Looking into Jets with Machine Learning

Kyle Cranmer & **Sebastian Macaluso**
New York University

Duccio Pappadopulo
Bloomberg LP, New York

NYU Physics x ML
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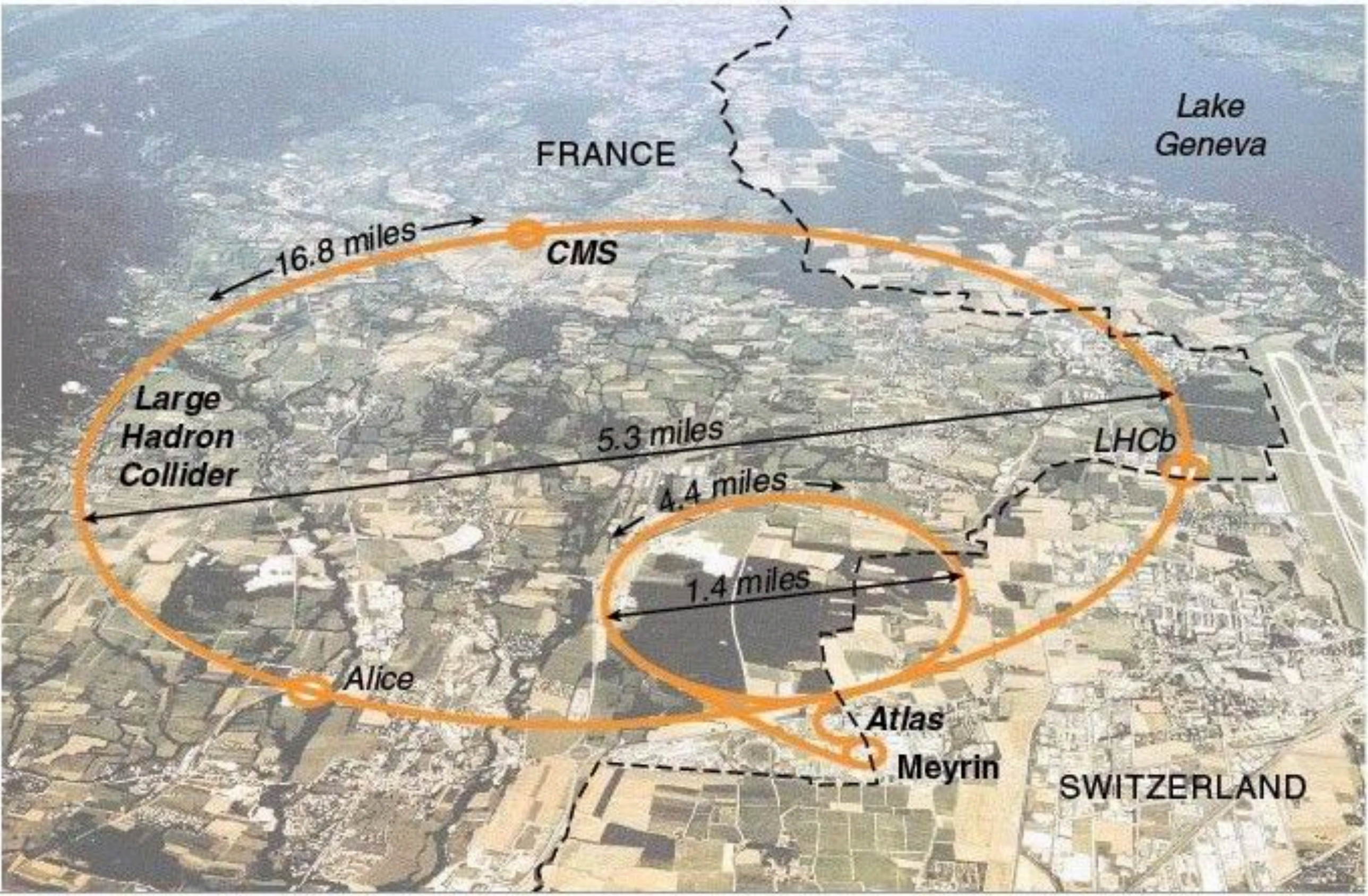
The Large Hadron Collider

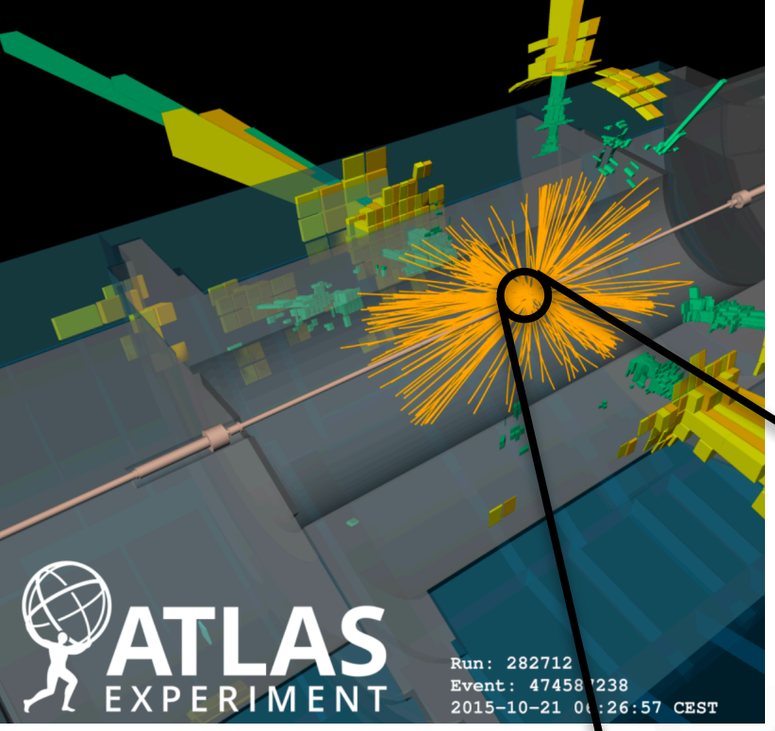


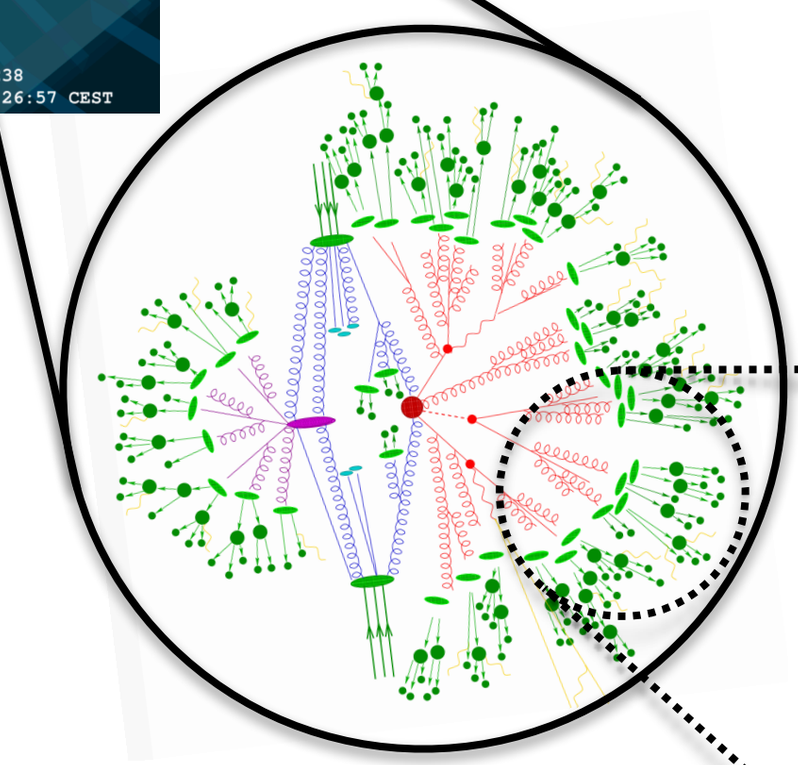
JETS

Collimated spray of energetic charged and neutral hadrons

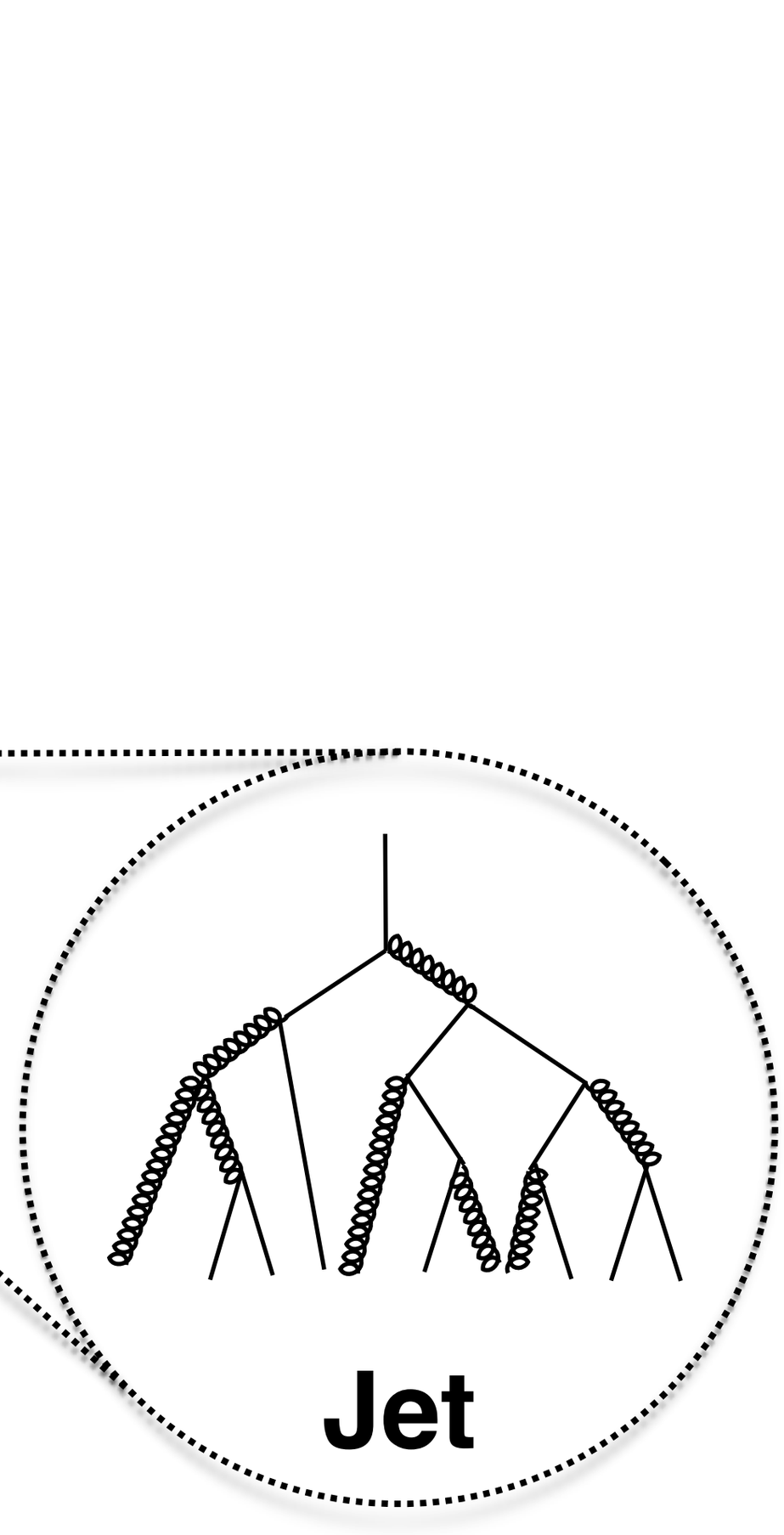
ATLAS EXPERIMENT

Run: 282712
Event: 474587238
2015-10-21 06:26:57 CEST

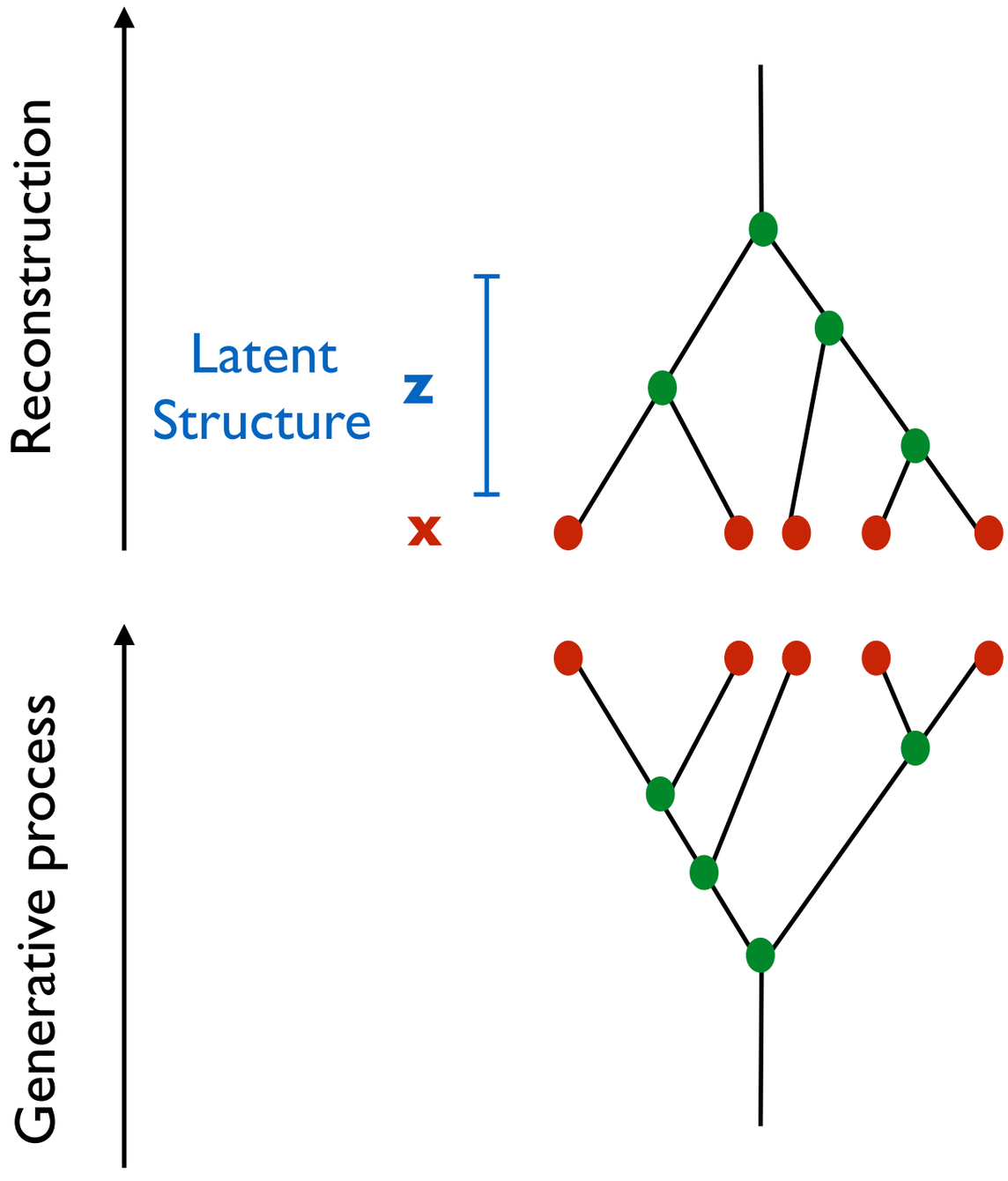




[Stefan Hoche 1411.4085]



Jet clustering

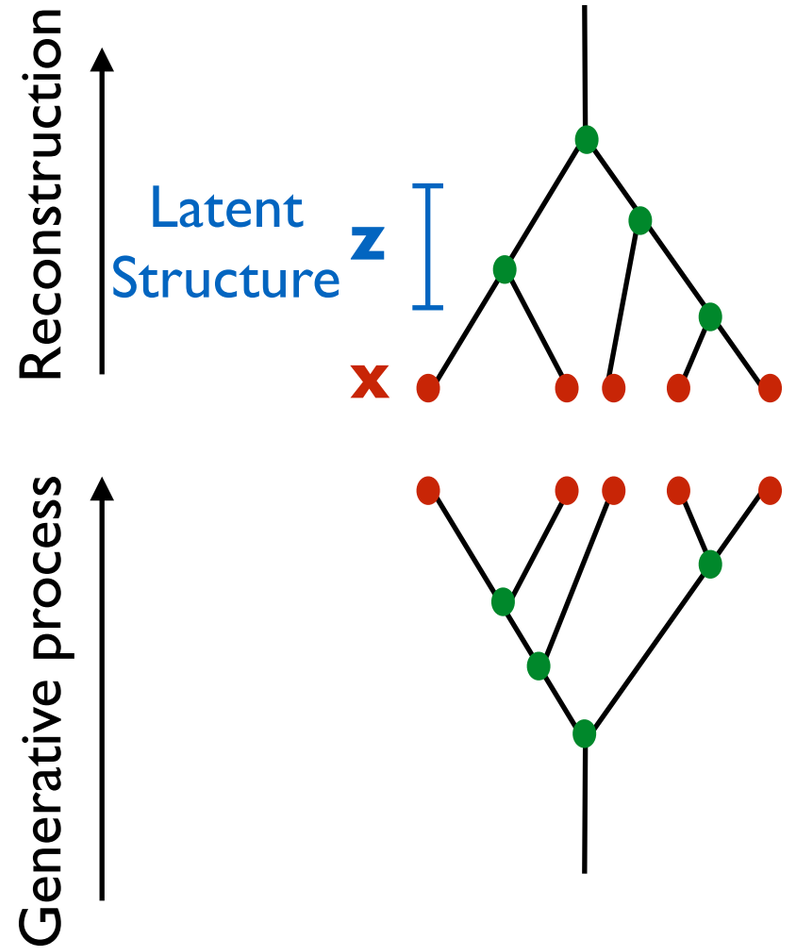


Problem settings

Classification

Maximum likelihood estimate

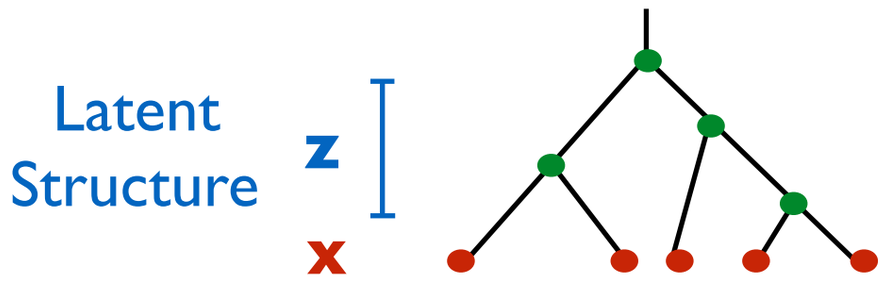
Posterior distribution on histories



Generation and inference unification

Aim to invert the generative model:

E.g. estimate the posterior distribution on histories conditioned on the observed particles.



$$p(z|x,\theta) = \frac{p(x|z,\theta)\ p(z|\theta)}{p(x|\theta)}$$

$$p(x|\theta) = \int dz\ p(x|z,\theta)\ p(z,\theta)$$

Sampling with MCMC or probabilistic programing techniques ?

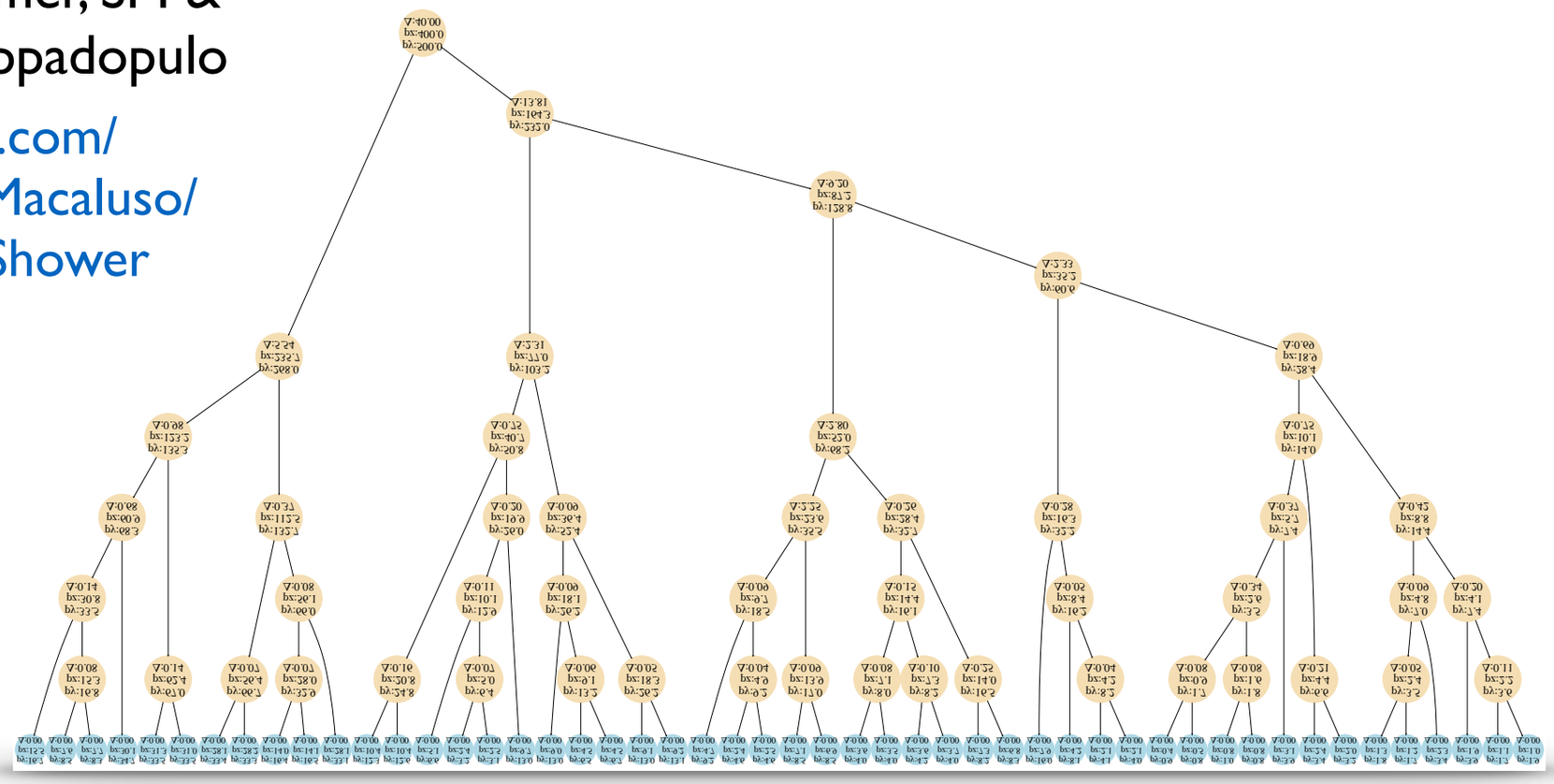
Assuming the toy model, attempt to find the most likely splitting history

- Reconstructing the splitting history is like inverting the generative model.
- **Hard**! There are a combinatorial number of histories to consider.
- Usually jet reconstruction algorithms don't use the probability model directly.
- We use the likelihood for the history as the optimization **objective.**

Ginkgo: Toy Generative Model for Jets

Kyle Cranmer, SM &
Duccio Pappadopulo

github.com/
SebastianMacaluso/
ToyJetsShower



Motivation

- Build a model to aid in ML research for jet physics.

Generation

- Tractable joint likelihood.
- Captures essential ingredients of parton shower generators in full physics simulations.
- Implements an analogue to a parton shower (no hadronization effects).
- Python implementation with few software dependencies.

Inference

- E.g. tuning of simulation parameters (PYTHIA TUNES) to optimize a fit to the data.

Model Specification

- Stand-alone mathematical **specification** of model.
- Document describing model to non-physicists.
- Algorithm described in computer science style.
- Python implementation with few software dependencies.

Toy Generative Model for Jets

Kyle Cranmer[1], Sebastian Macaluso[1] and Duccio Pappadopulo[2]

1 Center for Cosmology and Particle Physics & Center for Data Science, New York University, USA
2 Bloomberg LP, New York, NY 10022, USA.

1 Introduction

In this notes, we provide a standalone description of a generative model to aid in machine learning (ML) research for jet physics. The motivation is to build a model that has a tractable likelihood, and is as simple and easy to describe as possible but at the same time captures the essential ingredients of parton shower generators in full physics simulations. The aim is for the model to have a python implementation with few software dependencies.

Parton shower generators are software tools that encode a physics model for the simulation of jets that are produced at colliders, e.g. the Large Hadron Collider at CERN. Jets are a collimated spray of energetic charged and neutral particles. Parton showers generate the particle content of a jet, going through a cascade process, starting from an initial unstable particle. In this description, there is a recursive algorithm that produces binary splittings of an unstable parent particle into two children particles, and a stopping rule. Thus, starting from the initial unstable particle, successive splittings are implemented until all the particles are stable (i.e. the stopping rule is satisfied for each of the final particles). We refer to this final particles as the jet constituents.

As a result of this *showering process*, there could be many latent paths that may lead to a specific jet (i.e. the set of constituents). Thus, it is natural and straightforward to represent a jet and the particular showering path that gave rise to it as a binary tree, where the inner nodes represent each of the unstable particles and the leaves represent the jet constituents.

1

Model description

Recursive algorithm to generate a binary tree with jet constituents as the leaves.
Showering process: binary splittings + stopping rule.

Features

- Momentum conservation
- Running of the splitting scale

Algorithm 1: Toy Parton Shower Generator

function NodeProcessing $(\vec{p}_{\rm p}, \Delta_{\rm p}, \Delta_{\rm cut}, \lambda, \text{tree})$

Input : parent momentum $\vec{p}_{\rm p}$, parent splitting scale $\Delta_{\rm p}$, cut-off scale $\Delta_{\rm cut}$, rate for the exponential distribution λ, binary tree *tree*

Add parent node to tree.

if $\Delta_p > \Delta_{cut}$ **then**

draw ϕ from uniform distribution in $\{0, 2\pi\}$

$\vec{\Delta}_{\rm p} = \Delta_{\rm p}\ (\sin\phi_{\rm p}, \cos\phi_{\rm p})$

$\vec{p}_{\rm L} = \frac{1}{2}\vec{p}_{\rm p} - \vec{\Delta}_{\rm p}$

$\vec{p}_{\rm R} = \frac{1}{2}\vec{p}_{\rm p} + \vec{\Delta}_{\rm p}$

draw $\Delta_{\rm L}$, $\Delta_{\rm R}$ from the exponential distribution in Eq. 3.

NodeProcessing $(\vec{p}_{\rm L}, \Delta_{\rm L}, \Delta_{\rm cut}, \lambda, \text{tree})$

NodeProcessing $(\vec{p}_{\rm R}, \Delta_{\rm R}, \Delta_{\rm cut}, \lambda, \text{tree})$

Generative process

Start with $\Delta_{\mathrm{P}} = \Delta_{\mathrm{root}}$

Sample $\phi \sim \mathrm{Uniform}(0, 2\pi)$ to pick a direction for Δ_{P}

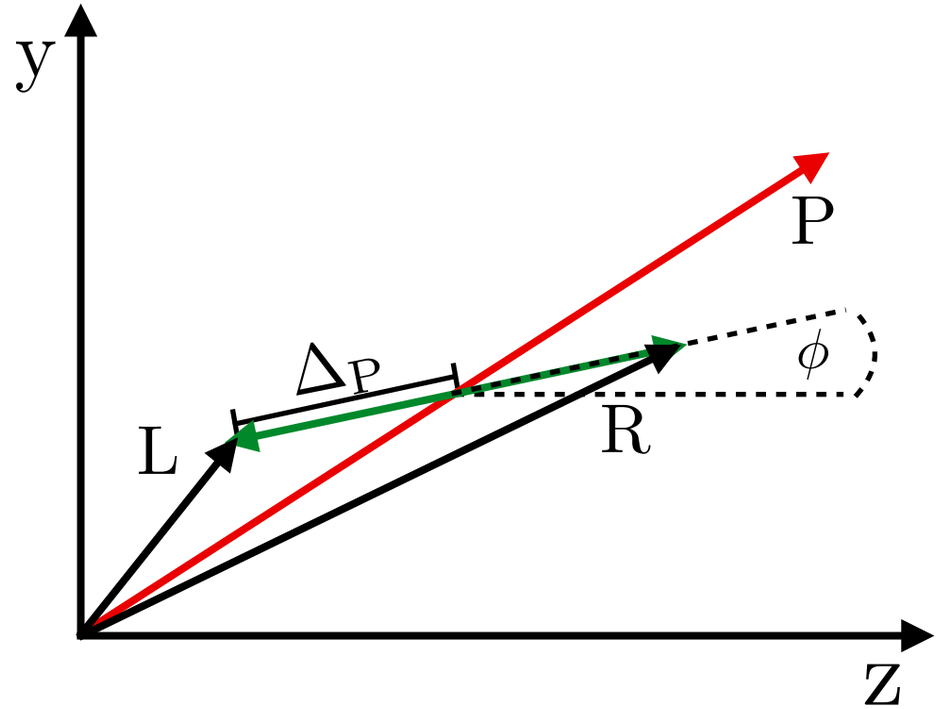
Heavy resonance X jet

$$\Delta_{\mathrm{root}} = \frac{m_X}{2}$$

Split parent node

$$\vec{p}_{\mathrm{L}} = \frac{1}{2}\vec{p}_{\mathrm{p}} - \vec{\Delta}_{\mathrm{p}}$$

$$\vec{p}_{\mathrm{R}} = \frac{1}{2}\vec{p}_{\mathrm{p}} + \vec{\Delta}_{\mathrm{p}}$$



Sample independently Δ_{L} and Δ_{R}

$$\Delta \sim f(\Delta|\lambda, \Delta_{\mathrm{p}}) = \frac{\lambda}{\Delta_{\mathrm{p}}} e^{-\frac{\lambda}{\Delta_{\mathrm{p}}}\Delta}$$

Promote (Δ_{L},L) and (Δ_{R},R) to (Δ_{P}, P).

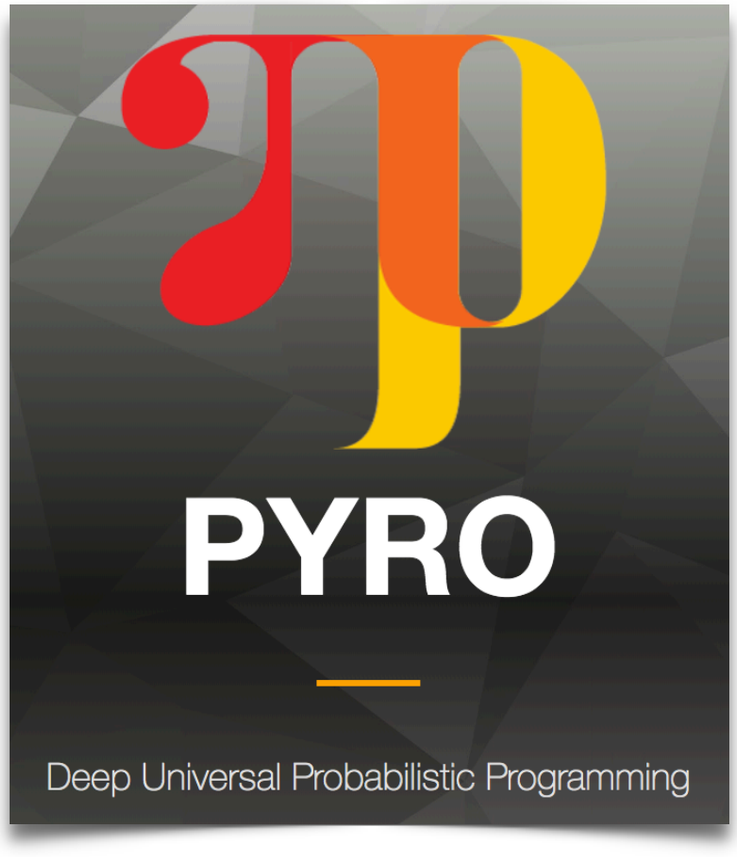
Augmented data

Additional information that characterizes the latent process can be extracted in Ginkgo:

- Joint likelihood
- Joint likelihood ratio
- Joint score

The model keeps track of the augmented data based on a **PYRO** implementation.

New techniques for likelihood-free inference can be applied.
[J. Brehmer, G. Louppe, J. Pavez & K. Cranmer 2018]

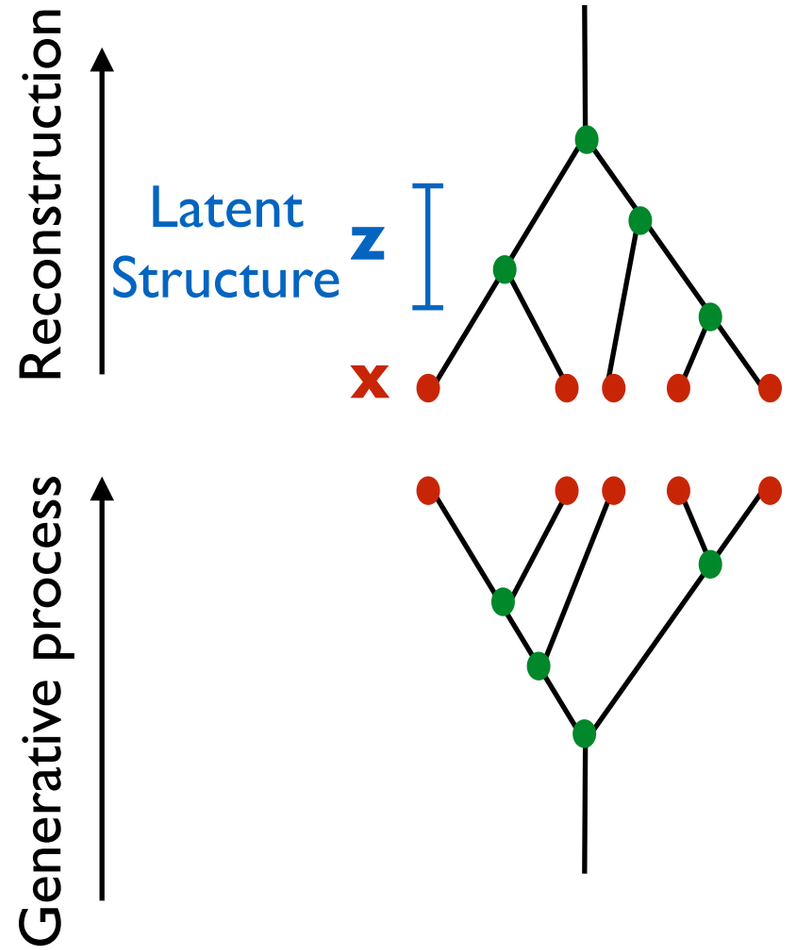


Problem settings

Classification

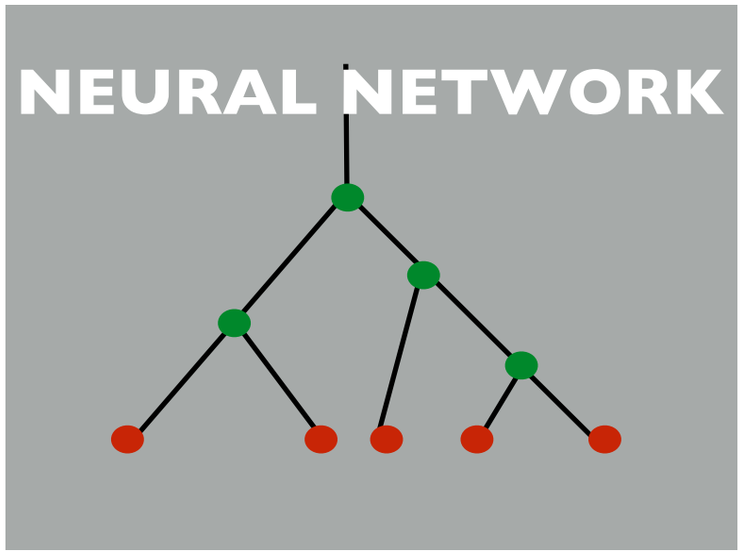
Maximum likelihood estimate

Posterior distribution on histories

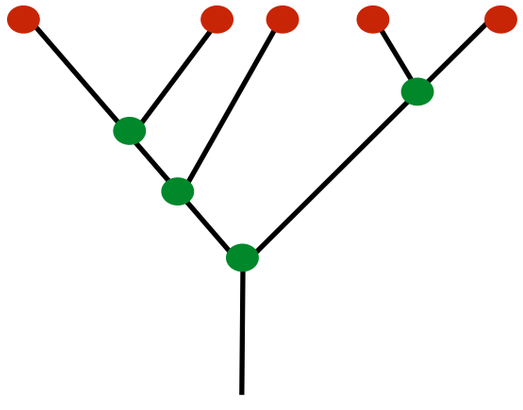


Neural Networks that conserve the tree structure

Classification/Regression



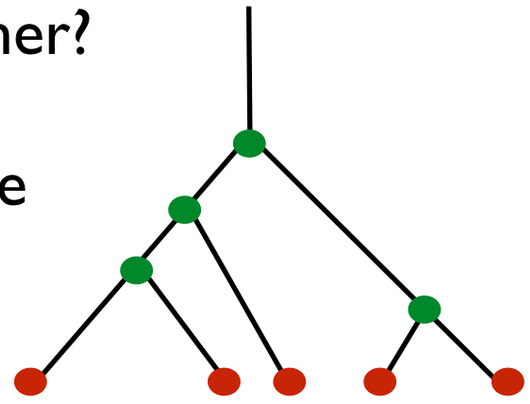
Generative process

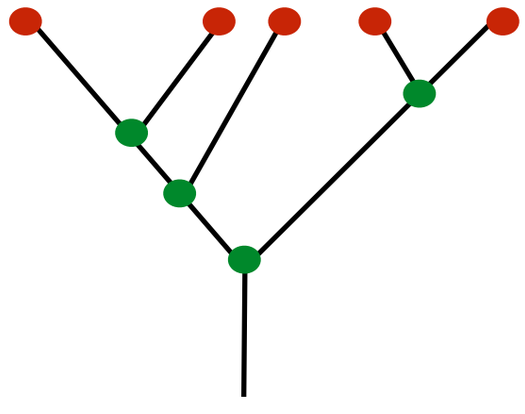


Can we solve both tasks together?

Find the right latent structure
+
classification/regression

Classification/Regression

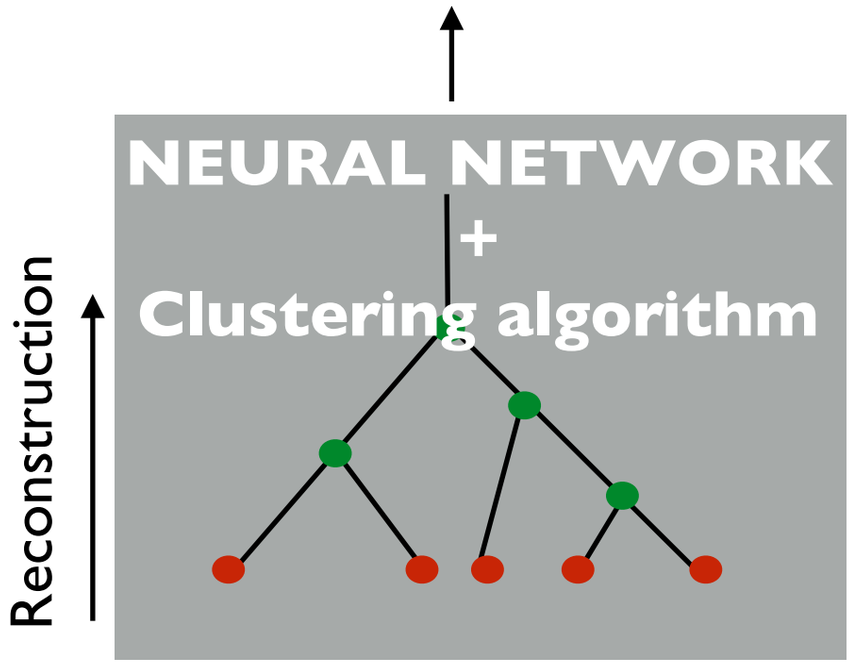


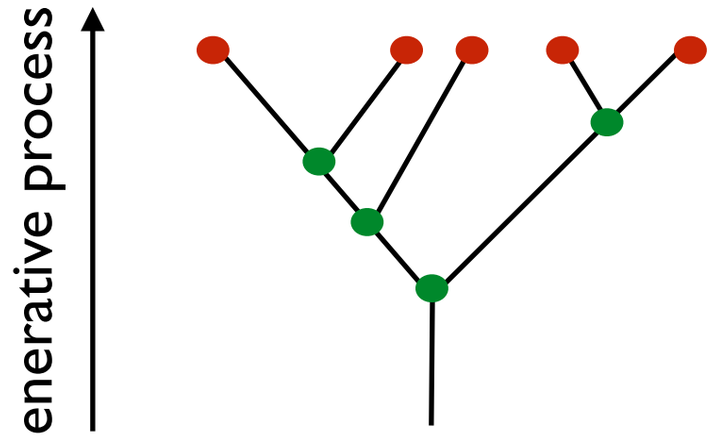


Neural Networks that conserve the tree structure

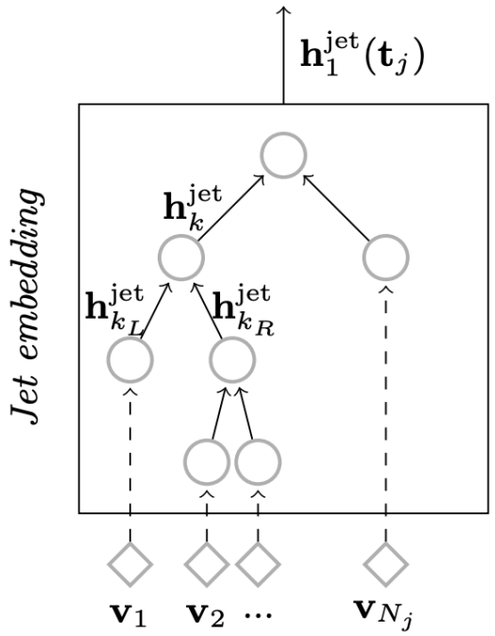
RecNN [Louppe, Cho, Becot & Cranmer '17]
TreeNiN [Macaluso & Cranmer '19]

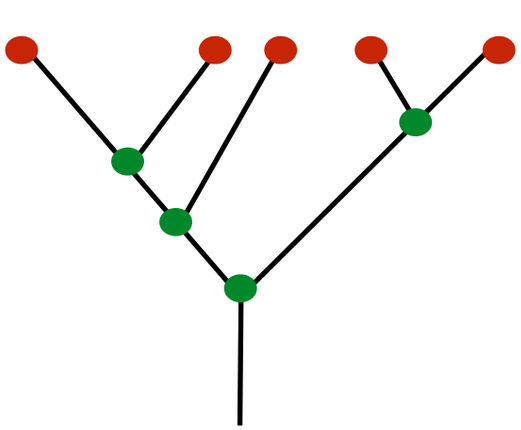
Classification/Regression





Classification/Regression





Generalized kt clustering algorithms

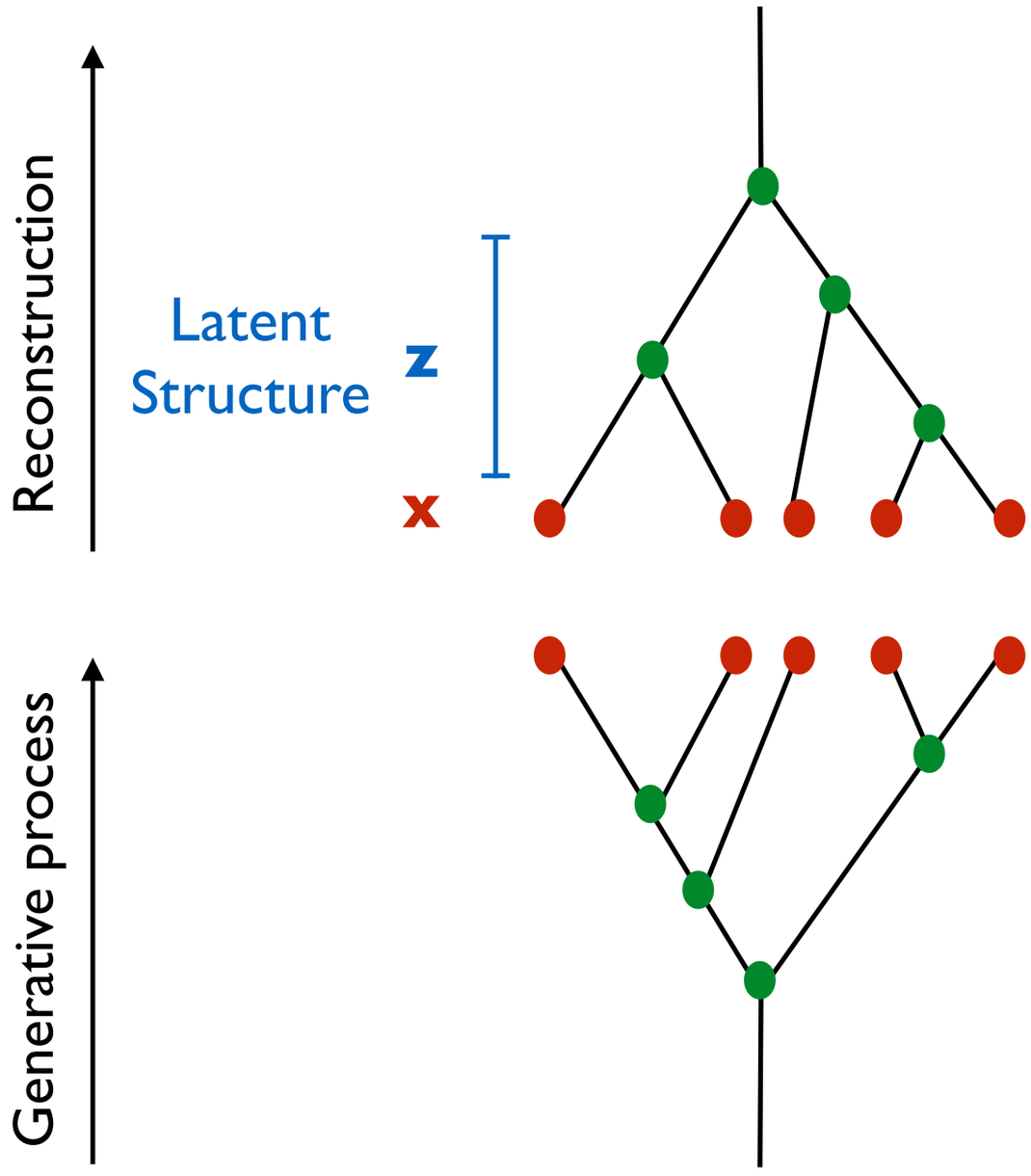
- Idea: sequentially cluster jet constituents.
- Permutation invariance: add 4-momenta of each pair that is clustered.
- Merge closest pair based on the distance measure:

$$d_{ij} = \min(p_{ti}^{2\alpha}, p_{tj}^{2\alpha}) \frac{\Delta R_{ij}^2}{R^2}$$

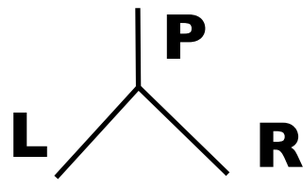
$$\Delta R_{ij}^2 = (y_i - y_j)^2 + (\phi_i - \phi_j)^2$$

$\alpha = \{1, 0, -1\}$ specifies the the kt, Cambridge/Aachen and anti-kt algorithms respectively.

Jet clustering



Can we cluster jets based on the likelihood of each splitting?



Joint likelihood:

$$p(x, z|\theta) = \prod_i p(\mathrm{L}_i, \mathrm{R}_i|\mathrm{P}_i, \theta)$$

Split likelihood:

$$p(\mathrm{L}_i, \mathrm{R}_i|\mathrm{P}_i) \equiv p(\vec{p}_\mathrm{L}, \vec{p}_\mathrm{R}|\vec{p}_\mathrm{P})$$

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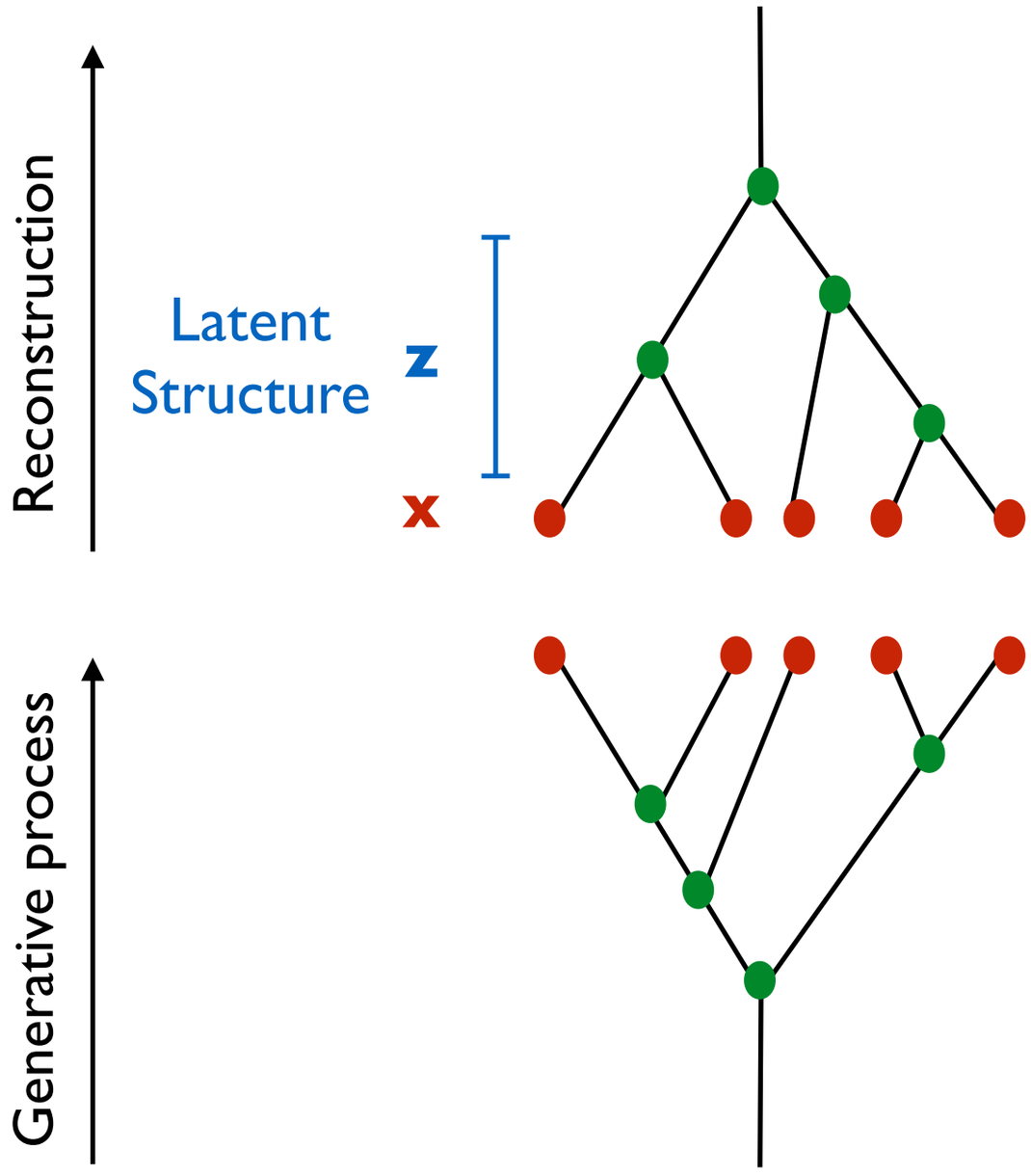
k_t distance measure

$$d(\mathrm{L}_i, \mathrm{R}_i) \equiv d(\vec{p}_\mathrm{L}, \vec{p}_\mathrm{R})$$

Jet clustering



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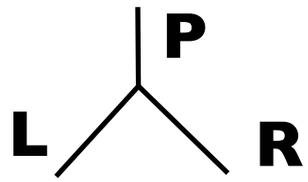


Joint likelihood:

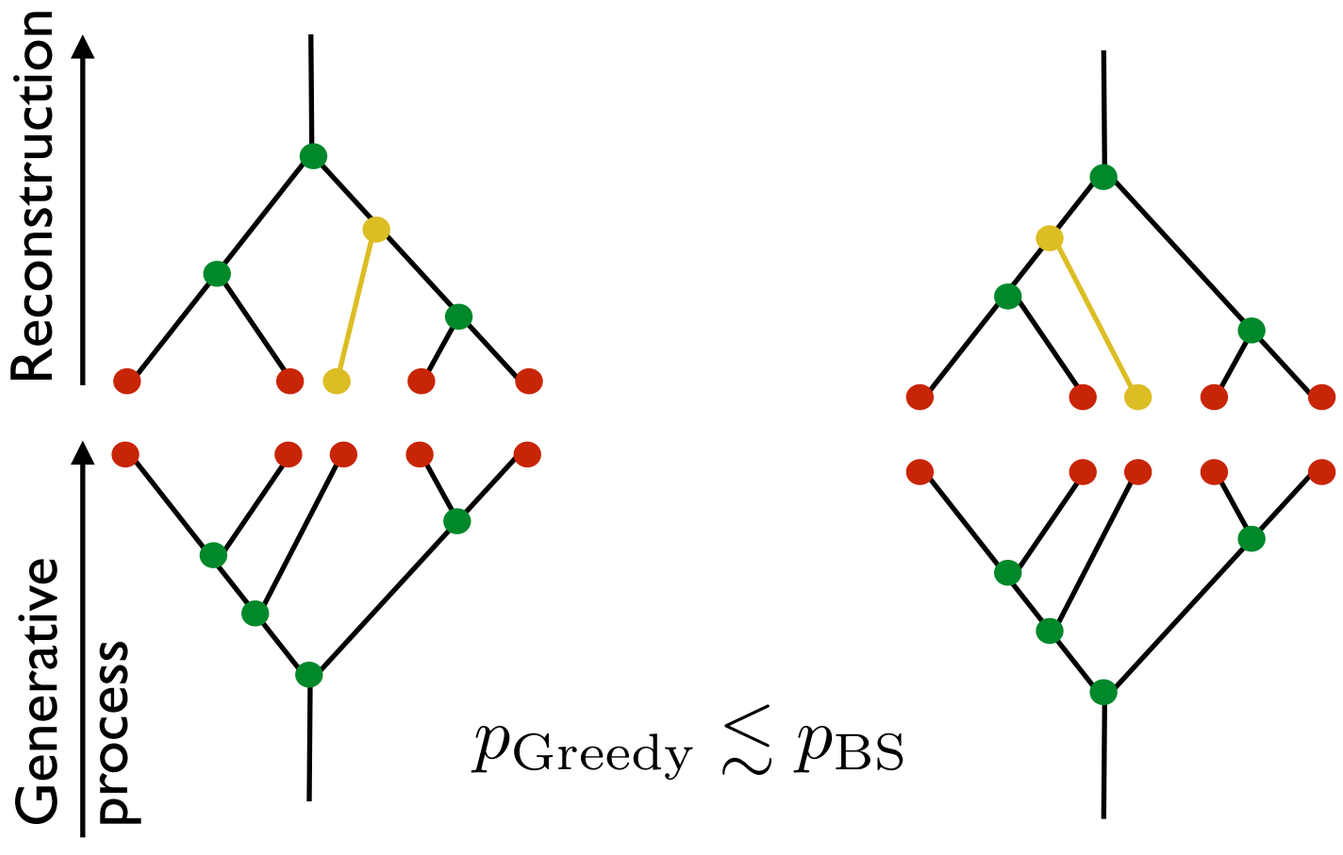
$$p(x, z|\theta) = \prod_i p(\mathrm{L}_i, \mathrm{R}_i|\mathrm{P}_i, \theta)$$

- Hard to do with full physics simulators, e.g. PYTHIA
- To prototype we built our own toy model!

Likelihood-based jet clustering

Greedy
Joint likelihood from locally maximizing the likelihood at each step.

Beam Search
Maximize the likelihood of multiple steps before choosing the latent path. Maybe we could fix mistakes?



Joint likelihood:

$$p(x, z|\theta) = \prod_i p(\mathrm{L}_i, \mathrm{R}_i|\mathrm{P}_i, \theta)$$

Goal: find the latent structure that maximizes the jet likelihood (MLE).

Given an algorithm, z is fixed.

$\hat{z}_{\text{Greedy}}$

$\hat{z}_{\text{BS}}$

$\hat{z}_{\text{MLE}} = \text{argmax}_z\ p(x|z)$

Viterbi algorithm
Computationally "infeasible" for jets with ~ 100 constituents

Greedy algorithms

Choose the optimal decision locally at each step.

Ginkgo jets properties

- Permutation invariance
- Distance measure

Generalized kt clustering algorithms

- Locally minimize the distance measure d_{ij}
- An analogue of the generalized k_t clustering algorithms can be defined for Ginkgo jets.

Greedy likelihood-based algorithm

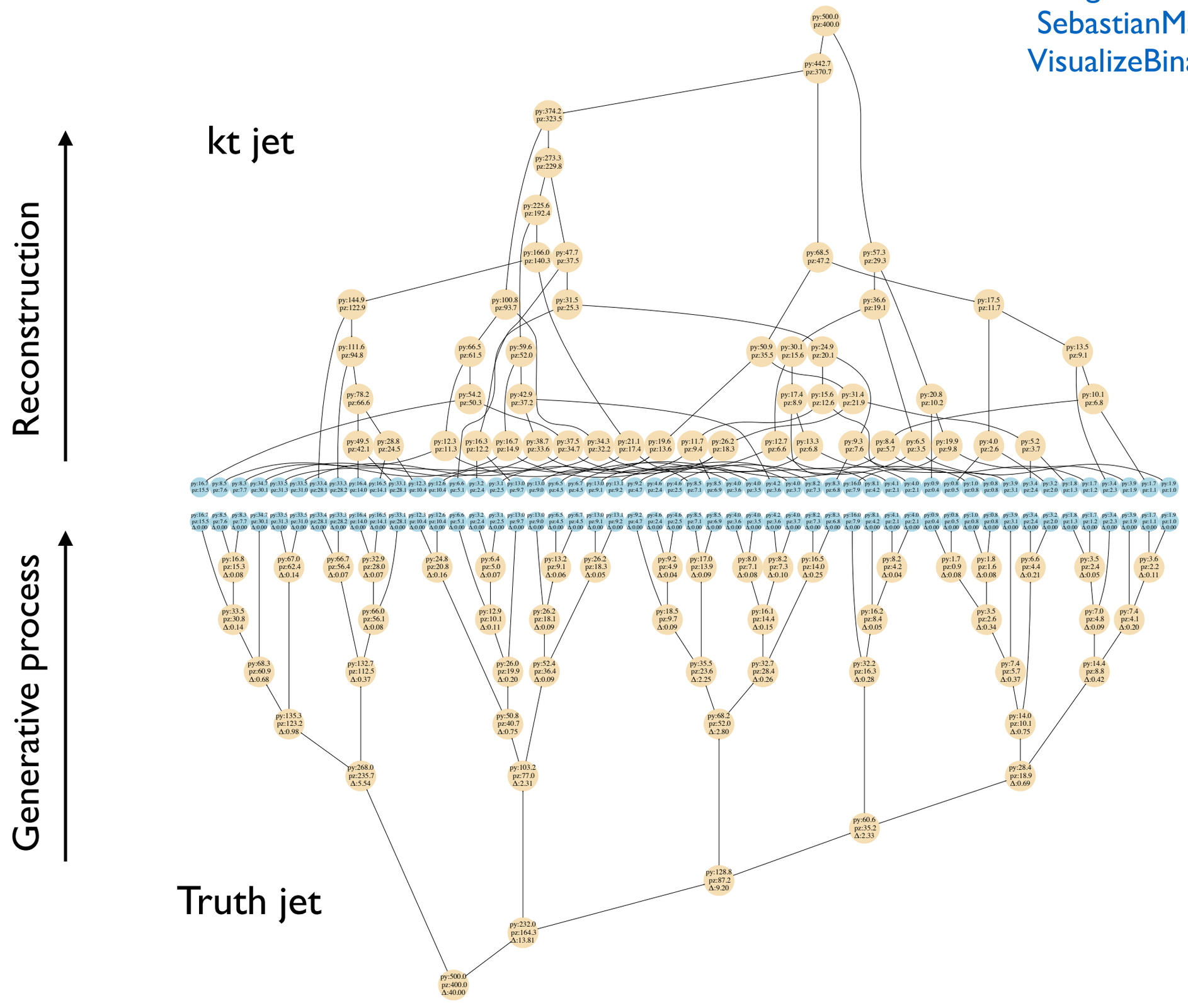
- Choose the nodes pairing that locally maximizes the likelihood at each step given by

$$p(\Delta_{\mathrm{L}}, \Delta_{\mathrm{R}} | \Delta_{\mathrm{p}})$$

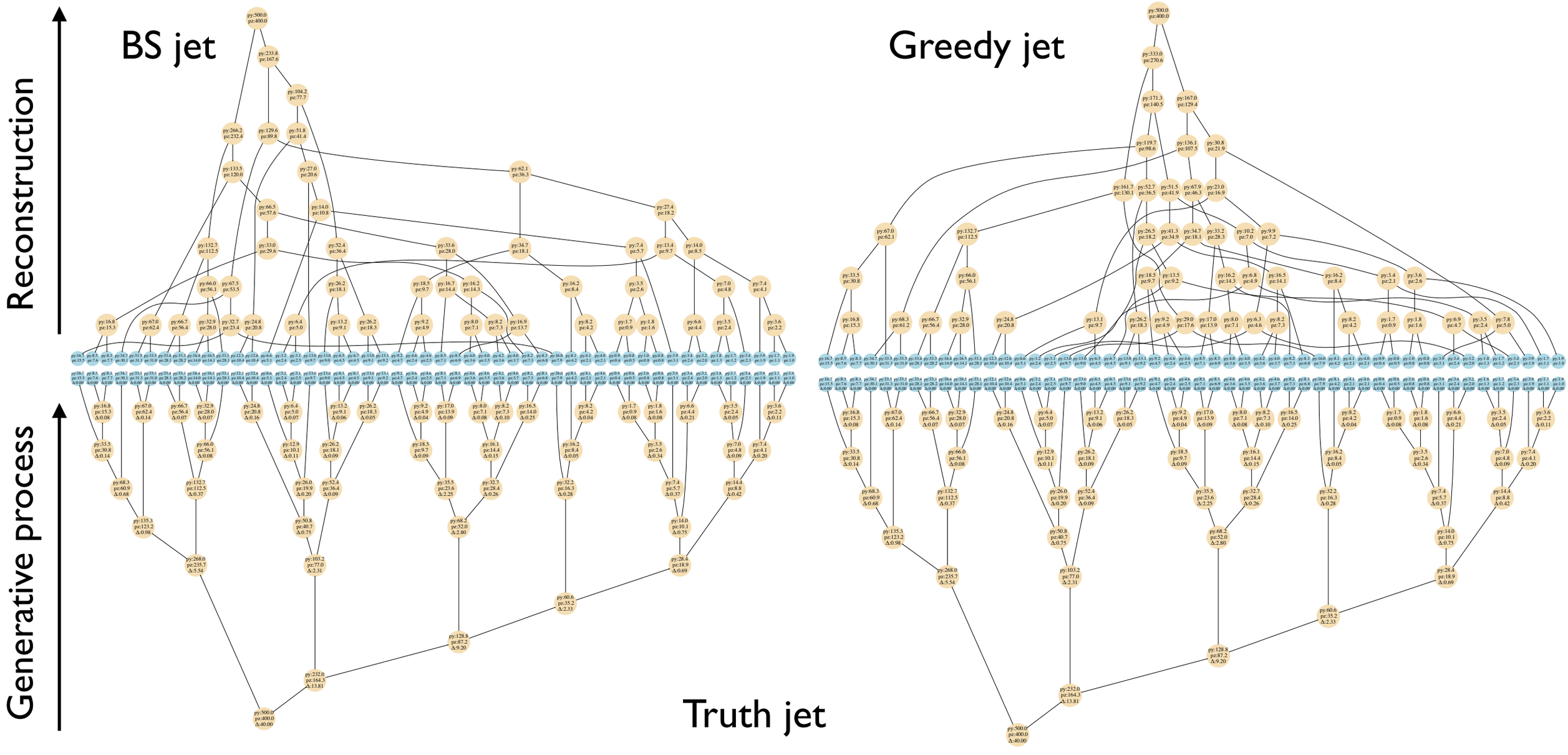
Our implementation improves the N^3 brute force time complexity to N^2.
Approach based on nearest neighbors introduced in FastJet
[hep-ph/0512210, G. Salam and M. Cacciari LPTHE-06-02].

1-D Tree only visualizations

Kyle Cranmer, SM &
Duccio Pappadopulo
github.com/
SebastianMacaluso/
VisualizeBinaryTrees



1-D Tree only visualizations



Heat cluster maps visualizations

Kyle Cranmer, SM &
Duccio Pappadopulo

github.com/SebastianMacaluso/
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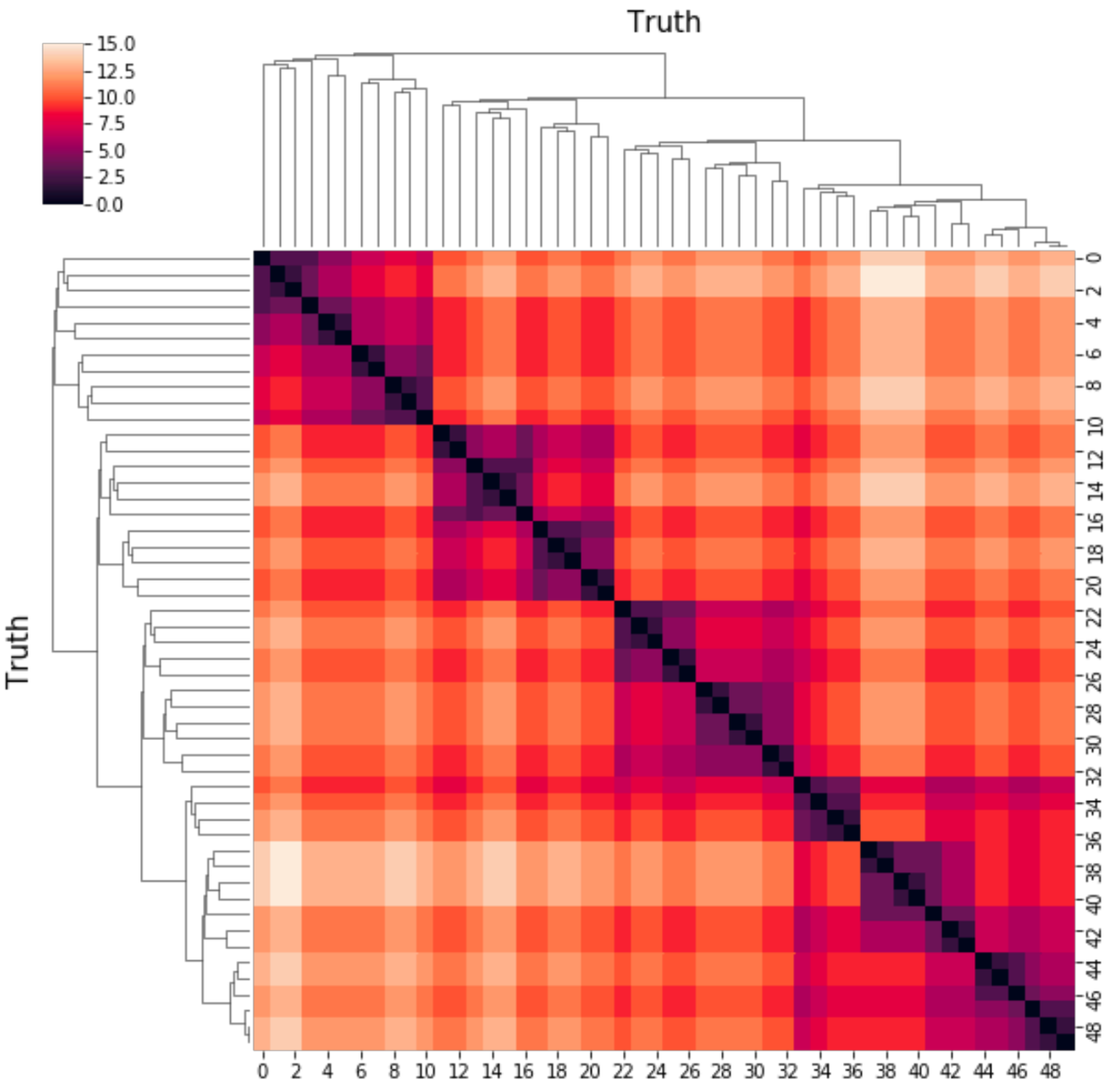

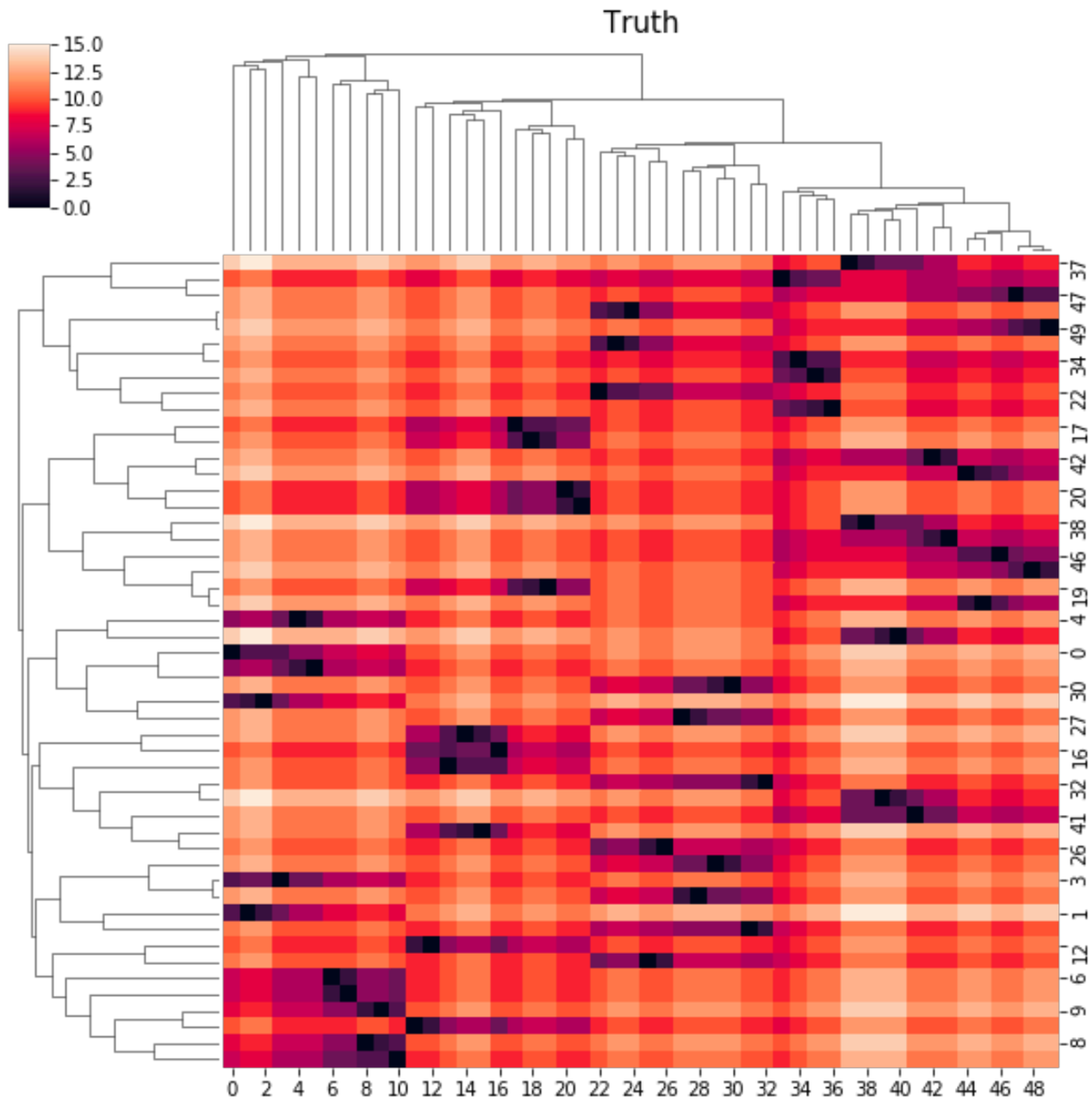

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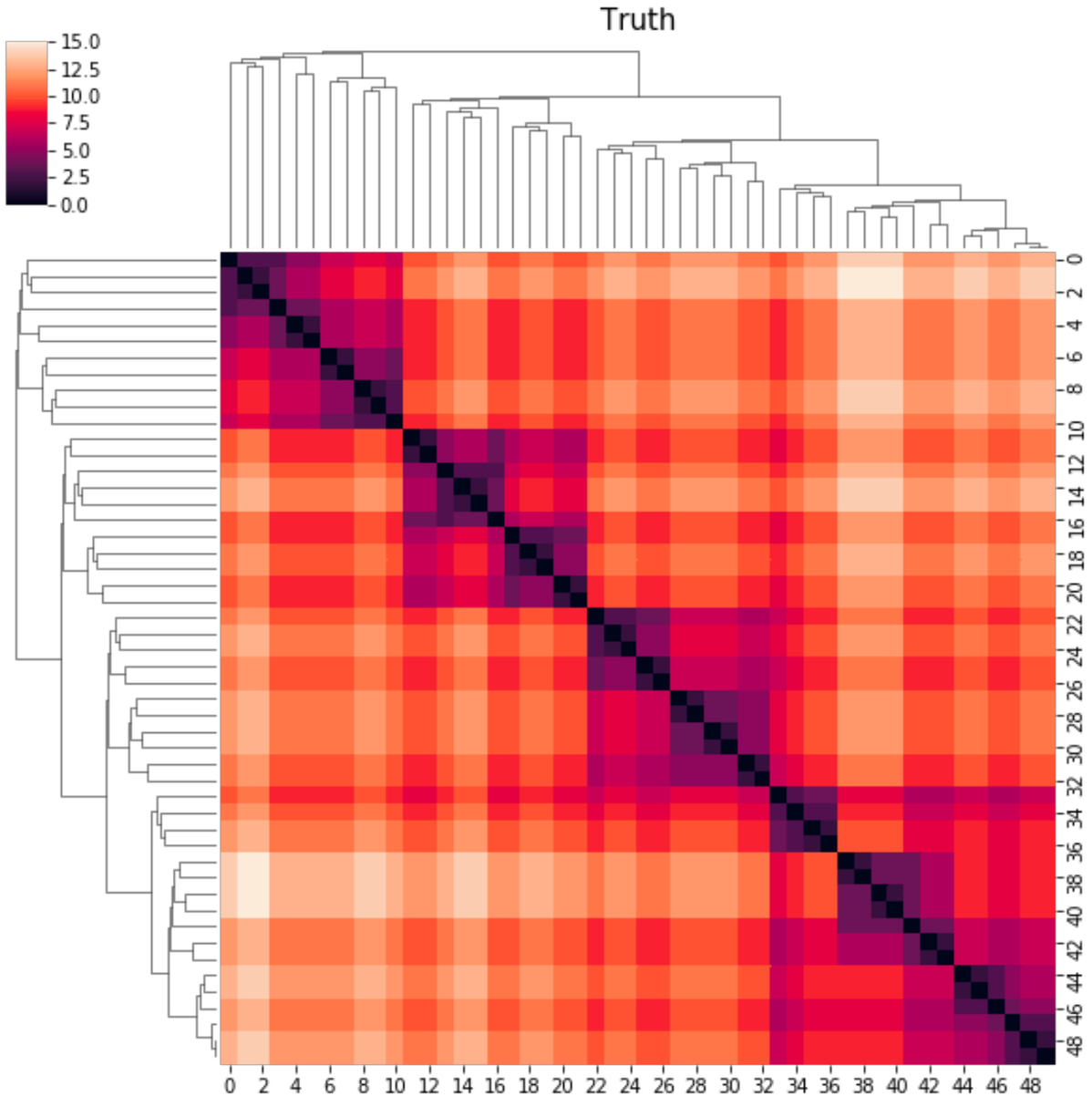
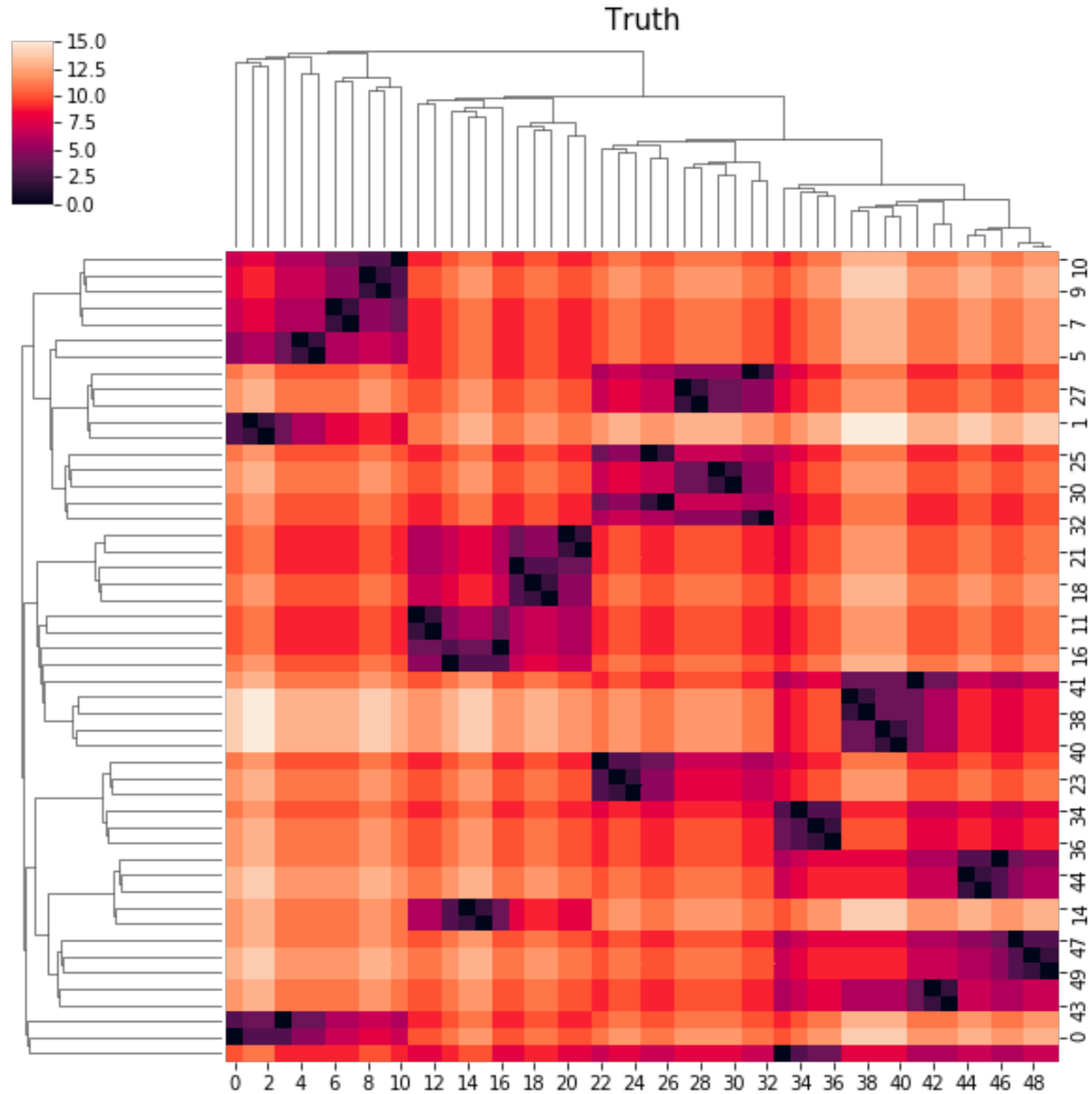




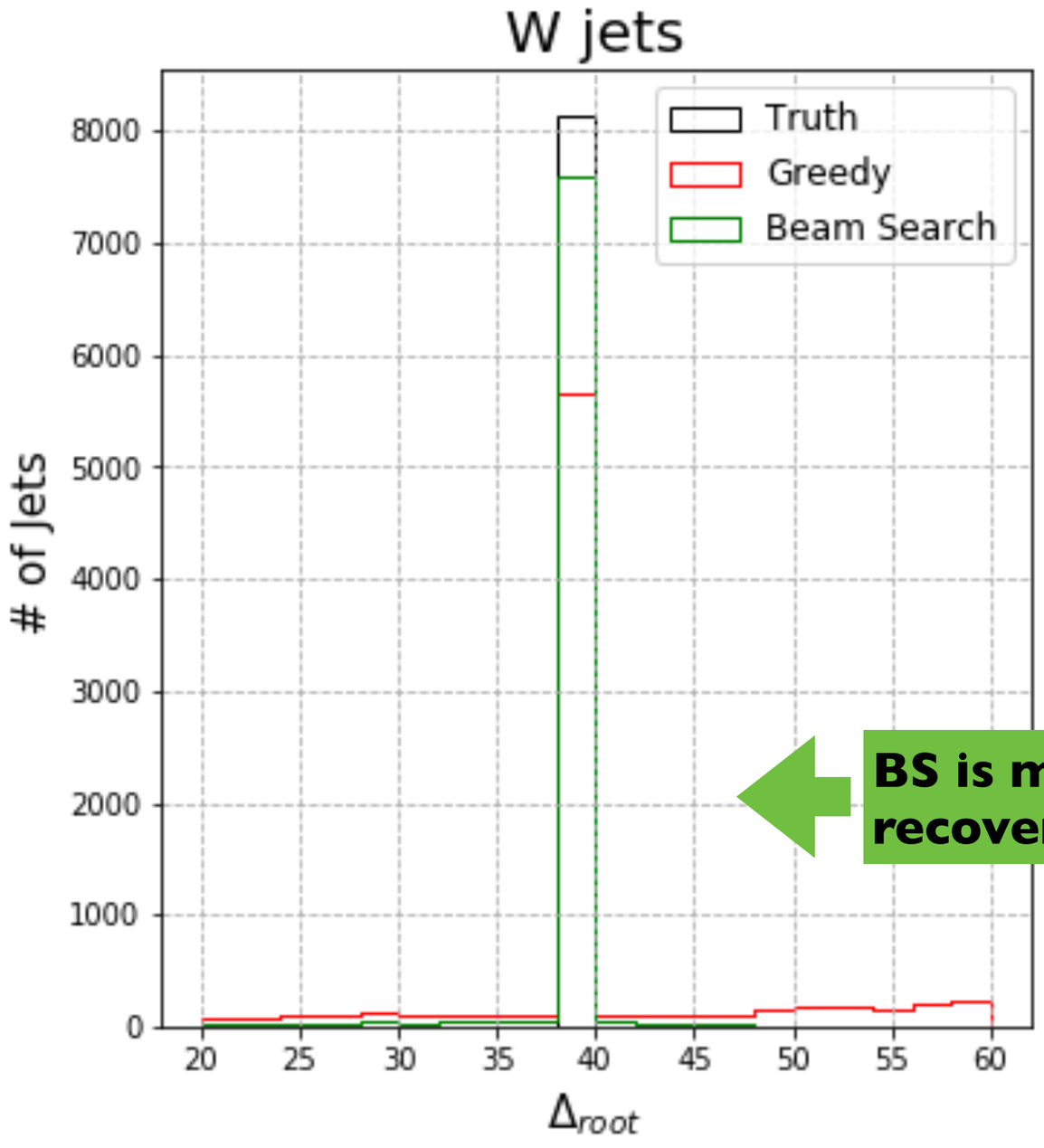
Reconstruction of Δ_{root}

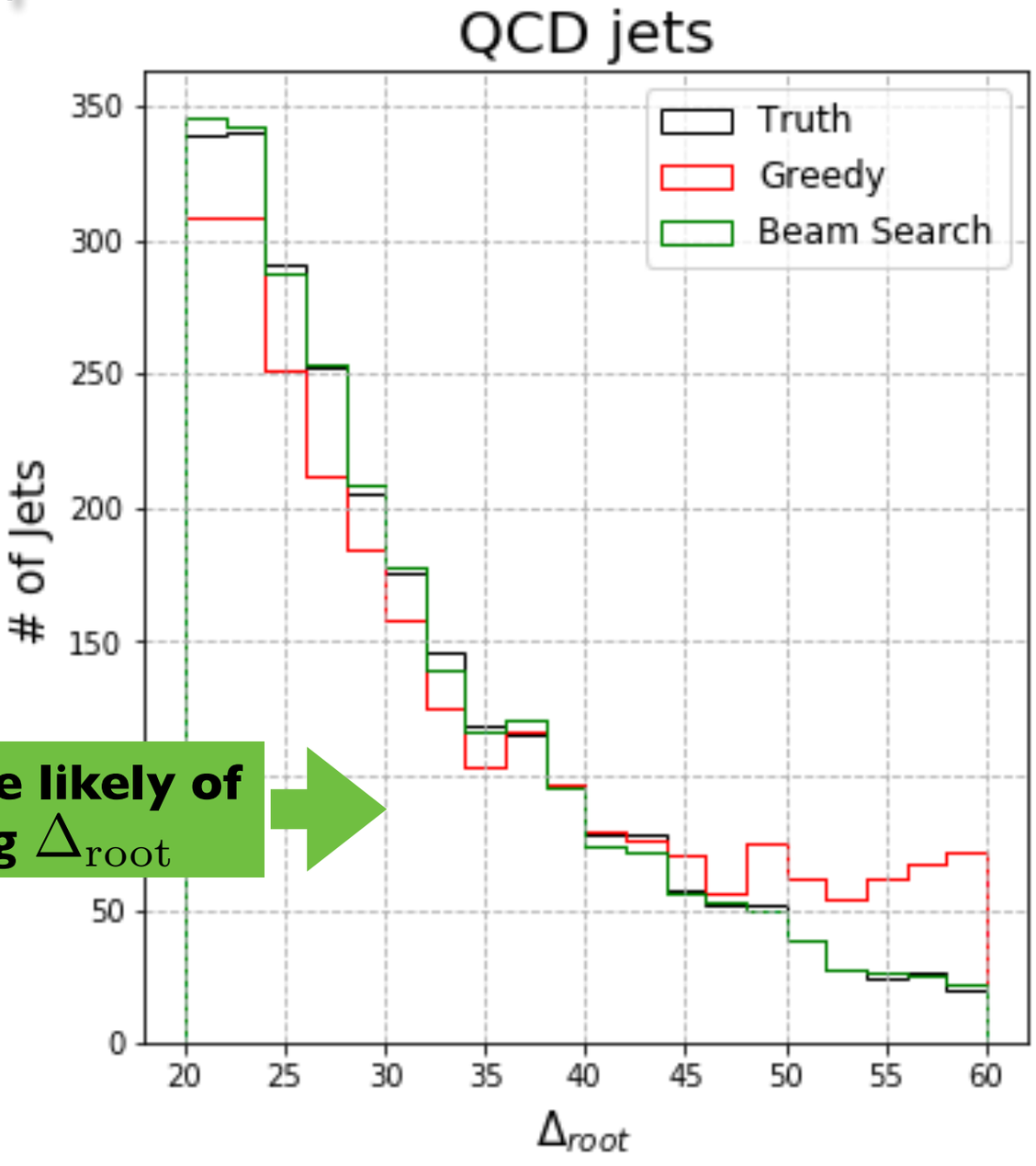
Ginkgo W jets

$$\Delta_{\text{root}} = \frac{m_W}{2}$$

Ginkgo QCD jets

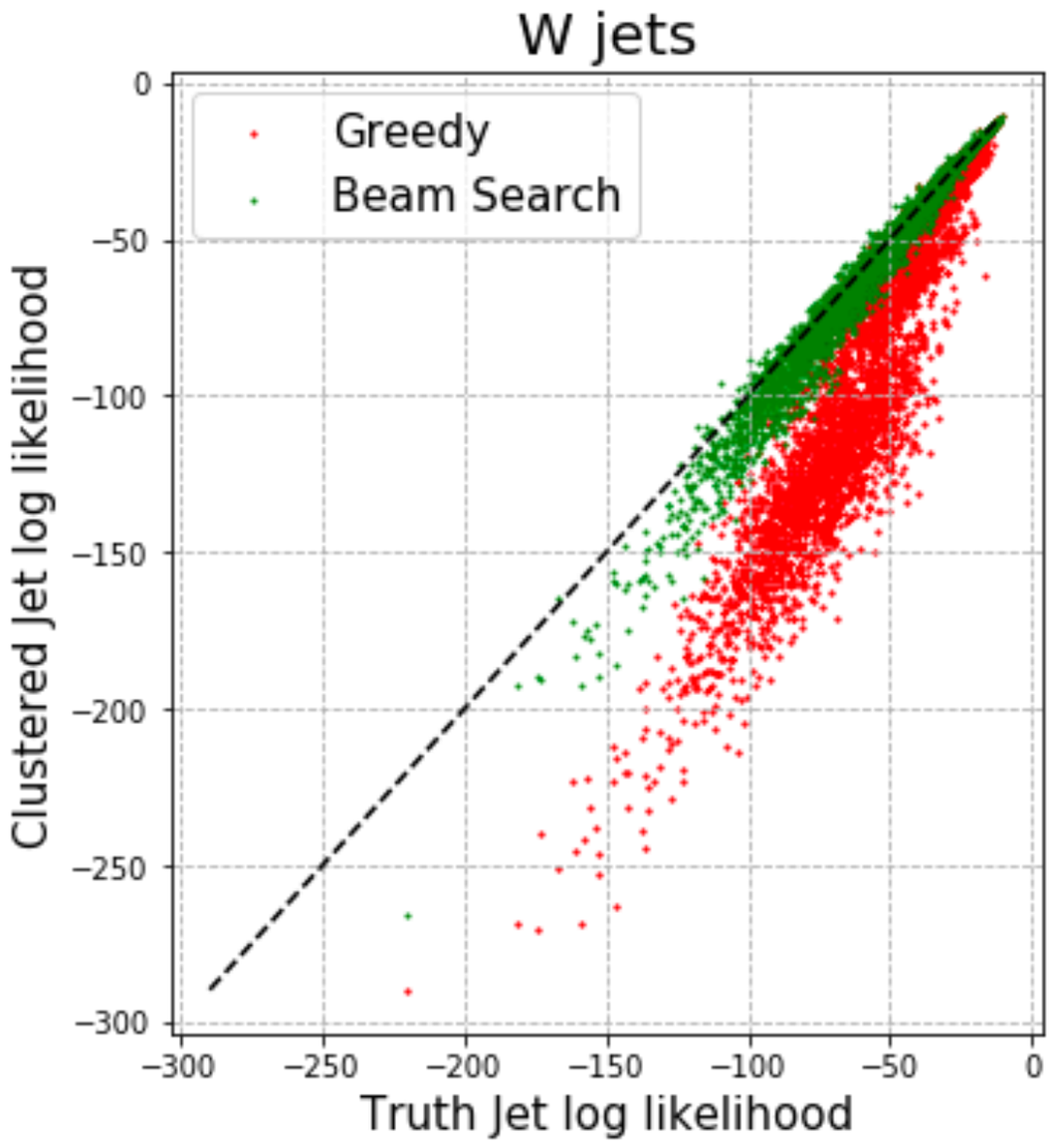
$$\Delta_{\text{root}} \sim f(\Delta|\lambda, \Delta_0) = \frac{\lambda}{\Delta_0} e^{-\frac{\lambda}{\Delta_0}\Delta}$$

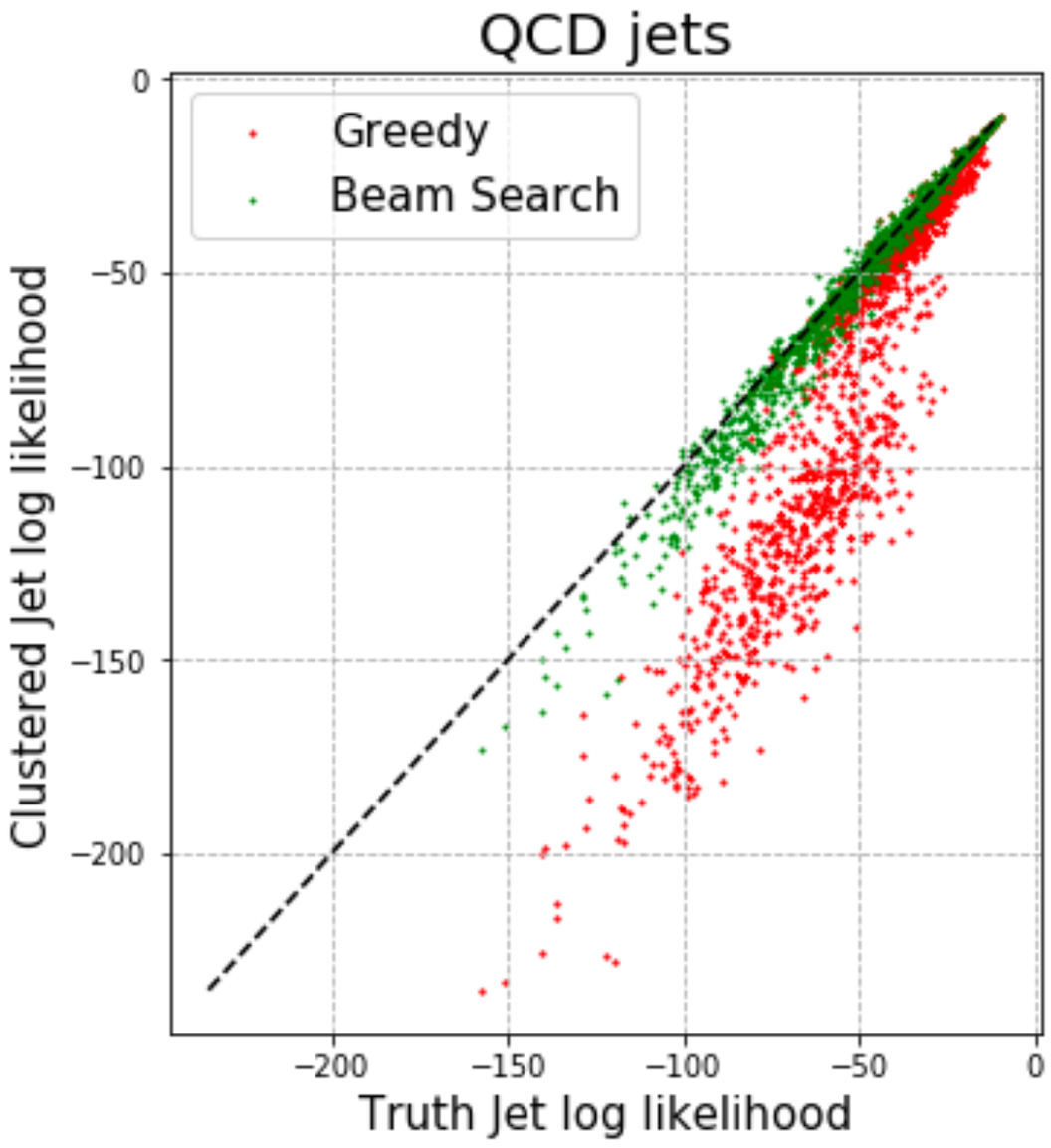




BS is more likely of recovering Δ_{root}

Jets log likelihood



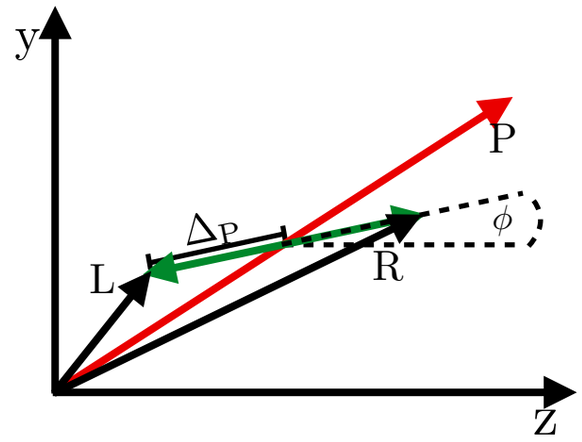


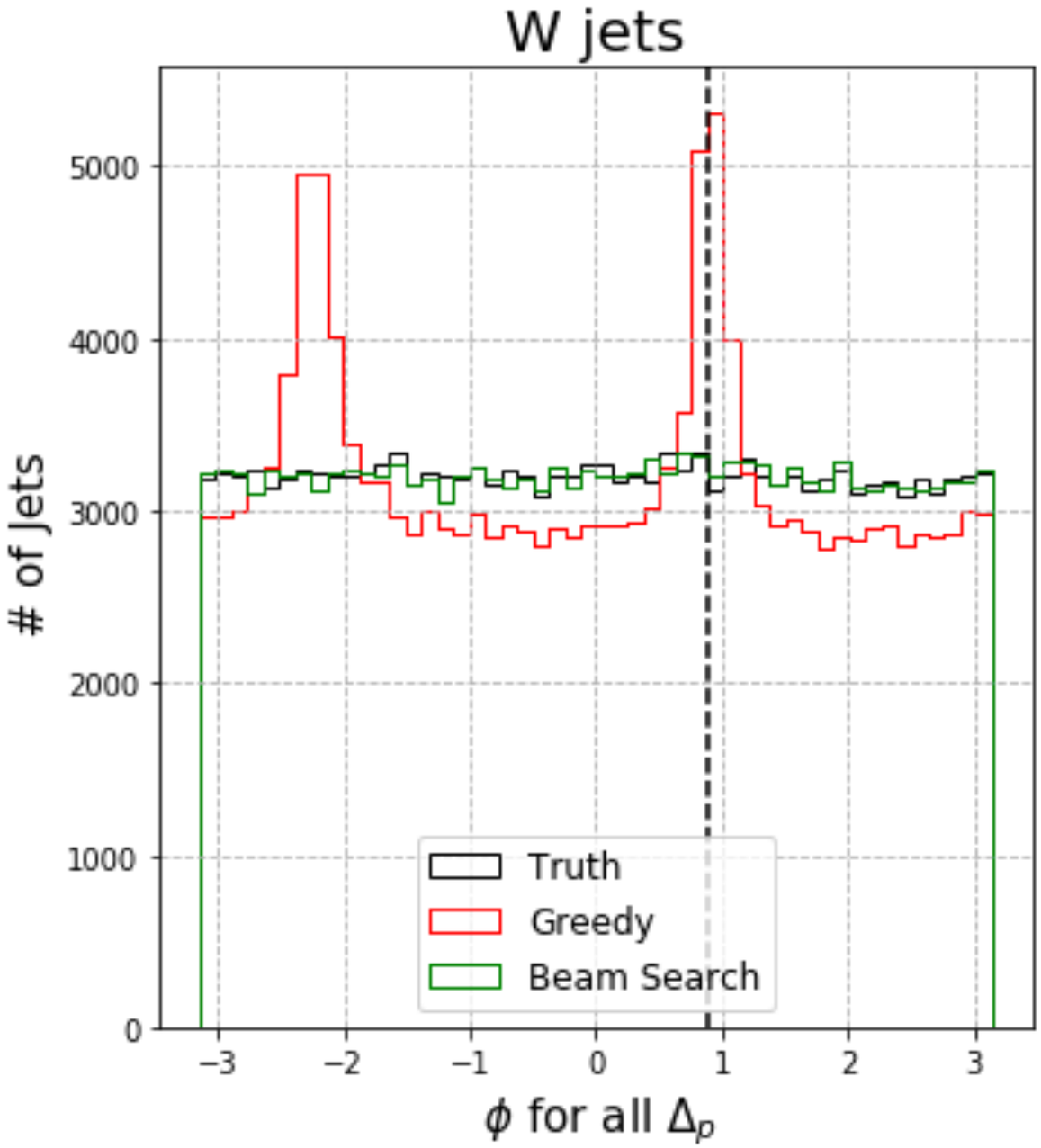
Mean values:

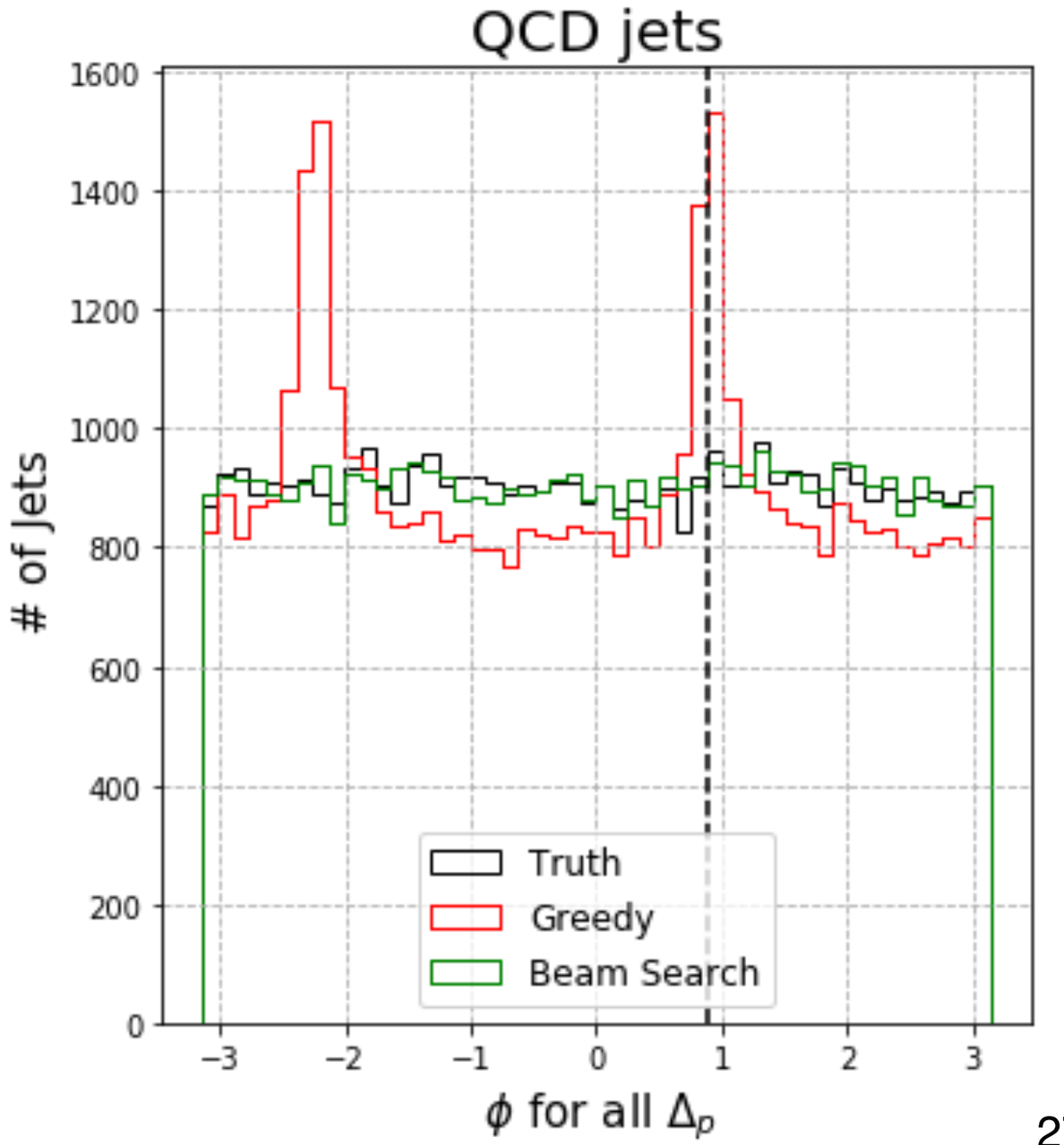
$$\log p_{\text{truth}} = -45.5 \pm 3.1$$
$$\log p_{\text{BS}} = -46.7 \pm 3.2$$
$$\log p_{\text{Greedy}} = -60.9 \pm 5.2$$

$$\log p_{\text{truth}} = -40.8 \pm 2.9$$
$$\log p_{\text{BS}} = -41.4 \pm 3.3$$
$$\log p_{\text{Greedy}} = -53.5 \pm 5.6$$

ϕ angle

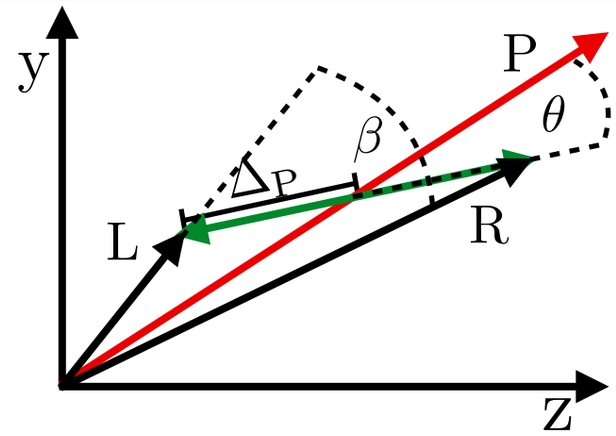

y
P
Δ_P
ϕ
L
R
z

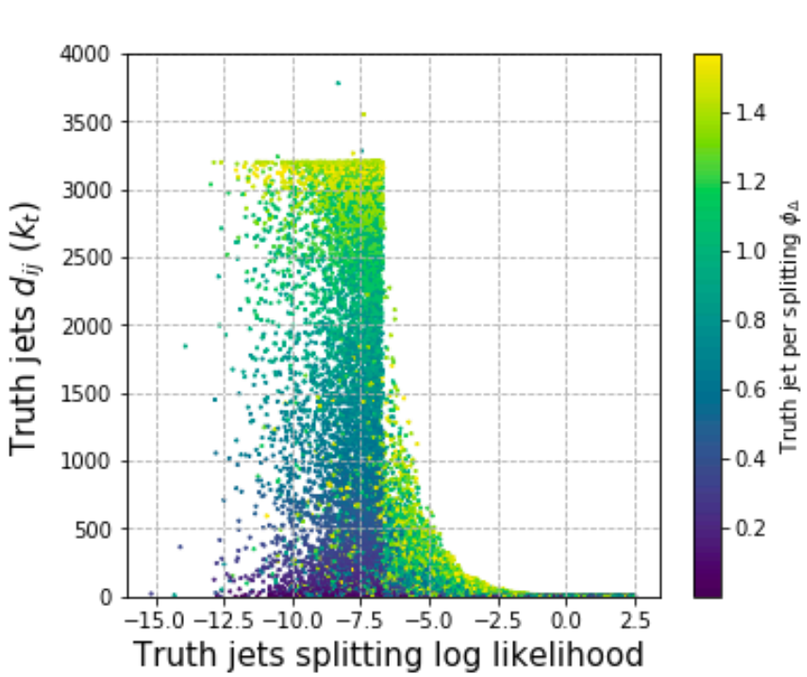

W jets
# of Jets
ϕ for all Δ_p
Truth
Greedy
Beam Search

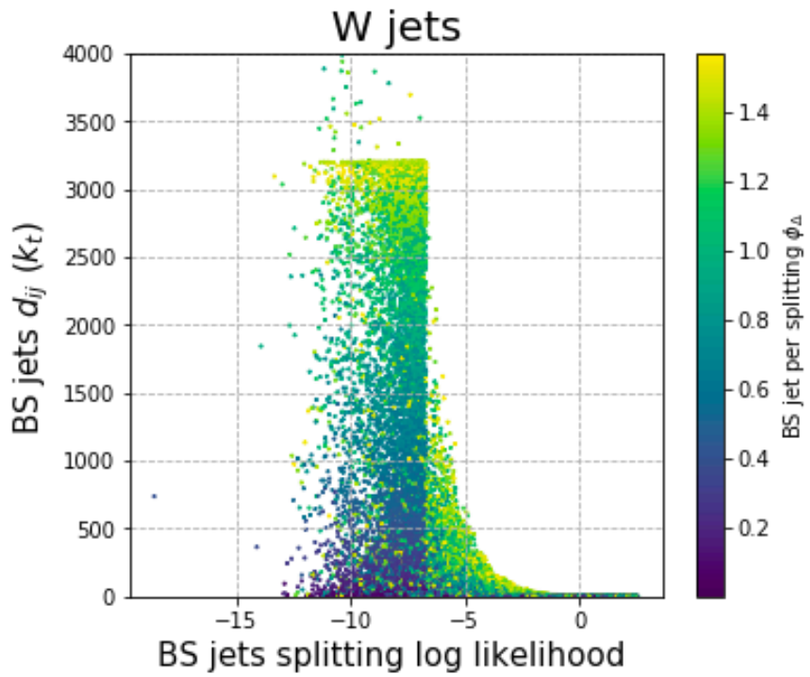

QCD jets
# of Jets
ϕ for all Δ_p
Truth
Greedy
Beam Search

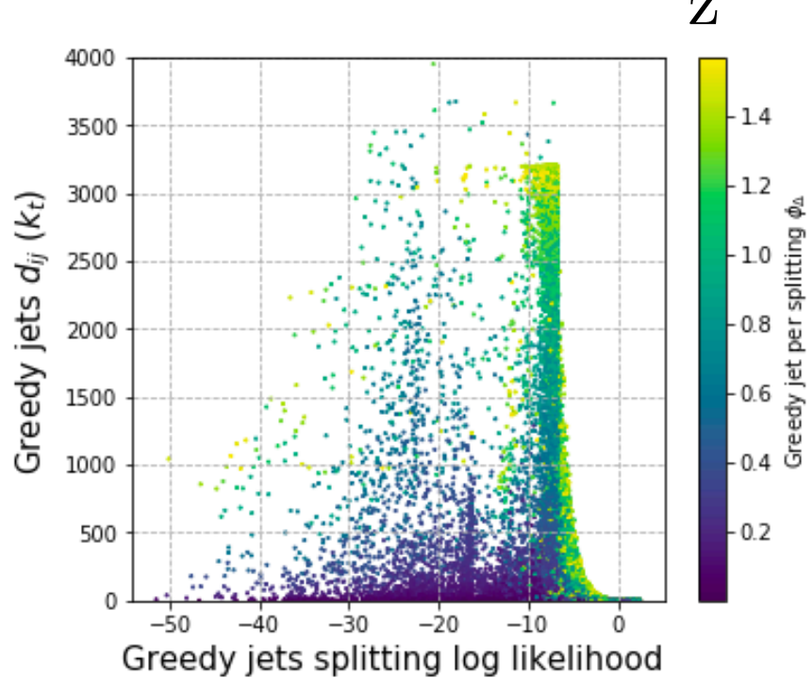
Splitting log LH vs kt distance metric dij

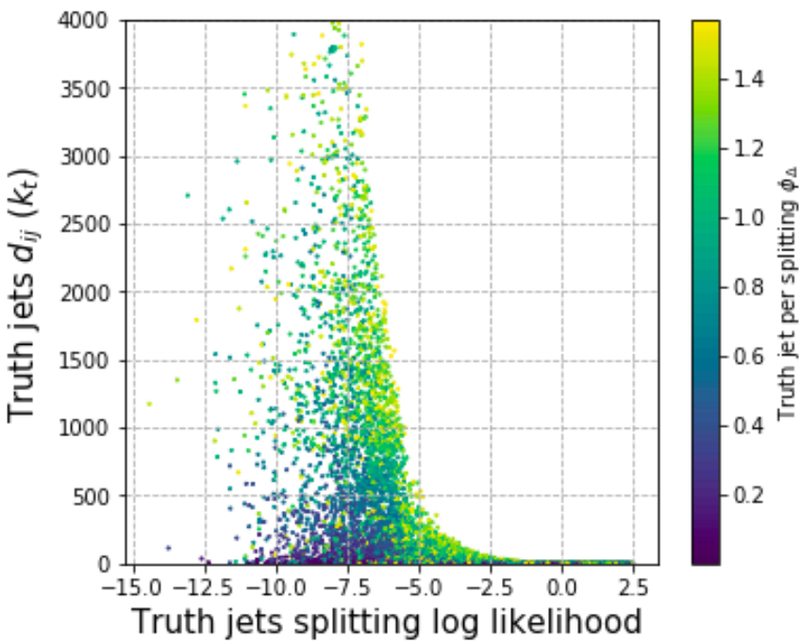
$$d_{ij} \sim \beta^2$$

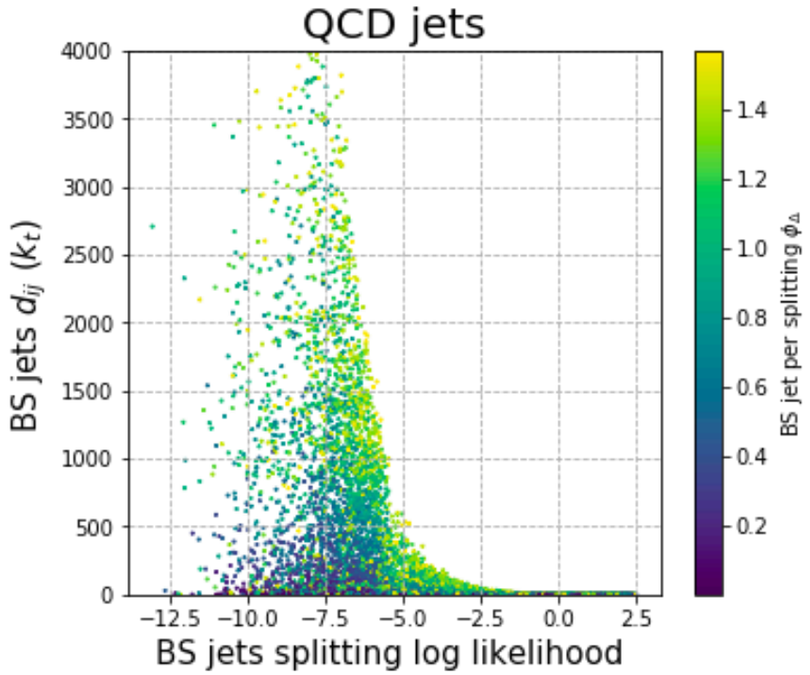


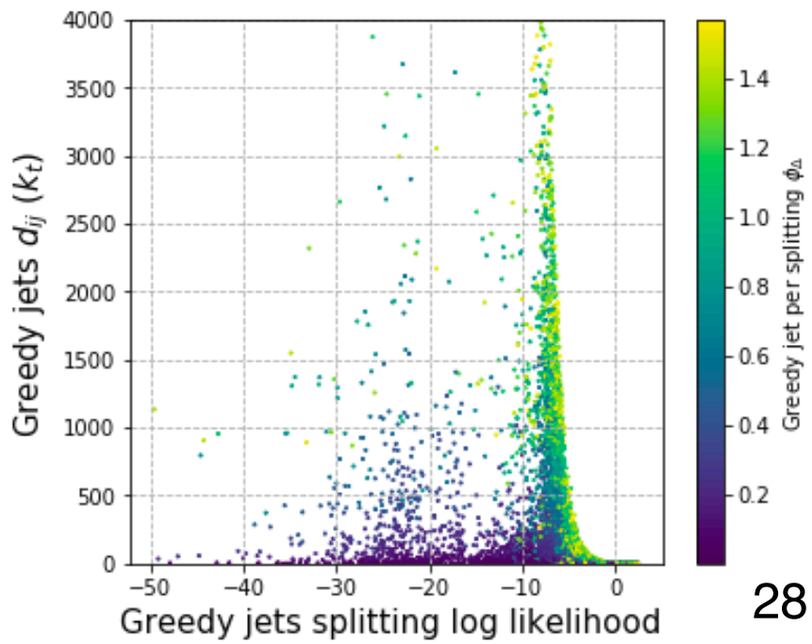






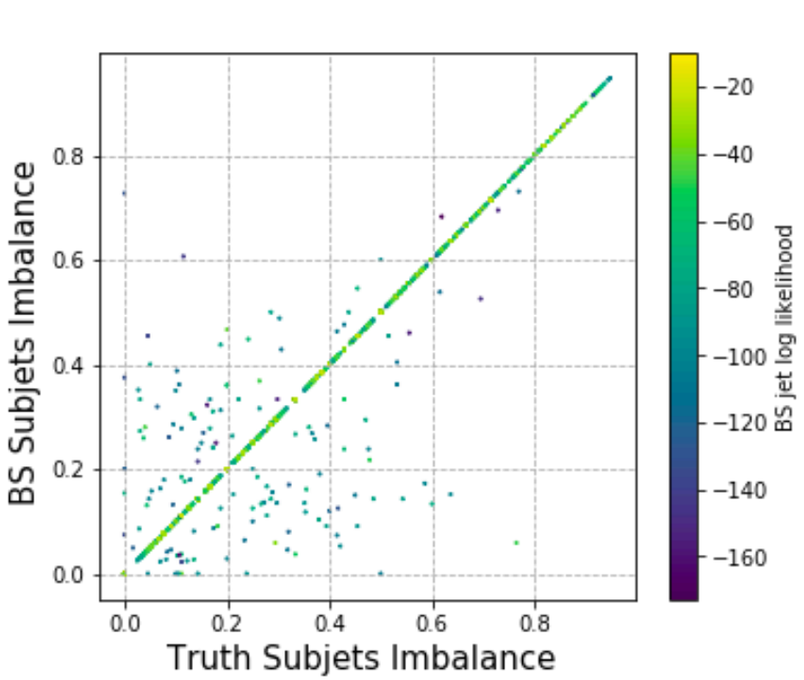


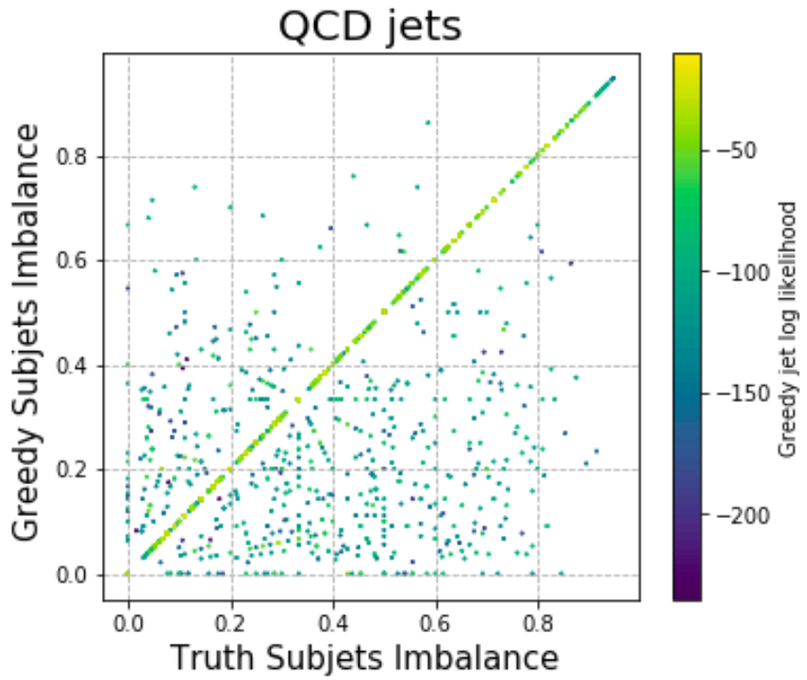


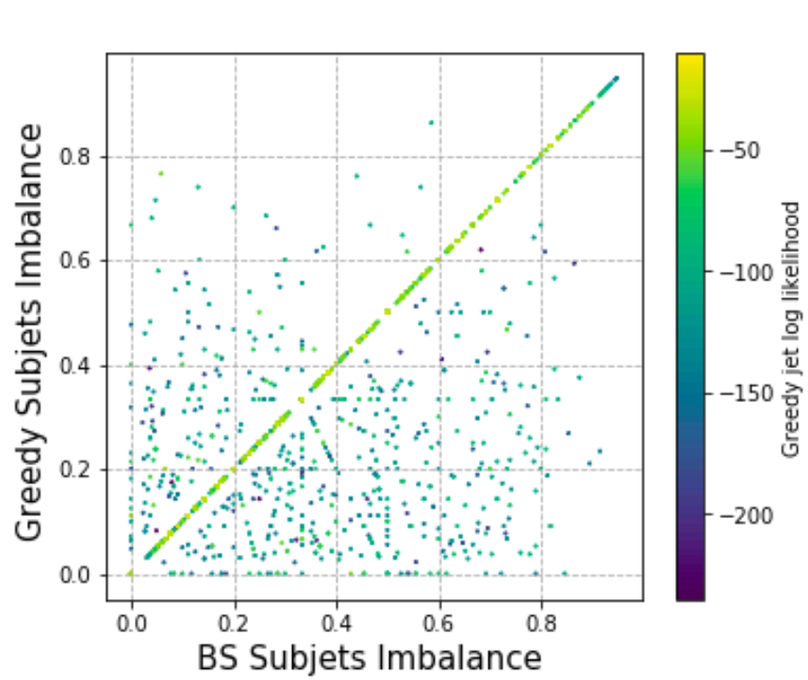


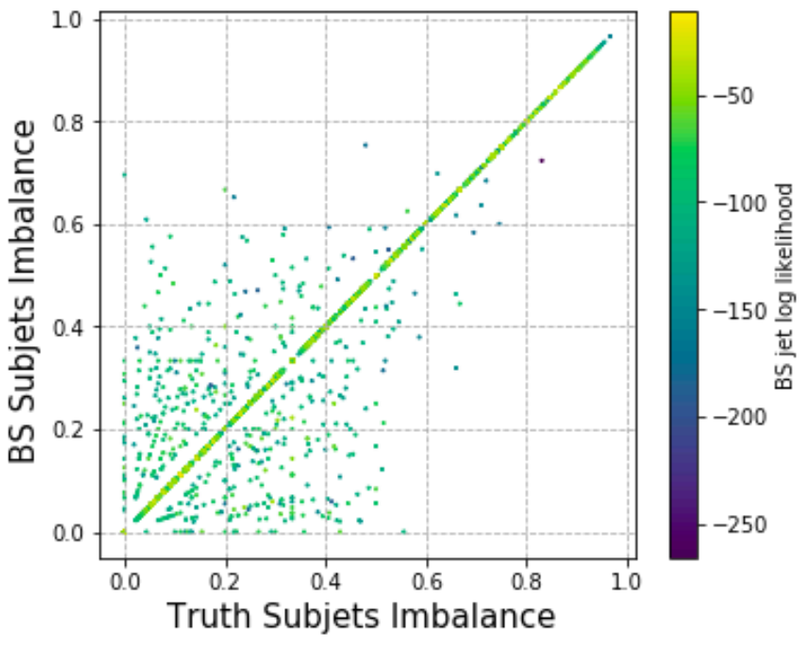
Subjets imbalance

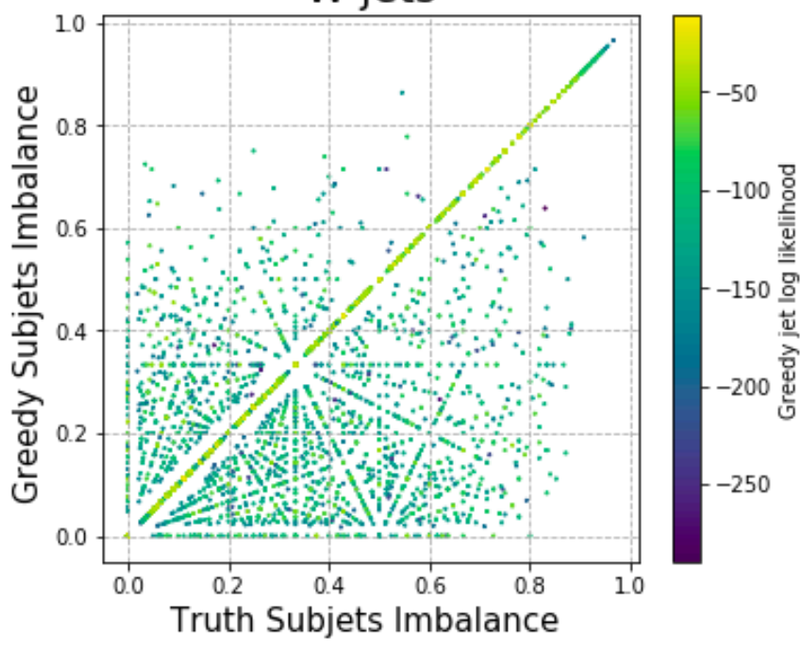
$$\mathcal{I} = \mathrm{abs}\left(\frac{N_L - N_R}{N_L + N_R}\right)$$

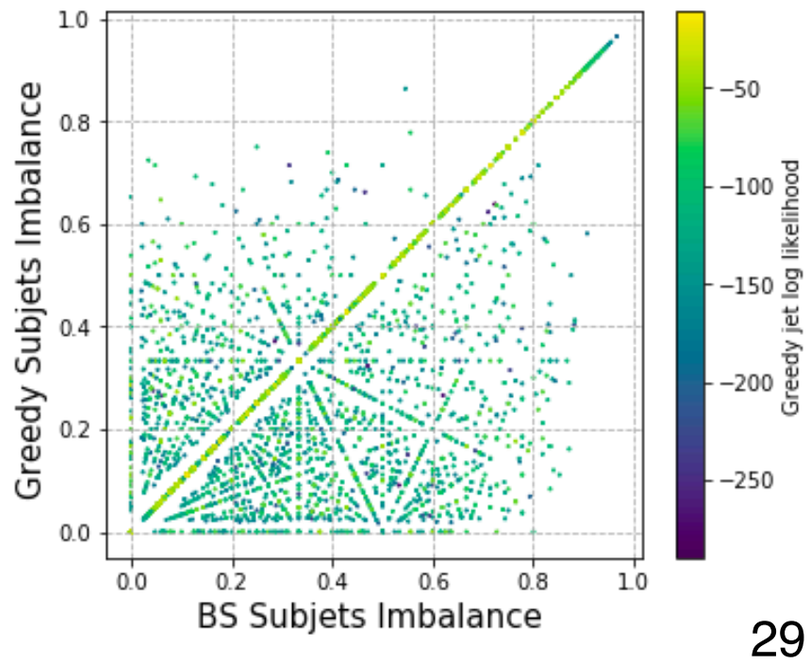






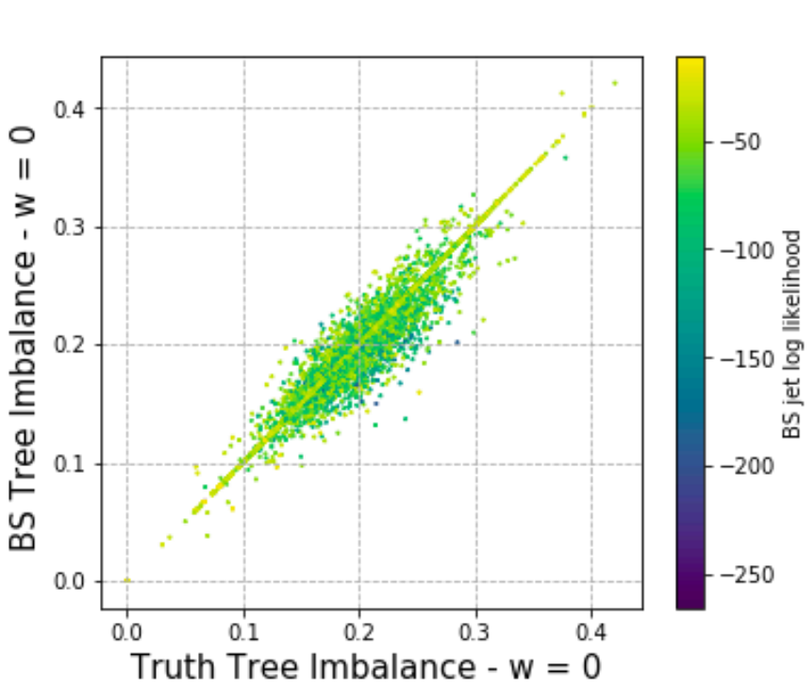


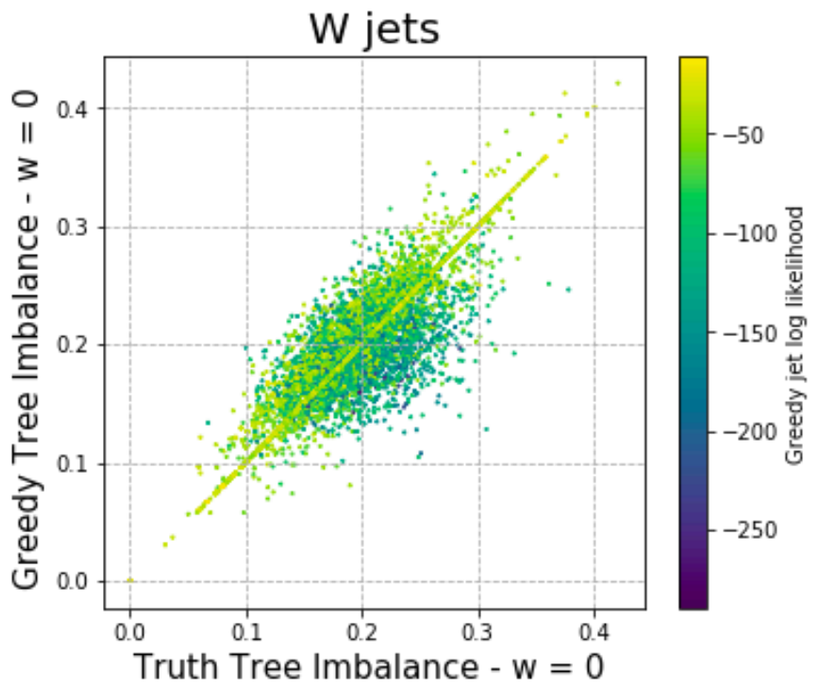


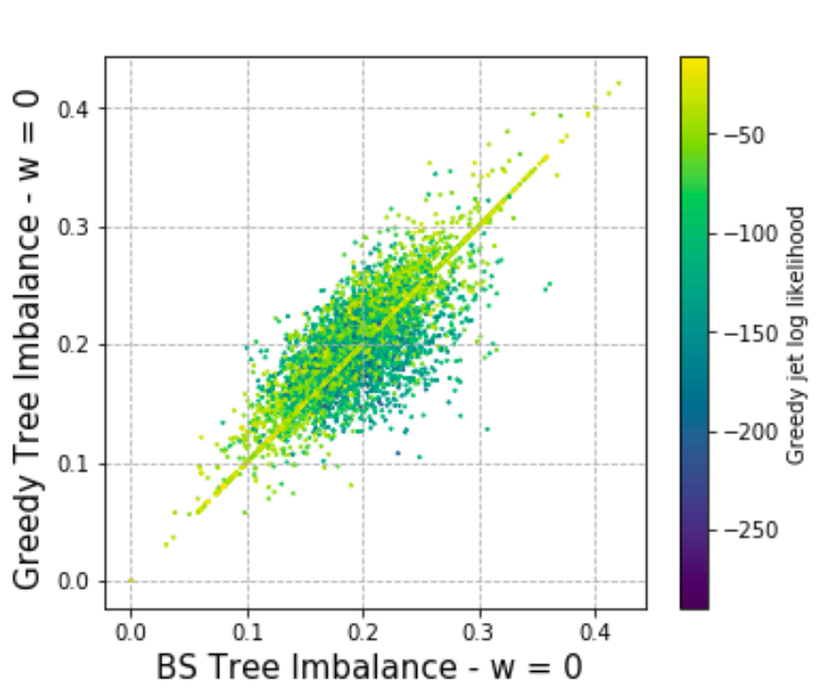


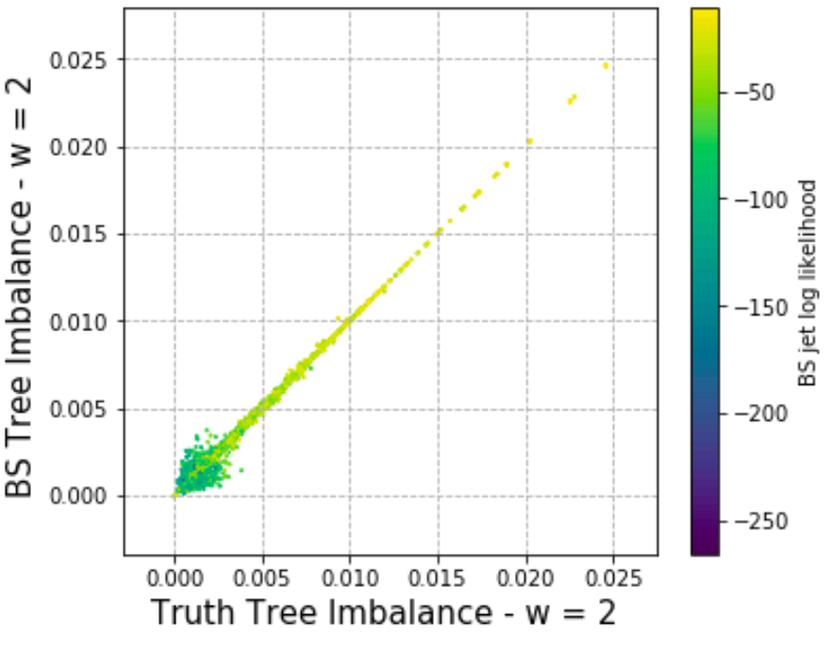
Tree imbalance

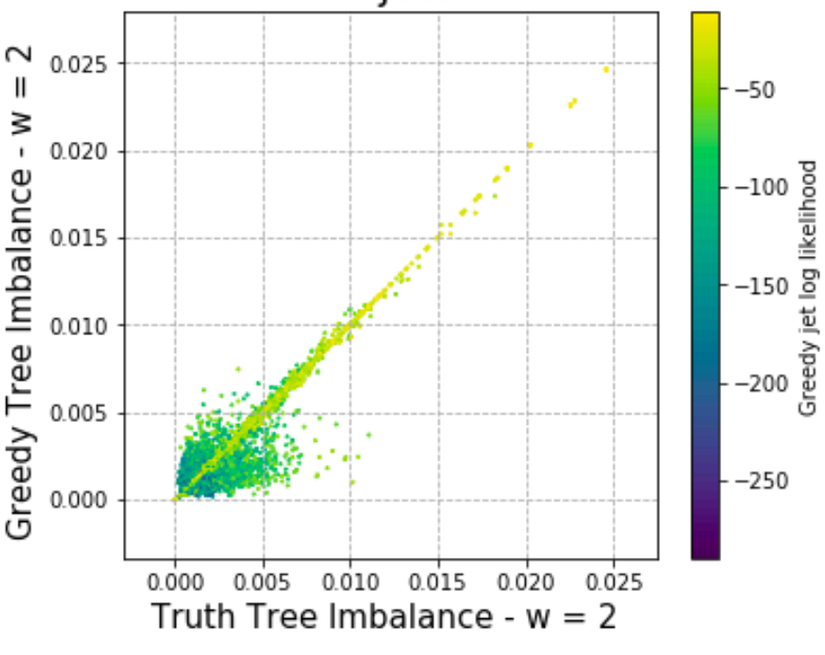
$$\mathcal{T} = \frac{1}{N_{\text{inner}}} \sum_i \exp(-wN_\ell)\, \mathcal{I}_i$$

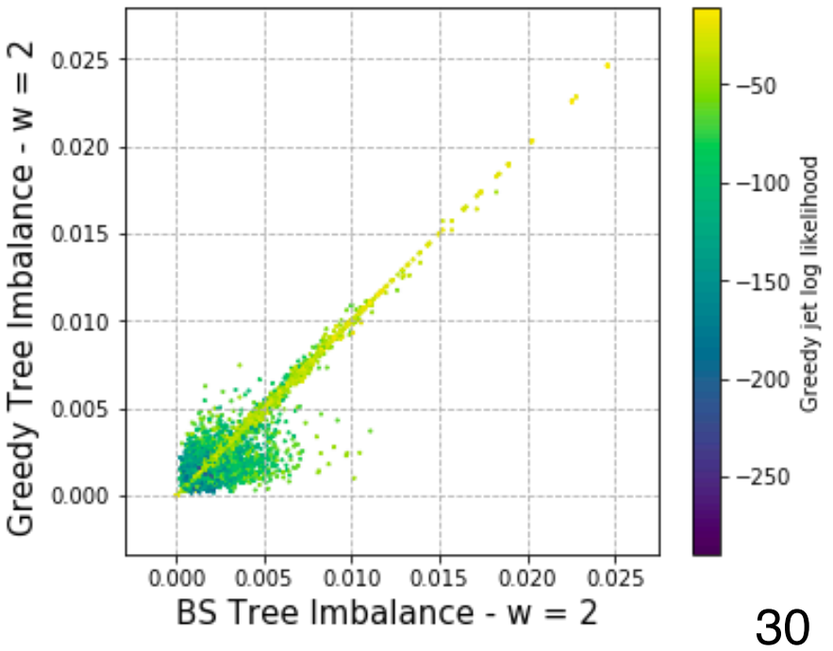












Final remarks and future directions

- Goal: Unification of generation and inference.
- Beam search is strictly better than the greedy algorithm (e.g. kt) in terms of estimating the most likely tree.
- Study algorithms for subject reconstruction and soft radiation removal, e.g reinforcement learning based algorithms.
- Study the posterior distribution $p(z|x,\theta)$ on clustering histories, conditioned on the observed particles.
  Obtain an estimate from sampling with MCMC or probabilistic programing techniques?
- Could we learn the node splitting from fitting to data and systematically improve the generative model?
- Study metrics to compare binary trees latent structures.
- Study the implementations of new results on parton shower generators in full physics simulations.

Thanks for your attention!