

# Leveraging Physics-informed GNN for enhanced Combinatorial Optimization

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loc. 17

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Ministero  
dell'Università  
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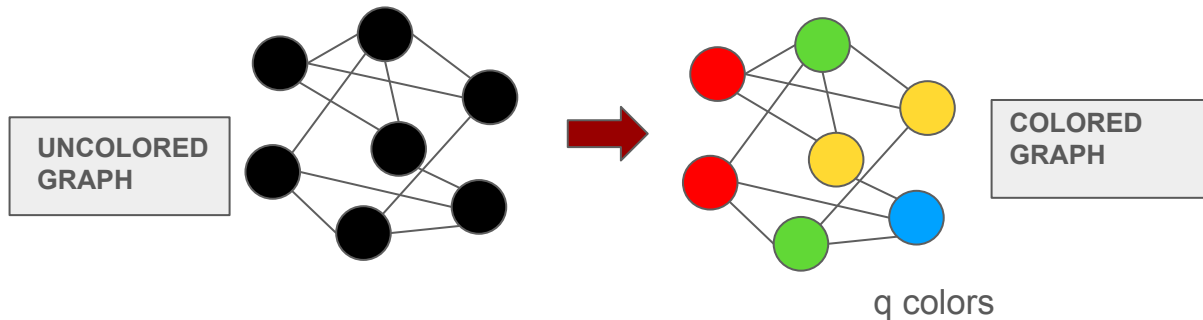
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Future  
Artificial  
Intelligence  
Research

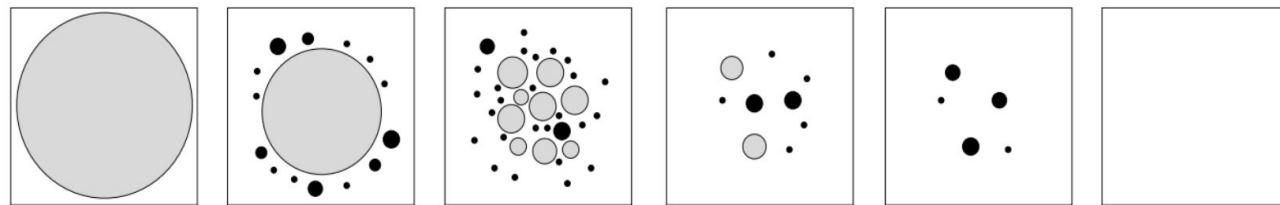


# GRAPH COLORING



- NP-Hard problem
- Numerous applications (eg. scheduling, register allocation)
- Can be studied using statistical mechanics.

$$\mathcal{H} = \sum_{(i,j) \in E} \delta_{\sigma_i \sigma_j}$$



Average connectivity

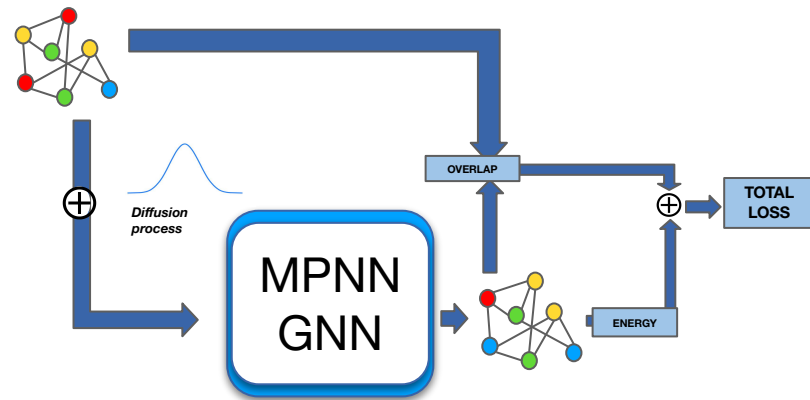
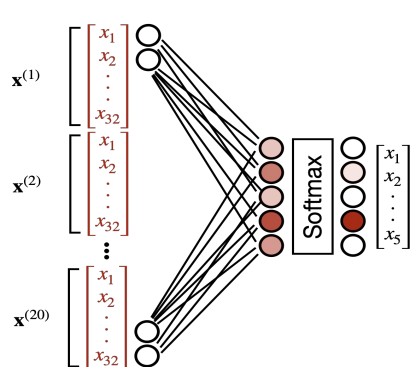
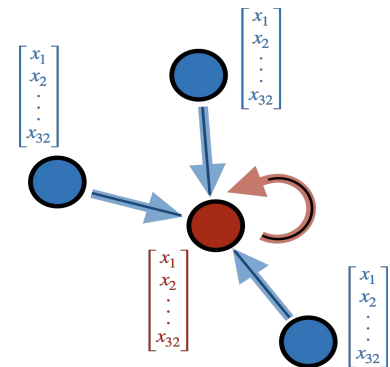
Clustering  
 $c_d$

Condensation  
 $c_c$

Rigidity  
 $c_r$

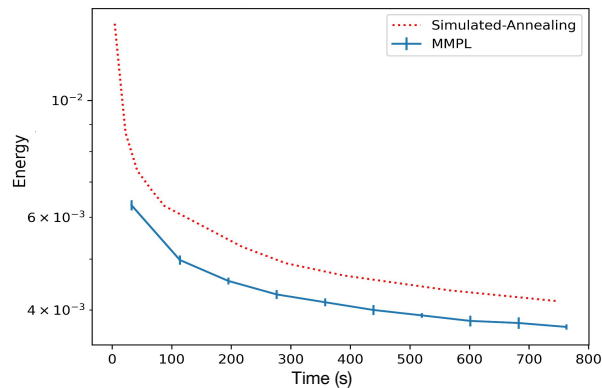
COL/UNCOL  
 $c_s$

# PI-GNN

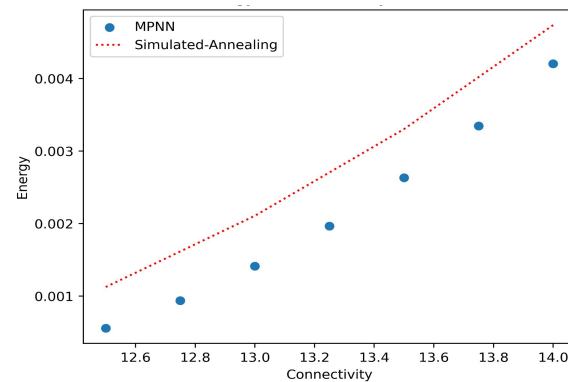


## Preliminary results

Energy vs time (N=10e5, c=14.0)

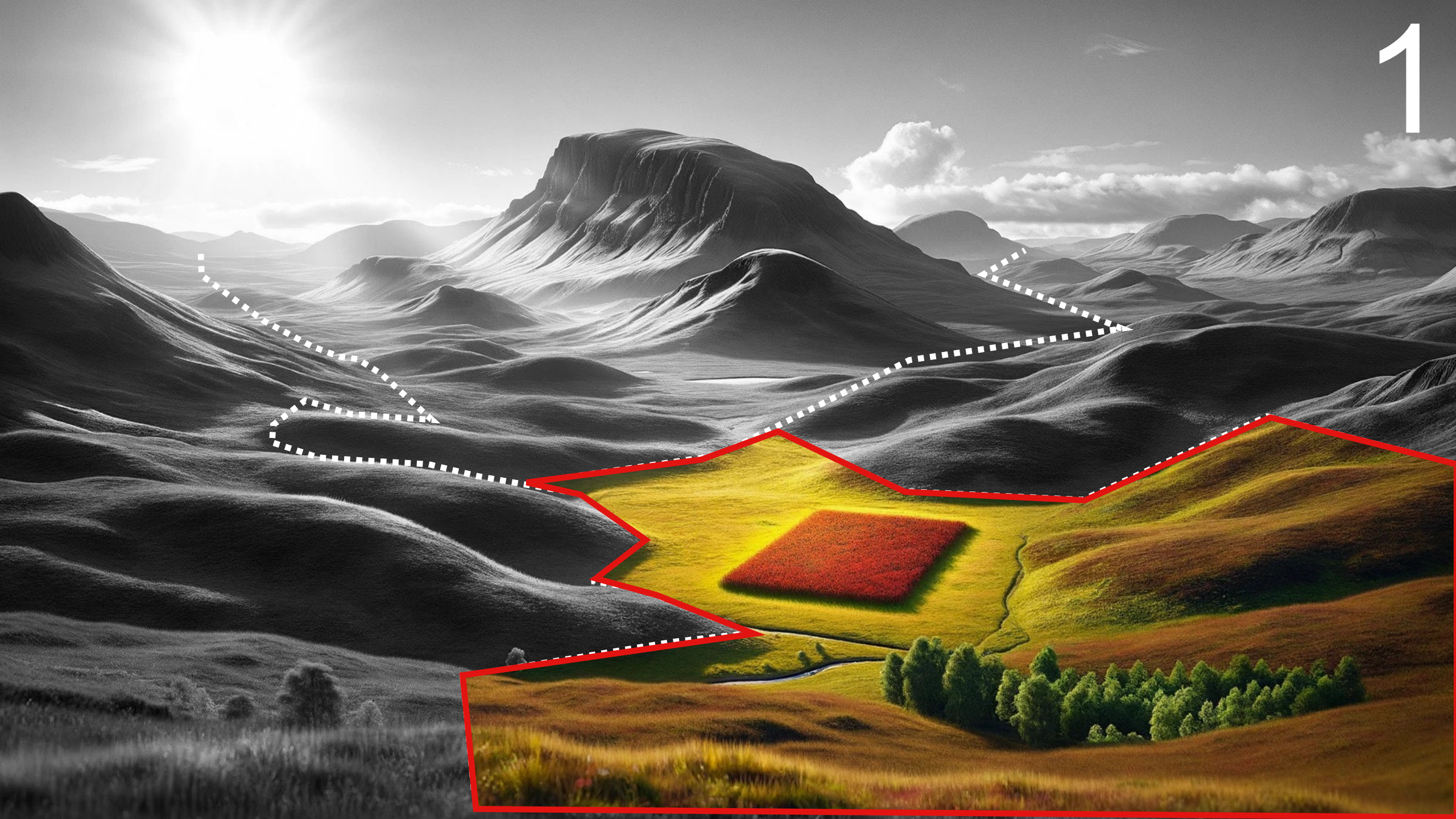


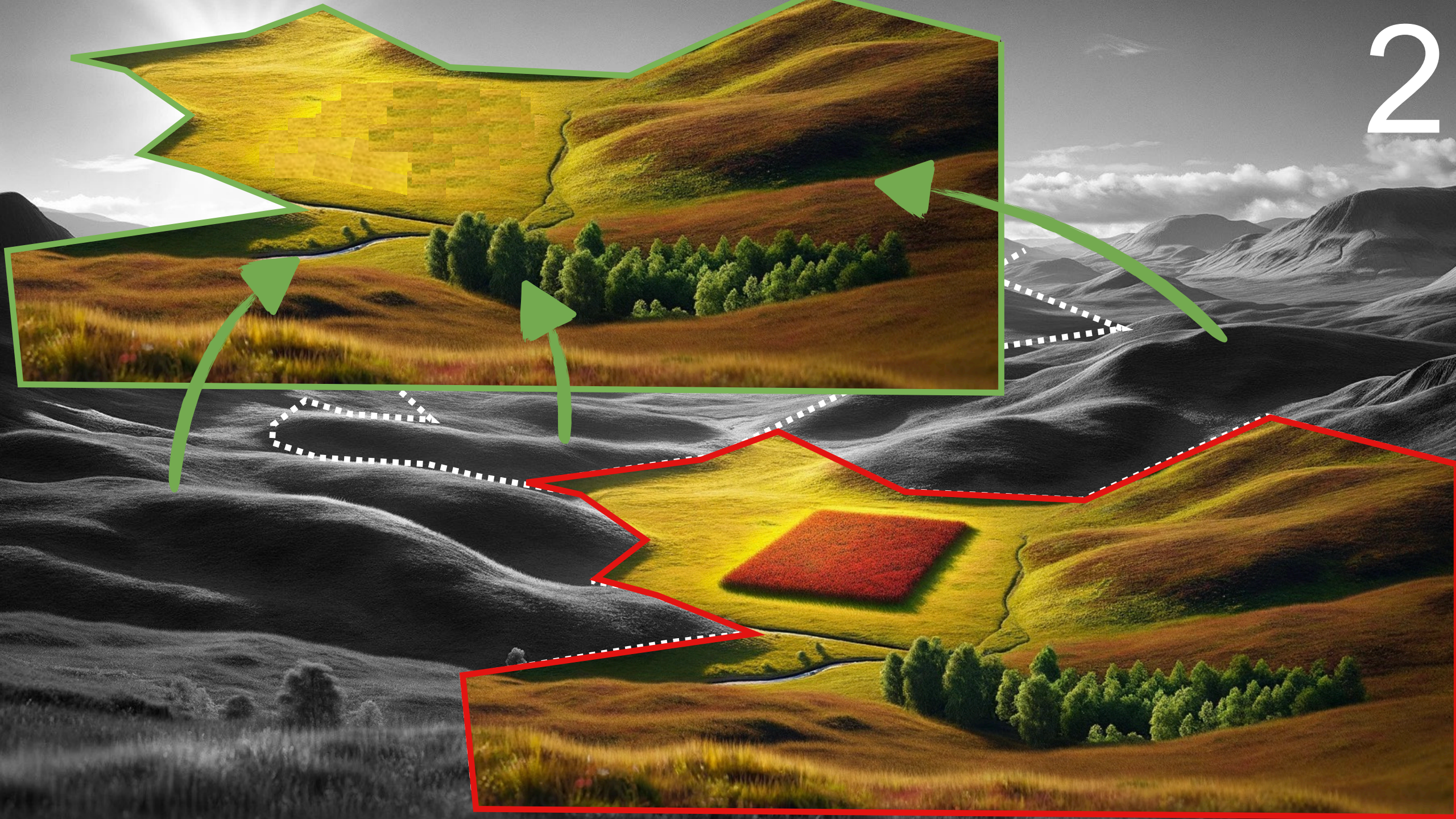
Energy vs Connectivity (N=2e5)

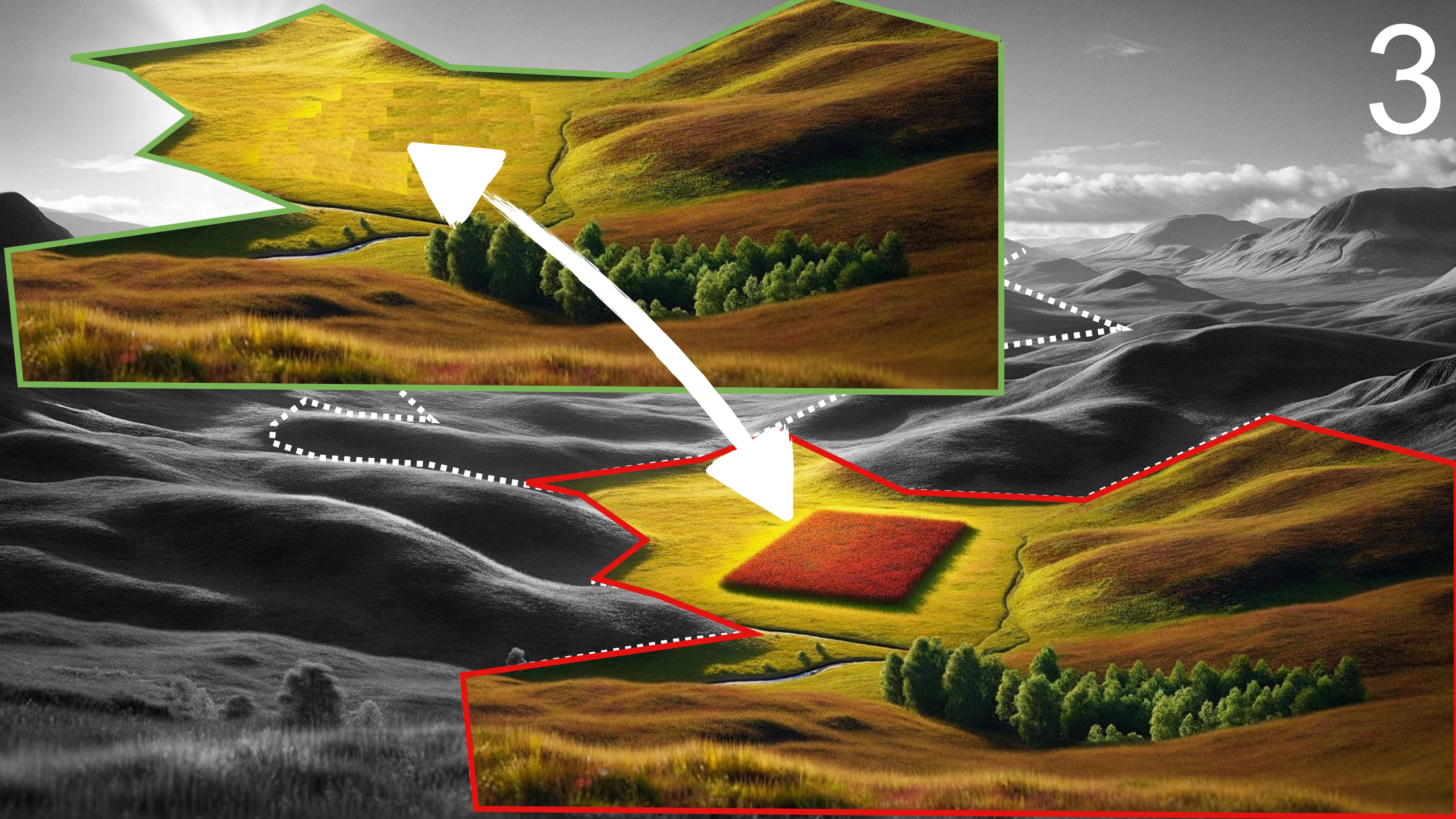
















# HyLAnD

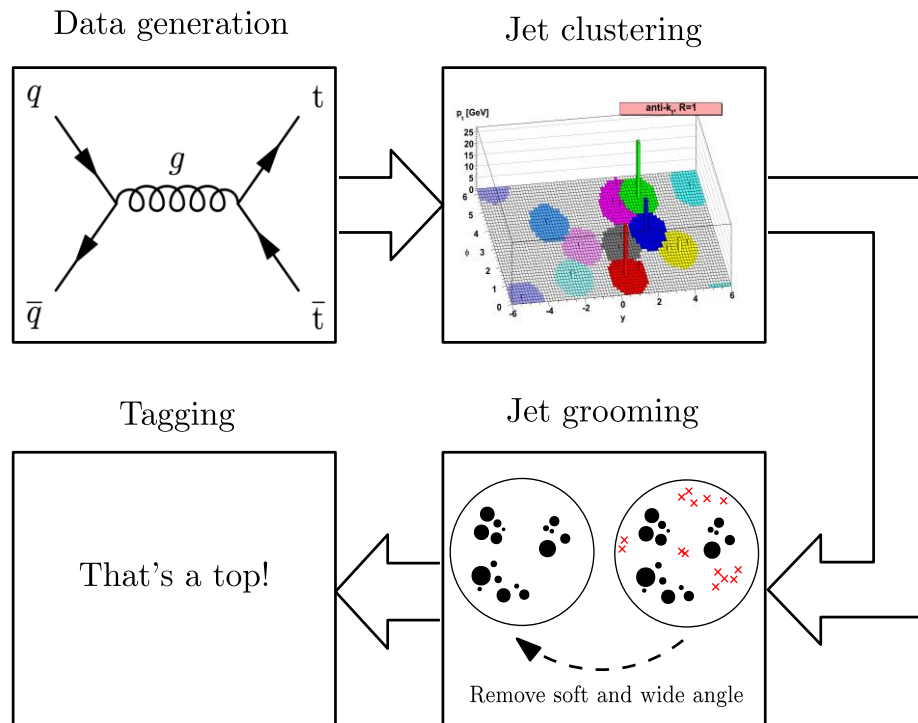
Hybrid Learning for Anomaly Detection

# BOOSTED PARTICLE RECONSTRUCTION WITH GRAPH NEURAL NETWORKS

Jacan Chaplais, Srinandan Dasmahapatra, Stefano Moretti



## TRADITIONAL RECONSTRUCTION PIPELINES

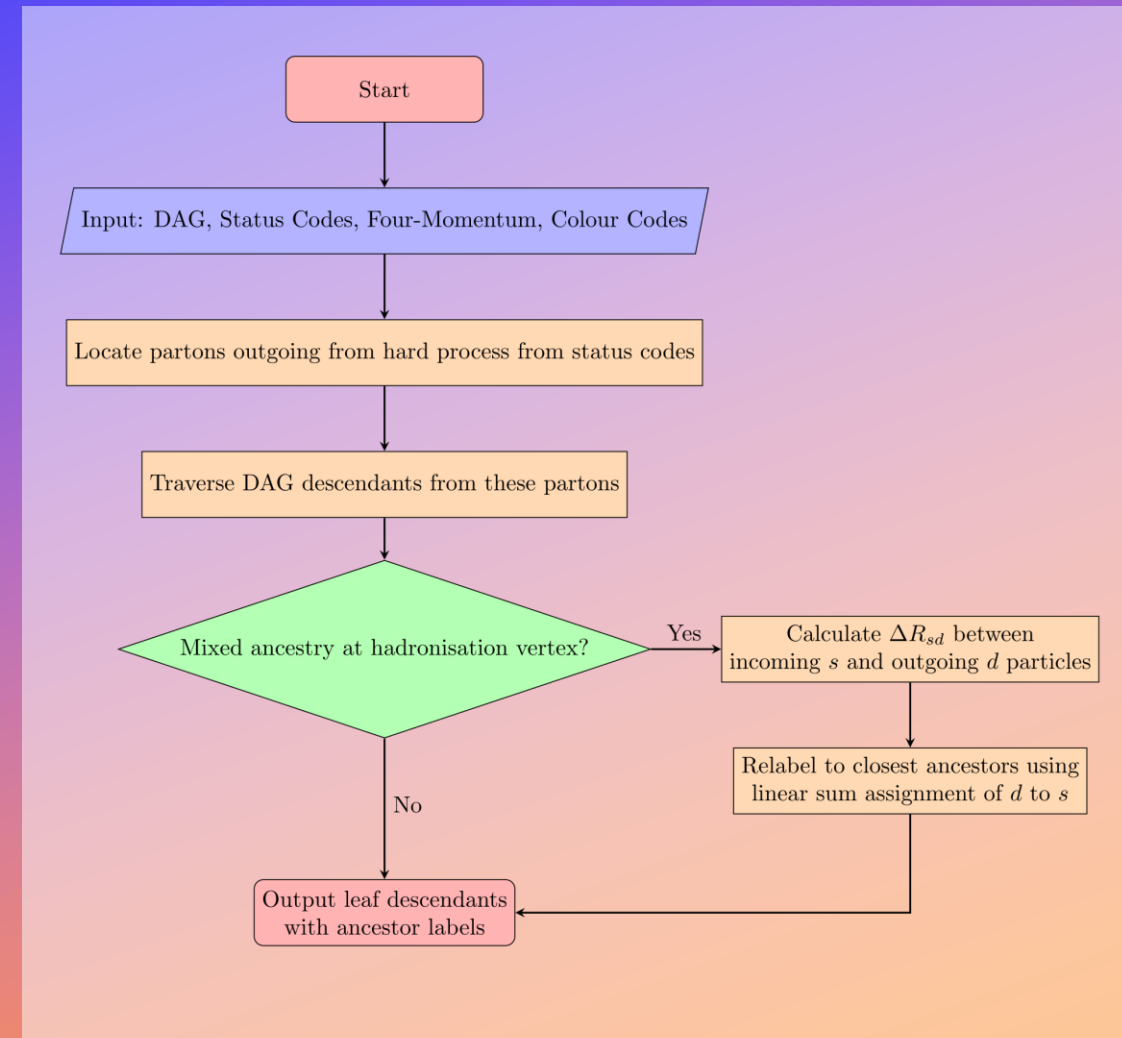
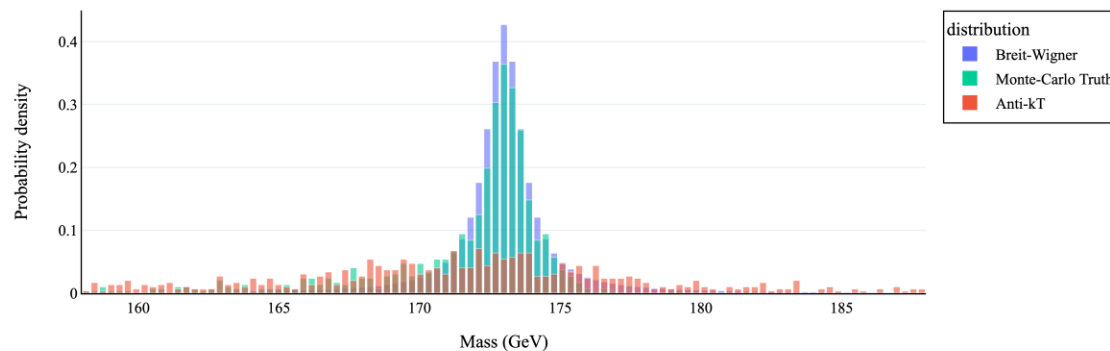


- Data is generated by simulation or experiment
- Tight, high momentum clusters (jets) of light particles form on detector walls
- Jets let us study particles which they decayed from
- Current methods based on physics theory, but only utilise momentum data

# LABELS FROM SIMULATIONS

- Simulation gives us full knowledge
- Possible to track back from detected particles to original
- Challenging when colours hadronise
  - Mixed ancestry
- Our novel method (right) combines more simulation data to fix this

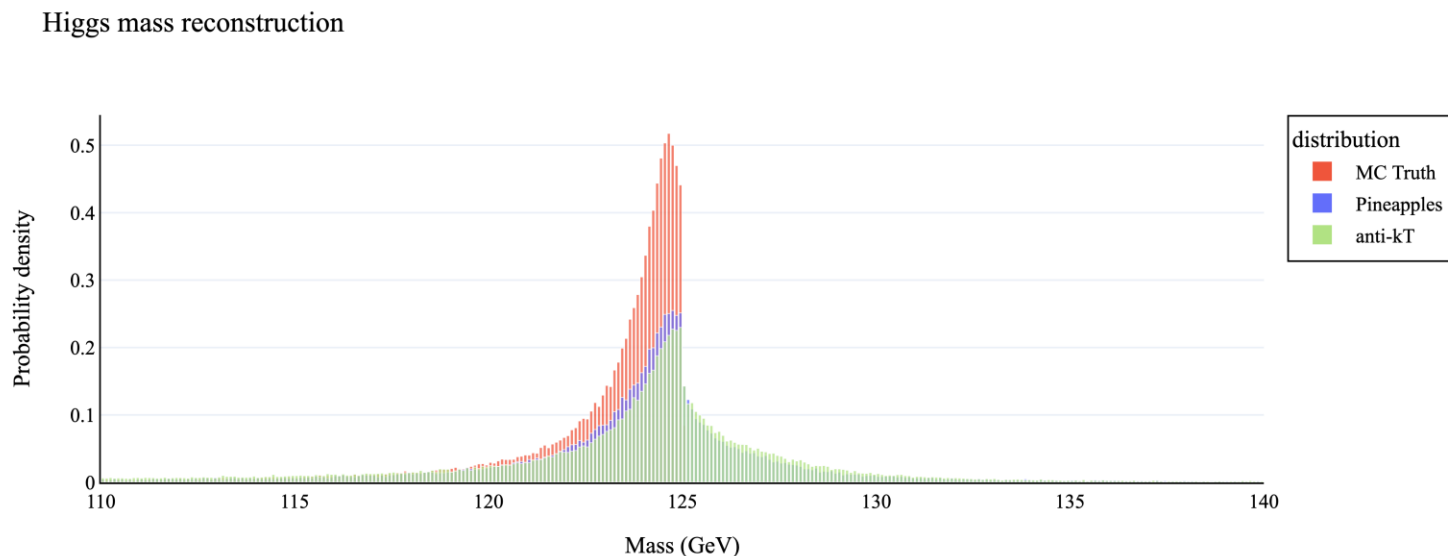
Top quark mass distribution



# GRAPH NEURAL NETWORK PIPELINE

Feeding our GNN models simulation-informed labels for the simpler case of Higgs datasets shows improved performance over anti- $k_T$ .

There is no need for combining, pruning, and tagging, as these are learned implicitly!



## OUTLOOK

- Investigate training on top quarks
- Check performance against taggers



Get the code!

For more information, visit my poster on  
Wednesday, during Session A, in Location 20!

# THANK YOU

# Accelerating the search for mass bumps using the Data-Directed Paradigm

Jean-François Arguin

Georges Azuelos

Émile Baril

Fannie Bilodeau

Bruna Pascual Dias

Muhammad Usman

Samuel Calvet

Julien Noce Donini

Eva Mayer

Shikma Bressler

Maryna Borysova

Michael Chu

Etienne Dreyer

Elad Kliger

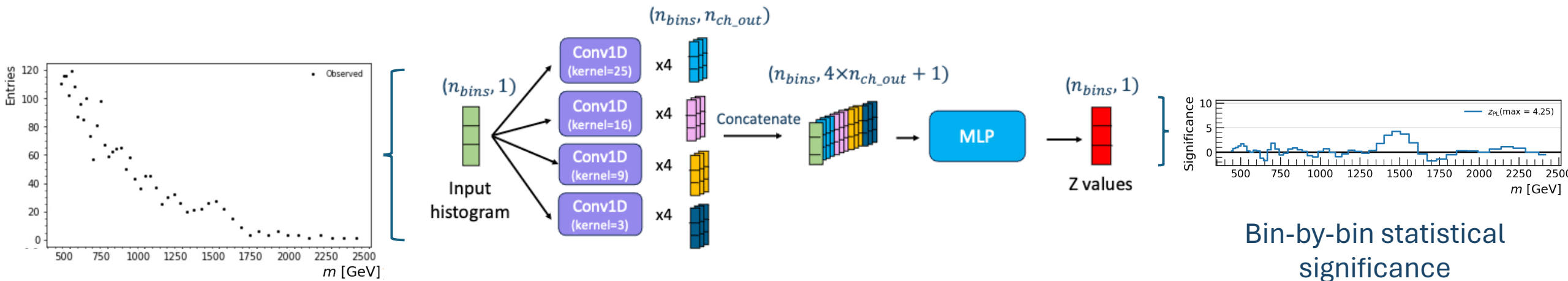
Nilotpall Kakati

Amit Shkuri



# What ?

- We want to maximize our chances to **find new physics** in collider data
- Train a neural network to **identify mass bumps in real data** without the need of simulation or analytical fit to estimate the background



Invariant mass histogram

Bin-by-bin statistical significance

# Why ?

- Exploit the **discovery potential of the data**
  - Impossible to check all final states with a traditional analysis
  - Many possible resonances in unexplored final states → bumps

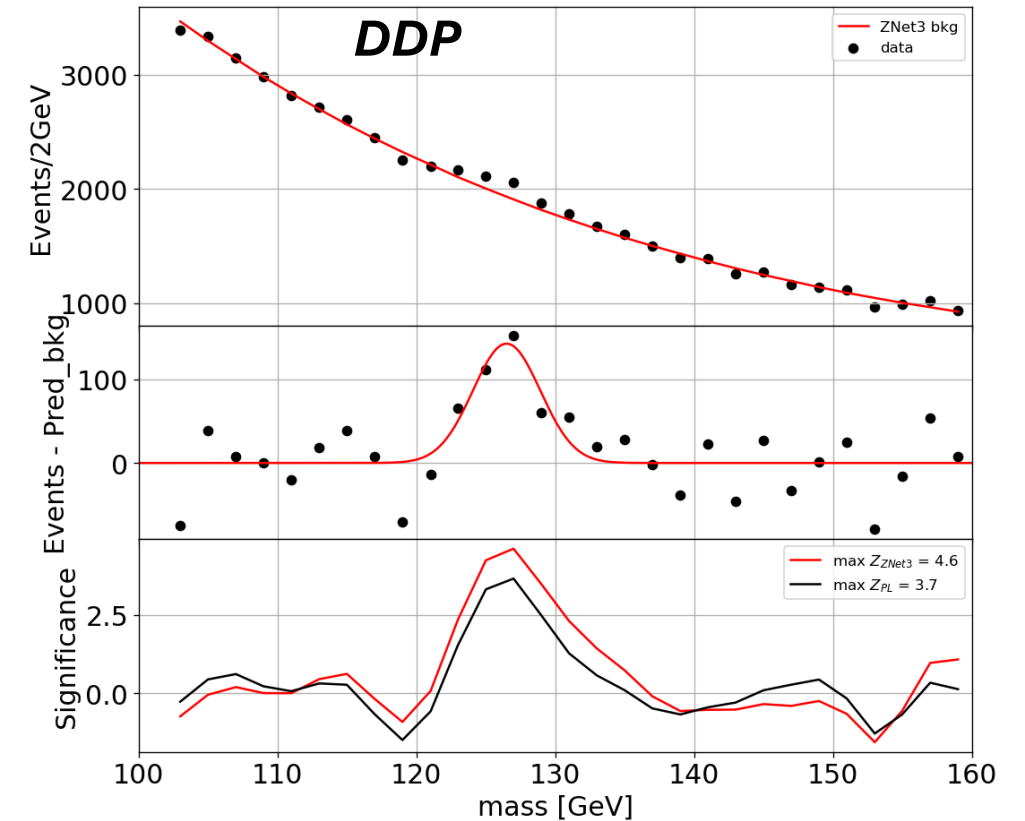
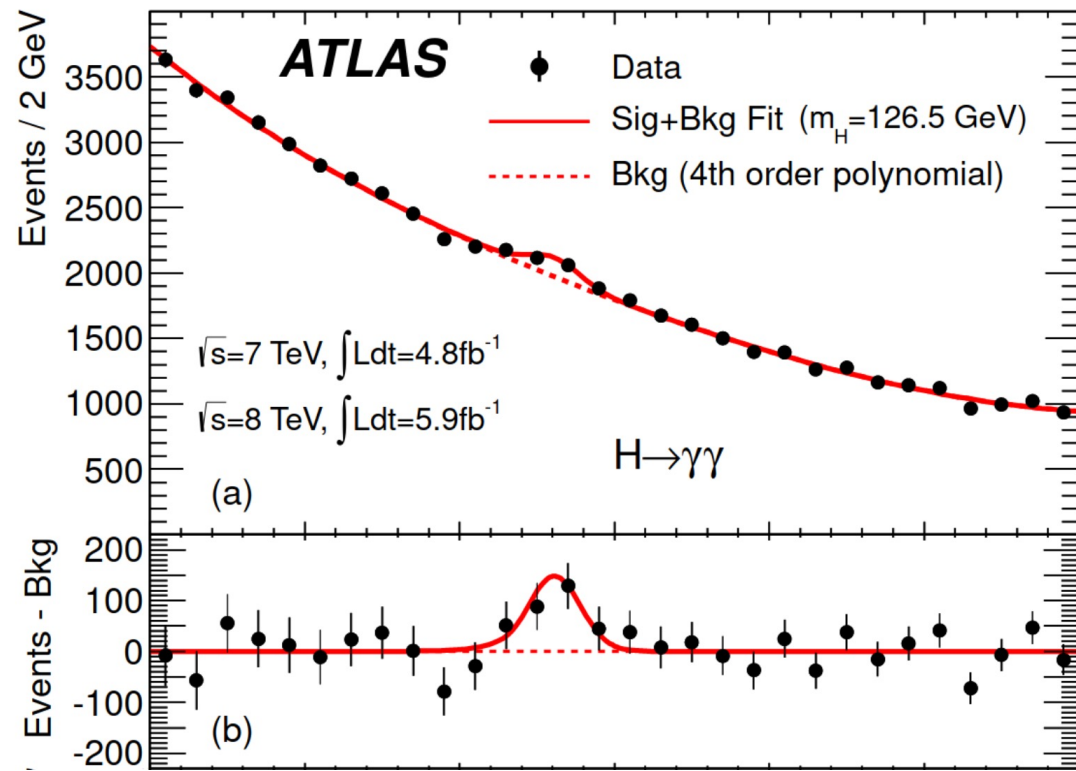
Existing searches for two-body resonances<sup>[1]</sup>

	$e$	$\mu$	$\tau$	$q/g$	$b$	$t$	$\gamma$	$Z/W$	$H$	BSM $\rightarrow$ SM <sub>1</sub> $\times$ SM <sub>1</sub>				BSM $\rightarrow$ SM <sub>1</sub> $\times$ SM <sub>2</sub>			BSM $\rightarrow$ complex			
										$q/g$	$\gamma/\pi^0$ 's	$b$	...	$tZ/H$	$bH$	...	$\tau q q'$	$e q q'$	$\mu q q'$	...
$e$	[37,38]	[39,40]	[39]	$\emptyset$	$\emptyset$	$\emptyset$	[41]	[42]	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	[43,44]	$\emptyset$	
$\mu$		[37,38]	[39]	$\emptyset$	$\emptyset$	$\emptyset$	[41]	[42]	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	[43,44]	
$\tau$			[45,46]	$\emptyset$	[47]	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	[48,49]	$\emptyset$	
$q/g$				[29,30,50,51]	[52]	$\emptyset$	[53,54]	[55]	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	
$b$					[29,52,56]	[57]	[54]	[58]	[59]	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	[60]	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	
$t$						[61]	$\emptyset$	[62]	[63]	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	[64]	[60]	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	
$\gamma$							[65,66]	[67-69]	[68,70]	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	
$Z/W$								[71]	[71]	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	
$H$									[72,73]	[74]	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	
BSM $\rightarrow$ SM <sub>1</sub> $\times$ SM <sub>1</sub>	$q/g$									$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	
	$\gamma/\pi^0$ 's										[75]	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	
	$b$											[76,77]	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	
	$\vdots$													$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	$\emptyset$	
$\vdots$																				

[1] J. H. Kim et al., version 1, 10.48550/ARXIV.1907.06659 (2019), <https://arxiv.org/abs/1907.06659>

# Promising result

- **Finding the Higgs bump**
  - Predicted significance matches the ATLAS significance within error [2]





# Please visit our poster !

More promising results !

More on the training data !



## Accelerating the search for mass bumps using the Data-Directed Paradigm

Jean-Francois Arguin<sup>1</sup>, Georges Azuelo<sup>1</sup>, Émile Baril<sup>1</sup>, Farzad Bilodeau<sup>1</sup>, Maryna Borysova<sup>1</sup>, Shikma Bressler<sup>1</sup>, Samuel Calvet<sup>1</sup>, Michael Chu<sup>2</sup>, Julien Noce Domini<sup>1</sup>, Etienne Dreyer<sup>2</sup>, Nilotpal Kakati<sup>1</sup>, Elad Kliger<sup>2</sup>, Eva Mayer<sup>3</sup>, Bruno Pascual Dias<sup>1</sup>, Amit Shkurip<sup>1</sup>, Muhammad Usman<sup>1</sup>

<sup>1</sup>Université de Montréal, <sup>2</sup>Weizmann Institute of Science, <sup>3</sup>Laboratoire de Physique de Clermont – UCA – CRNS/IN2P3

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### Motivation

What ? Train a neural network to **identify mass bumps in real data** without the need of simulation or analytical fit to estimate the background

Why ? Exploit the **discovery potential of the data**.

- Impossible to check all final states with the traditional analysis
- Many possible resonances in unexplored final states → bumps

### Data Directed Paradigm for bump searches

The **Data-Directed Paradigm (DDP)** is a search strategy to efficiently identify regions of interest in the data. It requires two ingredients:

- Property of the Standard Model (SM) on which deviations can be searched for
- Tool to scan the observable-space in search for deviations

Smoothly falling invariant mass      NN mapping invariant mass to statistical significance for bumps

### Neural network architecture

Use of 1D convolution layers followed by a dense layer

Intuitive and agnostic to the number of bins in the histogram

Mixes all representations for each bin independently

### Training data

Synthetic data generated by injecting a Gaussian signal on two types of backgrounds:

- Analytical functions
- Fits to simulation data (e.g. Dark Machines sample)

### Histogram processing and calibration

- Using the **Dark Machines dataset** [2]
  - Designed to test anomaly detection techniques
  - Dataset equivalent to 10 fb<sup>-1</sup> with highest cross section processes at the LHC
- Mass histograms with **all possible combinations** of the following objects:
  - Electron    Photon    Reconstructed leptonic Z    Boosted top
  - Muon    Jet    Boosted hadronic W/Z    High mass jet (m > 200 GeV)
- Additional kinematics cuts on missing energy (MET) and transverse momentum (p<sub>T</sub>) of leading objects
- Split the data according to jet multiplicity to improve S/B ratio and reduce the look-elsewhere effect
- Total of 30 000 mass histograms
- Rebinning that reflects the detector resolution**, using  $p_T \approx m/2$ 
  - Resolution is higher for m(4j) than m(3j), and for smaller masses
  - Binning reflects this with larger bin width when resolution is smaller

### Performance and finding Beyond the Standard Model (BSM) signals

- Accurately predicts maximum significance with no bias and a variance of  $\pm 0.64$
- Excellent discriminating performance with an AUC of 0.900

### Promising results when finding the Higgs bump

- Predicted significance matches the ATLAS significance within error [3]

### Successfully finds theorized BSM signals over the Dark Machines background

**RPV stop → bl**

$m(\mu) \text{ at } 1\mu + 1b + 6j$

**W' → WZ**

$m(W, E_{T \text{ miss}}) \text{ at } 1Wk + 1j$

Other BSM signals found include  $LQ \rightarrow beh_{\mu}, bebe$  and  $Z' \rightarrow 3l$

**0.1% false positive rate over background-only sample**

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### Acknowledgements

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### References

- [1] Volkovich, S., Hialeq, F. D. V. and Bressler, S. (2021). doi:10.48550/ARXIV.2107.11573
- [2] Aarrestad, T. et al. SciPost Phys. 12, 043 (2022). doi:10.21468/SciPostPhys.12.1.043
- [3] ATLAS Collaboration. Physics Letters B 716 (2012). doi:10.1016/j.physletb.2012.08.020

More on the pre-processing of the histograms !

Come ask questions !