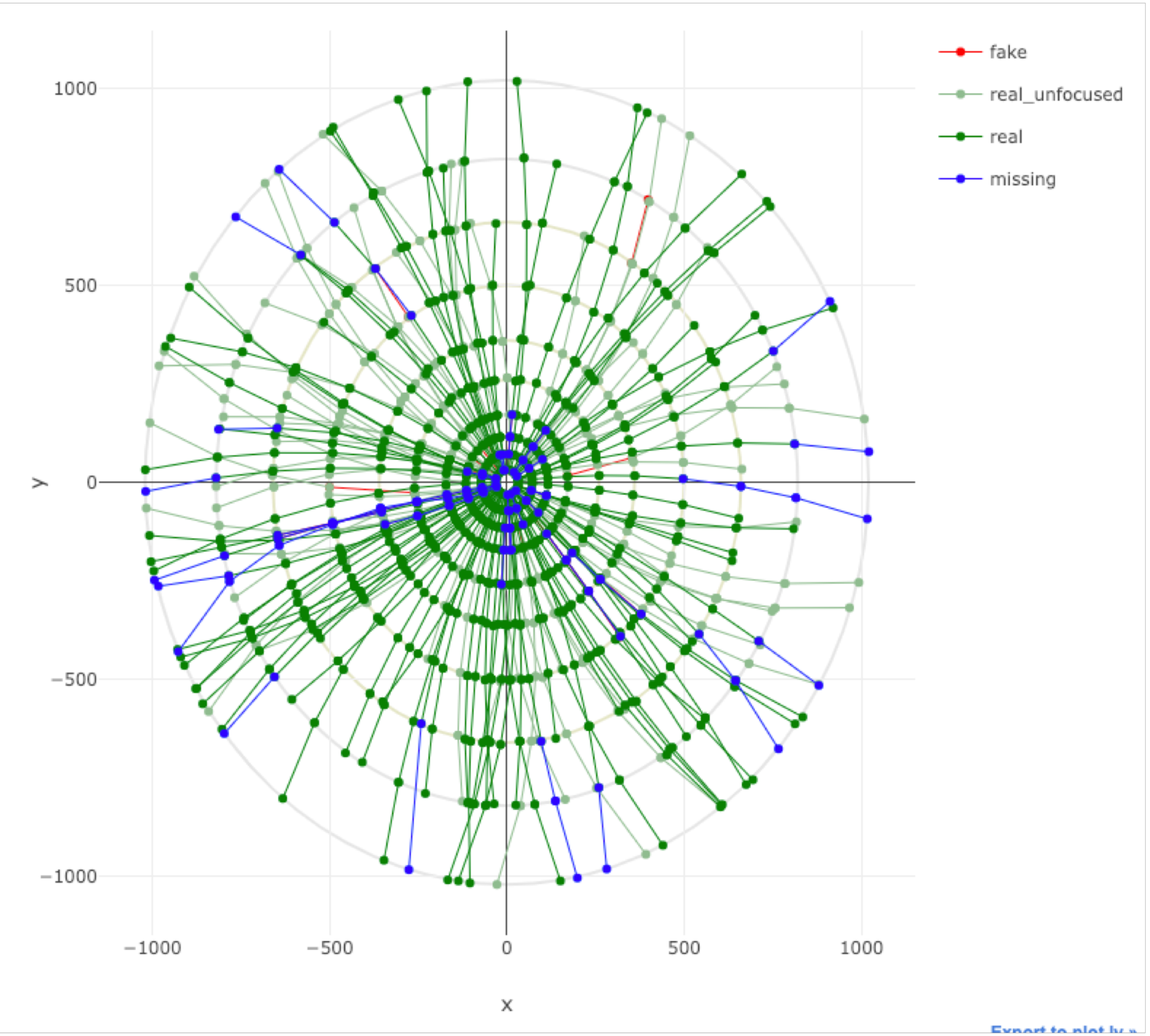
Doublet-Hit QUBO

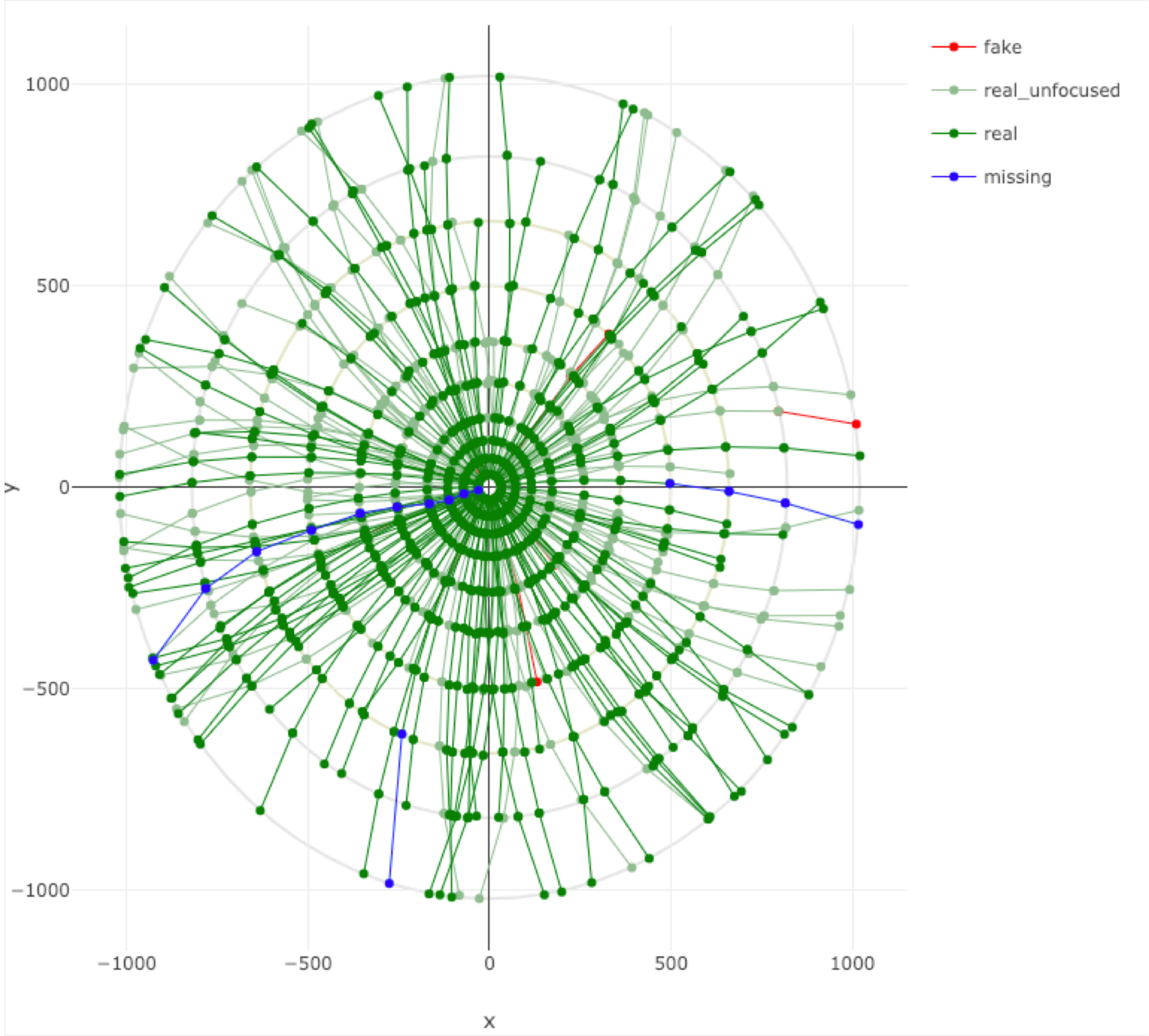


$$\text{N of QUBO} = N_{doublet} \times N_{hit}$$

Use “origin” constraint + triplet/quadruplet filter

qallseMp

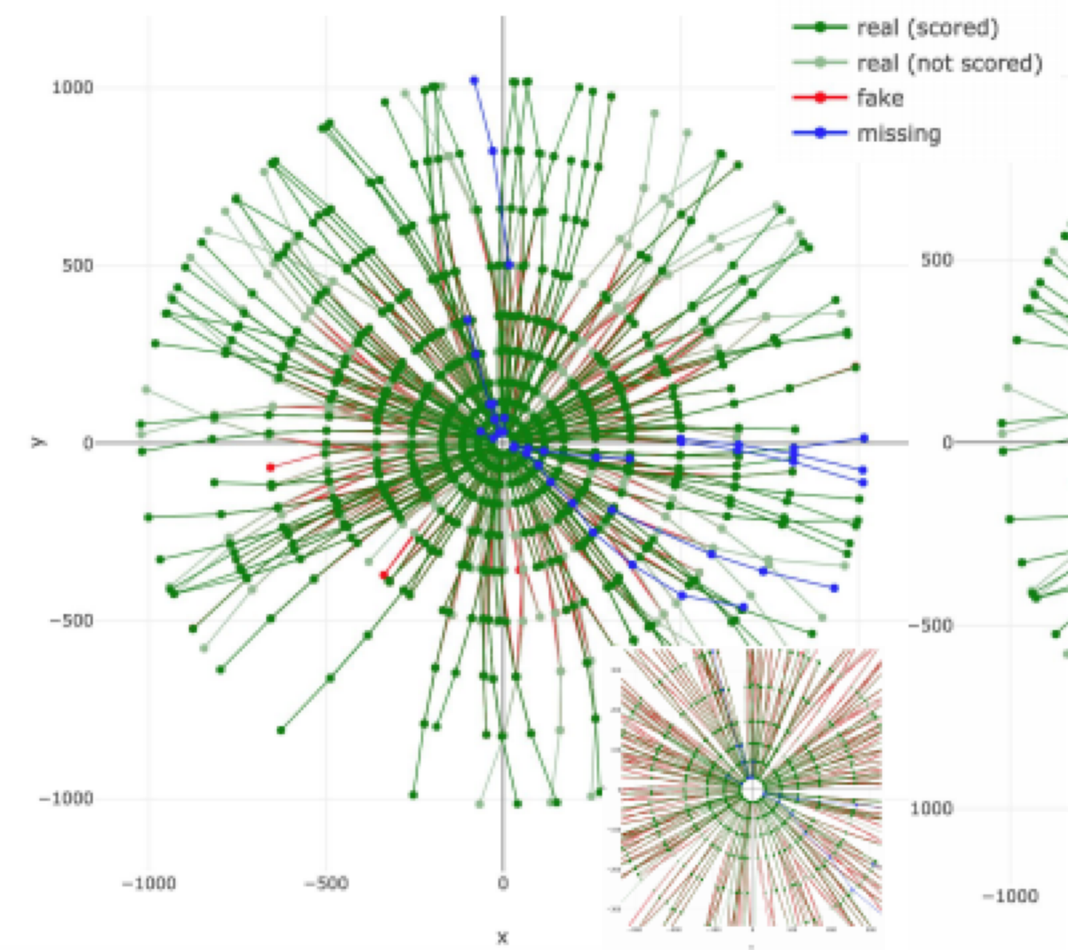


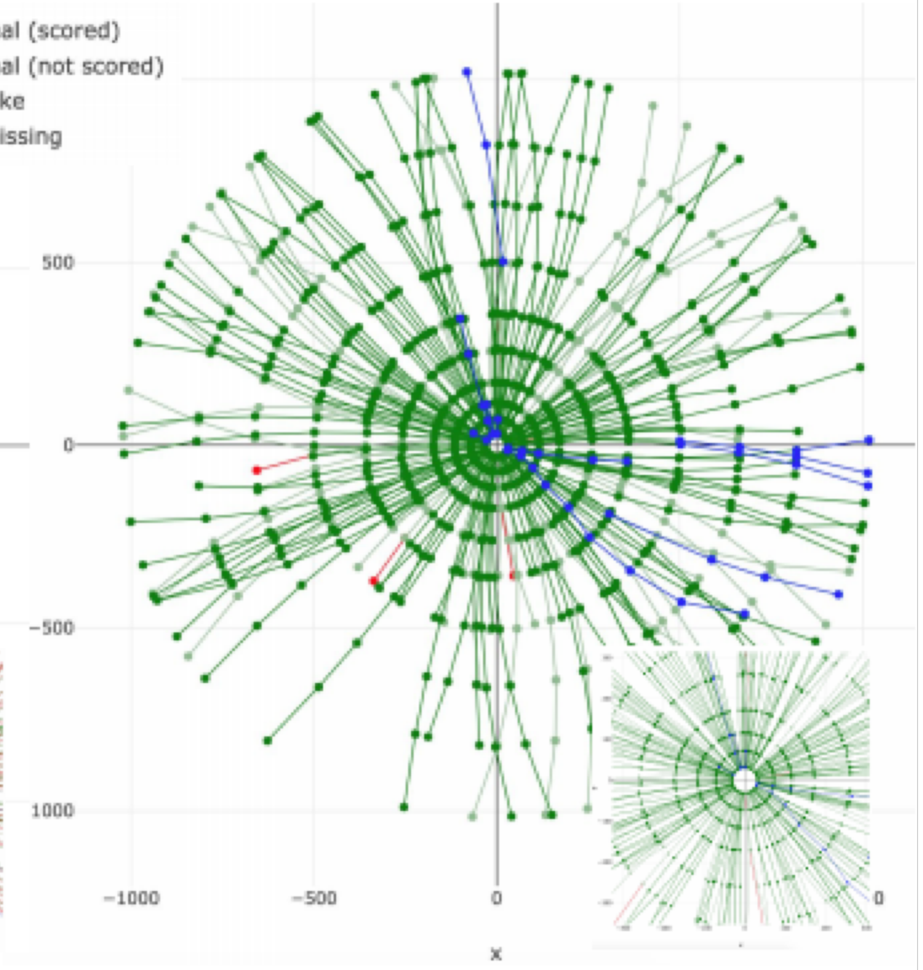


Results

dataset size: ~20%
1,637 particles, 11,030 hits

plotting error: too many doublets 392529





392,529 doublets
p=**0.26**%, r=**99.15**%

57.3s
build QUBO

2,546 doublets
(2,964 triplets)
QUBO size: 14,345

17.1s
sample QUBO
running on CPU

1,512 doublets
p=**99.13**%, r=**97.06**%

trackml score **97.55%**