

CoCo: Contrastive Framework for Combinatorics

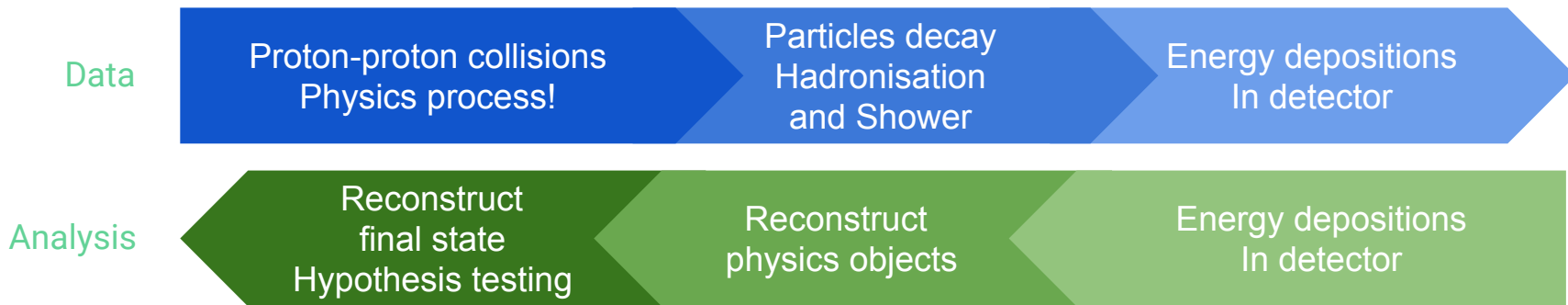
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ML4Jets, Hamburg 2023



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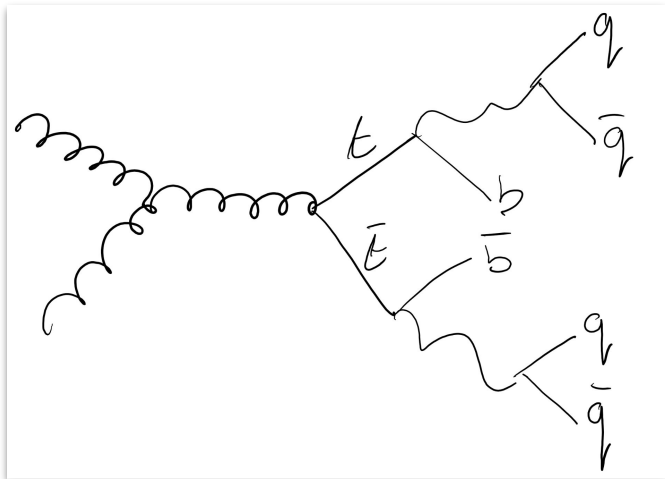
Reconstructing collisions

- In our detectors, all the interesting physics happens within $\sim 3\text{mm}$
 - The detector exists to capture the remnants
 - But we never see exactly what happened!



- One of the biggest challenges in our physics programme is
Reconstruction and inference

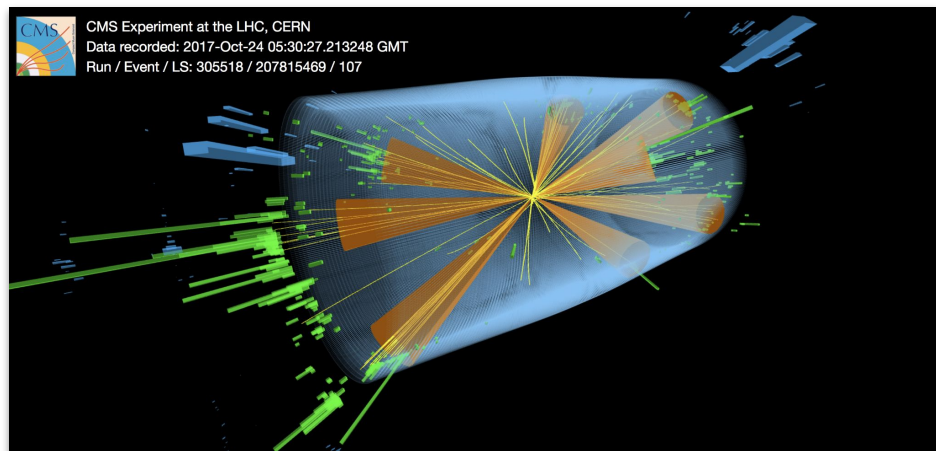
Problems with high multiplicity processes!



What we observe

Six jets, two b-tagged

All pointing back to interaction point



But which jet is which?

Need to match jets to correct quarks

Simple approaches

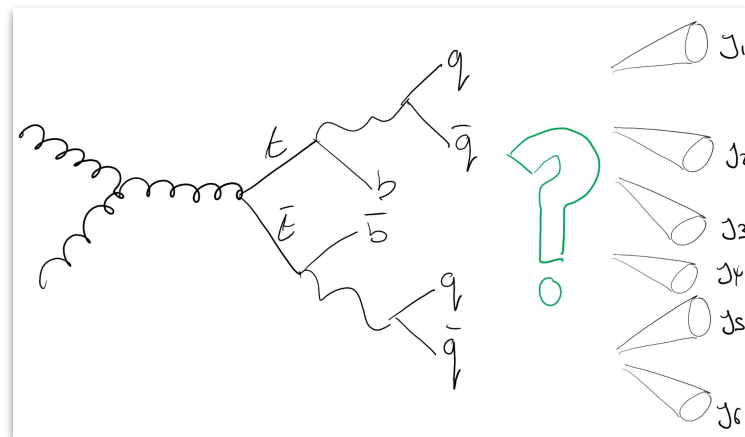
For top quark reconstruction very common approach:

Solve combinatorics of assigning jets to quarks

The standard method is to test every possible combination and pick “most likely”

nJets	6	7	8	9
nChoose6 (removing symmetries)	92	644	2576	7728

Huge combinatorial explosion!



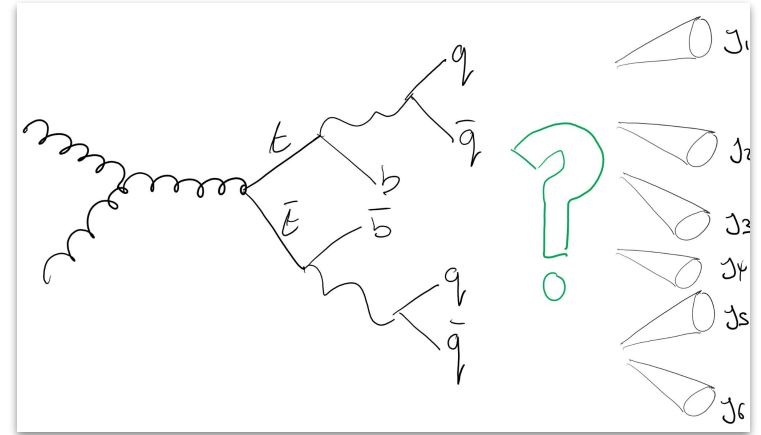
Simple approaches

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$$\chi^2 = \frac{(m_{b_1 q_1 q_2} - m_t)^2}{\sigma_t^2} + \frac{(m_{b_2 q_3 q_4} - m_t)^2}{\sigma_t^2} + \frac{(m_{q_1 q_2} - m_W)^2}{\sigma_W^2} + \frac{(m_{q_3 q_4} - m_W)^2}{\sigma_W^2},$$

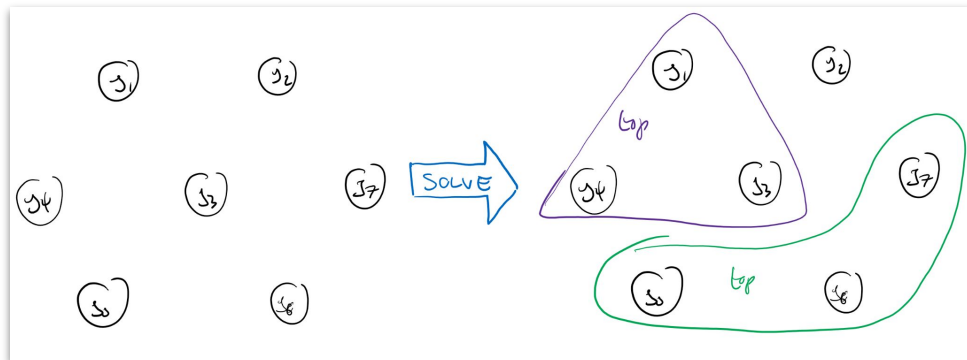


“Most likely” often chosen to minimise this

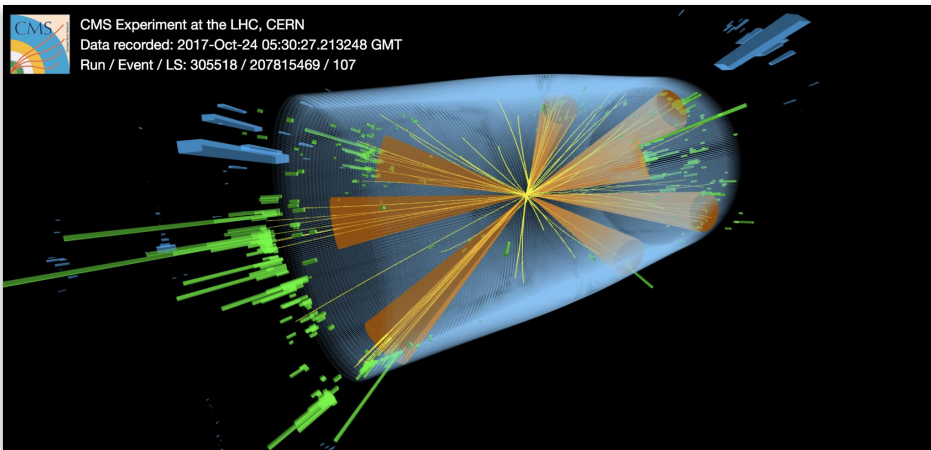
Modern ML techniques

Graphs and sets natural way to represent physics data

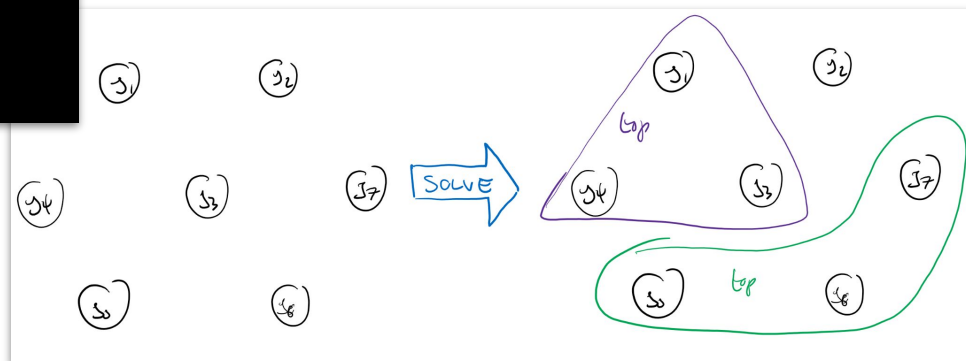
- Use graph networks to identify objects (jets/tracks) from same origin
 - Connect every object together $N(N-1)$ edges, **identify “true” edges**
- Attention transformers on sets
 - Evaluate all triplets directly
- Notable literature:
 - [SPANet](#)
 - [Topograph](#)



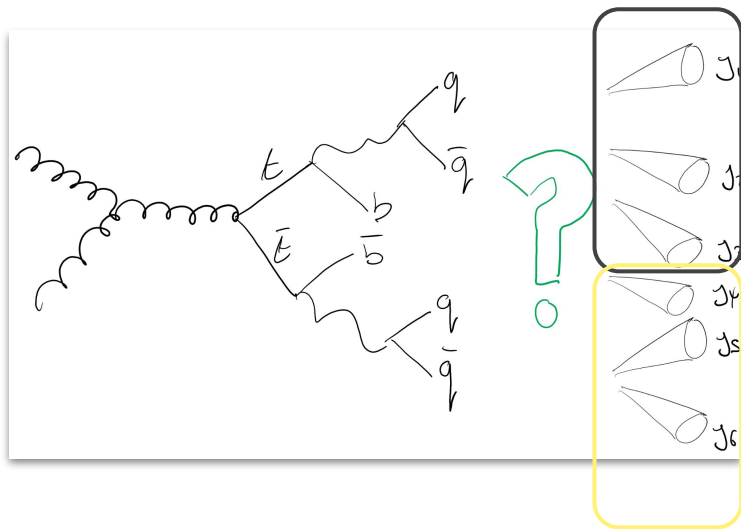
Unfortunately...



... detector environment doesn't end up with jets spatially grouped based on origin



Can we still do this?



YES!

Take inspiration from Feynman diagram

Can just cluster this space:

- Learn an embedding that groups based on decay tree

How can we do this?

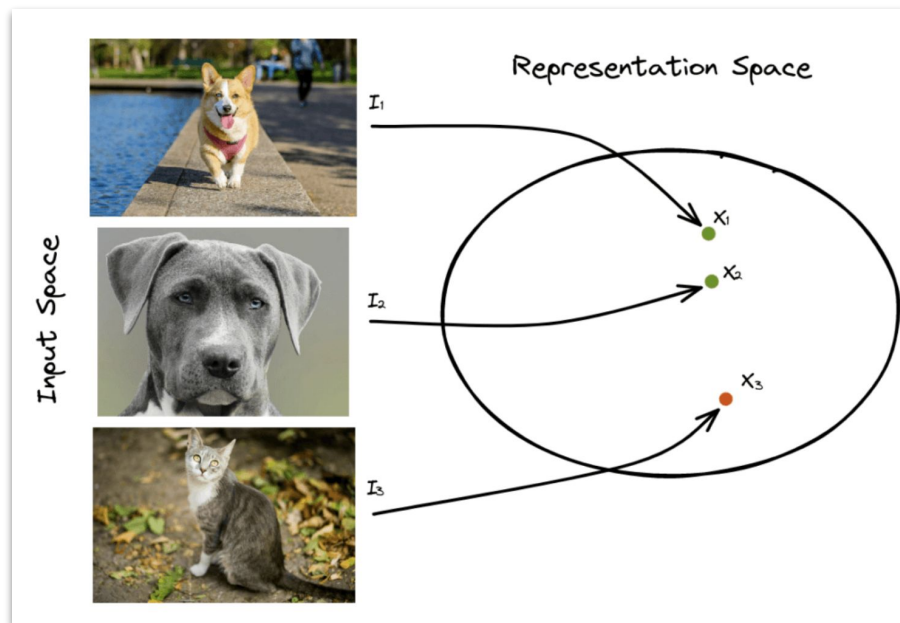
Contrastive learning!

Learn an embedding/feature space

For some definition of ‘sameness’, pull positive pairs, push negative pairs apart.

$$l_{i,j} = -\log \frac{\exp(\text{sim}(\mathbf{z}_i, \mathbf{z}_j)/\tau)}{\sum_{k=1}^{2N} \mathbb{1}_{[k \neq i]} \exp(\text{sim}(\mathbf{z}_i, \mathbf{z}_k)/\tau)},$$

The contrastive loss function



[Image credits](#)

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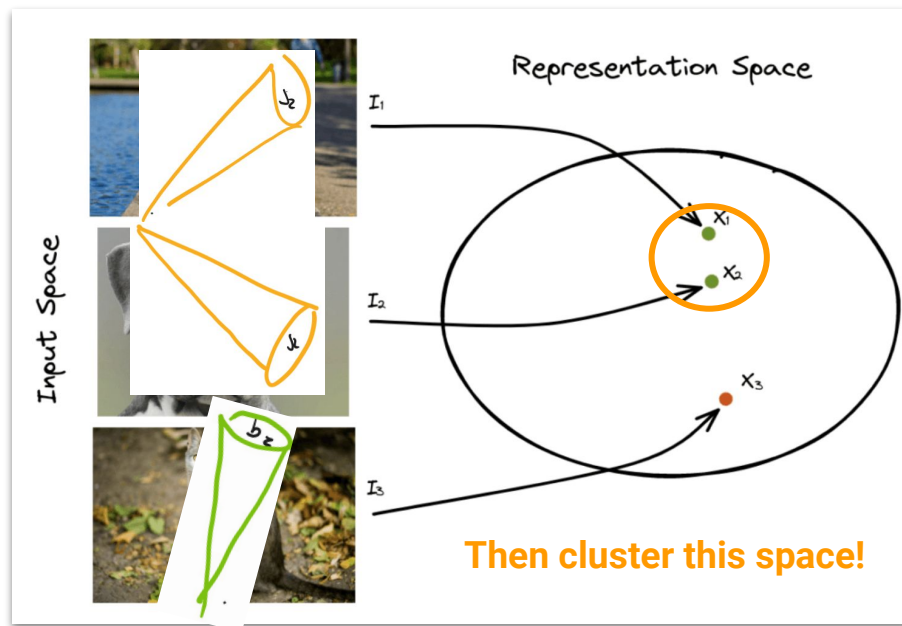
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The contrastive loss function

Embed jets instead



[Image credits](#)

Advantages

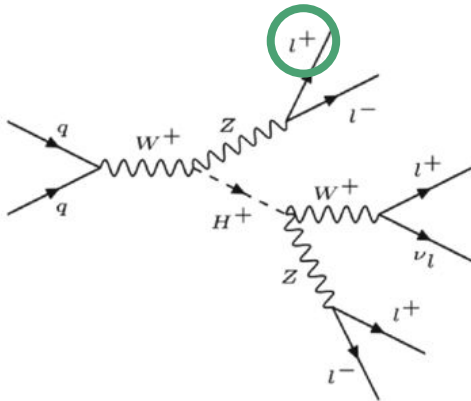
- Any Feynman diagram can be cast into this setup:
 - Method requires labels to identify common parents

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 - Method requires labels to identify common parents
- Missing objects are fine:
 - No kinematic reconstruction required → Method just learns to group things together
 - Can deal with asymmetric decay structures.

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(c)

Say - this object is somehow outside the acceptance, and missing.

No positive partner → But is still regularised by all the other negative partners.

An example case

$t\bar{t}$ hadronic channel

Casting the problem

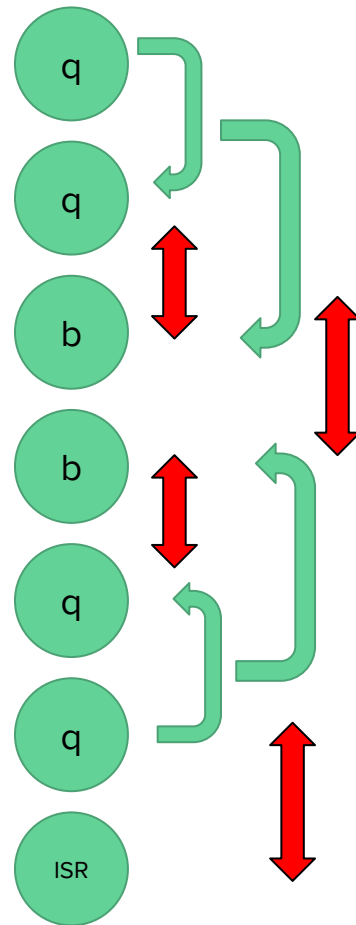
For $t \rightarrow W(qq) b$

Level 0:

1. Pull q's and b from same top together. Push the other q's and b from the other top apart.

Level 1:

1. Pull q's together, push b apart within this cluster.
2. Push everything else apart.
 - Train an encoder with: $\text{Loss} = \text{Level 0} + w * \text{Level 1}$
 - After training an encoder \rightarrow **Perform a bottom up clustering.**

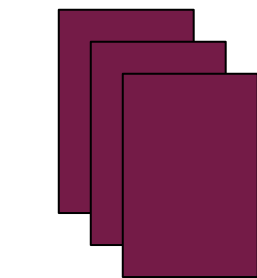


Workflow

Features:

1. features: jet kinematics, b-tag
2. Condition on number of jets in events.

Encoder used: Transformer



batch, jets, features



batch, jets, embedding

The clustering

Perform a bottom up clustering

- Merge two objects into a cluster, closer than a preset threshold
- If Cluster reaches a preset cardinality → remove from process.
- If Cluster exceeds cardinality → undo last merge and remove from process.
- Stop: When no two points are closer than preset threshold.

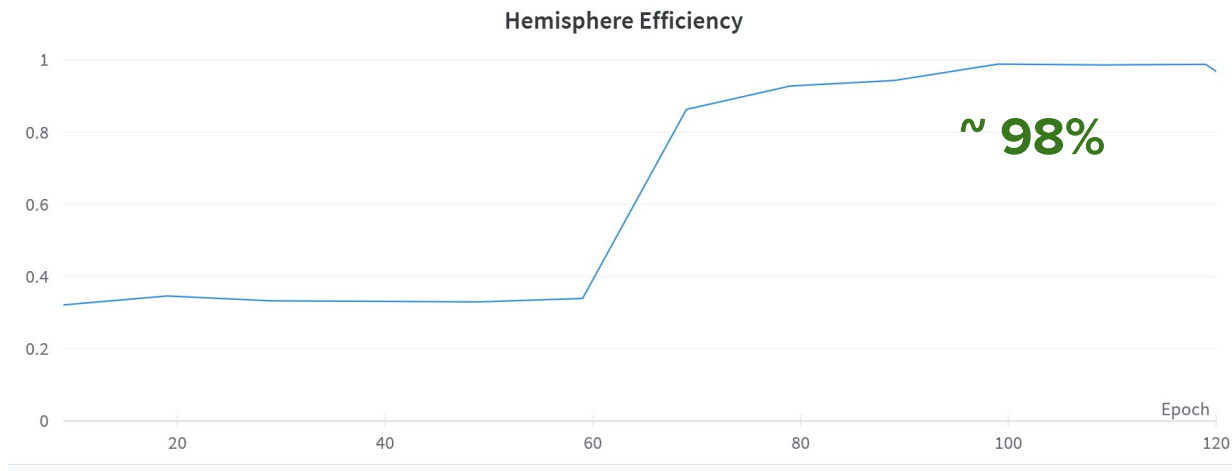
```
Define N: max cluster size
Define t: max distance threshold
Define  $e_i$ : embedding of object  $i$ 
Define  $\ell_i$ : cluster label
Define  $N_\ell$ : cluster number
 $d_{ij} = \text{pairwise\_distance}(e_i, e_j)$ 
 $C = \text{identity}(\text{len}(i))$ 
 $N_\ell \leftarrow 0$ 
 $d_{ij} = \text{mask\_lower\_triangle}(d_{ij})$ 
 $d_{ij} = \text{mask\_diagonal}(d_{ij})$ 
while any  $d_{ij} < t$  do:
  find (i,j) for  $\min(d_{ij})$ 
  if hard N requirement is True then
     $C' \leftarrow C$ 
  end if
   $C[i,j] \leftarrow 1$ 
   $C[i,:] \leftarrow C[i,:] \vee C[j,:]$ 
   $C[j,:] \leftarrow C[j,:] \vee C[i,:]$ 
   $C = \text{transpose}(C)$ 
  if  $\text{sum}(C[i,:]) \geq N$  then
    if hard N requirement and  $\text{sum}(C[i,:]) > N$  then
       $C' \leftarrow C'$ 
    end if
     $k \leftarrow 0$ 
    for  $v$  in  $C[i,:]$  do
      if  $v$  is 1 then
         $\ell_k \leftarrow N_\ell$ 
         $\text{mask}(d_{ij}[k,:])$ 
      end if
       $k \leftarrow k + 1$ 
    end for
     $N_\ell \leftarrow N_\ell + 1$ 
  if hard N requirement and  $\text{sum}(C[j,:]) > N$  then
     $k \leftarrow 0$ 
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  end if
end if
end while
```

▷ Set element i,j to 1
▷ Set nonzero elements in j to 1 in i
▷ Set nonzero elements in i to 1 in j
▷ Transpose to make symmetric on diagonal

The ideal clustering limit

Given a set of 'informed' encodings:

- If you could seed a centre → group the nearest neighbours
- In practice, we do a bottom up clustering.
- Performance to be gained here.



Top reconstruction efficiencies:

- Performs better than Chi Squared, approaching SotA.

	CoCo	Topograph	Chi Squared
6 jets = 2b	85.3%	88.3%	79.1%
6 jets \geq 2b	84.3%	87.8%	79.2%
7 jets = 2b	62.5%	70.6%	57.9%
7 jets \geq 2b	61.1%	69.7%	57.1%

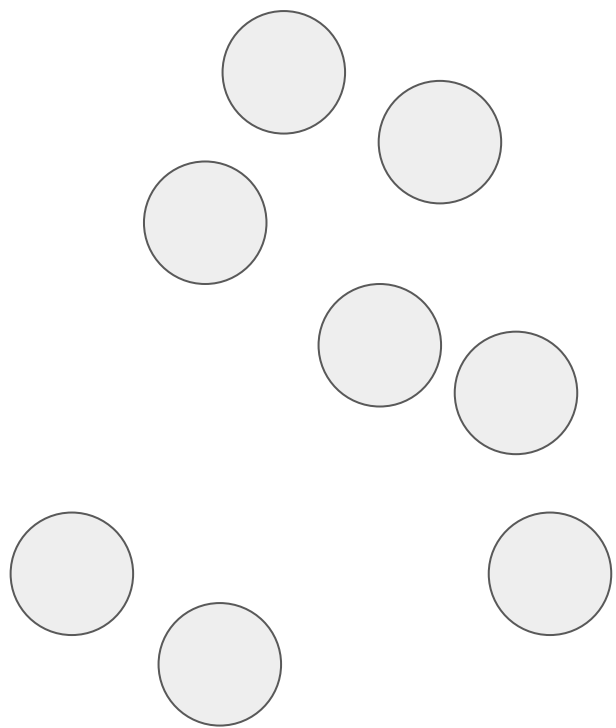
Top reco. eff. as a function of number of jets.

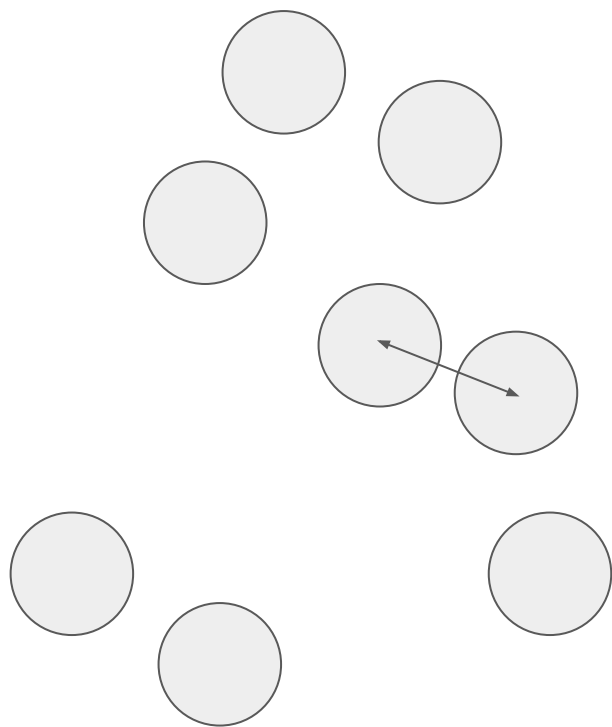
Outlook

- Contrastive losses a natural framework for combinatoric solving.
 - Flexible, generisable, performant

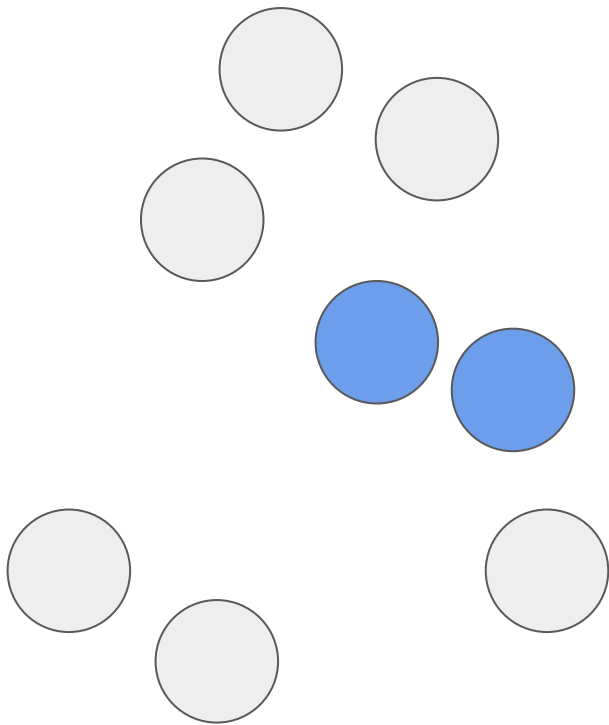
Backup

- Clustering demo





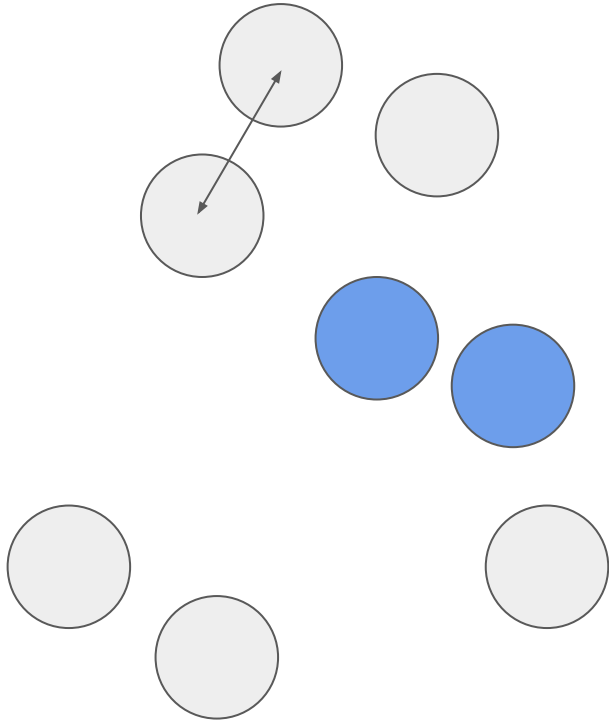
Find nearest two embeddings



Find nearest two embeddings

Merge into same cluster

- If already in a cluster, merge clusters

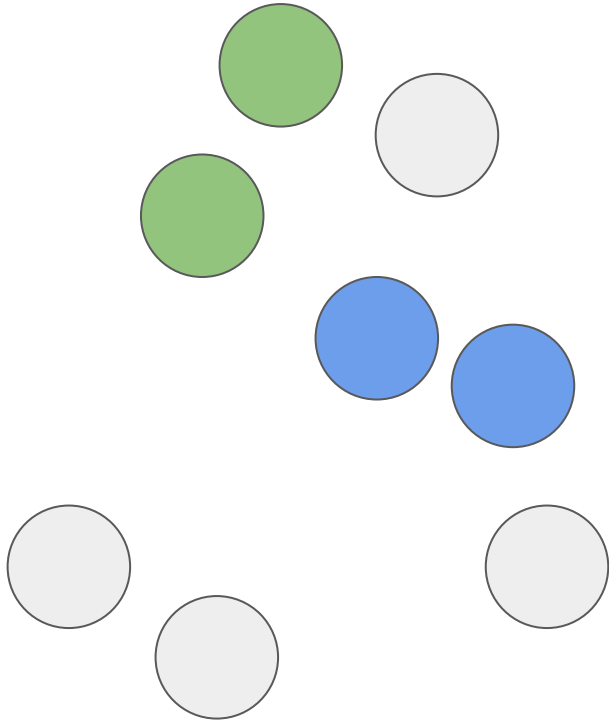


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Repeat until hit max cluster size

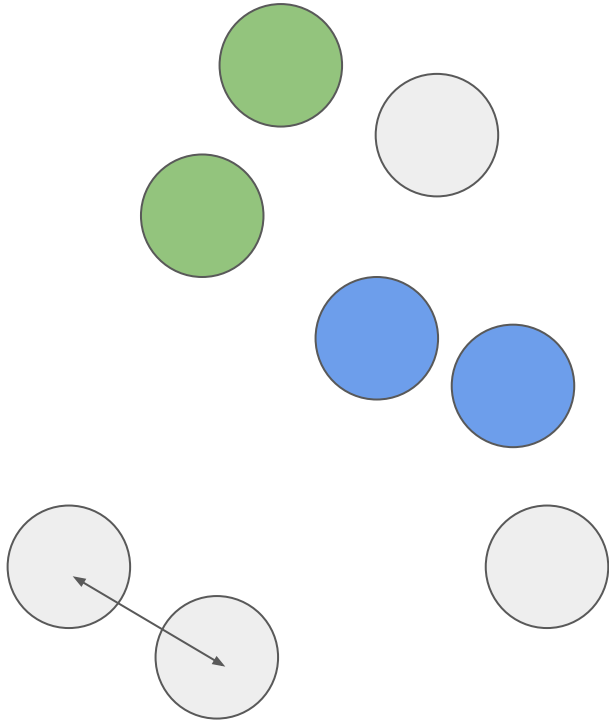


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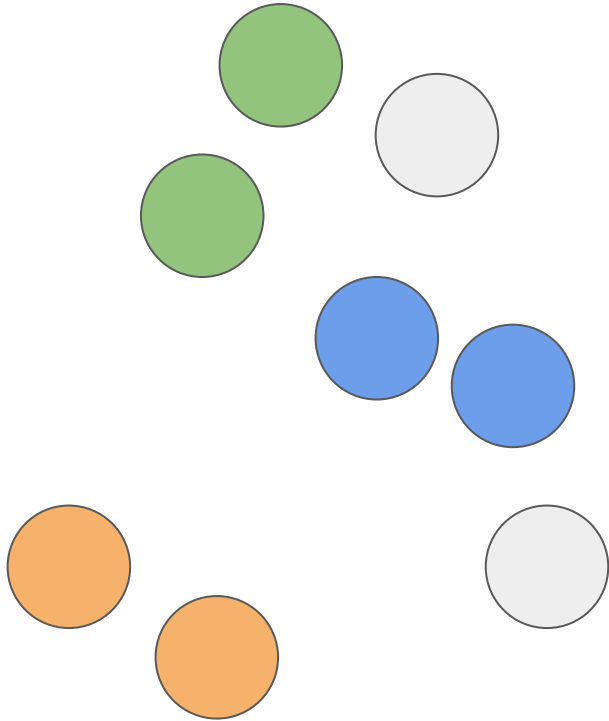


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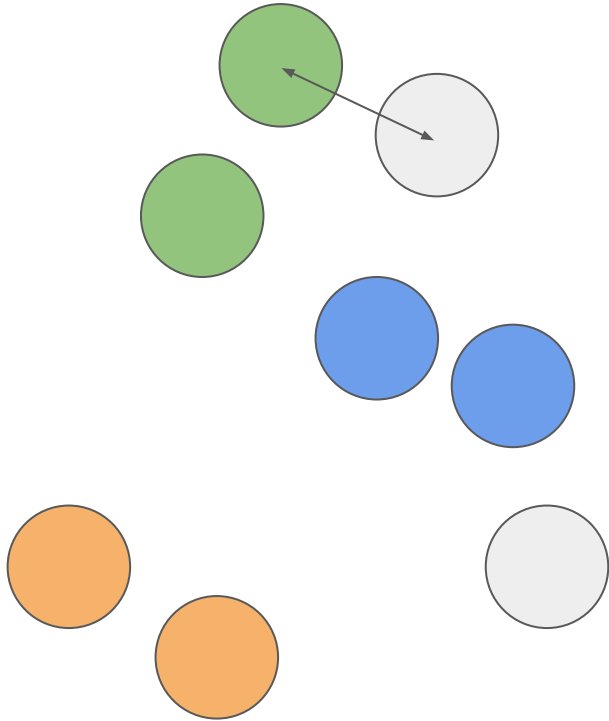


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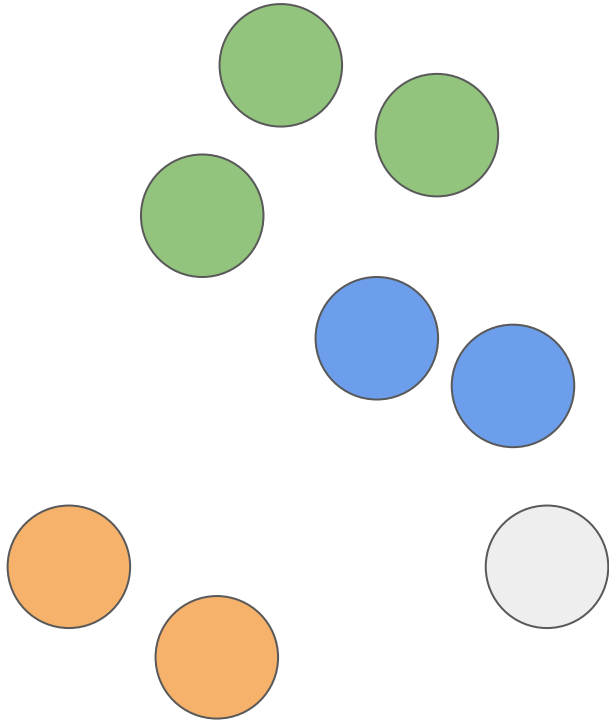


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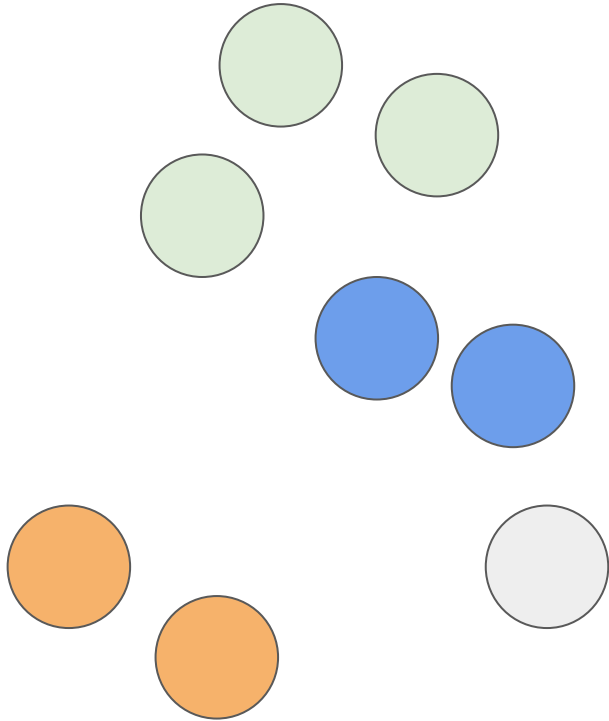


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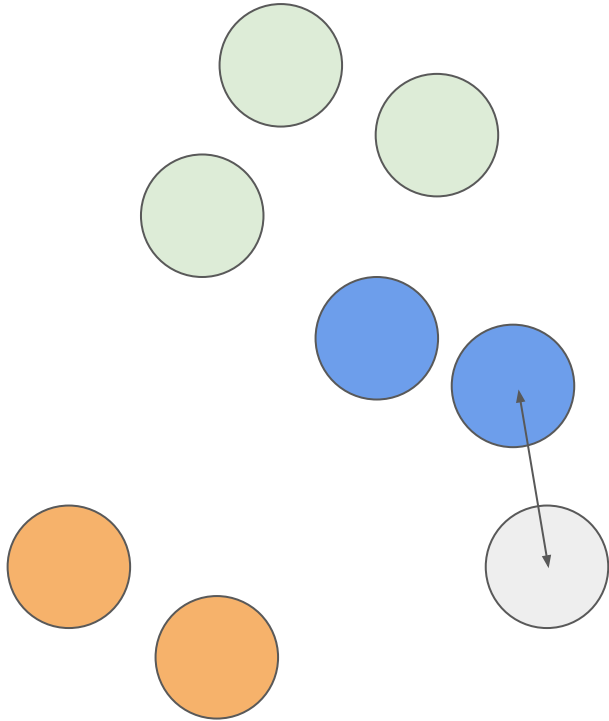
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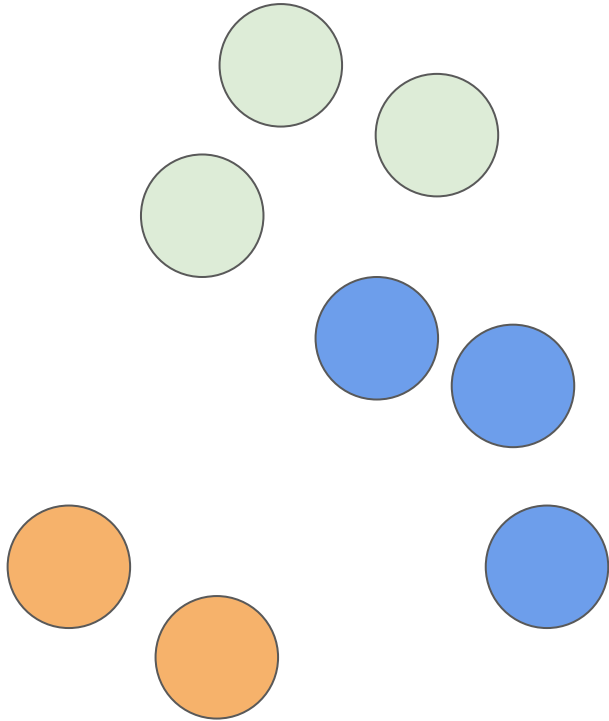
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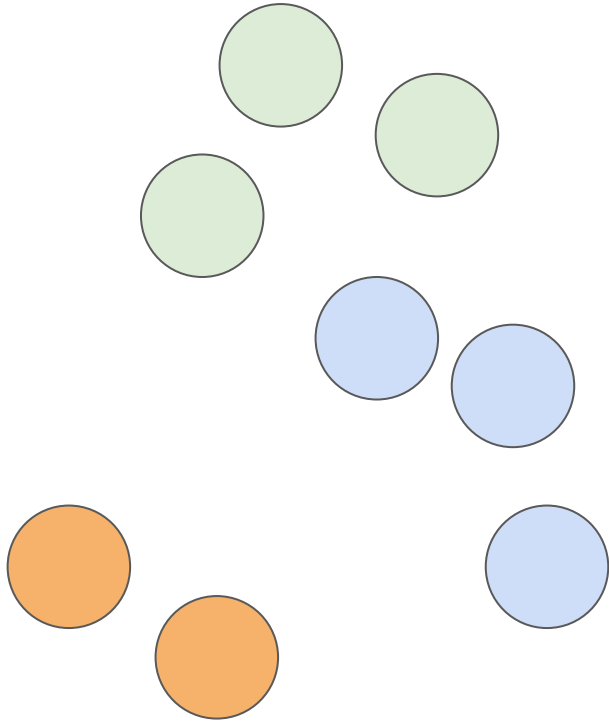
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