Training machines, training people

- Associate Research
  - **Tracking with Graph Neural Networks** (GNNs)
  - Organizing **software training events** with HSF and IRIS-HEP
  - With CMS

- till July ‘23: PhD with **Belle 2**
  - Calibrating the FEI (aka Belle 2’s Skynet candidate) for a V_{cb} measurement
  - Maintaining Belle 2’s integration/performance test (“validation”) framework
  - Rebuilt Belle 2’s onboarding training

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iris hep

Discuss in #7

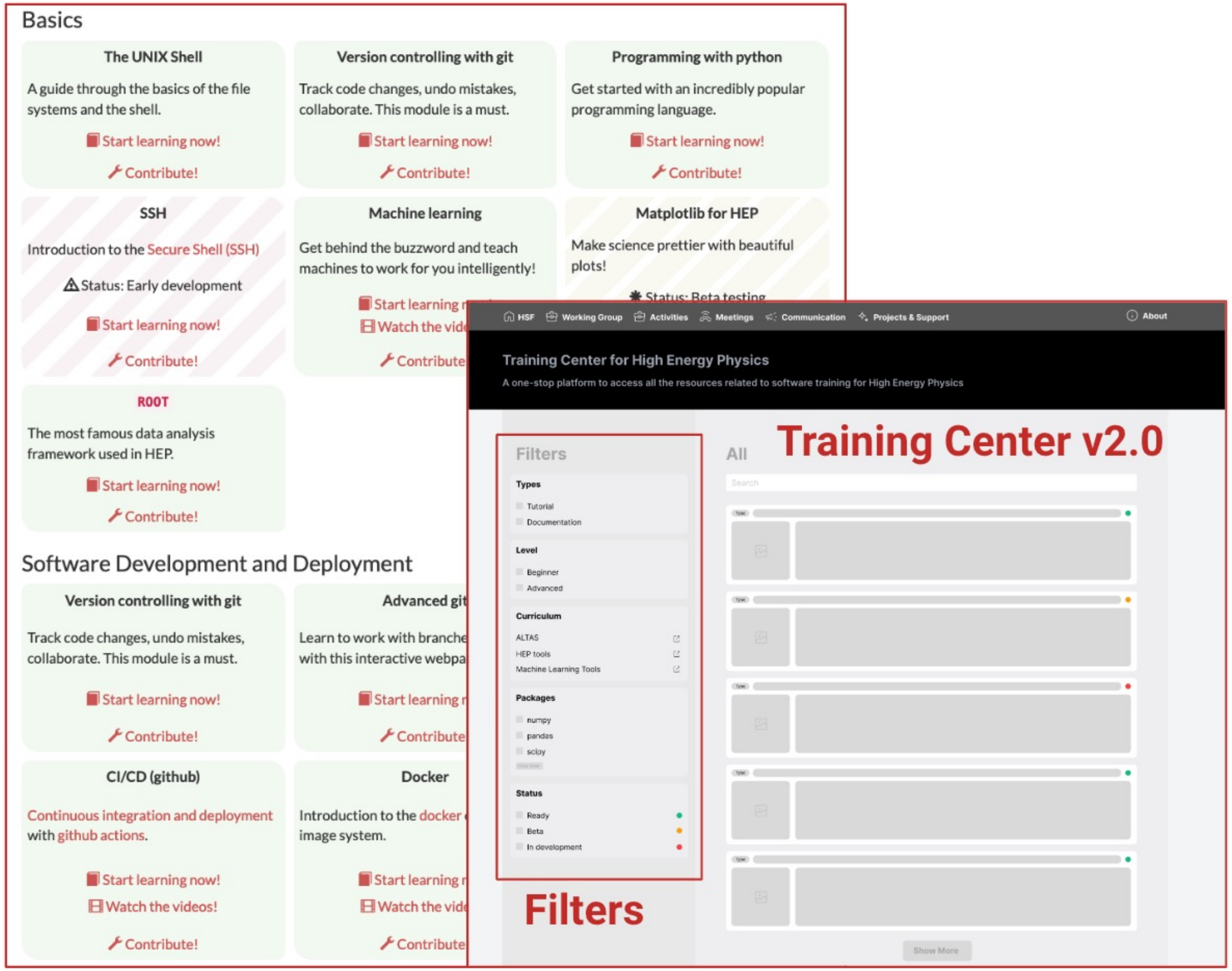
Training people

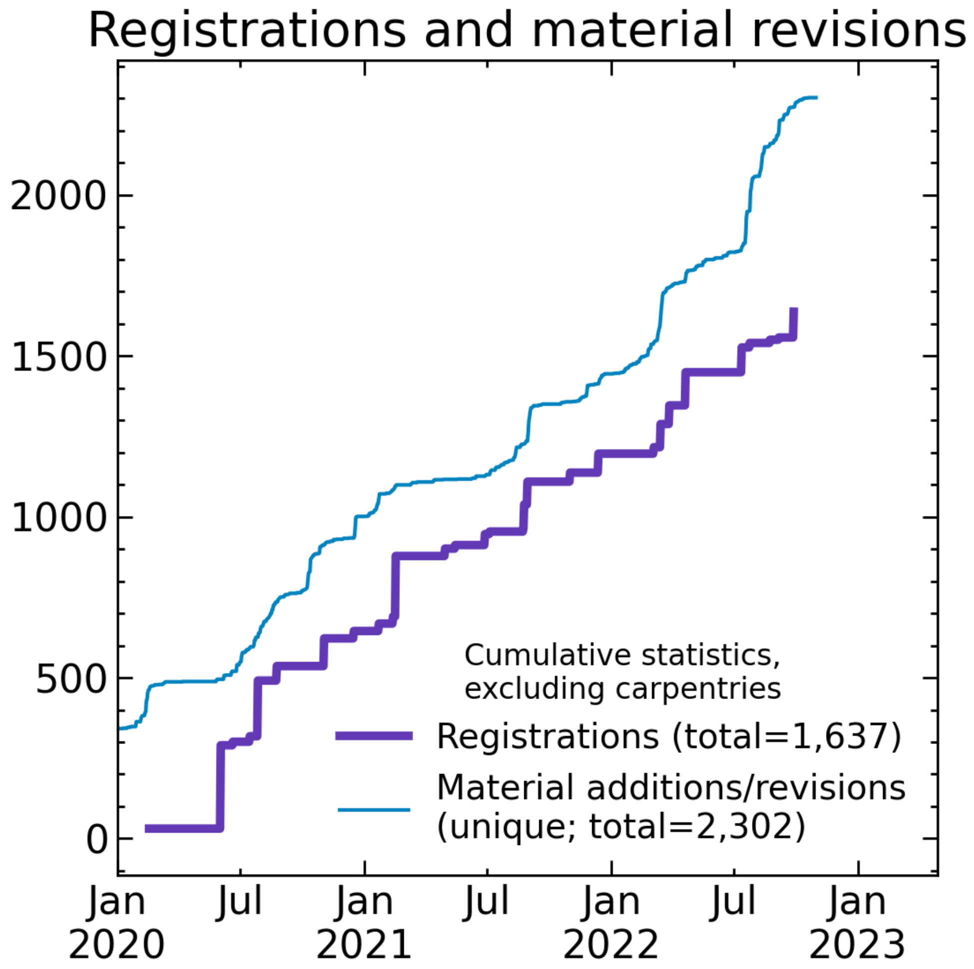
Training people in cross-experiment software skills

Discuss in #7

How can we collaborate & be efficient?

Unified training center hepsoftwarefoundation.org/training/curriculum.html



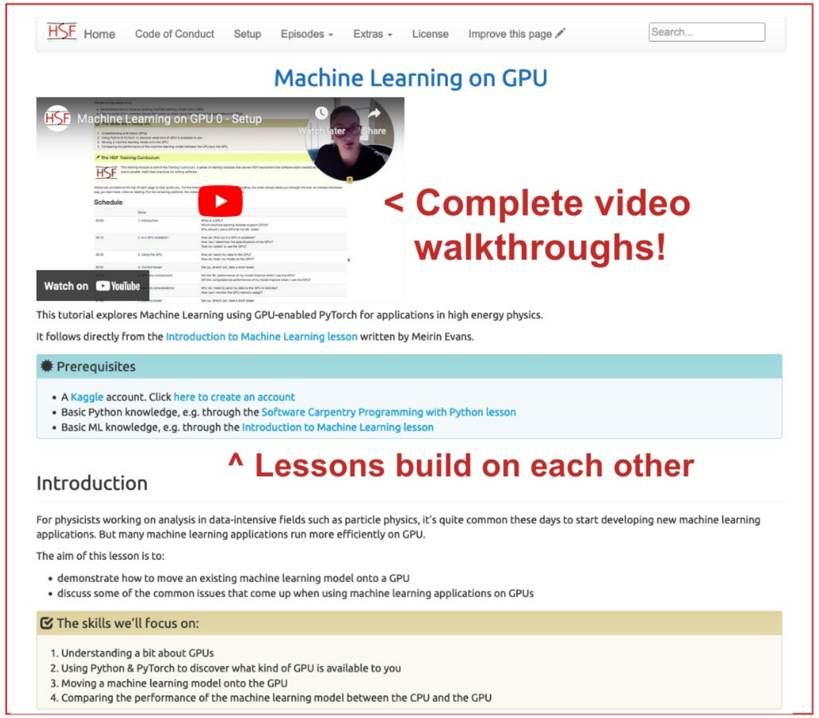


Training material (technical side)

Discuss in #7

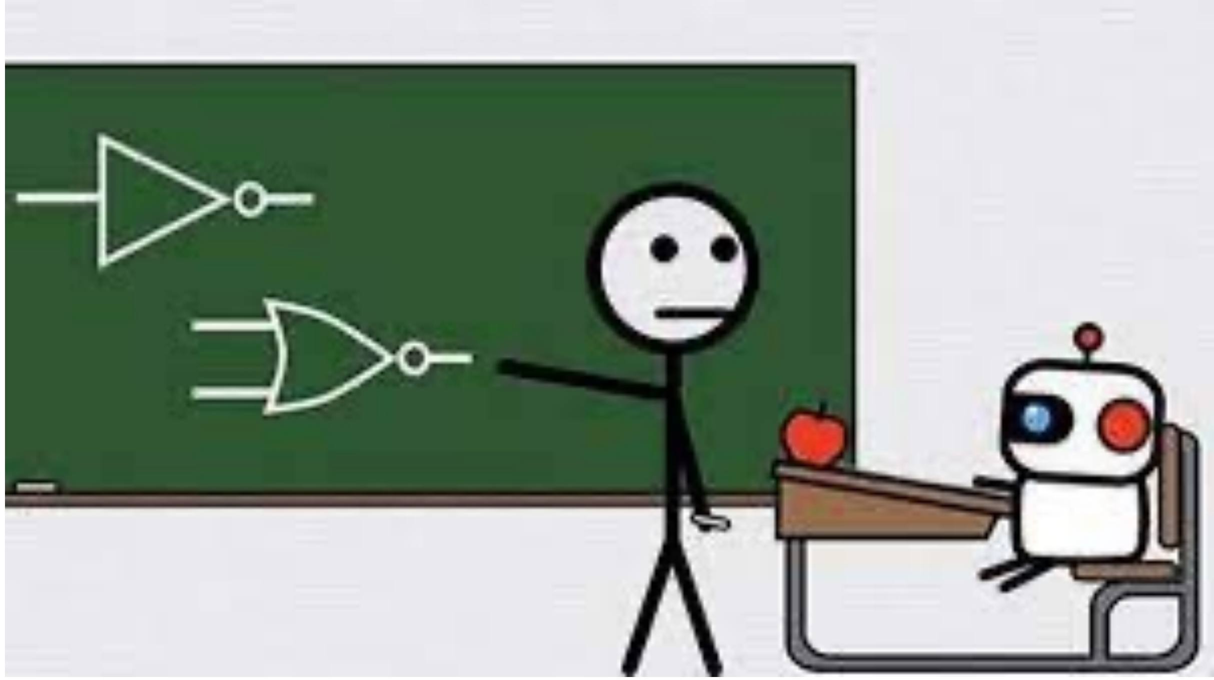
- **How to write material:**
  - HSF uses a lot of **“carpentry-style”** websites (built in Jekyll)
  - SW Carpentry recently switched to new framework (in R): **Good time to reevaluate our choices!**
  - In an ideal world, there would be >=3 versions of each course:
    - Self-study writeup/notebook (verbose & complete)
    - Workshop presentation slides/notebook
    - Workshop student notebooks (for exercises)

  ==> Not feasible? How to approach
- **Running code in the browser:**
  - Binder is now low on resources
  - Google collab will work for anything without big dependencies
  - GitHub codespaces looks very promising
- Cool idea (via Jim): Include **feedback buttons** directly in exercise notebook



Discuss in #26, #19

Training machines

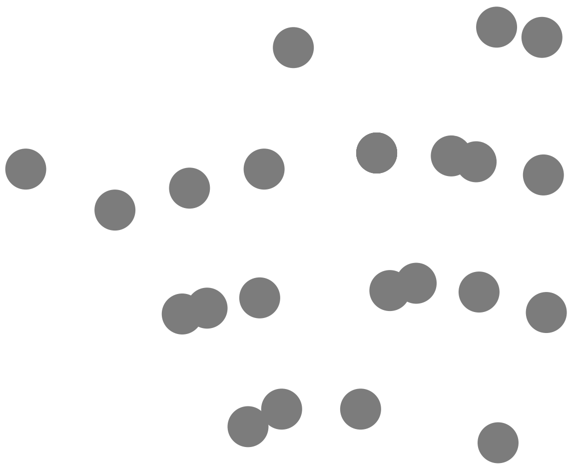


(from CGP Grey)

Tracking with object condensation

Point cloud

(coordinates of hits in detector)

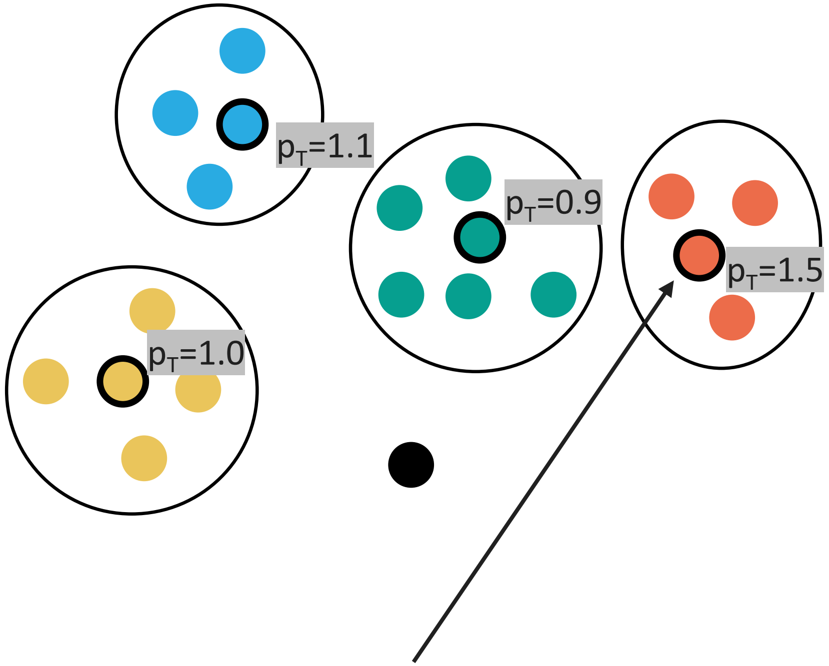


Repulsion & attraction

of points in latent space

Learnt latent space

Hits already clustered by particle;
Clusters can be collected trivially



Condensation point

Represents the track, can learn track parameters like p_T (WIP)

No time resolution of points
==> Everything everywhere all at once

Tech stack & implementation

PyTorch Talking to the GPU

PyG
Dealing with graphs & GNNs

PyTorch Lightning Cut boilerplate, checkpoints, hyperparams

Weights & Biases
Online dashboard

Fully open source framework:
github.com/gnn-tracking

klieret Ruff fixes ... ✓ 12 hours ago 1,055

View code

README.md

GNNs for Charged Particle Tracking

docs passing | pre-commit.ci passed | Python package passing | Check Markdown links passing | codecov 70%

This repository holds the main python package for the GNN Tracking project. See the readme of the organization for an overview of the task.

Ongoing fights: SLURM & ML

Perhaps to discuss in #19

- Our infrastructure (in my case, **SLURM**) is often not a first class citizen for ML frameworks: How can we get them to play nice together?

Example 1: SLURM + Weights & Biases

Weights & Biases

- Batch nodes usually don't have internet, but Weights & Biases syncs to a cloud.
- Solution (self-advertisement): Trigger synchronizations from the login node github.com/klieret/wandb-offline-sync-hook
- Alternative: Use ray

Example 2: SLURM + Ray Tune

RAY tune

- SLURM example from Ray docs is probably not what you want
- But can start ray head on login node, then allocate ray workers (example)
- But how to handle timeout of nodes with long training jobs? Ideally would like to not accept job if we cannot finish it and instead resubmit request for new node

Positive example: SLURM + Lightning

SLURMEnvironments can checkpoint + resubmit itself

Collaborating on ML R&D

Discuss in #26

How can we structure **ML frameworks for R & D** such that we can get multiple developers & scientists **develop models together**

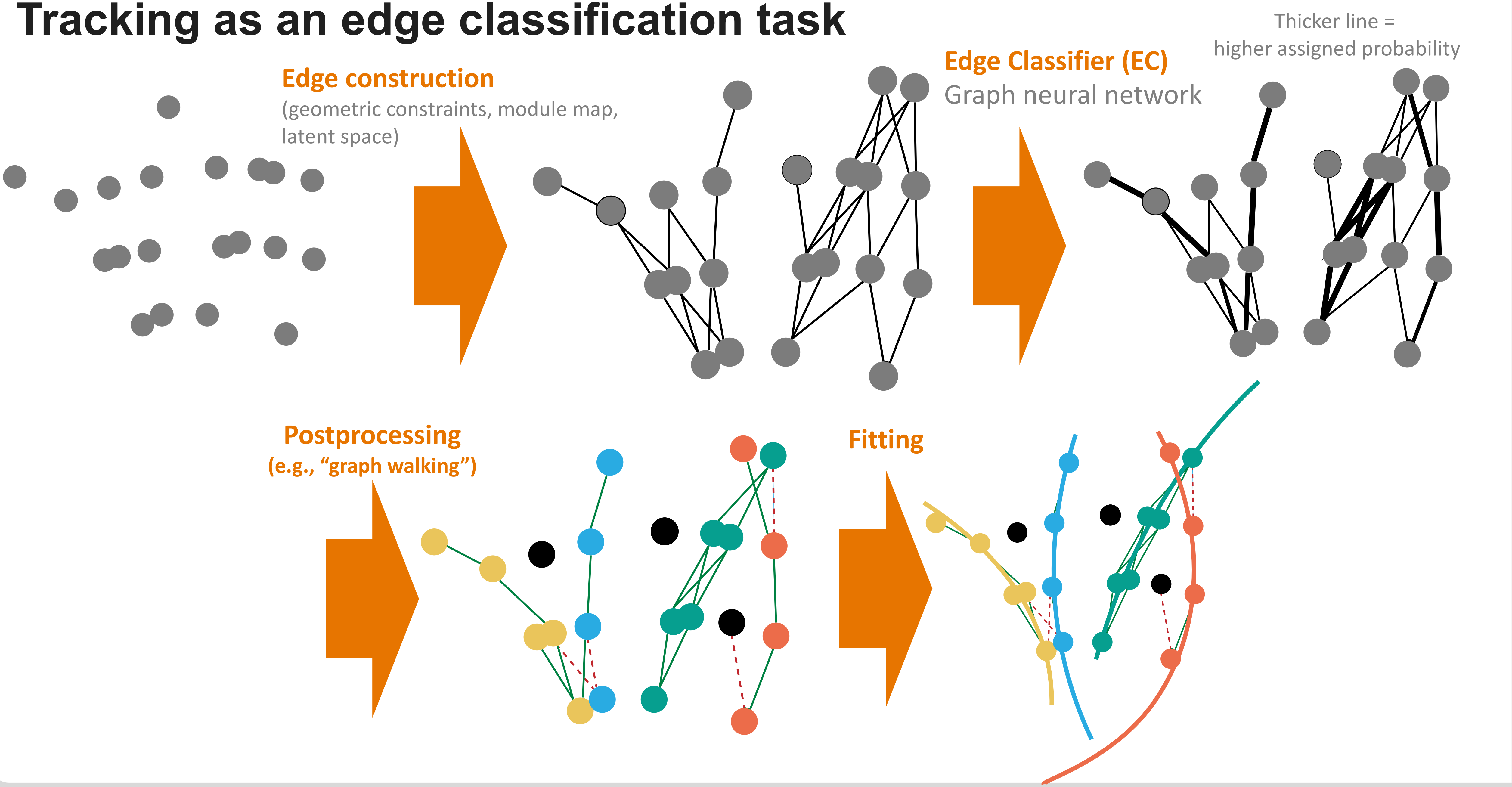
1. Want: **Cutting boiler plate** & making it fun
2. Want: **Mix & match models**
3. Don't want: **"Fork & forget"**, people starting forks for some experiment that never contribute back to the original project
4. Don't want: **Constrain creativity**

Bottom line:

- This very different from the requirements ML in production
- Both a "soft topic" and a framework question

Backup

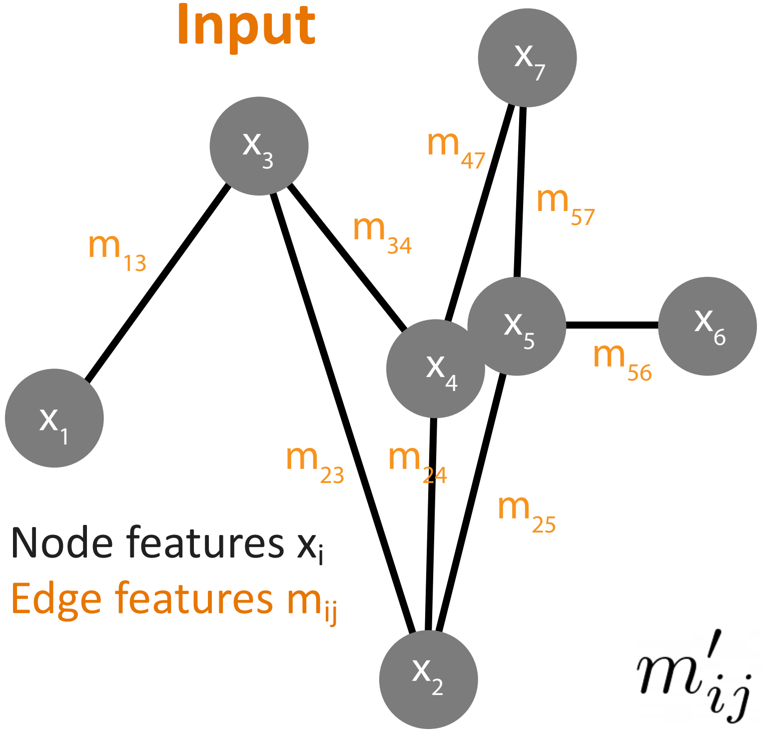
Tracking as an edge classification task



Graph Neural Networks

In our case: Input, latent and output is (almost) the same graph (but different features)

Input

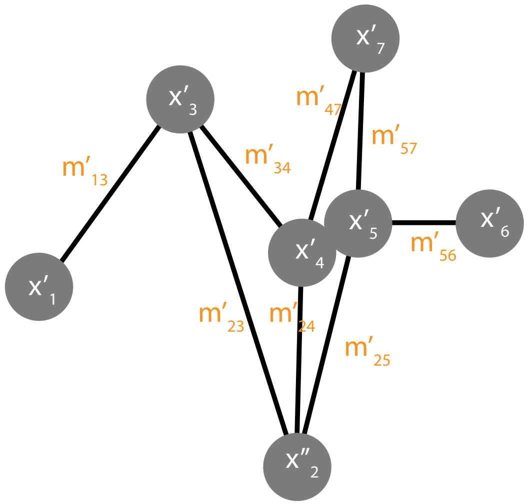


Node features x_i

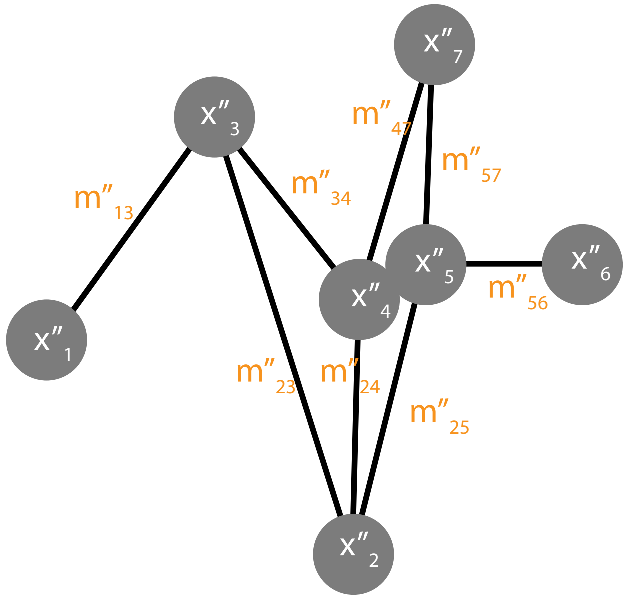
Edge features m_{ij}

Latent

(usually more than one graph)



Output



$$m'_{ij} = \mathrm{NN}(x_i, x_j, m_{ij})$$

$$x'_i = \mathrm{NN}\Big(x_i, \bigoplus_{j \in \mathcal{N}_i} m_{ij}\Big)$$

all neighboring nodes

some permutation invariant aggregation

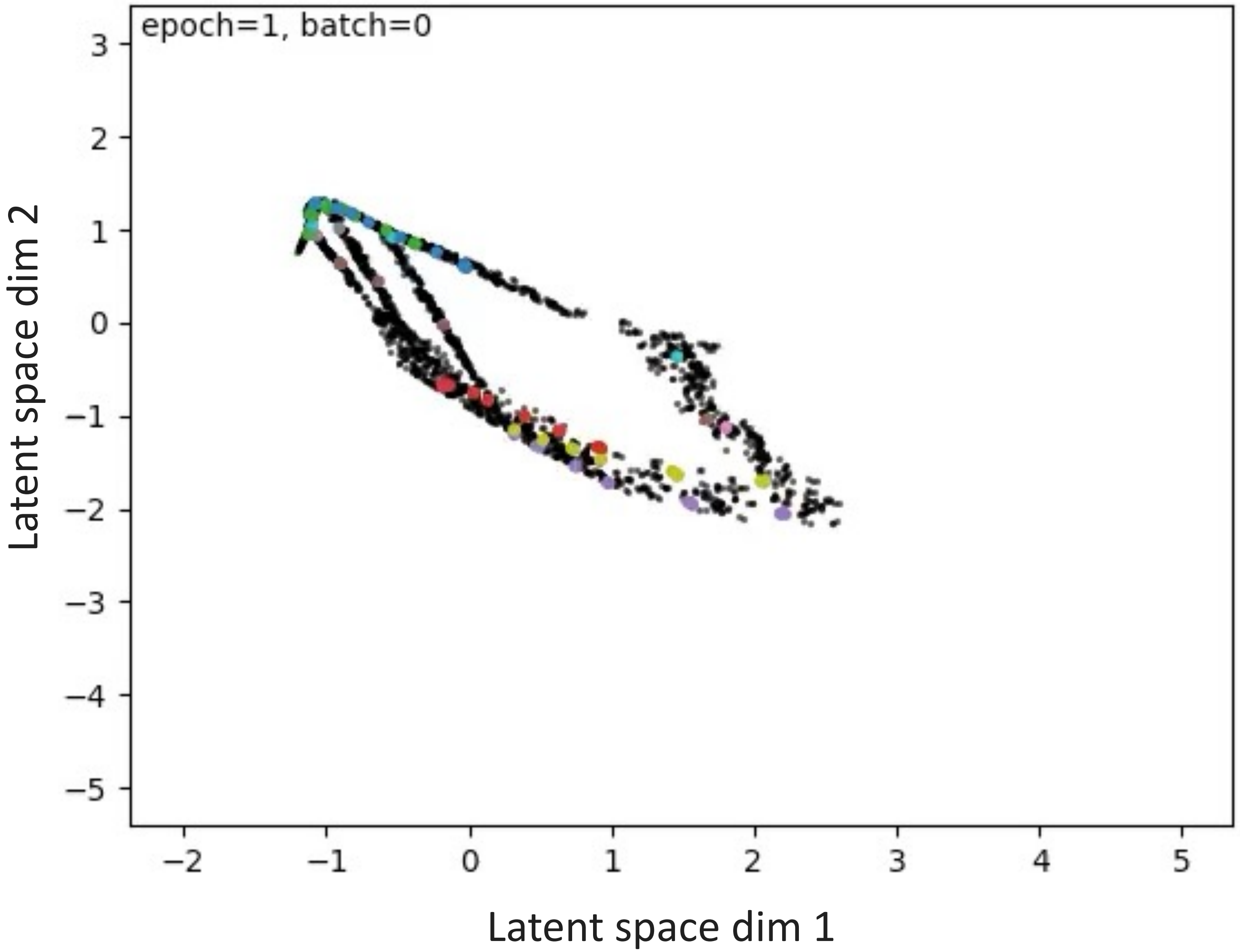
Edge classification: Final edge features are probability that edge is correct (connects hits that belong to the same particle)

Object condensation in action

2D latent space; random selection of particles colored

Early simplified study (much fewer hits than in real life)

Click here if video doesn't play



Object condensation: Training losses

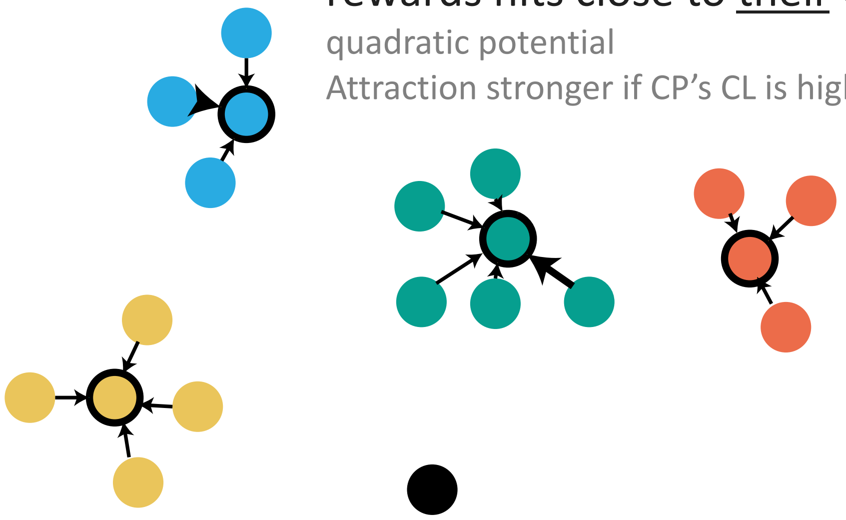
Latent space
before training

GNN predicts **condensation likelihoods (CL)** for every hit.
Hit with max CL for particle* is **condensation point (CP)**

*during inference: for cluster

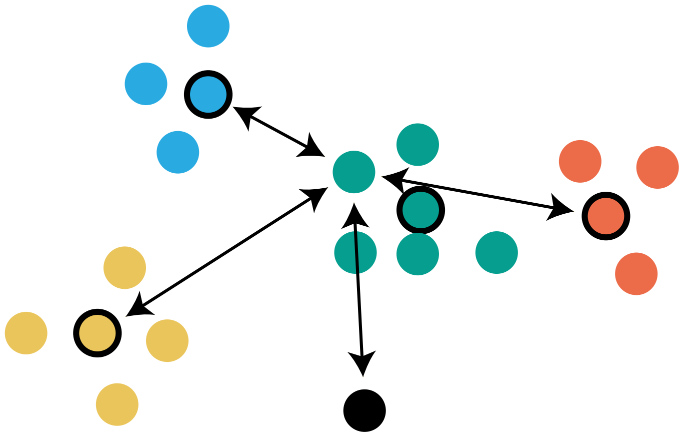
Attractive loss function

rewards hits close to <u>their</u> CP
quadratic potential
Attraction stronger if CP's CL is high



Repulsive loss function

penalizes hits close to <u>other</u> CP
hinge loss: no more repulsion after certain distance
repulsion stronger for strong CP CLs



Background loss function

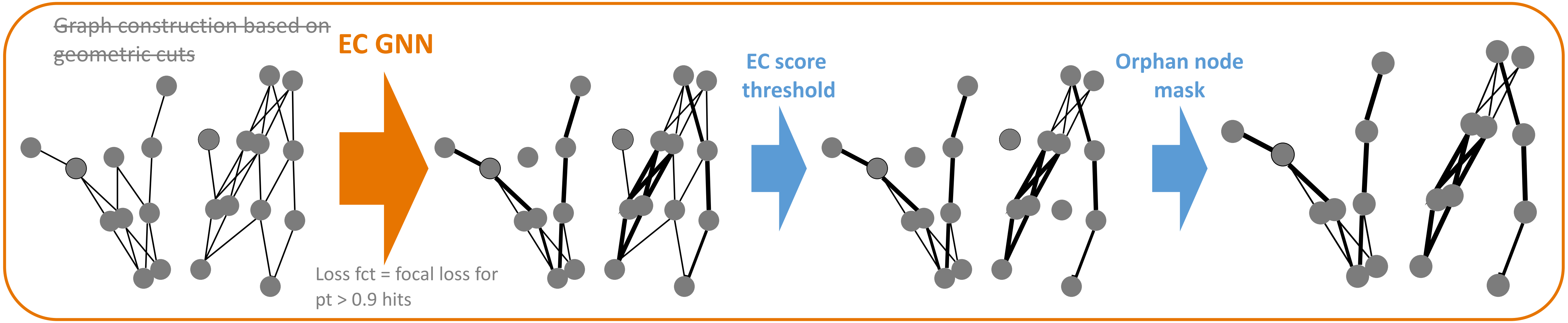
noise hits should have low CL

Loss functions implemented from Kieseler 2020 (2002.03605)

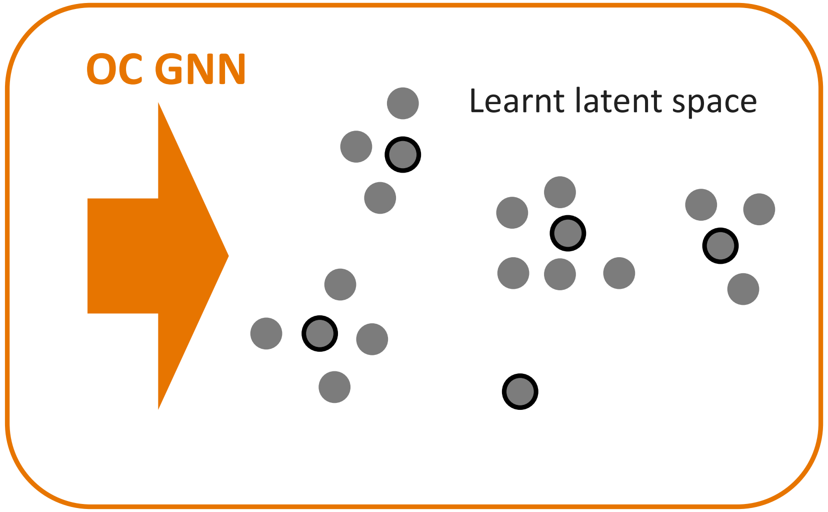
Object condensation: Our current pipeline

STAGE 1: EC

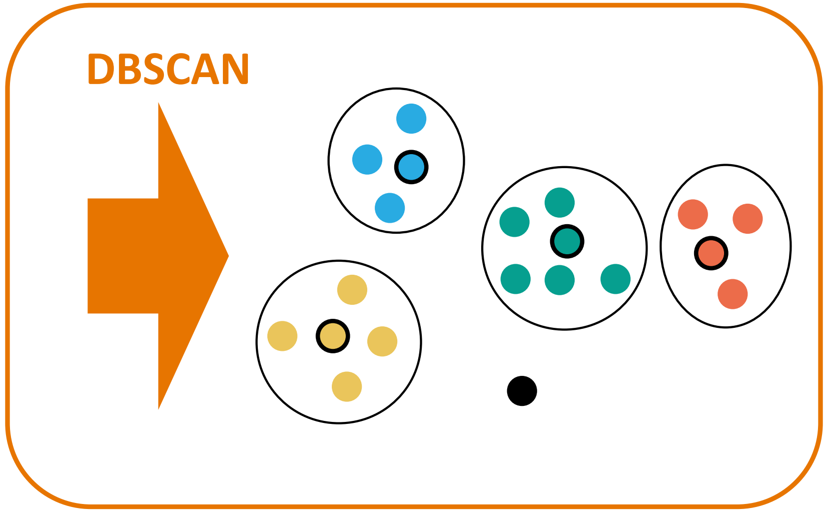
→ Working on replacing this with dynamic edge creation "Point cloud network"



STAGE 2: OC



STAGE 3: Collect clusters



- All three stages have their own hyperparameters
- Can be trained/optimized separately (fixing the previous stage)