

# Learning Symmetry-Independent Jet Representation via Jet Joint **Embedding Predictive Architecture**

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Larger than Larger Ep1 2025 Jan 7

†: equal contribution



https://arxiv.org/abs/2412.05333



# Outline

- Motivation
- Introduction to JEPA
- Our J-JEPA approach
- Dataset
- Pretraining + fintuning setup
- Pretraining result
- Pretraining + fine-tuning result
- Ongoing and Future work

## **Motivations for Self-Supervised Learning (SSL)** Learning without labels

- representations from unlabeled data
- data such as images or sounds, rather than from manually assembled labeled datasets.



Self-Supervised Learning: A type of machine learning where models learn useful features and

• To learn effectively (like human), system must learn these representations directly from unlabeled • With the HL-LHC upgrade [1] in the near future, we will need to simulate an order of magnitude more events with a more complicated detector geometry to keep up with the recorded data [2].



### SSL for foundation model

- 1. [HL-LHC] https://arxiv.org/abs/1705.08830
- 2. [Computing for HL LHC] https://doi.org/10.1051/epjconf/201921402036



# **JEPA: Different SSL Architectures**



- not mask the input

Difference between JEPA and (b): JEPA predicts in the latent space and does



# **JEPA: Joint Embedding Predictive Architecture**





- Predict the masked parts in the representation space
- Augmentation free to minimize bias



### Example: The I-JEPA Architecture I: Image



**J (Jet) - JEPA** 





### **J-JEPA** Cluster subjets with radius 0.2

### An AK8 Jet



### J-JEPA: Define Target and Context Subjets Randomly divide subjets into target/context categories

An AK8 Jet



### J-JEPA: Define Target and Context Subjets Randomly divide subjets into target/context categories



### Target Subjets







Context Subjets







Particle: $p_T, \eta, \phi, E$
Particle N: $p_T, \eta, \phi, E$

Particle 1: $p_T, \eta, \phi, E$
Particle: $p_T, \eta, \phi, E$
Particle N: $p_T, \eta, \phi, E$

Particle 1: $p_T, \eta, \phi, R$	
Particle: $p_T, \eta, \phi$ ,	Ε
Particle N: $p_T, \eta, \phi, J$	E

Particle 1: $p_T, \eta, \phi, E$
Particle: $p_T, \eta, \phi, E$
Particle N: $p_T, \eta, \phi, E$

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Particle 1: $p_T, \eta, \phi, E$
Particle: $p_T, \eta, \phi, E$
Particle N: $p_T, \eta, \phi, E$

### J-JEPA: Subjet Embedding Layer (SEL) Each subjet creates its embedding independently



### **Other options:**



### Subjet Embedding Layer (SEL)





## **J-JEPA: Calculate Subjet Representations Using Transformer Encoder Blocks**





### **J-JEPA: Predict in the Representation Space** Providing the target subjets' coordinates to the predictor **Target subjets'** representations







# J-JEPA: Pretraining



SEL: Subjet Embedding Layer



### Questions?



# Datasets

### We use JetClass for pretraining and TopTagging for finetuning

Dataset name	Size	Description	Portions we used	Role in transfer learning
JetClass	100 Million AK8 Jets	Contains 10 classes of jets	500K Top jets 500k q/g jets	Stand in for the large pretaining unlabeled dataset
Top Tagging	1.2 Million AK8 Jets	Only Top and QCD jets	760K mixed jets*	Stand in for the small fine- tuning dataset



\* We only used jets with more than 10 subjets



### Top Tagging Dataset 1902.09914





Information collapse: The model fails to capture the meaningful variations in the data, leading to poor performance in tasks like classification or regression.

### Latent after Pre-training: Not Collapsing J-JEPA model learned a diverse latent space

- 0.8

- 0.6

- 0.4

- 0.2

0.0



Let A be the features of Jet 1, and B be the features of Jet 2, then the cosine similarity is defined as

 $\cos(\theta) = \frac{\mathbf{A} \cdot \mathbf{B}}{\|\mathbf{A}\| \|\mathbf{B}\|}$ 

- 1. Randomly select 128 Jets.
- 2. Represent each jet by their flattened subjet representations
- 3. Calculate cosine similarity between each pair of jets

**Average Cosine Similarity: 0.457** 



## **J-JEPA: Finetuning Setup** From subjet representation to jet representation



### **Aggregation Methods for Fine-tuning** 3 Different methods of attaching the latent space to a classification head



# Our training and evaluation setup

Baseline refers to the same model directly trained on the finetuning dataset without pretraining



# Metrics

### Accuracy: correctly predicted / total number of samples **Rejection: inverse of background rejection (FPR) at 50% signal efficiency (TPR)**



background rejection

Significance: In a background dominant dataset, how much background can you reject while letting in a certain number of signal samples (the more the better)

1.0

### **J-JEPA Performance Pretrain on JetClass and finetune on Top Tagging**



Attention-based SEL

**MLP-based SEL** 



### Visualizing learned features **UMAP** and direct comparison show that the features have good separation power







### **Our results** 1. J-JEPA improves the downstream performance compared with from scratch (for most models)

Model	Aggregation	Baseline 10%	Baseline Full	Finetuned 10%	Finetuned Full
		Accuracy [%]			
SjT-T	Flatten	$87.52\pm0.16$	$89.13\pm0.10$	$88.21\pm0.55$	$89.95\pm0.13$
SjT-T	Cls Attn	$88.30 \pm 0.18$	$89.67 \pm 0.13$	$88.67\pm0.02$	$90.00\pm0.07$
AE-SjT-T	Flatten	$88.92\pm0.15$	$90.01\pm0.08$	$88.94 \pm 0.13$	$90.03 \pm 0.07$
AE-SjT-T	Cls Attn	$88.84 \pm 0.21$	$90.03 \pm 0.05$	$88.82\pm0.11$	$90.00\pm0.12$
		$1/\varepsilon_B(\varepsilon_S=0.5)$			
SjT-T	Flatten	$40.50 \pm 1.26$	$70.70 \pm 1.46$	$53.67 \pm 9.97$	$90.06 \pm 3.80$
SjT-T	Cls Attn	$52.56 \pm 1.54$	$79.75 \pm 5.12$	$61.32\pm0.66$	$91.51 \pm 1.20$
AE-SjT-T	Flatten	$67.34 \pm 1.40$	$97.79 \pm 3.90$	$70.47 \pm 1.09$	$97.52 \pm 1.71$
AE-SjT-T	Cls Attn	$67.19 \pm 1.54$	$99.38 \pm 2.80$	$68.25 \pm 1.64$	$95.47 \pm 1.83$



# 

### **Our results** 2. Class attention blocks are more effective than simply flattening (for most models)

Model	Aggregation	Baseline 10%	Baseline Full	Finetuned 10%	Finetuned Full
		Accuracy [%]			
SjT-T	Flatten	$87.52\pm0.16$	$89.13\pm0.10$	$88.21\pm0.55$	$89.95 \pm 0.13$
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# 785767 Number of Labeled Training Samples

### **Our results** 3. Our custom attention-based embeddings offer a significant improvement in downstream performance compared with the traditional MLP-based embeddings

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SjT-T	Flatten	$87.52 \pm 0.16$
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AE-SjT-T	Cls Attn	$67.19 \pm 1.54$





# /85/6/ Number of Labeled Training Samples

# Summary

- J-JEPA: A subject-based Joint-Embedding Predictive Architecture
- Pre-train J-JEPA on a large dataset and finetune the target encoder on a small dataset achieves better performance than training the encoder from scratch,
- Different encoder architectures has different response to the J-JEPA pretraining, but overall positive.



# **Ongoing Work**

- Implementing a particle-based JEPA lacksquare
- Training shorter models to reduce overfitting
- Experiment different ways to provide information to the predictor
- Generalize the JEPA scheme to different physics objects: particles, events, detector readout, etc.



# Large-Scale Pretraining and **Finetuning for Efficient Jet** Classification **Zihan Zhao**, Farouk Mokhtar, Raghav Kansal, Billy Li, Javier Duarte

Larger than Larger Ep1 2025 Jan 7



https://arxiv.org/abs/2408.09343



# Intro to SSL strategies

### As opposed to supervised learning, which is limited by the availability of labeled data, self-supervised approaches can learn from vast unlabeled data (2304.12210)

### To learn useful features from the data itself without using labels





### Masked Modeling

2401.13537

JEPA

2108.04253

2412.05333



# **Necessity of SSL in LHC Physics**

- Simulations don't model the data perfectly: need a way to directly train on data
- It will be even harder and more computationally expensive to produce high-quality simulations for High Luminosity LHC (1803.04165)


# First Goal of the Project

features directly from vast unlabeled data.



**Current workflow using only Supervised Learning** 

• To show that we can leverage SSL to learn powerful, generic, and transferable



Workflow incorporating SSL

# **Toward Foundation Model**









# **Towards Foundation Model in HEP**

Contrastive Learning: Symmetry Augmentation



Dillon, Kasieczka, Olischlager Plehn, Sorrenson, Vogel, 2108.04253

Masked Particle Type Prediction



Kishimoto, Morinaga, Saito Tanaka, 2312.06909

#### Masked Particle Modeling



Contrastive Learning: **Re-Simulation** 



Harris, MK, Krupa, Maier, Woodward, 2403.07066

Supervised Pre-training and Joint Optimization



#### Supervised Classification and Generation

2401.13537



Vigl, Hartman, Heinrich, 2401.13536

Mikuni, Nachman 2404.16091

Credit: This slide is copied from Michael Kagan's talk in the FM Mini Workshop in October 2024

#### Next Token Predictoin



A set of

object

component

Target 2

Target .

Birk, Hallin, Kasieczka, 2403.05618

#### Context repr. **Context encode** Context 2 Representation Space Target

**Target encode** 

J-JEPA

Katel, Li, Zhao, et al. https://arxiv.org/abs/2412.05333



#### https://indico.cern.ch/event/1386125/contributions/6139666/

#### Large-Scale Fine-Grained Classification



Li, Li, et al. 2405.12972





# **Towards Foundation Model in HEP**

Contrastive Learning: Symmetry Augmentation



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Supervised Pre-trai and Joint Optimization





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Mikuni, Nachman 2404.16091

Credit: This slide is copied from Michael Kagan's talk in the FM Mini Workshop in October 2024

Li, Li, et al. 2405.12972

https://indico.cern.ch/event/1386125/contributions/6139666/



# **Primary Goal of the Project**

performance of foundation model.



## • Focus on studying the effect of scaling up the sizes of pretraining datasets on the



# Outline

- Toward Foundation Model in HEP
- Goals of the Project
- Intro to JetCLR
- Transfer Learning: from JetClass to Top Tagging
- Scaling up pretraining dataset size
- Some technical details
  - Classification head for finetuning: MLP vs Linear Projection
  - Techniques to speed up training
- Ongoing and Future work

# Intro to JetCLR



$$\mathcal{L}_i = -\log rac{e^{s(z_i,z_i)/ au}}{\sum_{j 
eq i \in ext{batch}} \left[ e^{s(z_i,z_j)/ au} + e^{s(z_i,z_j')/ au} 
ight]}$$

2108.04253

## Augmentations



# **Model Architecture for encoder**

- Started with a simple Transformer encoder



#### **Transformer Encoder** 1706.03762

Working on switching to more advanced architectures such as Particle Transformer

**Particle Transformer** 2202.03772

## Datasets

## JetClass for unlabeled pretraining, Top Tagging for labeled finetuning



2202.03772

Description	Role in transfer learning
Contains 10	Stand in for unlabeled "data",
classes of jets	use for pretraining
Only Top and	Stand in for labeled
QCD jets	"simulation", use for fine-tuning



#### Top Tagging Dataset 1902.09914

## Metrics

## Accuracy: correctly predicted / total number of samples **Rejection: inverse of background rejection (FPR) at 50% signal efficiency (TPR)**



background rejection

Significance: In a background dominant dataset, how much background you can reject while letting in a certain fraction of signal samples (the more the better)

1.0

# **Pretraining on JetClass and fine-tuning on Top Tagging**

## The pre-trained model requires significantly fewer samples to achieve high accuracy and rejection rate: higher data efficiency

uncertainty bands, respectively



• The averages and standard deviations over 5 trainings are shown in solid lines and



# **Pretraining on JetClass and fine-tuning on Top Tagging**

## The pre-trained model converges much faster: higher computational efficiency

uncertainty bands, respectively



• The averages and standard deviations over 5 trainings are shown in solid lines and



## Scaling up pretraining dataset size By scaling up the pretraining dataset, the model demonstrated enhanced performance and faster convergence: both data and computational efficiency improve as we use larger datasets for pretraining

Background rejection at 50% signal efficiency



Rejection: inverse of background rejection at 50% signal efficiency



# Conclusion

- Through large-scale pretraining followed by finetuning, our SSL approach has demonstrated
  - superior performance compared to the fully supervised approach.
  - faster than its fully supervised counterpart.
  - Both efficiencies increase as the pretraining dataset size increases.
- understanding of the potential of SSL for scientific discovery.

• Enhanced data efficiency—requiring fewer labeled training samples to achieve

• Greater computational efficiency—enabling the model to converge significantly

• This paves the way for the use of unlabeled data in HEP and contributes to a better

# **Ongoing and Future work**

Ongoing work

•

- encoder
- Pretrain on JetClass v2, an even larger dataset, or the <u>Aspen Open Jets</u> dataset, a real CMS dataset
- Evaluate on different SSL strategies beyond JetCLR lacksquare
- Explore other physically motivated augmentations
  - Pairing the two jets from dijet events
  - Using two subjets clustered with smaller radii  $\bullet$
  - Using tracks and clusters as two views of the same jet

• Study the effectiveness of more advanced architectures like the ParticleTransformer as the backbone

## Support **Thank you for listening!**

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- This work was performed using the National Research Platform Nautilus HyperCluster supported by NSF





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# Back Up (Part 1)

## Example: The I-JEPA Architecture I: Image



# **Details of the Top Tagging Dataset**

$$p_{T,j} = 55$$

For the signal only, we further require a matched parton-level top to be within  $\Delta R = 0.8$ , and all top decay partons to be within  $\Delta R = 0.8$  of the jet axis as well. No matching is performed for the QCD jets. We also require the jet to have  $|\eta_j| < 2$ . The constituents are extracted through the Delphes energy-flow algorithm, and the 4-momenta of the leading 200 constituents are stored. For jets with less than 200 constituents we simply add zero-vectors.

The top signal and mixed quark-gluon background jets are produced with using Pythia8 [25] with its default tune for a center-of-mass energy of 14 TeV and ignoring multiple interactions and pile-up. For a simplified detector simulation we use Delphes [26] with the default ATLAS detector card. This accounts for the curved trajectory of the charged particles, assuming a magnetic field of 2 T and a radius of 1.15 m as well as how the tracking efficiency and momentum smearing changes with  $\eta$ . The fat jet is then defined through the anti- $k_T$  algorithm [27] in FastJet [28] with R = 0.8. We only consider the leading jet in each event and require

> $550 \dots 650 \text{ GeV}$  . (1)

#### 1902.09914

# **Details of the JetClass Dataset**

Simulation setup. Jets in this dataset are simulated with standard Monte Carlo event generators used by LHC experiments. The production and decay of the top quarks and the W, Z and Higgs bosons are generated with MAD-GRAPH5\_aMC@NLO (Alwall et al., 2014). We use PYTHIA (Sjöstrand et al., 2015) to evolve the produced particles, i.e., performing parton showering and hadronization, and produce the final outgoing particles<sup>1</sup>. To be close to realistic jets reconstructed at the ATLAS or CMS experiment, detector effects are simulated with DELPHES (de Favereau et al., 2014) using the CMS detector configuration provided in DELPHES. In addition, the impact parameters of electrically charged particles are smeared to match the resolution of the CMS tracking detector (CMS Collaboration, 2014). Jets are clustered from DELPHES E-Flow objects with the anti $k_{\rm T}$  algorithm (Cacciari et al., 2008; 2012) using a distance parameter R = 0.8. Only jets with transverse momentum in 500–1000 GeV and pseudorapidity  $|\eta| < 2$  are considered. For signal jets, only the "high-quality" ones that fully contain the decay products of initial particles are included<sup>2</sup>.

#### 2202.03772 56

## **Transformer Embedding Layer Effects Correlation between subjets is reduced**



Correlation Matrix of Subjets for Jet 102, mean=0.6697532534599304



- 1.0 - 0.8 - 0.6 - 0.4 - 0.2

0.0

## WIP: Study of how to provide the additional info Pre-train and fine-tune on Top Tagging

Experiments	Encode subjet coordinates at both (encoder and predictor)	Encode coordinates only at predictor	Encode pT ranking at both	Use a MLP to encode subjet coordinates
Inverse Rejection Power	63.99	45.33	45.02	Converging



## **Study of subjet embedding** Pre-training and fine-tuning on Toptagging dataset

Inverse Rejection Power	<b>Dimension Reduction</b>	<b>Dimension Expansion</b>
Attention	86.42	73.81
MLP	73.55	63.99
Linear	44.31	

# Strategies to prevent collapse

- Targets being padded subjets
- Most particles are padded so all subjets look the same to the model
- Information bottleneck in the predictor is too big
- Dataset was not normalized

- We only select targets from non-empty subjets
  - We implemented Attentionbased embedding
  - We decreased the size of the predictor dimension
- We normalized the dataset
- Plus: EMA updating the Target Encoder



## J-JEPA: Splitting jets into subjets number of subjets per jet

Percentage of Subjets per Jet (10% Sample) by Algorithm



## J-JEPA: Splitting jets into subjets number of particles per subjet

Percentage of Constituents per Subjet (10% Sample) by Algorithm





# Back Up (Part 2)

## **Techniques to speed up training** Steps we took to ensure the model finished pretraining within a reasonable amount of time

- Removed unnecessary CPU-GPU synchronizations, especially read-out from GPU for recording losses
- Modified the default model dimensions to be multiples of 8 to make use of CUDA matrix multiplication kernels more efficiently
- Fused point-wise operations into a single CUDA kernel when computing the contrastive loss.
- Utilized the Automatic Mixed Precision (AMP) package
  - Measures to mitigate the numerical instability caused by using AMP in backup.



# LHC and Jet Tagging

#### Proton beams

Outgoing particles: tracks ..... electromagnetic energy. hadron energy

### Collision point

÷.....

### Collision event













# Measures to mitigate the numerical instability caused by using AMP

- Monitor loss and gradient values regularly with tensorboard
- Gradient clipping with a maximum norm of 0.1
- Set the  $\epsilon$  parameter to 10<sup>(-4)</sup> in the Adam optimizer.
- Manually run certain parts of the code in full precision

## **Pretraining on JetClass and fine-tuning on Top Tagging**

### The pre-trained model shows a much clearer separation between signal and background



Trained from scratch

68



## Pretraining on JetClass and fine-tuning on Top Tagging

### The pre-trained model shows a much clearer separation between signal and background



Trained from scratch



#### **Pre-trained**



## **Pretraining on JetClass and fine-tuning on Top Tagging** Despite limited data, the pre-trained model achieves higher accuracy and converges faster



- A linear layer was added to the encoder for fine-tuning.
- Blue curve was pre-trained on 1% of the JetClass dataset (1 Million jets) with SimCLR
- Red curve was trained from scratch
- Both models share the same hyperparameters
- Both models are trained with 100k jets (1/12 of the Top Tagging Dataset)

## Accuracies of two trials trained with 1000 labeled samples







# The CMS detector coordinate system



 $\eta \equiv -\ln \left| an \left( rac{ heta}{2} 
ight) 
ight|$ 

### https://tikz.net/axis3d\_cms/


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## 2202.03772

## **Training on Top Tagging** Are the features correlated?



