Construction and Fitting of a Deep Generative Hadronization Model

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Matter To The Deepest 2023

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Motivation - Monte Carlo Event Generators (MCEG)

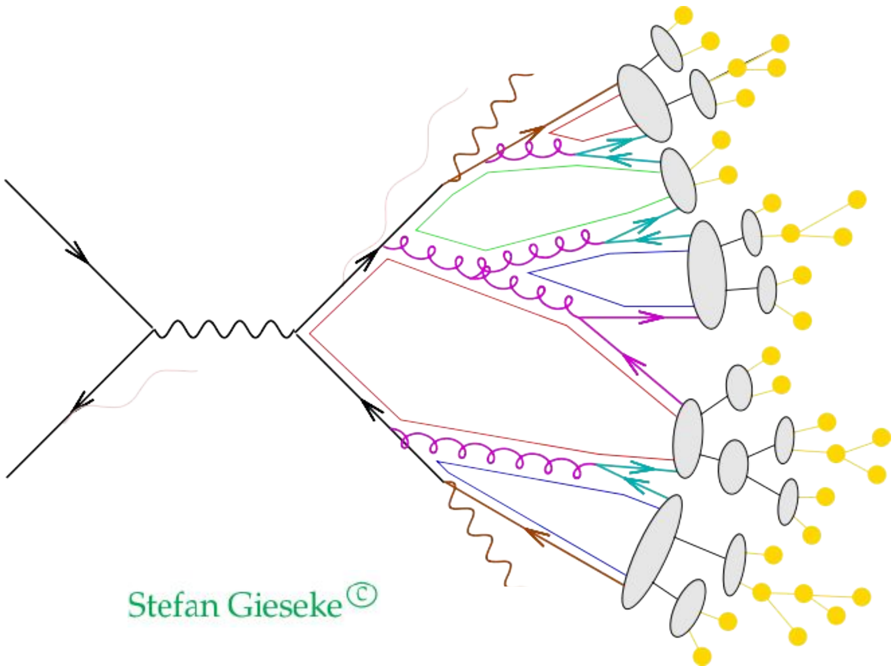
QCD correctly describes strong interactions in each energy range but its complex mathematical structure makes it very difficult to obtain precise predictions (Millennium Prize Problem $1,000,000)

High energy

- **perturbative QCD**
- **in theory we know what to do**
- **in practice very difficult**
  [see Gabor's talk]

Low energy

- **non-perturbative QCD**
- **we don't know what to do**
- **phenomenological models (with many free parameters)**



[see J. Whitehead's talk for the perturbative part]

Why hadronization?

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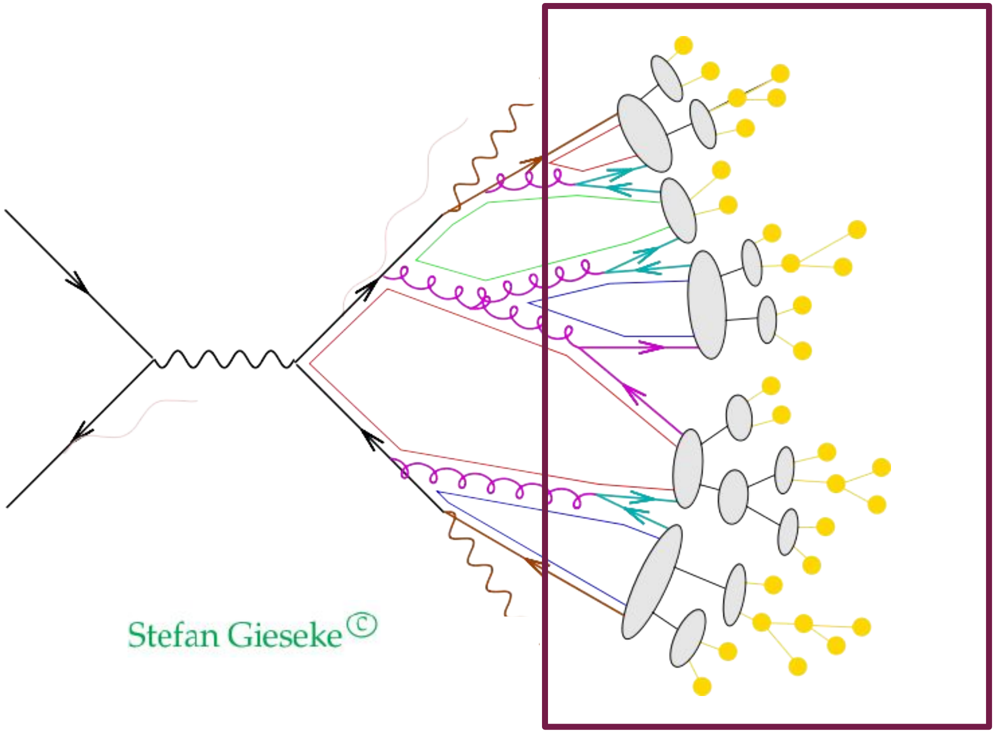


Hadronization:
one of the least understood elements of MCEG

Motivation - Hadronization

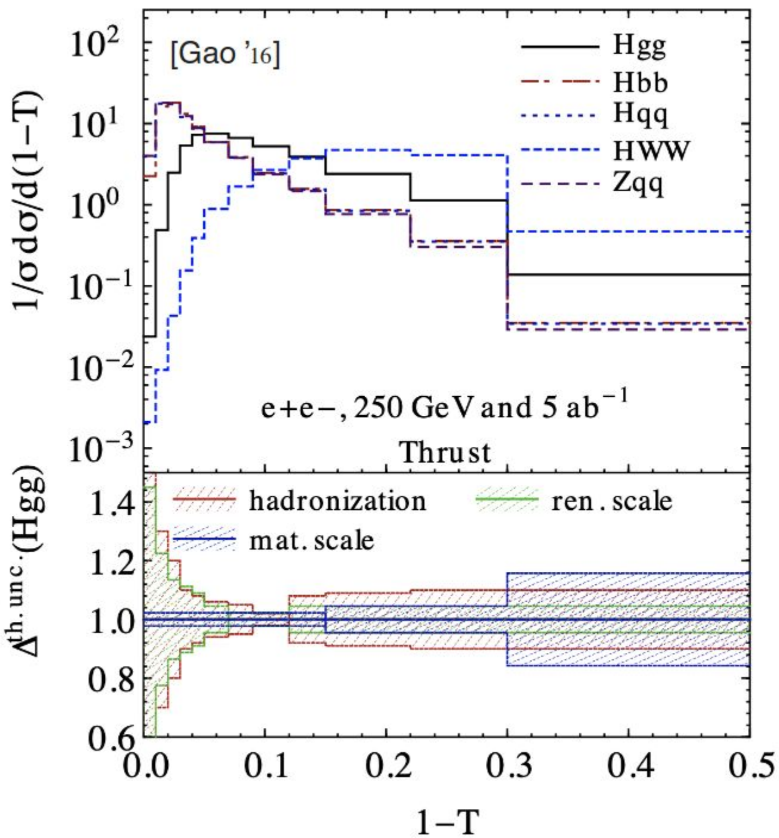
Hadronization:

➔ Increased control of perturbative corrections ⇒ more often LHC measurements are limited by non-perturbative components, such as hadronization.

- W mass measurement using a new method [Freytsis at al. JHEP 1902 (2019) 003]
- Extraction of the strong coupling in [M. Johnson, D. Maître, Phys.Rev. D97 (2018) no.5]
- Top mass [S. Argyropoulos, T. Sjöstrand, JHEP 1411 (2014) 043]
- ...

Pier Moni's talk
FCC Physics Workshop 2023

- However, hadronisation remains the main bottleneck
  - e.g. thrust in Higgs decays (MC variation in plot)
- Increase in energy insufficient for suppression ($Q \sim m_H$)
- Runs at lower energies are essential for a robust tuning of NP models in MCs
  - Also crucial for training of ML algorithms for jet tagging, instrumental in extraction of Higgs couplings



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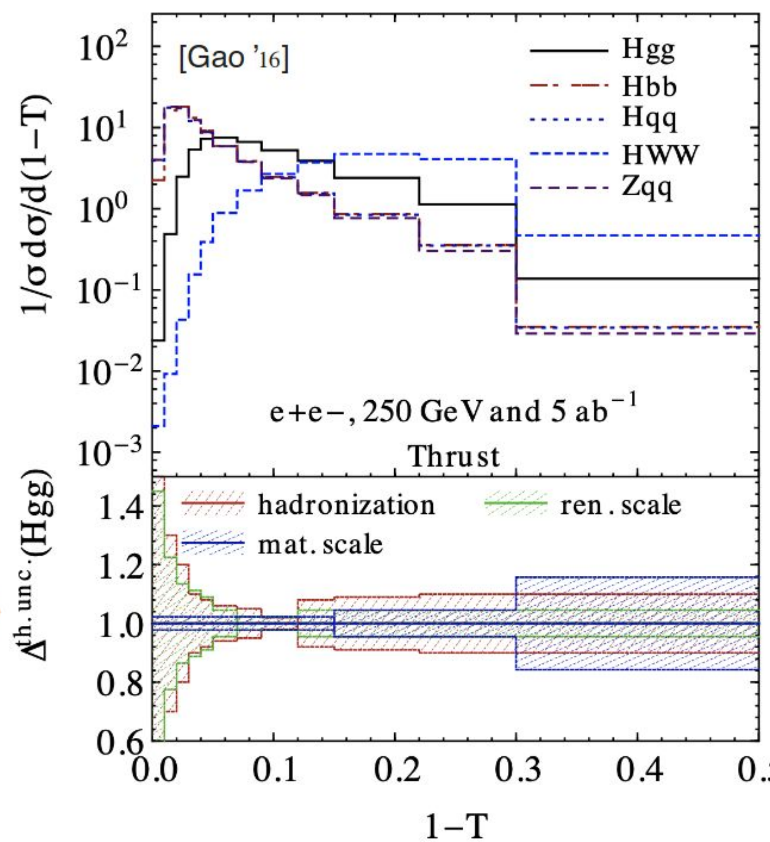
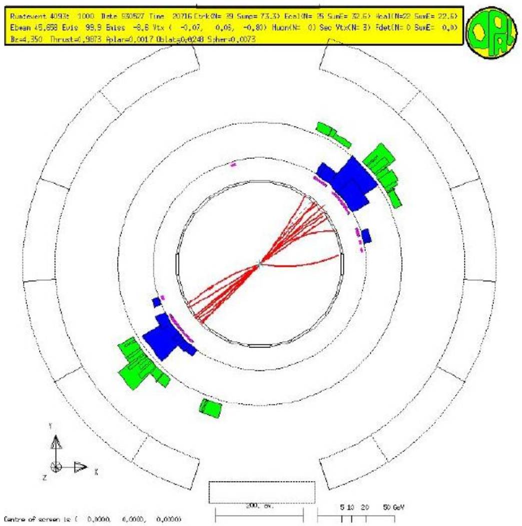


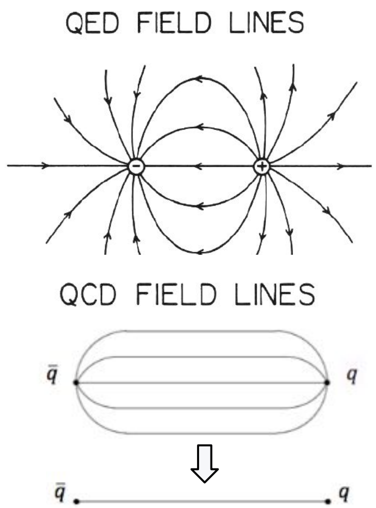
String Model in nutshell [Andersson, Gustafson, Ingelman, Sjostrand, Phys.Rept.97(1983)31]

Originally invented without perturbative physics of parton showers in mind.

We start with 2-jet events in
$e^+ e^- \to$ hadrons.



Self coupling of gluons
“attractive field line”

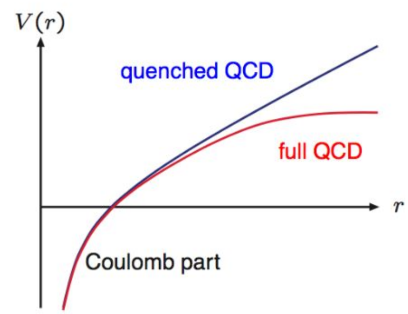


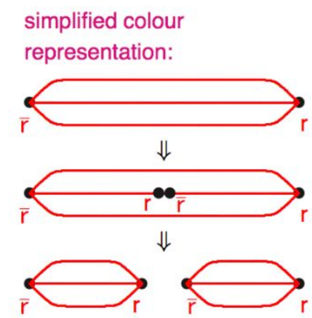
1+1 - dim. object: **string**

Linear static potential:

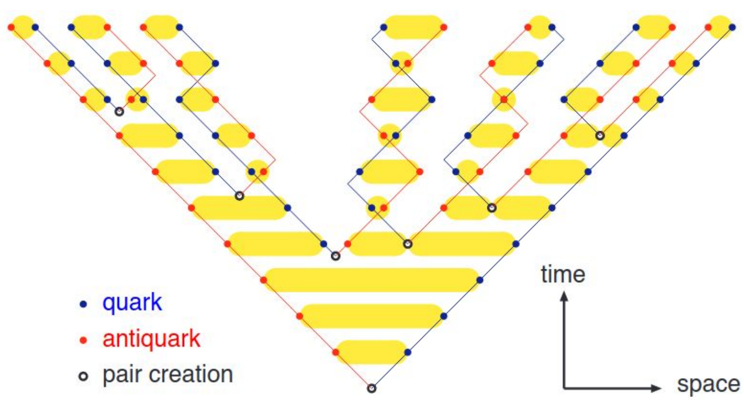
$$F(r) \approx \text{const} = \kappa \approx 1\ \text{GeV/fm} \quad \Longleftrightarrow \quad V(r) \approx \kappa r$$

Picture supported by lattice QCD





Lund string model: like rubber band that is pulled apart and breaks into pieces



Plots from T. Sjostrand

String Model in nutshell

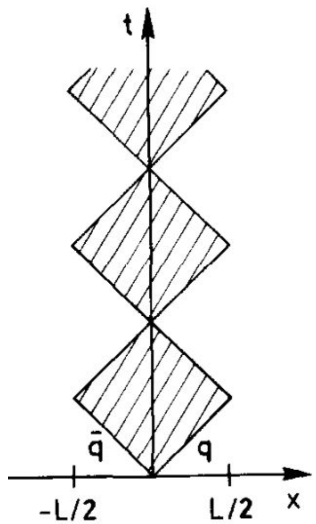
[Andersson, Gustafson, Ingelman, Sjostrand, Phys.Rept.97(1983)31]

String motion

From linear static potential $V(r) \approx \kappa r$ and linearity between space–time and energy–momentum:

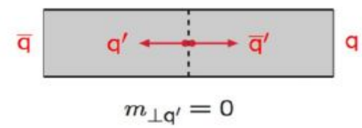
$$\left|\frac{\mathrm{d}E}{\mathrm{d}z}\right| = \left|\frac{\mathrm{d}p_z}{\mathrm{d}z}\right| = \left|\frac{\mathrm{d}E}{\mathrm{d}t}\right| = \left|\frac{\mathrm{d}p_z}{\mathrm{d}t}\right| = \kappa$$

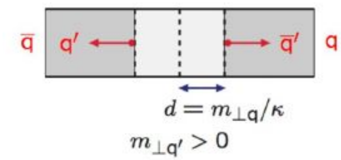
We get a “YoYo“ state which we interpret as a meson.



String breakdowns

The quarks obtain a mass and a transverse momentum in the breakup through a tunneling mechanism





with a probability:

$$\mathcal{P} \propto \exp\left(-\frac{\pi m_{\perp q}^2}{\kappa}\right) = \exp\left(-\frac{\pi p_{\perp q}^2}{\kappa}\right) \exp\left(-\frac{\pi m_{q}^2}{\kappa}\right)$$

- Suppression of heavy quarks: uu : dd : ss : cc ≈ 1 : 1 : 0.3 : 10^{-11}
- Common Gaussian pT spectrum, <pT>~ 0.4 GeV
- Diquark (qq - q̄q̄ breakups) ~ antiquark ⇒ simple model for baryon production.

Iterative process (left-right symmetry) leads to distribution of momentum fraction taken by each hadron as:

$$f(z) \propto \frac{(1-z)^a}{z} \exp\left(-\frac{bm^2}{z}\right)$$

Summary:

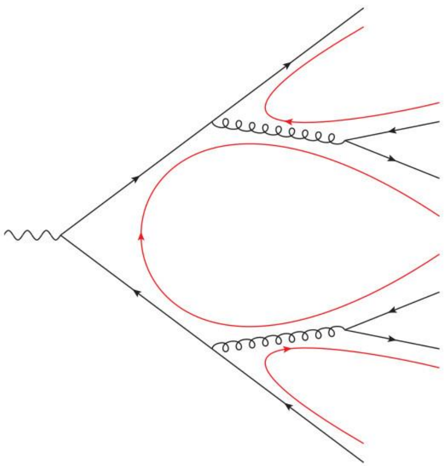
String model has very good energy-momentum picture however it is unpredictive in understanding of hadron mass effects ⇒ many parameters, 10-30 depending on how you count.

Cluster model in nutshell

[Webber NPB238(1984)492]

What if we have PS (more perturbative input before hadronization).

The philosophy of the model: use information from perturbative QCD as an input for hadronization. QCD **pre-confinement** discovered by Amati & Veneziano [*Phys.Lett.B* 83 (1979) 87-92]:



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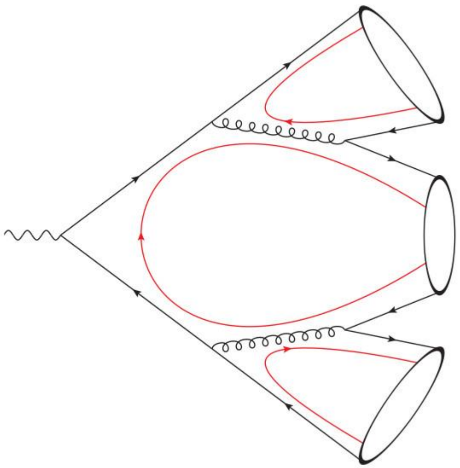

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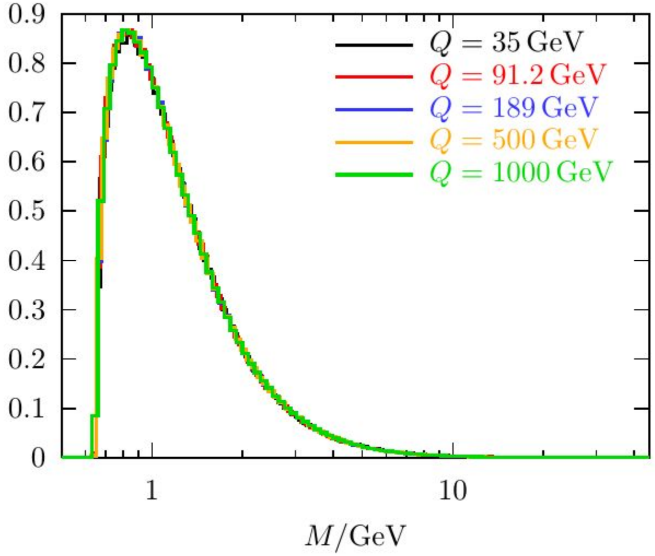

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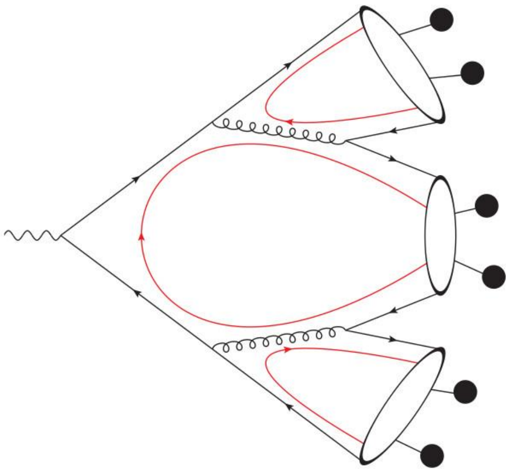

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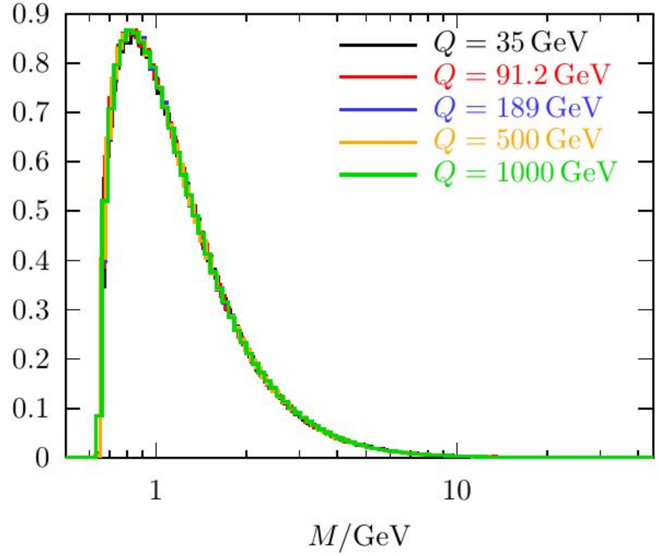

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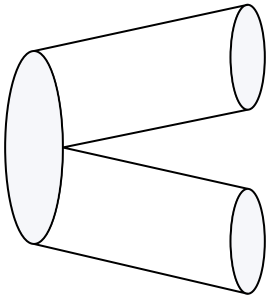
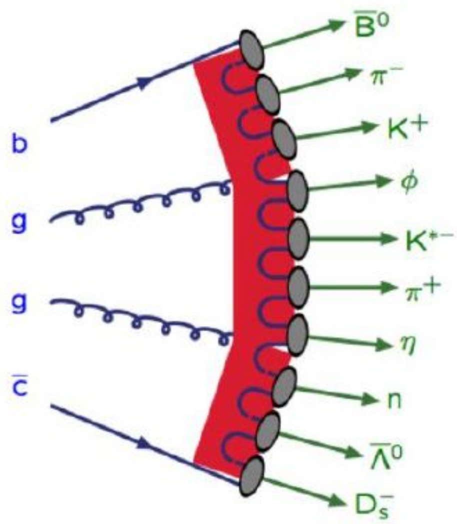
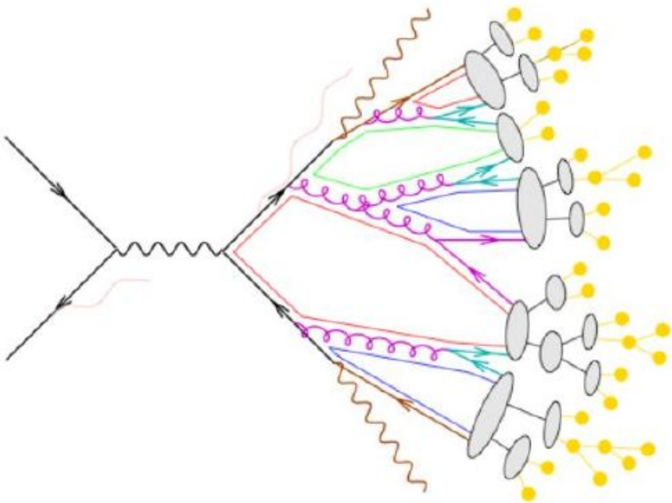
- Small fraction of clusters too heavy for isotropic two-body decay, heavy cluster decay first into lighter cluster C → CC, or radiate a hadron C → HC, it is rather string-like.
- ~ 15% of primary clusters get split but ~ 50% of hadrons come from them!



String vs Cluster model





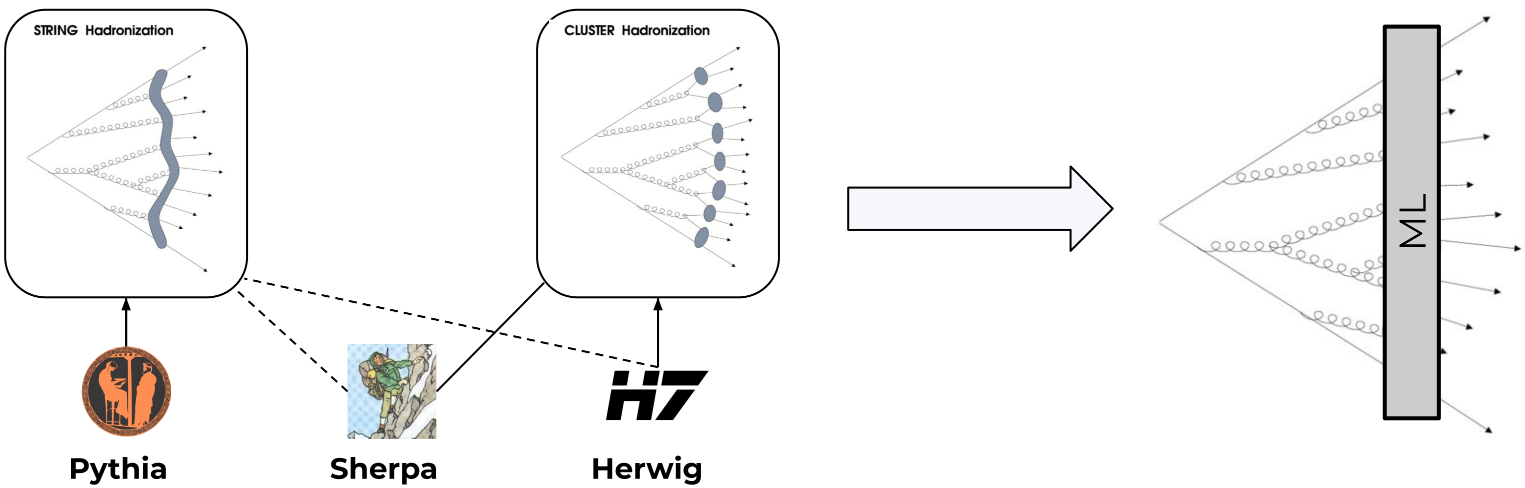
program	PYTHIA	Herwig
model	string	cluster
energy–momentum picture	powerful	simple
	predictive	unpredictive
parameters	few	many
flavour composition	messy	simple
	unpredictive	in-between
parameters	many	few

Taken from T. Sjostrand

Hadronization:

Early 1980's
(not much progress)

Early 2020's
(lot of progress in ML)



Idea of using Machine Learning (ML) for hadronization.

Motivation for Machine learning hadronization

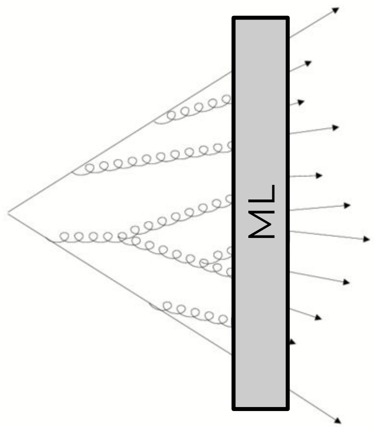
Idea of using Machine Learning (ML) for hadronization.

- Existing hadronization models are highly parameterized functions.
- Hadronization is a fitting problem [see P. Sarmah talk]

  - Can ML hadronization be more flexible?

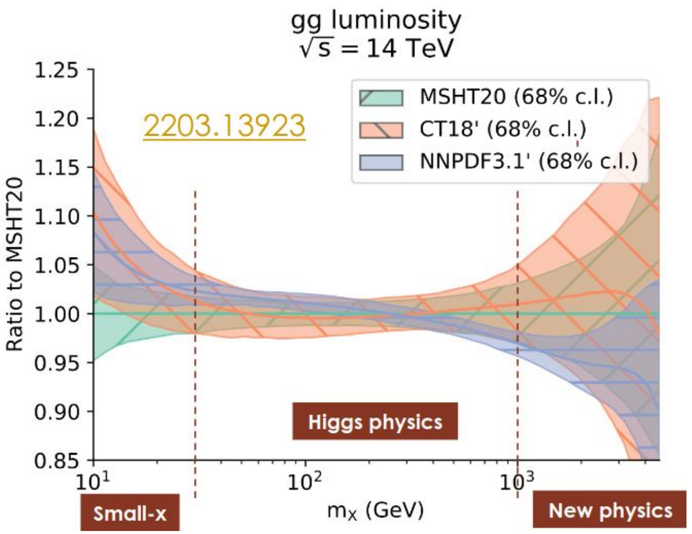
  - Can ML hadronization extract more information from the data?

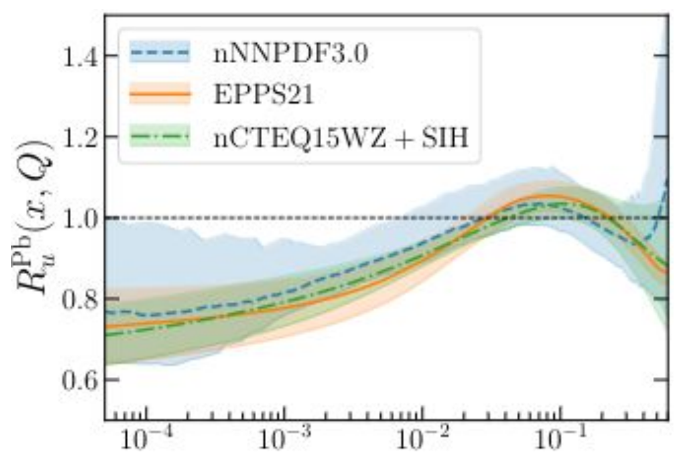
  [can accommodate unbinned and high-dimensional inputs]



- NNPDF

NNPDF used successfully ML to nonperturbative Parton Density Functions (PDF). Hadronization is closely related to fragmentation functions (FF) which were considered the counterpart of PDFs.



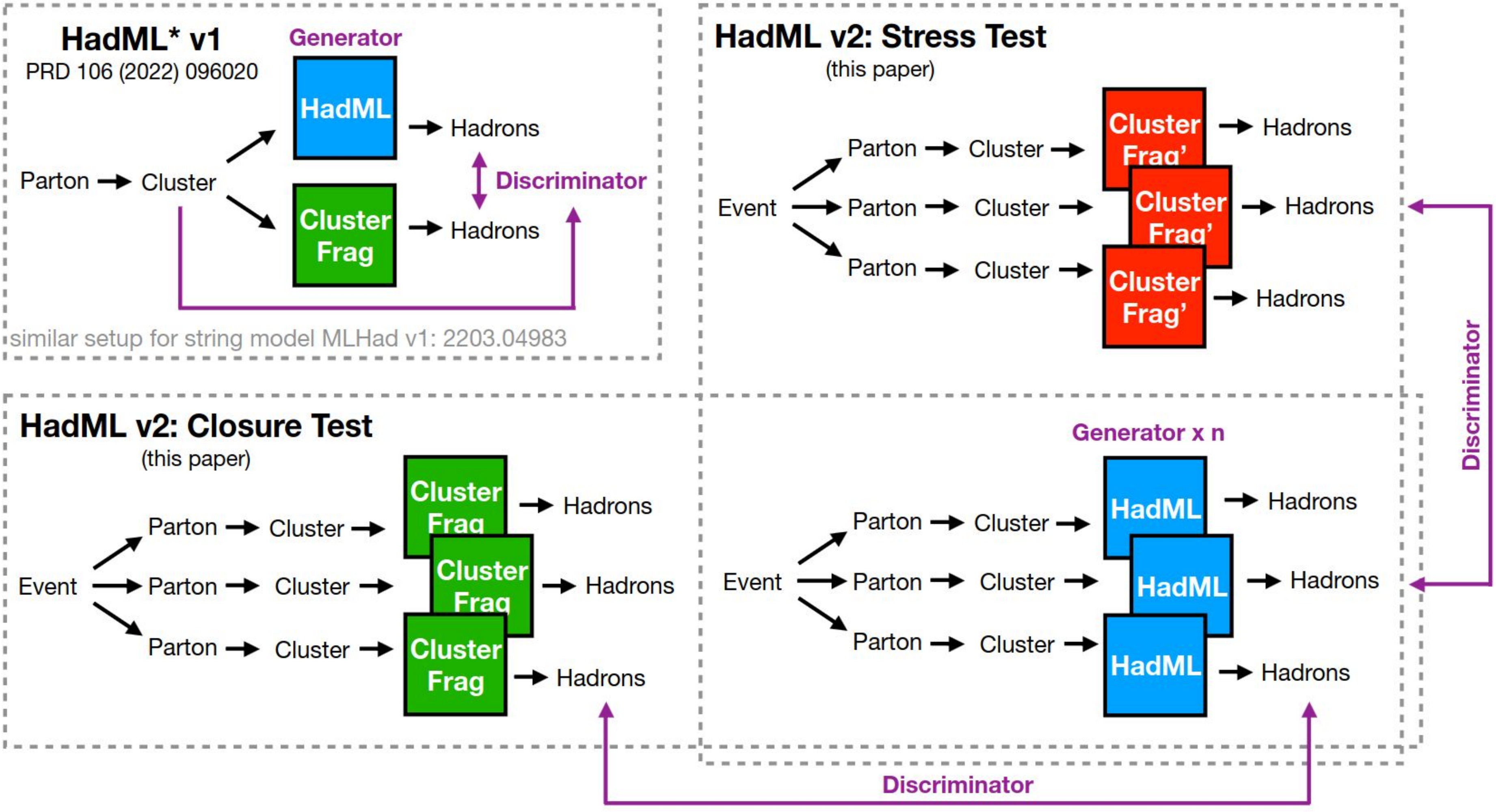


First steps for ML hadronization:

- HADML - [A. Ghosh, Xi. Ju, B. Nachman **AS**, *Phys.Rev.D* 106 (2022) 9]
- MLhad - [P. Ilten, T. Menzo, A. Youssef and J. Zupan, SciPost Phys. 14, 027 (2023)]

	MLhad	HADML
Deep generative model:	Variational Autoencoder	Generative Adversarial Networks
Trained on:	String model	Cluster model
Recent progress:	*"Reweighting Monte Carlo Predictions and Automated Fragmentation Variations in Pythia 8"* [Bierlich, Ilten, Menzo, Mrenna, Szewc, Wilkinson, Youssef, Zupan, 2308.13459]	*"Fitting a Deep Generative Hadronization Model"* [J. Chan, X. Ju, A. Kania, B. Nachman, V. Sangli and **A.S,** JHEP 09 (2023) 084]

Road map for today



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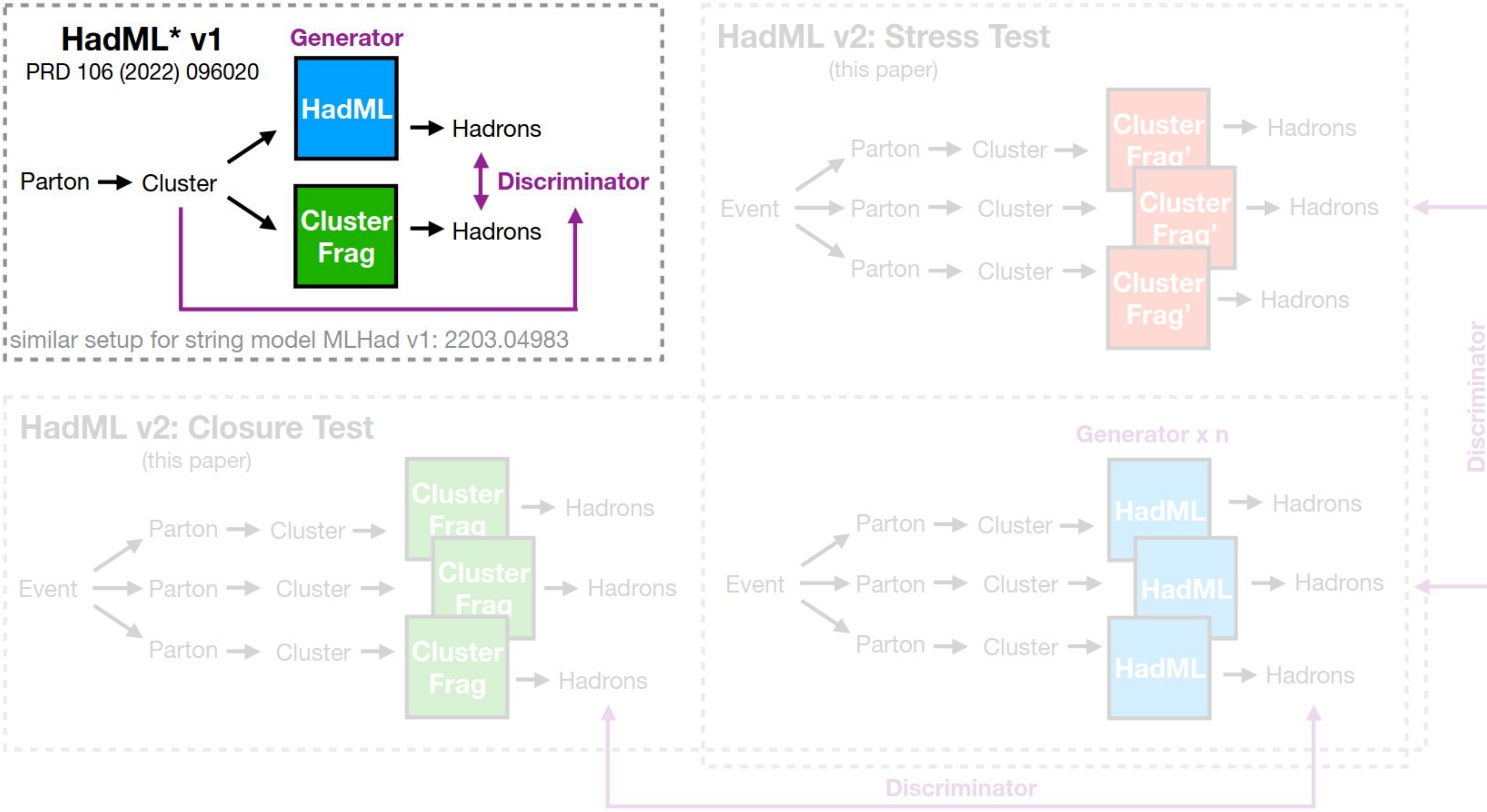

Cluster hadronization model

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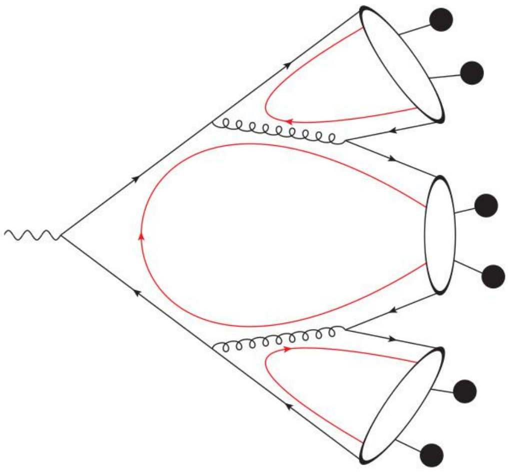

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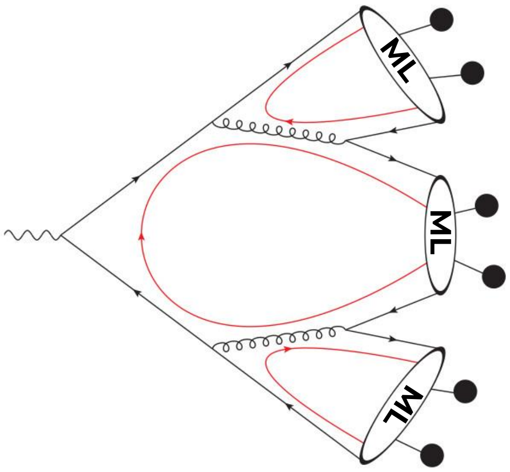

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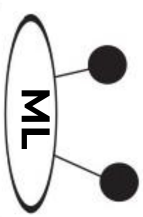
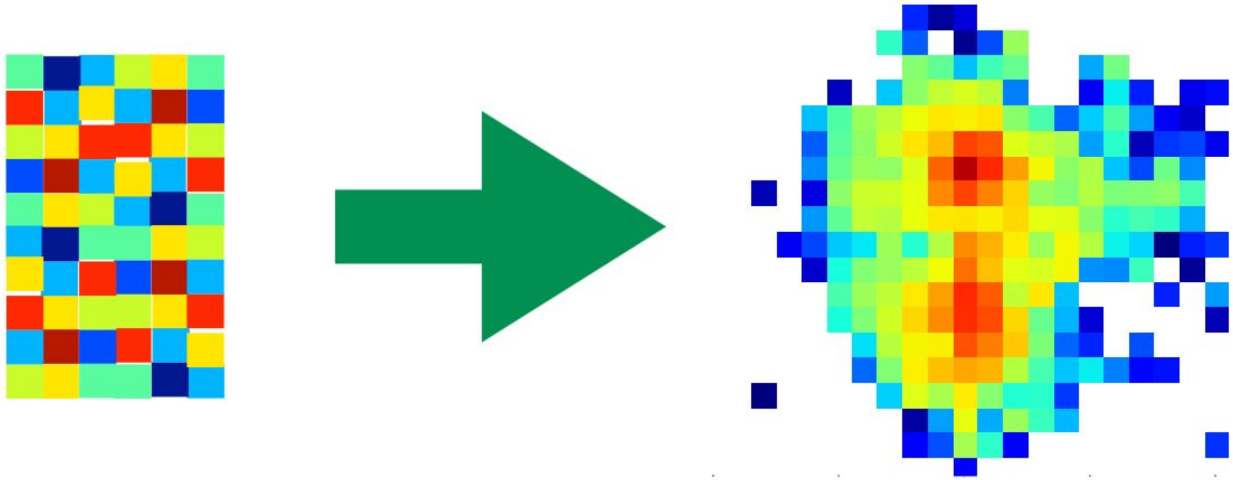
- **ML hadronization**
  1st step: generate kinematics of a cluster decay:



- **How?**
  Use Generative Adversarial Networks (**GAN**)

What is a deep generative model?

A **generator** is nothing other than a function that maps random numbers to structure.

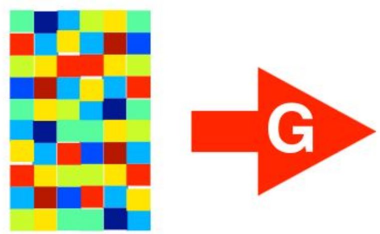


Deep generative models: the map is a deep neural network.

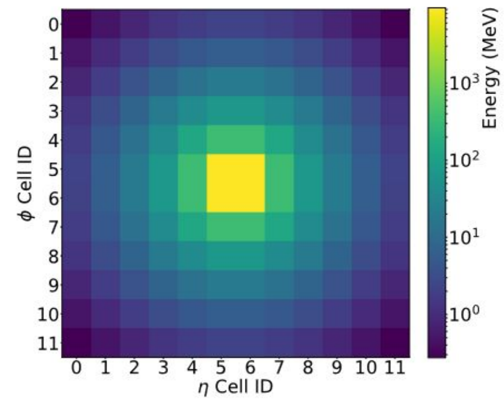
Our tool of choice: GANs

[Goodfellow et al. "Generative adversarial nets". arxiv:1406.2661]

Generative Adversarial Networks (GANs):
A two-network game where one ***maps noise to structure*** *and one* ***classifies images as fake or real****.*



noise

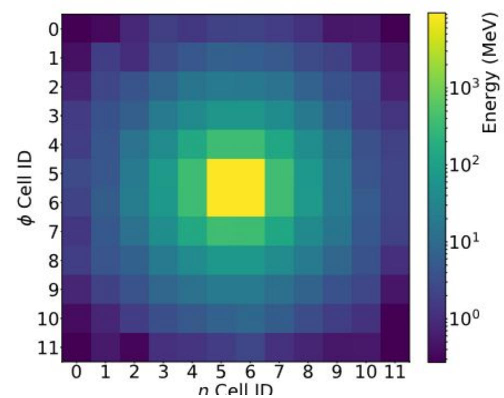


D

{real,fake}

D

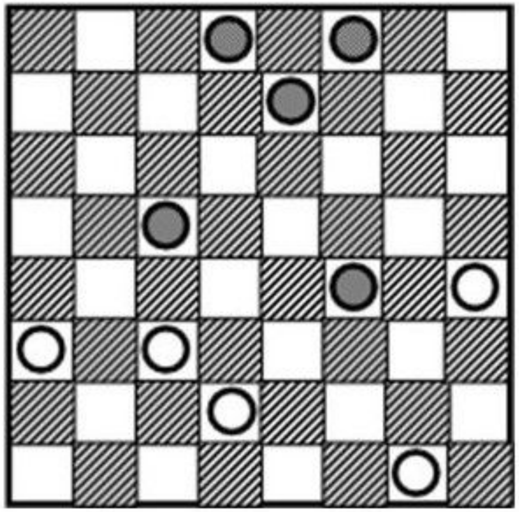
When **D** is maximally confused, **G** will be a good generator



Physics-based simulator or data

Adversarial Networks

Arthur Lee Samuel (1959) wrote a program that learnt to play checkers well enough to beat him.



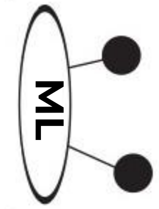
- He popularized the term **"machine learning"** in 1959.
- The program chose its move based on a **minimax** strategy, meaning it made the move assuming that the opponent was trying to optimize the value of the same function from its point of view.
- He also had it play thousands of **games against itself** as another way of learning.

Adversarial Networks

By playing **games against itself**, AlphaGo Zero surpassed the strength of <u>AlphaGo Lee</u> in three days by winning 100 games to 0.

ML hadronization

1st step: generate kinematics of a cluster decay to 2 hadrons



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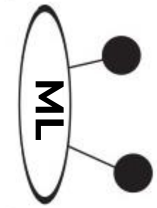
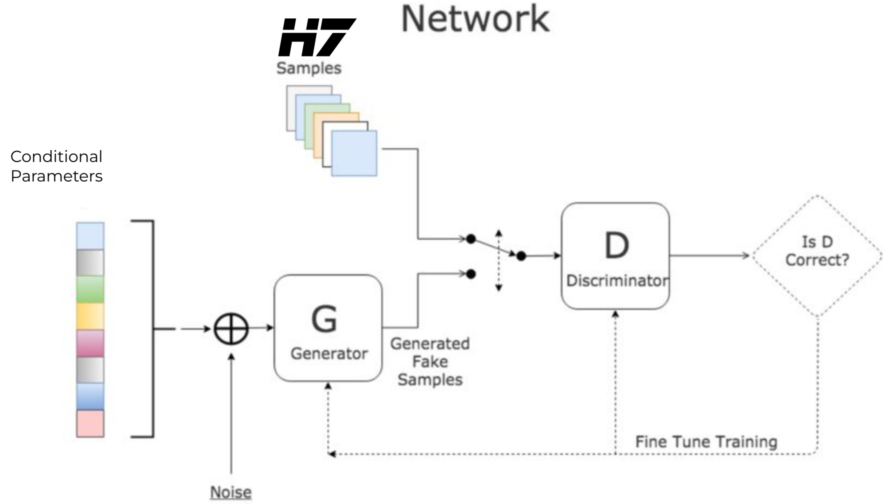


How?

We have a conditional GAN, with cluster 4-vector input and two hadron 4-vector outputs.

Generative Adversarial Network



Towards a Deep Learning Model for Hadronization

ML hadronization

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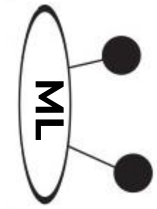

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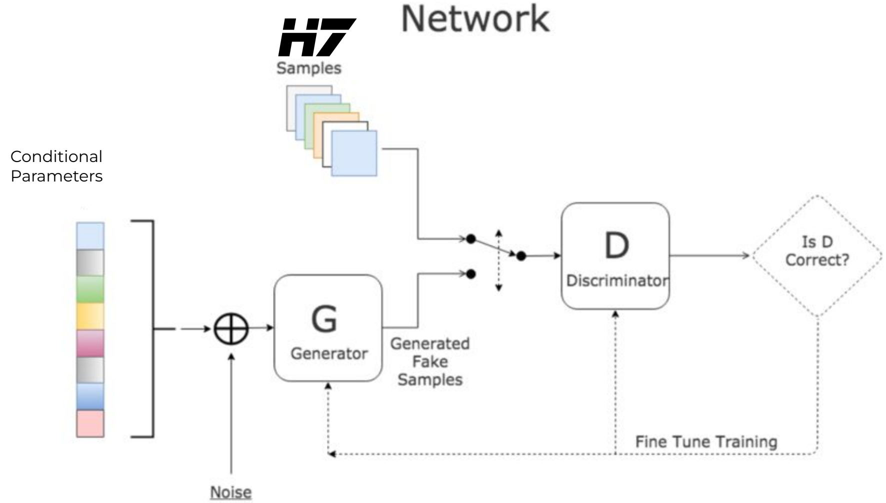
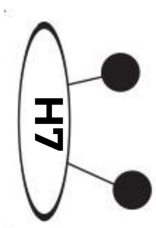


Training data:

e^+e^- collisions at $\sqrt{s} = 91.2$ GeV

Cluster $(E,\ p_x,\ p_y,\ p_z)$



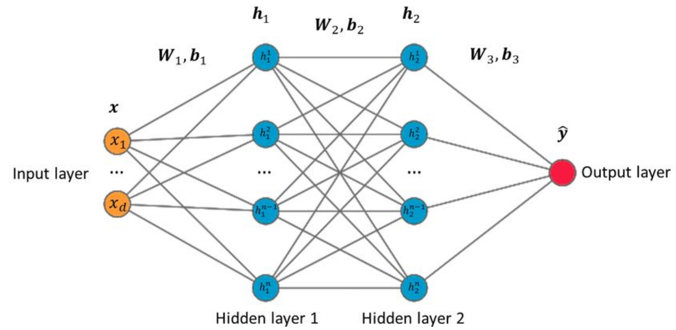
$\pi^0(E,\ p_x,\ p_y,\ p_z)$

$\pi^0(E,\ p_x,\ p_y,\ p_z)$

Simplification: considering only pions and generating two angles in the cluster rest frame.

Architecture: conditional GAN

Generator and the Discriminator are composed of two-layer perceptron
(each a fully connected, hidden size 256, a batch normalization layer, LeakyReLU activation function)



Generator

Input

Cluster $(E,\ p_x,\ p_y,\ p_z)$ and 10 noise features sampled from a Gaussian distribution

Output (in the cluster frame)

ϕ - polar angle
θ - azimuthal angle

we reconstruct the four vectors of the two outgoing hadrons

Discriminator

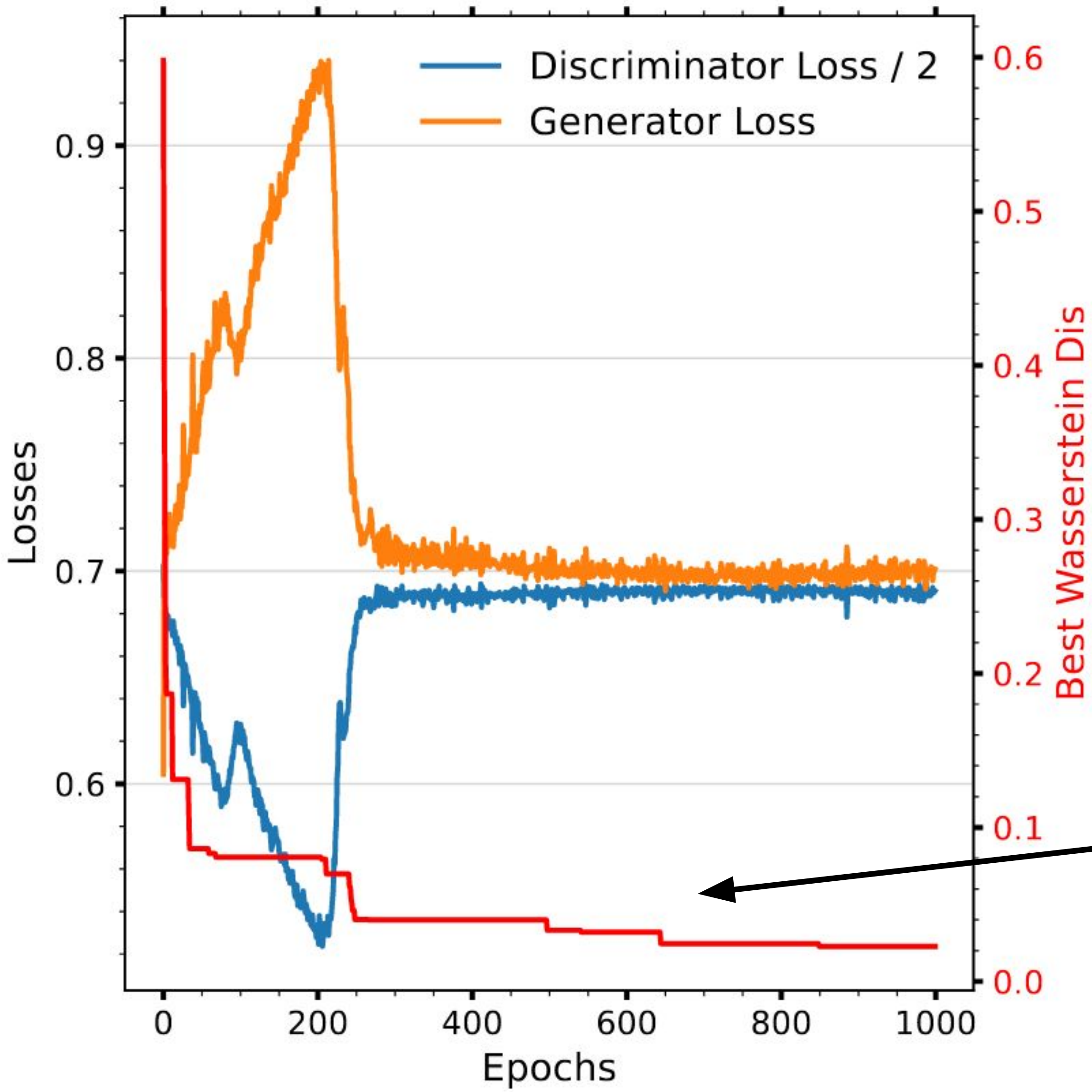
Input

ϕ and θ labeled as signal (generated by Herwig) or background (generated by Generator)

Output

Score that is higher for events from Herwig and lower for events from the Generator

Training HADML v1

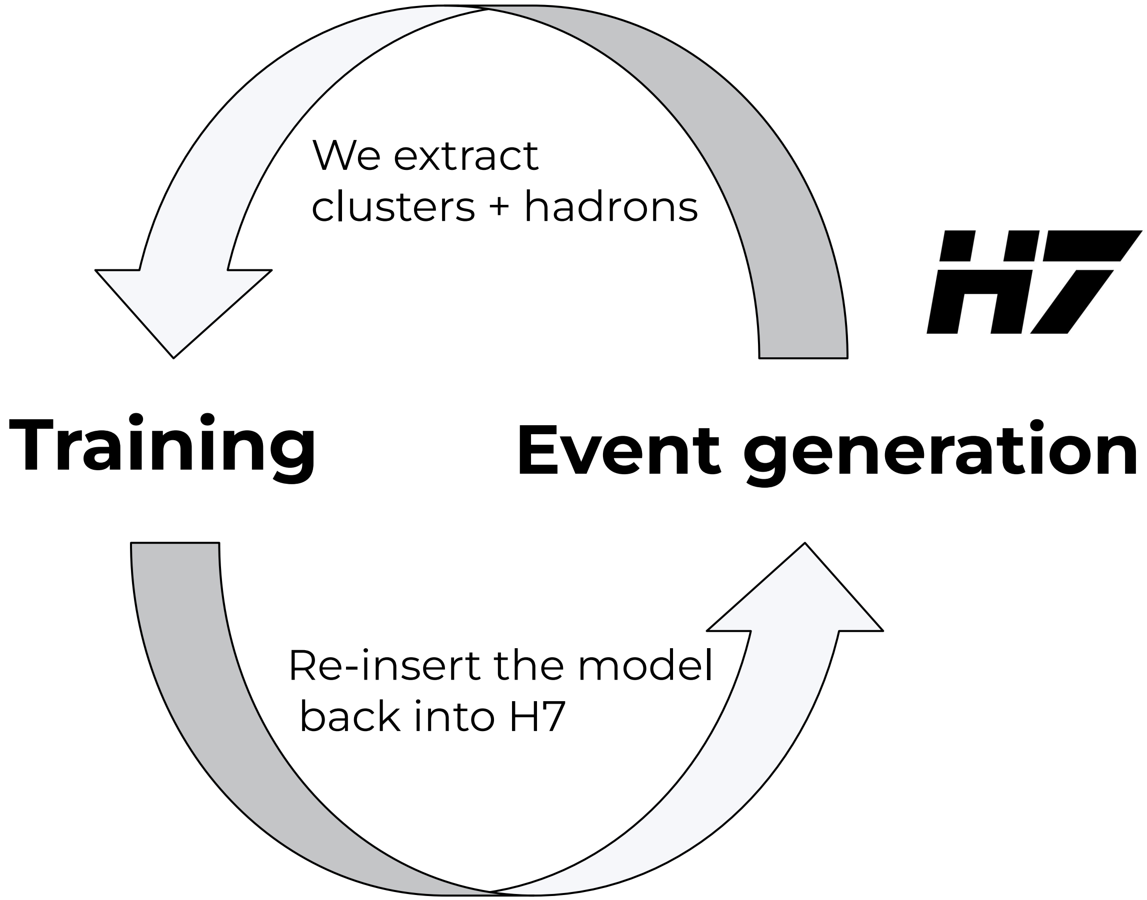


We have a conditional GAN, with cluster 4-vector input and two hadron 4-vector outputs.

<u>Simplification:</u> considering only pions and generating two angles in the cluster rest frame.

This is a typical learning curve for GAN training

Integration into Herwig

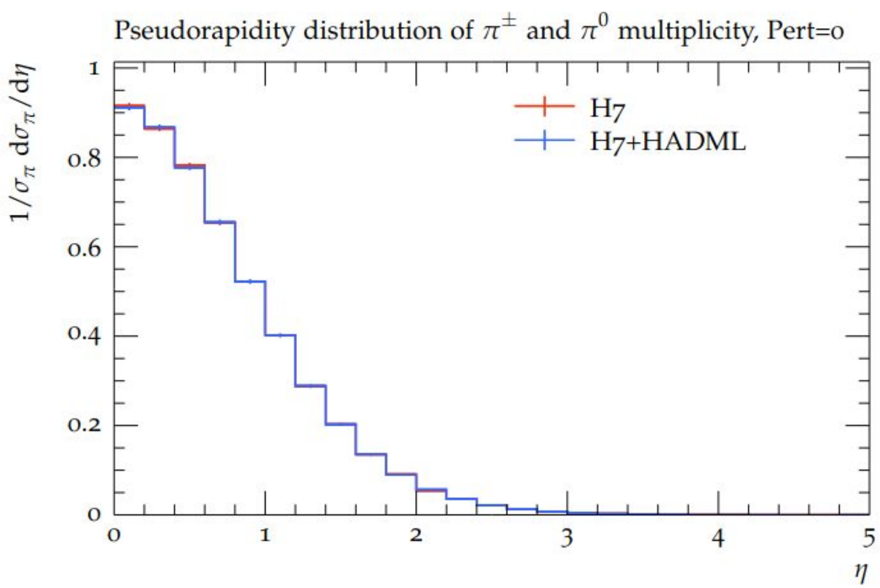


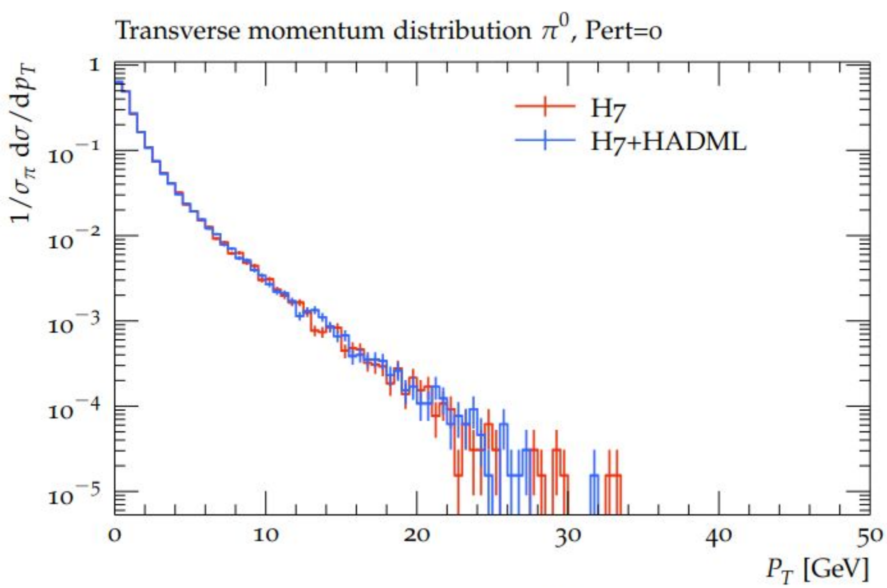
This then allows us to run a full event generator and produce plots

Low-level Validation
(similar to training data)

e^+e^- collisions at
$\sqrt{s} = 91.2$ GeV

π^0 kinematic variables

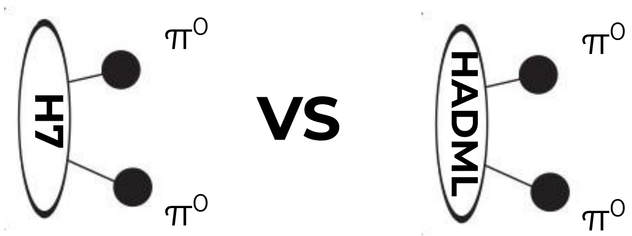




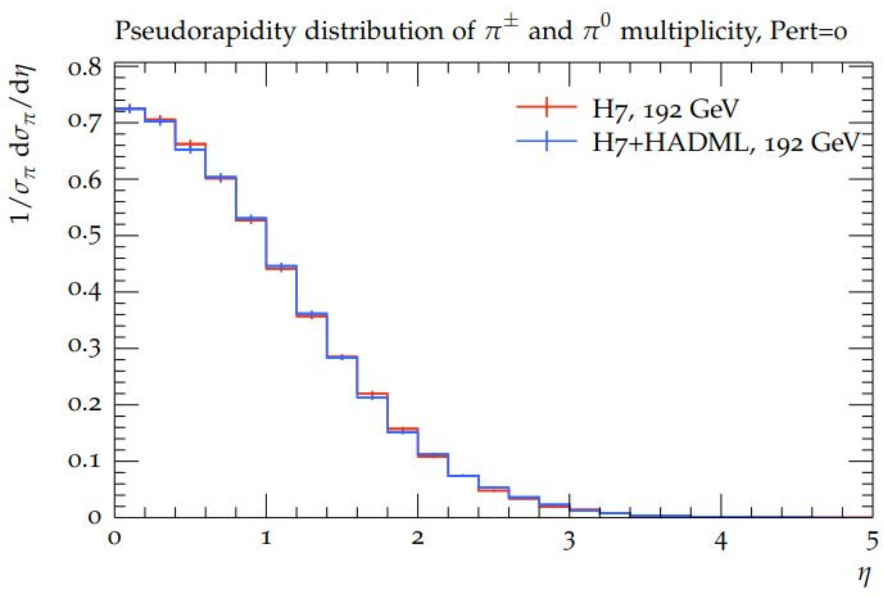
Performance: Energy of the collisions

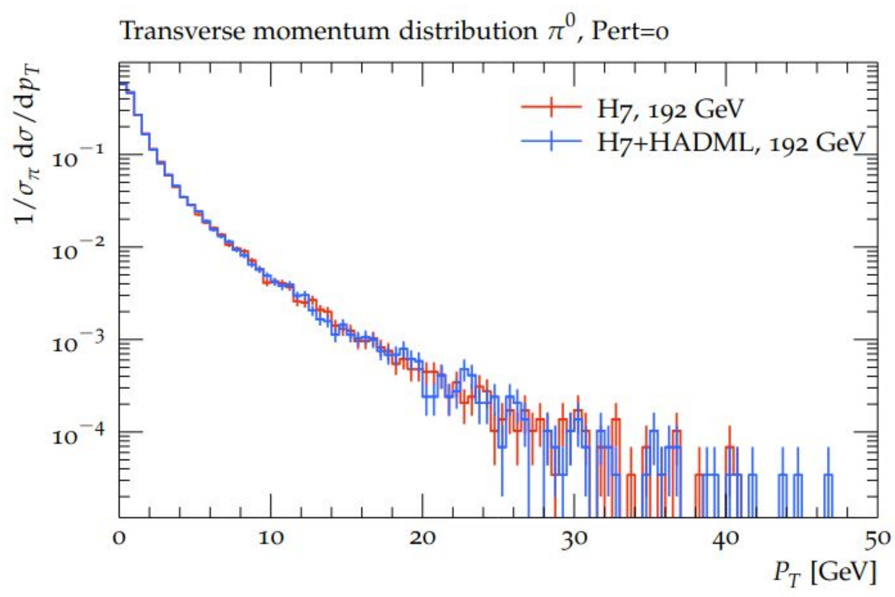
Low-level Validation
(**beyond** training data **different energy**)

e^+e^- collisions at
$\boxed{\sqrt{s} = 192\ \mathrm{GeV}}$



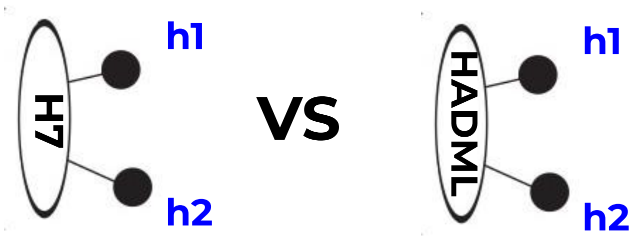
π^0 kinematic variables





Low-level Validation
(**beyond** training data **different hadrons**)

e^+e^- collisions at $\sqrt{s} = 91.2$ GeV

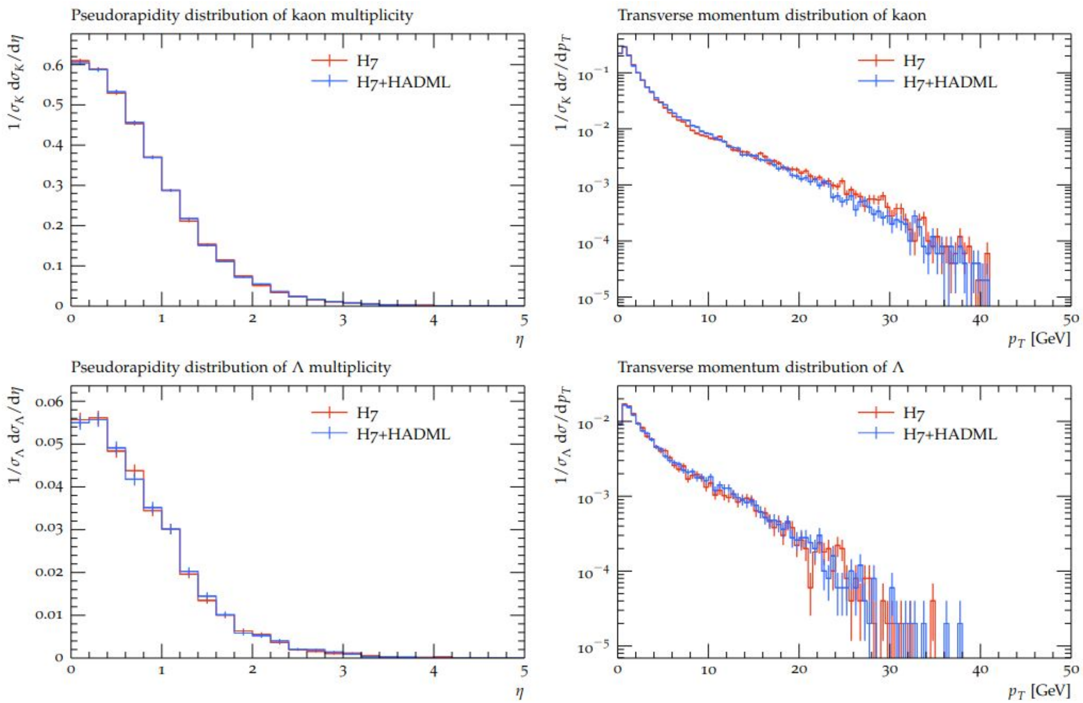


h kinematic variables

As a crude “full” model, we simply take the PIDs from Herwig and the kinematics from the GAN.

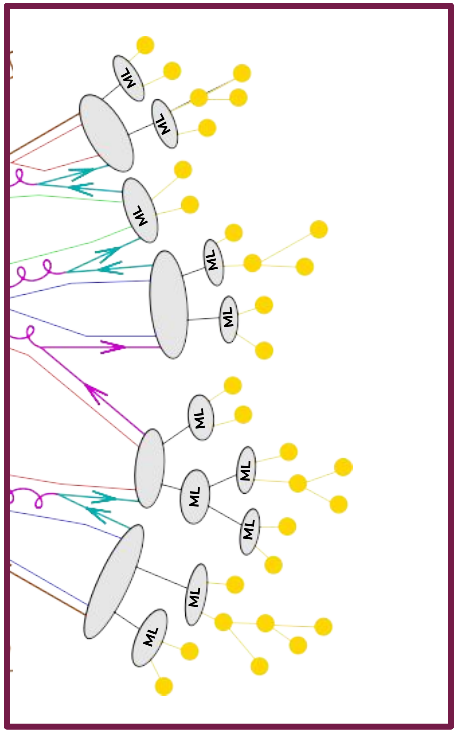
Kaons

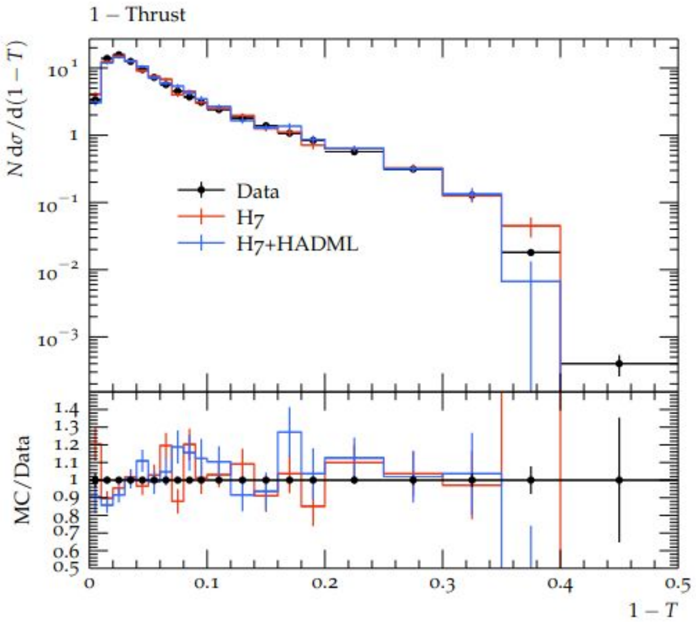
Lambda

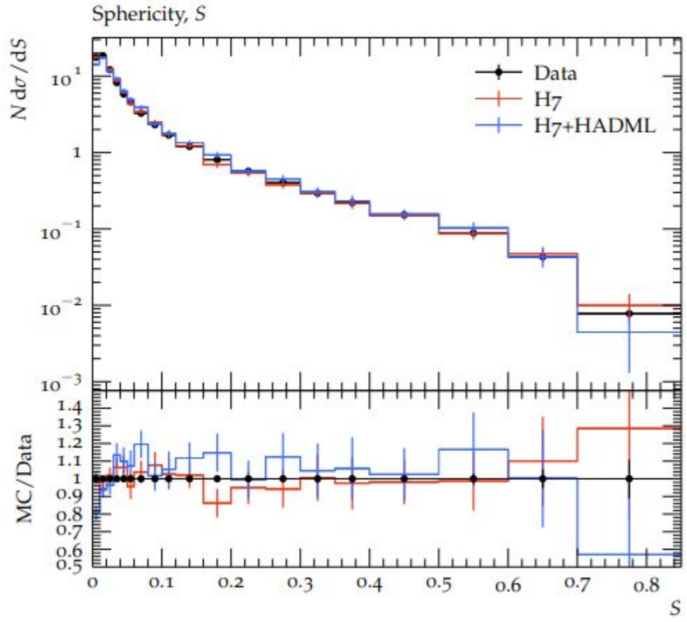


With a "full" model, we can compare directly to data!

LEP DELPHI **Data**

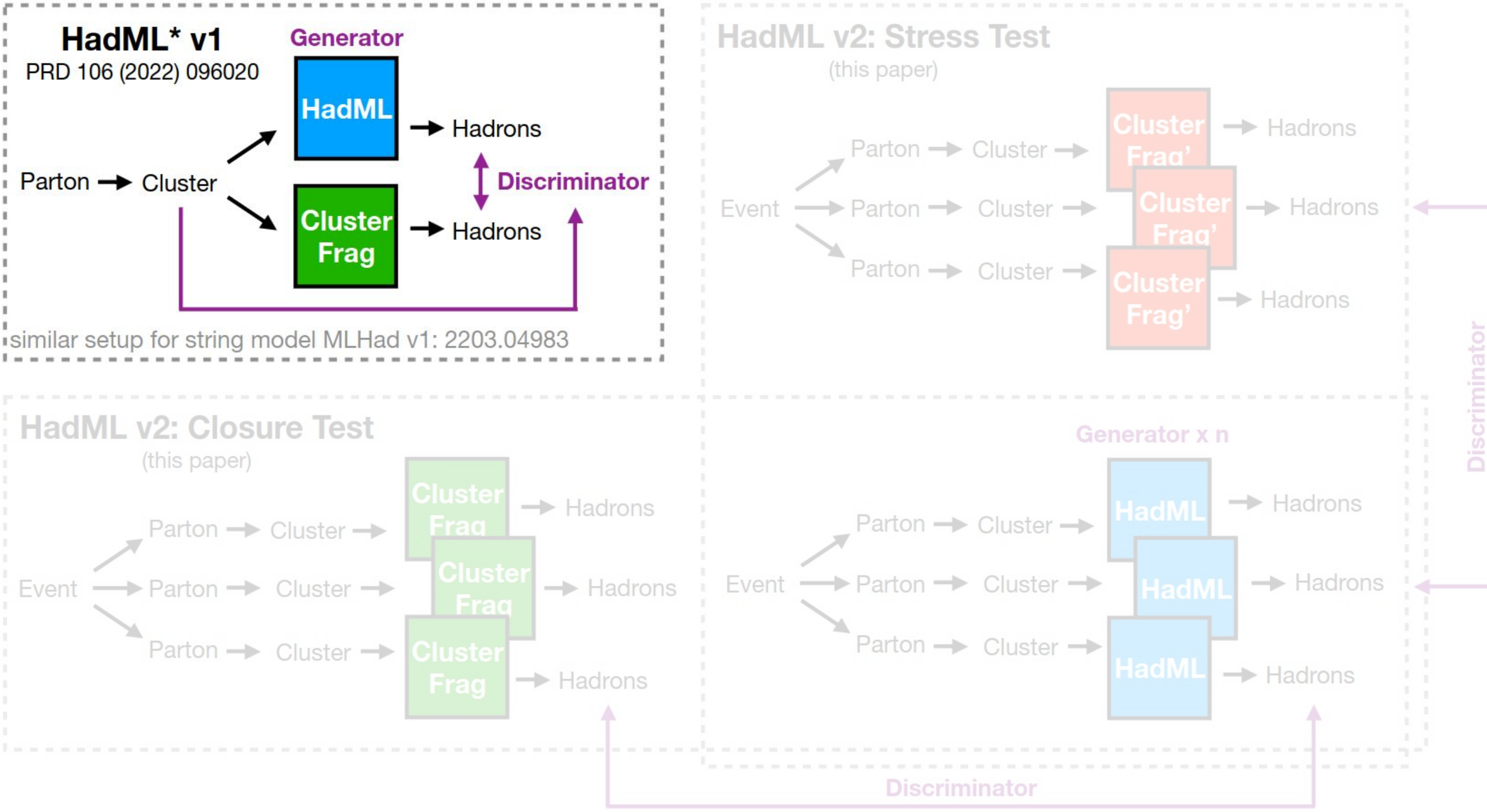




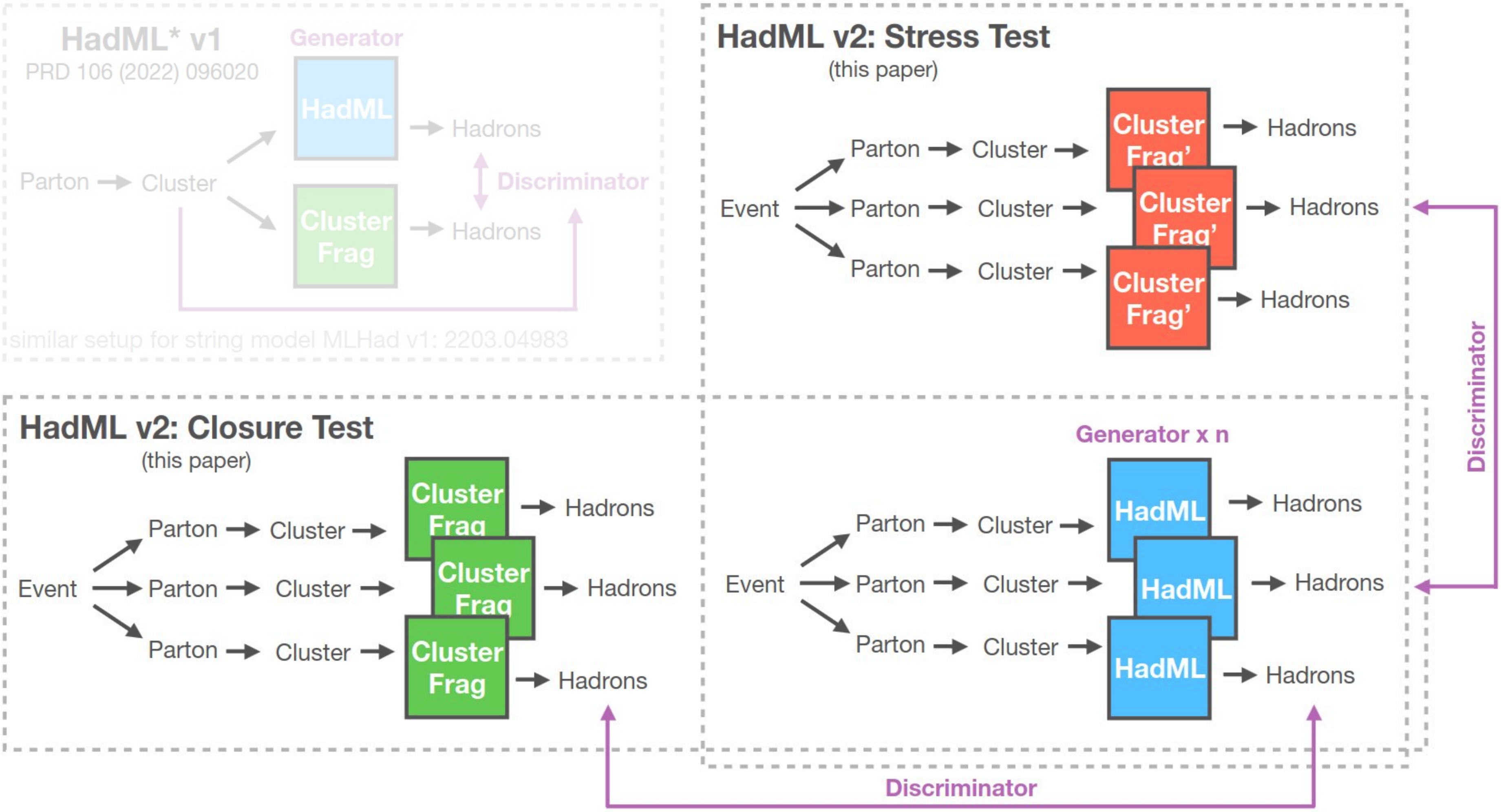


N.B. we have trained on H7, so we don't expect to be any better than it at modeling the data.

Road map for today

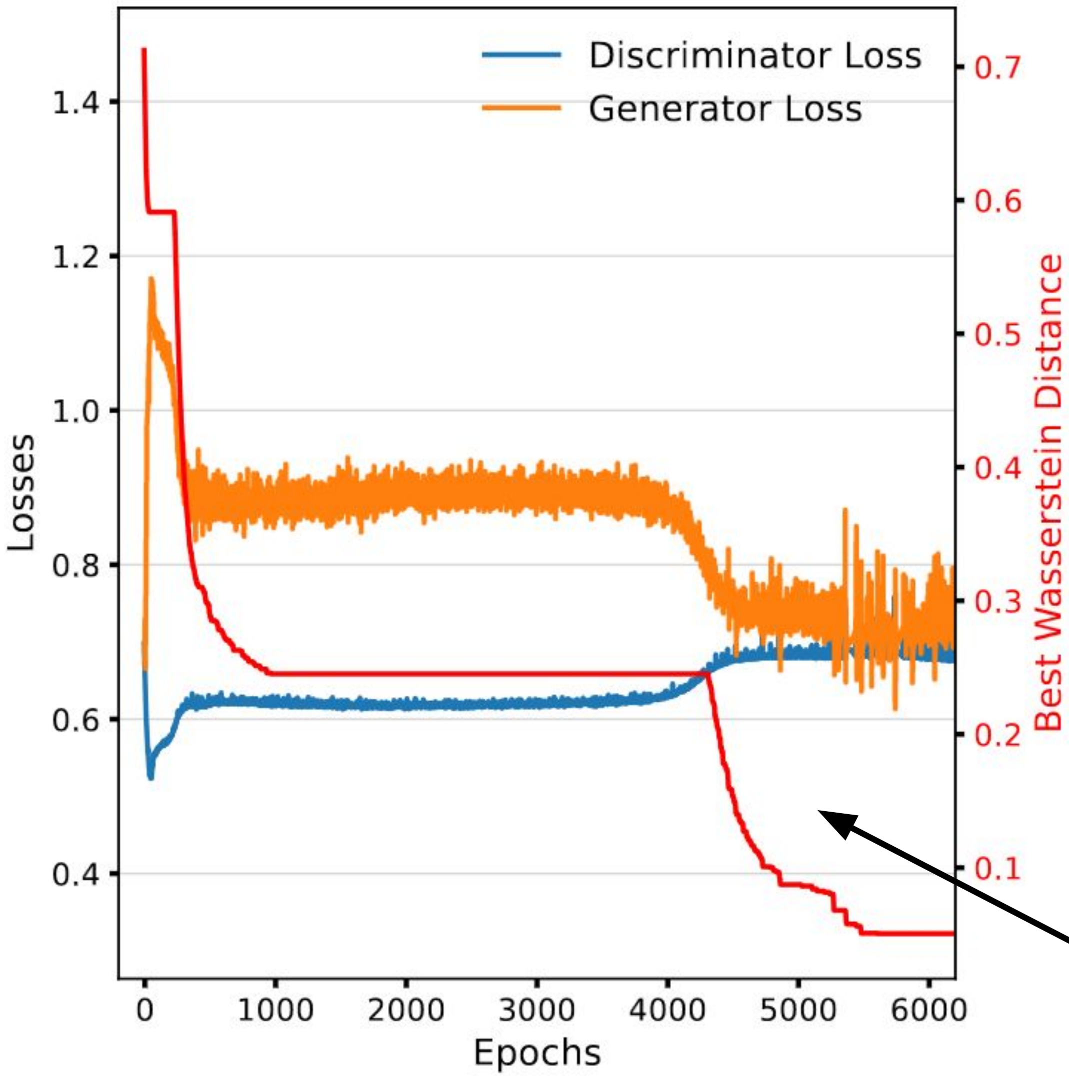


Road map for today



Protocol for fitting a deep generative hadronization model in a realistic data setting, where we only have access to a set of hadrons in data.

Training HADML v2



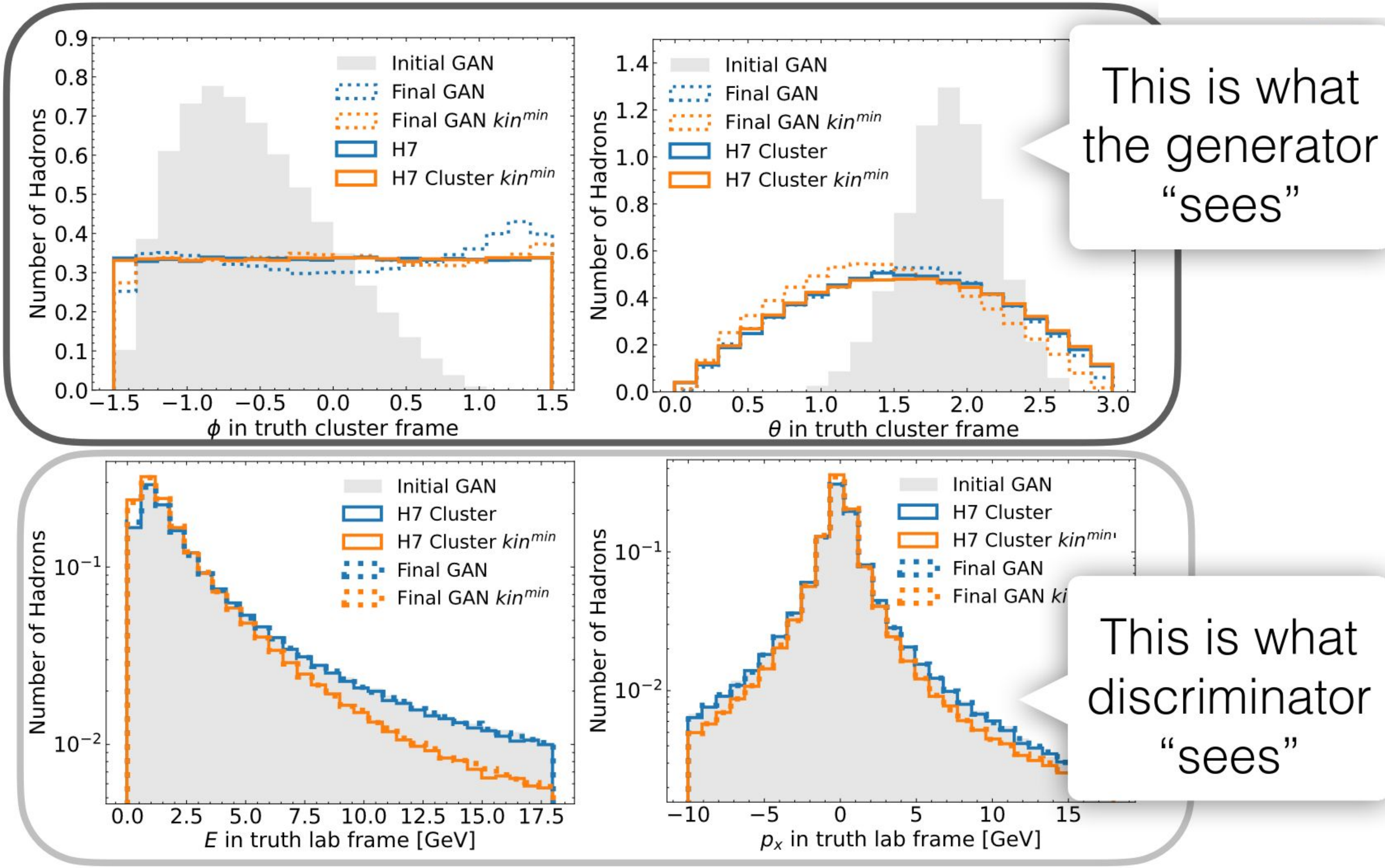
Now, the generator is local (per cluster), but the discriminator is global (whole event).

Discriminator is a permutation-invariant architecture called Deep Sets.

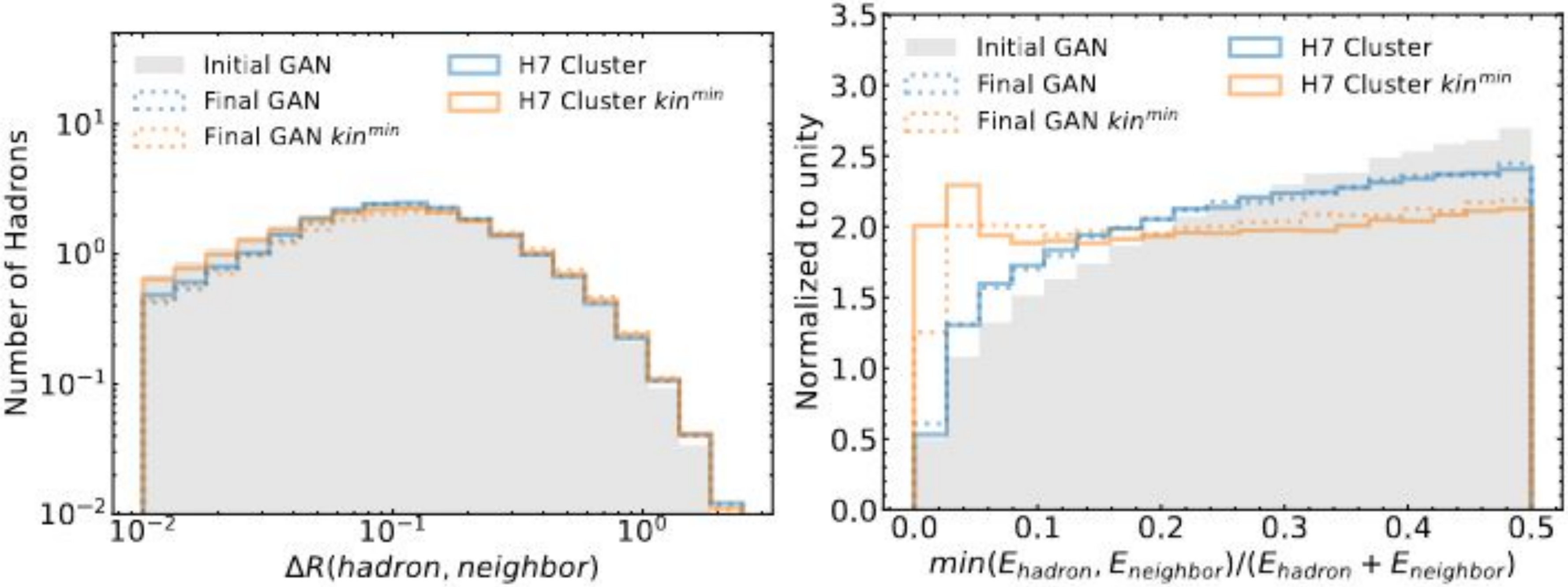
Simplification only Pions

Still works !

Performance



Performance: going beyond inputs and outputs

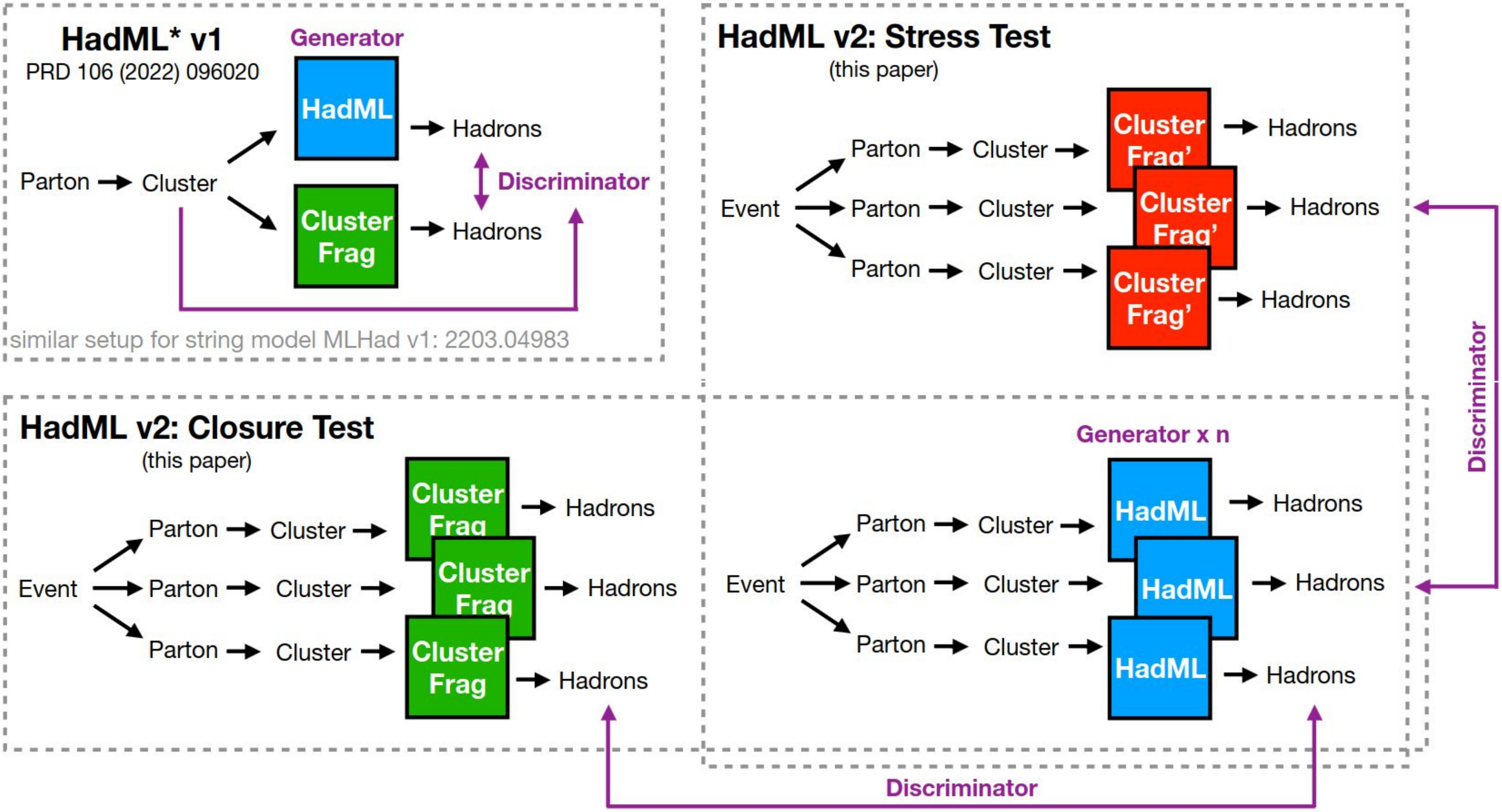


MINIMAL $\Delta R^2 = \Delta\phi^2 + \Delta\eta^2$

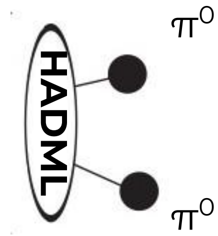
A key advantage of this fitting protocol over other methods is that it can accommodate unbinned and high-dimensional inputs.

The approach could also be used to fit (without binning) data to a parametric physics model (for example cluster) as well.
However, this would require making the cluster model differentiable.

Summary


HadML* v1
PRD 106 (2022) 096020
Generator
HadML
Hadrons
Parton
Cluster
Discriminator
Cluster Frag
Hadrons
similar setup for string model MLHad v1: 2203.04983
HadML v2: Stress Test
(this paper)
Event
Parton
Cluster
Cluster Frag'
Hadrons
HadML v2: Closure Test
(this paper)
Cluster Frag
Generator x n
HadML
Discriminator
Discriminator

- First ML hadronization models: HADML and MLHAD
- Recent progress:
  -HADML: “Data fitting protocol”
  - MLHAD: “Reweighting Monte Carlo Predictions and Automated Fragmentation Variations”

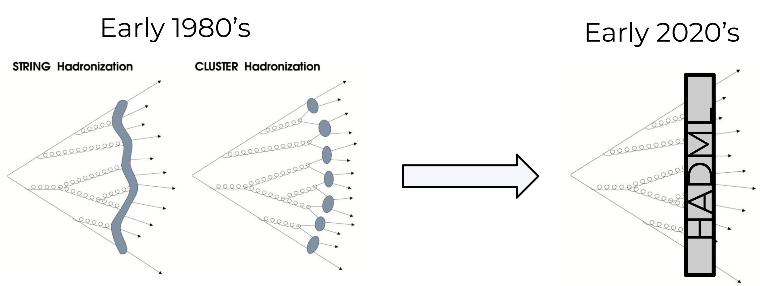


We have made significant progress, but there are still multiple steps to build and tune a full-fledged hadronization model.

What is next for HADML?

- Number of technical and methodological step needed:
  - ➔ Directly accommodate multiple hadron species with their relative probabilities
  - ➔ Hyperparameter optimization, including the investigation of alternative generative models
  - ➔ More flexible model with a capacity to mimic the cluster or string models as well as go beyond either model.

There is still a multi-year program ahead of us, but it will be worth it!



So Stay tuned!

A postdoc in ML/HEP position

JAGIELLONIAN UNIVERSITY
IN KRAKÓW

If you are interested please contact me:
andrzej.siodmok@cern.ch

Discriminator HadML v1 vs v2

HadML v1

The loss function:

$$L = -\sum_{\lambda \sim \textsc{Herwig},\, z \sim p(z)} \left(\log\left(D\left(\tau\left(\lambda\right)\right)\right) + \log\left(1 - D\left(G\left(z, \lambda\right)\right)\right)\right)$$

HadML v2

The discriminator function is modified, we parameterize is as a Deep Sets model

$$D_E\left(x\right) = F\left(\frac{1}{n}\sum_{i=1}^{n} \Phi\left(h_i, \omega_{D_\Phi}\right), \omega_F\right)$$

invariant under permutations of hadrons

Φ embeds a set of hadrons into a fixed-length latent space and F acts on the average

$$L = -\sum_{x \sim \text{data}} \log\left(D_E\left(x\right)\right) - \sum_{\{G\} \sim \textsc{Herwig},\, z \sim p(z)} \log\left(1 - D_E\left(\{G\left(z, \lambda\right)\}\right)\right)$$

The approach could also be used to fit (without binning) data to a parametric physics model (for example cluster) as well. However, this would require making the cluster model differentiable.

Wasserstein distance

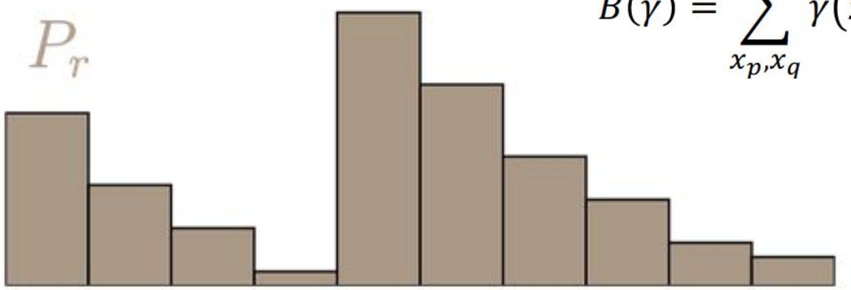
The Wasserstein distance

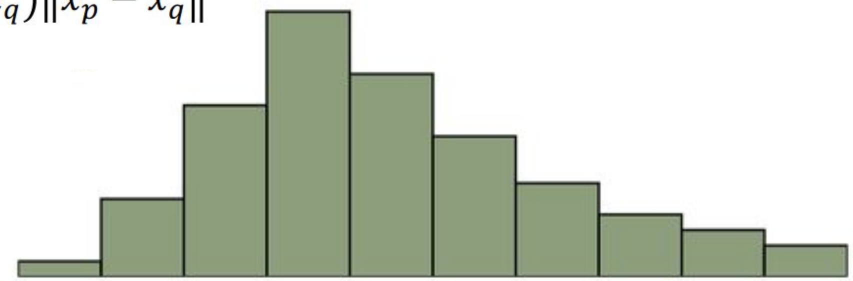
- For discrete probability distributions, the Wasserstein distance is called the earth mover's distance (EMD):
- EMD is the minimal total amount of work it takes to transform one heap into the other.

$$W(P,Q) = \min_{\gamma \in \Pi} B(\gamma)$$

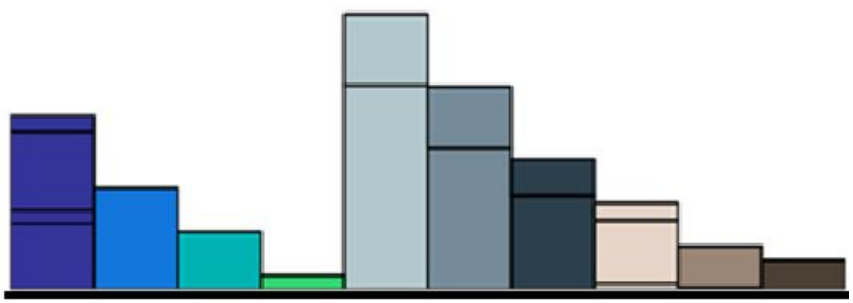
- Work is defined as the amount of earth in a chunk times the distance it was moved.

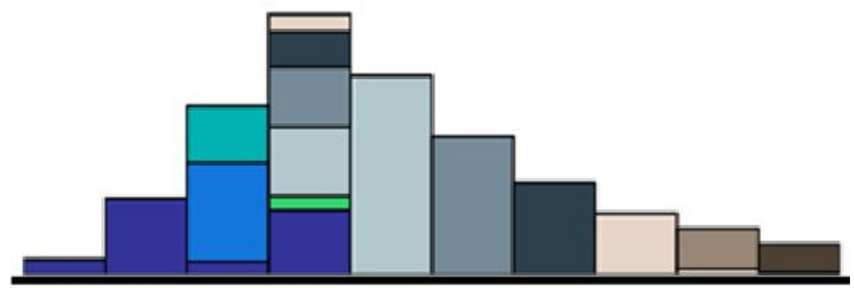
$$B(\gamma) = \sum_{x_p, x_q} \gamma(x_p, x_q) \|x_p - x_q\|$$





Best "moving plans" of this example





Minimax Loss

In the paper that introduced GANs, the generator tries to minimize the following function while the discriminator tries to maximize it:

$$E_x[log(D(x))] + E_z[log(1 - D(G(z)))]$$

In this function:

- `D(x)` is the discriminator's estimate of the probability that real data instance x is real.
- E_x is the expected value over all real data instances.
- `G(z)` is the generator's output when given noise z.
- `D(G(z))` is the discriminator's estimate of the probability that a fake instance is real.
- E_z is the expected value over all random inputs to the generator (in effect, the expected value over all generated fake instances G(z)).
- The formula derives from the cross-entropy between the real and generated distributions.

The generator can't directly affect the `log(D(x))` term in the function, so, for the generator, minimizing the loss is equivalent to minimizing `log(1 - D(G(z)))`.

AlphaGo

- AlphaGo's victory against Lee Sedol was a major milestone in artificial intelligence research.
- Go had previously been regarded as a hard problem in machine learning that was expected to be out of reach for the technology of the time.
- Most experts thought a Go program as powerful as AlphaGo was at least five years away;some experts thought that it would take at least another decade before computers would beat Go champions. Most observers at the beginning of the 2016 matches expected Lee to beat AlphaGo.
- Netflix document