PELICAN: deep jets with permutation and Lorentz equivariance

Joint work with: David Miller, Timothy Hoffman, Jan Offermann, Xiaoyang Liu (UChicago)



Alexander Bogatskiy **Research Fellow, Flatiron Institute**



ML4Jets 2022





Jet-images — deep learning edition

Luke de Oliveira, Michael Kagan, Lester Mackey, Benjamin Nachman 🖂 & Ariel Schwartzman

Journal of High Energy Physic 1558 Accesses | 180 Citati

A preprint version of the

ABSTRACT

•

Building on the notion of a high energy particles, or jet learning techniques based Modern deep learning algo motivated feature driven a these features are learned **k** performance. This interpla learning algorithms is gene discover new particles and jets.

Regular Article - Theoretical Physics Open Access Published: 25 January 2017 Deep learning in color: towards automated quark/gluon jet discrimination

Patrick T. Komiske, Eric M. Metoc

Journal of High Energy Physics 1764 Accesses | 162 Citations

A preprint version of the a

ABSTRACT

Artificial intelligence offers th collider physics. To establish i convolutional neural network designed by physicists. Our ap image, with intensity given by by adding color to the images, momentum in charged partic charged particle counts. Overa variables. We also find that, w the neural networks are surpl observables. This suggests that imperfect simulations.



ABSTRACT

We apply computer v (CNN) — to build a hi of Kasieczka et al) has performance to stateintroduce a number o image preprocessing, BDTs based on high-l wide range of tagging QCD background reje (non-merged) top jets straightforwardly exte here may be useful to

ABSTRACT

Machine learning from the LHC. To DeepTop approa a network archite Model production multivariate QCI performance, est multivariate hypo

Pulling out all the tops with computer vision and deep

Regular Article - Experimental Physics | Open Access | Published: 02 May 2017

Deep-learning top taggers or the end of QCD?

Gregor Kasieczka 🗠, Tilman Plehn, Michael Russell & Torben Schell

ournal of High Energy Phy				
30 Accesses 137 Cita				
• A <u>preprint version</u> o	Neural Message Passing for Jet Physics			
BSTRACT	Icoco Honrion, Johonn Drohmon, Joon	Drung Krunghun Cha Kulo Cronmor		
	Center for D	ata Science		
lachine learning based	New York I	University NY 10012 kyunghyun, kyle.cranmer*}@nyu.edu		
om the LHC. Top taggi	New York, {henrion* iohann.brehmer. bruna, }			
eepTop approach and				
network architecture to	Gilles Louppe	Gaspar Rochette		
lodel production chanr	Department of Computer Science University of Liège	Department of Computer Science École Normale Supérieure		
ultivariate QCD-based	Belgium	Paris, France		
erformance, establishir	g.louppe@ulg.ac.be	gaspar.rochette@ens.fr		
ultivariate hypothesis-				





QCD-aware recursive neural networks for jet physics

Gilles Louppe, Kyunghyun Cho, Cy [Submitted on 24 Nov 2017]

Journal of High Energy Physics 2 857 Accesses 78 Citations

Long Short-Term Memory (LSTM) networks with jet constituents for boosted top tagging at the LHC

A preprint version of the art •

ABSTRACT

Recent progress in applying ma between calorimeters and imag networks built instead upon an four-momenta are like words an

algorithms is like the parsing of a sentence. momenta of a variable-length set of particle event-by-event basis. Our experiments high specific jet embeddings and show that recu and data efficient than previous image-base individual jets (sentences) to full events (pa level classifier operating on all the stable pa

Multivaria identificat Recent De activation network. this work networks constituen achieves a than a fac trained on Regular Article Published: 17 July 2019

Shannon Egan Waisiach Fadarka, Alican Lister, Janniska Bearkes, Calin C

Pileup mitigation at the Large Hadron Collider with graph neural networks

J. Arjona Martínez, O. Cerri, M. Spi The European Physical Journal Plu 116 Accesses | 30 Citations |

Abstract.

At the Large Hadron Collider, t collaborations occur in coincide usually referred to as pileup. Pi event reconstruction as pileup a observables. We present a class particles coming from high-tra from pileup collisions. This mo Bertolini et al., JHEP 10, 059 (Thanks to an extended basis of considered network architectur with respect to state-of-the-art

geometry with distance-weighted graph networks Shah Rukh Qasim, Jan Kieseler 🖂, Yutaro liyama & Maurizio Pierini The European Physical Journal C 79, Articl

2903 Accesses 49 Citations 38 Altm

• A preprint version of the article is av

Abstract

We explore the use of graph networks to https://doi.org of particle reconstruction. Thanks to the networks can exploit the full detector gr and arbitrarily complex detector geome Abstract network architectures, dubbed GARNET The top-H reconstruction task. The performance o The precis simulated particle interactions on a toy beyond the inspired by the endcap calorimeter to b Luminosity LHC phase. We study the cl calorimetric particle reconstruction, an approaches. The proposed algorithms p LHC, with

Special Article - Tools for Experiment and Theory Open Access Published: 18 July 2019

Learning representations of irregular particle-detector





[Submitted on 27 Jul 2017 (v1), last revised 23 Apr 2018 (this version, v3)]

Deep-learned Top Tagging with a Lorentz Layer

Anja Butter, Gregor Kasieczka, Tilman Plehn, Michael Russell

Regular Article - Theoretical Physics | Open Access | Published: 15 January 2019

[Submitted on 8 Jun 2020]

Energy flow networks: deep sets for particle jets

Patrick T. Komiske, Eric M. Metodiev 28 Jesse Thaler

Journal of High Energy 1334 Accesses 101

Open Access

A preprint version

Matthew J. Dolan and Ayodele Ore Phys. Rev. D 103, 074022 – Published 27 April 2021

ABSTRACT

A key question for m and learn from collic particles, we build up or "point clouds". Ad introduce Energy Flc We also develop Part inclusion of addition feature a per-particle overall event-level la existing event repres demonstrate the pov the collider task of di

Lorentz Group Equivariant Neural Network for Particle Physics

Alexander Bogatskiy, Brandon Anderson, Jan T. Offermann, Marwah Roussi, David W. Miller, Risi Kondor

Equivariant energy flow networks for jet tagging

We present a neural network architecture that is fully equivariant with respect to transformations under the Lorentz group, a fundamental symmetry of space and time in physics. The architecture is based on the theory of the finite-dimensional representations of the Lorentz group and the equivariant nonlinearity involves the tensor product. For classification tasks in particle physics, we demonstrate that such an equivariant architecture leads to drastically simpler models that have relatively few learnable parameters and are much more physically interpretable than leading approaches that use CNNs and point cloud approaches. The competitive performance of the network is demonstrated on a public classification dataset [27] for tagging top quark decays given energy-momenta of jet constituents produced in protonproton collisions.

performance compared to existing methods. We also show how the learned event representation can be directly visualized, providing insight into the inner workings of the model. These architectures lend themselves to efficiently processing and analyzing events for a wide variety of tasks at the Large Hadron Collider. Implementations and examples of our architectures are available online in our **<u>EnergyFlow</u>** package.

Acc

[Submitted on 27 Jul 2017 (v1), last revised 23 Apr 2018 (this version, v3)]

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[Submitted on 5 Jul 2021] We present a neural network architecture that Particle Convolution for High Energy Physics

Acc

We introduce the Partic equivariant neural netw particle convolution lay Energy Flow network a operator is promoted t implemented for variou of rotation about the je tasks, q/g tagging and achieves performance of Moreover, we show that significantly outperforr We speculate that by g convolutional symmetr current state-of-the-a

[Submitted on 20 Jan 2022 (v1), last revised 29 May 2022 (this version, v5)]

An Efficient Lorentz Equivariant Graph Neural Network for Jet Tagging

Shiqi Gong, Qi Meng, Jue Zhang, Huilin Qu, Congqiao Li, Sitian Qian, Weitao Du, Zhi-Ming Ma Tio Van I

Deep learning n particle physics be an important in many applica spacetime symr incorporated in design is compl high-order tens

Particle Transformer for Jet Tagging

Huilin Qu, Congqiao Li, Sitian Qian Proceedings of the 39th International Conference on Machine Learning, PMLR 162:18281-18292, 2022.

Abstract

Jet tagging is a critical yet challenging classification task in particle physics. While deep learning has

• Euclidean symmetries in jet images (CNN's)

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Permutations of particles (particle clouds, Deep Sets, GNN, MPNN)

- Euclidean symmetries in jet images (CNN's)
- Rotational, boost, Lorentz symmetries

Permutations of particles (particle clouds, Deep Sets, GNN, MPNN)

• Linear: a restricted linear mixing operations acting on data stored as a collection of irreducible representations $\alpha A + \beta B$

- of irreducible representations $\alpha A + \beta B$
- Nonlinear: a tensor product combined with a Clebsch-Gordan decomposition

 $\otimes : R$

 $\rho_1(g) \otimes \rho_2(g) = C$

Linear: a restricted linear mixing operations acting on data stored as a collection

$$R_1 \times R_2 \to R_3$$

$$\Gamma_{\rho_1,\rho_2} \left[\bigoplus_{\rho \in 1}^{\mu(\rho)} \rho(g) \right] C^{\dagger}_{\rho_1,\rho_2}$$

- Linear: a restricted linear mixing operations acting on data stored as a collection of irreducible representations $\alpha A + \beta B$
- Nonlinear: a tensor product combined with a Clebsch-Gordan decomposition
- A covariant universal approximation theorem motivates the sufficiency of these operations for outputs belonging to arbitrary finite-dimensional representations.
 - $\otimes : R$
 - $\rho_1(g) \otimes \rho_2(g) = C_{\rho}$

$$R_1 \times R_2 \to R_3$$

$$\int_{\rho_1,\rho_2} \left[\bigoplus_{\substack{\rho \\ \rho }} \bigoplus_{\substack{1 \\ \rho }} \rho(g) \right] C^{\dagger}_{\rho_1,\rho_2}$$

What constraints does full Lorentz+Permutation symmetry impose?

Invariants of the Lorentz group

VECTOR INVARIANTS

6. Second example: unimodular group SL(n)

We shall take up the question of invariants of the unimodular group SL(n)at once for any number of covariant or Latin vectors x, y, \cdots and any number of contravariant or Greek vectors ξ , η , \cdots . THEOREM (2.6.A).

 $[xy \cdots z],$ (

is a complete table of typical basic invariants for the unimodular group. load to the ages where only

$$(\xi x), \qquad [\xi \eta \cdots \zeta]$$

[H. Weyl, The Classical Groups, 1939]

45

Invariants of the Lorentz group

functions of only the dot products $d_{ii} = \eta_{\mu\nu} p_i^{\mu} p_i^{\nu}$

All Lorentz-invariant symmetric functions of a set of 4-vectors p_i^{μ} can be expressed as

 $I(p_1, ..., p_N) = I\left(\{p_i \cdot p_j\}_{i,j}\right)$

 $p_i \cdot p_i = p_i^0 p_i^0 - \overrightarrow{p_i} \cdot \overrightarrow{p_i}$

Input to the network: matrix of dot products $d_{ij} = p_i \cdot p_j$

 \mathbf{N}

Permutation equvariant architecture with only edge data?

PEL CAN

PELICANPermutation Equivariant, Lorentz Invariant/Covariant Aggregator Net

• Basic approach — Deep Sets $\rho\left(\sum_{i} \phi(x_{i})\right)$

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- Basic approach Deep Sets $\rho\left(\sum_{i}\phi\right)$
- Common approach GNN/MPNN: v'_i
- For pure "edge data", look for the most $T_{ij} \mapsto T'_{ij}$

$$F\left(\pi\circ T_{i_1i_2\cdots i_r}\right)=\pi\circ F\left(T_{i_1i_2\cdots i_s}\right), \quad \pi\in S_N.$$

$$b(x_i))$$

= $f(v_i, \sum_j m_{ij}(v_i, v_j))$

For pure "edge data", look for the most general permutation-equivariant mapping

• Basic approach — Deep Sets $\rho\left(\sum_{i}\phi\right)$ Common approach — GNN/MPNN: v'_i $T_{ij} \mapsto T'_{ij}$

$$F\left(\pi\circ T_{i_1i_2\cdots i_r}\right)=\pi\circ F\left(T_{i_1i_2\cdots i_s}\right), \quad \pi\in S_N.$$

The space of such linear mappings between $N \times N$ matrices is 15-dimensional

$$b(x_i))$$

= $f(v_i, \sum_j m_{ij}(v_i, v_j))$

For pure "edge data", look for the most general permutation-equivariant mapping

Let's illustrate equivariant mappings $T_{ij} \mapsto T'_{ij}$ as rank 4 binary tensors (N = 2)

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Identity map

Let's illustrate equivariant mappings $T_{ij} \mapsto T'_{ij}$ as rank 4 binary tensors (N = 2)

$T'_{22} = \text{Agg}(\{T_{22}\})$

Let's illustrate equivariant mappings $T_{ij} \mapsto T'_{ij}$ as rank 4 binary tensors (N = 2)

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The aggregation function can be any symmetric function of a set of inputs. We choose weighted means $N^{\alpha} \sum_{i=1}^{N} x_{i}$ with learnable α . i=1

•		

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PELICAN equivariant block

PELICAN equivariant block

Linear mixing of the outputs of 15 aggregators
PELICAN Classifier



Classifier

$p_i \rightarrow d_{ij} \rightarrow \text{Embed} \rightarrow [\text{Eq}_{2\rightarrow 2}]^L \rightarrow \text{Eq}_{2\rightarrow 0} \rightarrow \text{MLP}$



PELICAN Classifier

$p_i \rightarrow d_{ij} \rightarrow \text{Embed} \rightarrow$



Classifier

$$\begin{bmatrix} Eq_{2\rightarrow 2} \end{bmatrix}^L \rightarrow \boxed{Eq_{2\rightarrow 0}} \rightarrow MLP$$



Top-tagging with PELICAN





Top-tagging performance

- State of the art top-tagger with 8x fewer params of the previous best tagger
- Exact invariance massively improves sample efficiency



Architecture	Accuracy	AUC	$1/\epsilon_B$	# Params
LGN	0.929(1)	0.964(14)	424 ± 82	4.5k
PFN	0.932	0.982	891 ± 18	82k
ResNeXt	0.936	0.984	1122 ± 47	1.46M
ParticleNet	0.938	0.985	1298 ± 46	498k
LorentzNet	0.942	0.9868	2195 ± 173	220k
PELICAN	0.9425(1)	0.9869(1)	2289±204	46k



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Sample efficiency

• Exact invariance improves sample efficiency



Regression with PELICAN



Lorentz equivariance

All Lorentz-equivariant mappings $F^{\mu}(p_1, ..., p_N)$ have the form

 $F(p_1, ...,]$

where $c_i(p_1, ..., p_N)$ are Lorentz-invariant, i.e. only functions of d_{ij} .

$$p_N) = \sum_i c_i p_i,$$

Lorentz equivariance

All Lorentz-equivariant mappings $F^{\mu}(p_1, ..., p_N)$ have the form

 $F(p_1, ..., p_n)$

What about permutation invariance?

$$p_N) = \sum_i c_i p_i,$$

where $c_i(p_1, ..., p_N)$ are Lorentz-invariant, i.e. only functions of d_{ii} .



Lorentz-equivariant

 $F^{\mu}(p_1, ..., p_N)$



Lorentz-equivariant

 $F^{\mu}(p_1,...,p_N)$

Permutation-equivariant $C_i\left(\left\{d_{jk}\right\}\right)$



Lorentz-equivariant

 $\overline{F^{\mu}(p_1,\ldots,p_N)}$

Permutation-equivariant $C_i\left(\left\{d_{jk}\right\}\right)$

 $F^{\mu}(p_1, \dots, p_N) = \sum c_i p_i^{\mu}$



PELICAN 4-momentum Regressor

 $p_i \rightarrow d_{ij} \rightarrow \text{Embed} \rightarrow [\text{Eq}_{2\rightarrow}]$



4-momentum regressor

$$_{2}$$
 \rightarrow $Eq_{2 \rightarrow 1}$ \rightarrow $MLP \rightarrow \{c_i\}_{i=1}^N$

PELICAN 4-momentum Regressor

4-momentum regressor

 $p_i \rightarrow d_{ij} \rightarrow \text{Embed} \rightarrow [\text{Eq}_{2-i}]$



PELICAN weights

$$_{2}$$
 \rightarrow $Eq_{2 \rightarrow 1}$ \rightarrow $MLP \rightarrow \{c_i\}_{i=1}^{N}$

PELICAN 4-momentum Regressor

 $p_i \rightarrow d_{ii} \rightarrow \text{Embed} \rightarrow \text{Eq}_{2-1}$

The 4-momentum is reconstructed

The loss function is a linear combination of $|m_{\text{predict}} - m_{\text{target}}|$ and $|\vec{p}_{\text{predict}} - \vec{p}_{\text{target}}|$



4-momentum regressor

PELICAN weights

$$_{2} \rightarrow \mathbb{E}q_{2 \rightarrow 1} \rightarrow \mathbb{MLP} \rightarrow \{c_i\}_{i=1}^N$$

$$as p_{predict} = \sum_{i=1}^{N} c_i p_i$$



Dataset similar to the top-tagging one:





Dataset similar to the top-tagging one:

Only top jets 1.







Dataset similar to the top-tagging one:

- Only top jets 1.
- Only hadronic decays $t \rightarrow bW(qq)$ 2.







Dataset similar to the top-tagging one:

- Only top jets 1.
- Only hadronic decays $t \rightarrow bW(qq)$ 2.
- Two versions: truth level and DELPHES 3. reconstructed from calorimeter towers







Dataset similar to the top-tagging one:

- Only top jets 1.
- 2. Only hadronic decays $t \rightarrow bW(qq)$
- Two versions: truth level and DELPHES 3. reconstructed from calorimeter towers
- 4. Non-ML baseline: built-in method of the Johns Hopkins top-tagger (37%/31% efficiency on these datasets)

top_candidate.structure_of<TopTaggerBase>().W()

[Kaplan, Rehermann, Schwartz, Tweedie 2008]







W

b

 \mathcal{N}



JH = Johns Hopkins Top Tagger [Kaplan, Rehermann, Schwartz, Tweedie 2008]

PELICAN | JH = PELICAN on JH-tagged events





JH = Johns Hopkins Top Tagger [Kaplan, Rehermann, Schwartz, Tweedie 200

PELICAN | JH = PELICAN on JH-tagged ever

Γ (%)	σ_m (%)	σ_{ψ} (centirad)	
0.65%	1.27%	0.156	
0.82%	1.20%	0.384	
0.27%	0.59%	0.088	
0.3 %	8.3 %	8.73	
5.51%	3.22%	4.16	
3.81%	2.86%	2.67	//
			7
[80			1
nts			→ \$\overline{q}\$









DELPHES





Explaining PELICAN

Distribution of output PELICAN weights on truth-level dataset (~100k events)



Explaining PELICAN

200 events



Energy of constituents

Explaining PELICAN

200 events



PELICAN weight

PELICAN learns to separate out the b-quark cluster













PELICAN-reconstructed W



Truth



Truth level

JH

PELICAN weight



Truth



Truth level

JH

PELICAN weight


Truth



Truth level

JH

PELICAN weight



Truth



Truth level

JH

PELICAN weight

And these are only events successfully tagged by JH (~37%)!





Truth level

PELICAN is consistently better at identifying the W clusters



Truth level

PELICAN is consistently better at identifying the W clusters

DELPHES dataset



Distribution of output PELICAN weights on DELPHES dataset





200 random events













JH

DELPHES





PELICAN is consistently better at identifying the W clusters



PELICAN is consistently better at identifying the W clusters



• What is the function of non-binary weights in the DELPHES case?

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Hypothesis:

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Hypothesis:

• to undo the effect of multiple decay products hitting the same calorimeter cell

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• to correct the mass of the reconstruction

- What is the function of non-binary weights in the DELPHES case?
- Hypothesis:
 - to undo the effect of multiple decay products hitting the same calorimeter cell
 - to correct the mass of the reconstruction

Define
$$r_i = E_i^{W_{\text{true}}}/E_i$$
. Note that $E^{W_{\text{true}}} = \sum_i r_i E_i$

Therefore expect high correlation $c_i \sim r_i$





Pb+Pb, 5.02 TeV
Run: 365681
Event: 1064766274
2018-11-11 22:00:07 CEST

 $\Sigma E_{\rm T}^{\rm FCal} = 71 \text{ GeV} (left), 0.9 \text{ GeV} (right)$ 71 tracks, $p_{\rm T} > 0.4 \text{ GeV}$

ATLAS Experiment © 2022 CERN



Don't beam axes break SO(3) symmetry?



Pb+Pb, 5.02 TeV Run: 365681 Event: 1064766274 2018-11-11 22:00:07 CEST

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Don't beam axes break SO(3) symmetry?

No! Rather than giving up symmetry, provide complete inputs.



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 $p_1, ..., p_N$



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Detector breaks symmetry? Don't beam axes break SO(3) symmetry?

No! Rather than giving up symmetry, provide complete inputs.

$$e_{z+}, e_{z-}, p_1, \dots, p_N$$

 $e_{z+} = (1,0,0,1), e_{z-} = (1,0,0,-1)$



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Detector breaks symmetry? Don't beam axes break SO(3) symmetry?

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$$e_{z+}, e_{z-}, p_1, \dots, p_N$$

 $e_{z+} = (1,0,0,1), e_{z-} = (1,0,0,-1)$

Now PELICAN knows E_i, m_i, p_i^T, p_i^Z .



Pb+Pb, 5.02 TeV Run: Event: 1064766274 2018-11-11 22:00:07 CEST

 $\Sigma E_{\rm T}^{\rm FCal} = 71 \,\,{
m GeV} \,\,({
m left}) , \,\,0.9 \,\,{
m GeV} \,\,({
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Mass reconstruction



Truth level



m_{true}

m_{true}

Truth level

PELICAN uses beams to adjust mass



Delphes







Delphes

PELICAN uses beams to adjust mass



Mass regression



Transfer Learning: W mass measurement

Truth level

Trained on 80GeV jets Evaluated on 72GeV jets



Transfer Learning: W mass measurement

Delphes

Trained on 80GeV jets Evaluated on 72GeV jets



Truth level modified W mass (GeV)

Truth level modified W mass (GeV)



• IRC safe PELICAN



IRC safe PELICAN

Looking inside jets: parent reconstruction

- IRC safe PELICAN
- Looking inside jets: parent reconstruction
- Integrated pipeline: tagging \rightarrow regression

- IRC safe PELICAN
- Looking inside jets: parent reconstruction
- Integrated pipeline: tagging \rightarrow regression
- Polarization tagging (helicity angle distributions)
Other applications

- IRC safe PELICAN
- Looking inside jets: parent reconstruction
- Integrated pipeline: tagging \rightarrow regression
- Polarization tagging (helicity angle distributions)
- Jet combinatorics?



