#### Deep Learning at the LHC: Tagging Resonances & Discovering New Physics

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Bundesministerium für Bildung und Forschung



CMS Experiment at the LHC, CERN Data recorded: 2012-May-27 23:35:47.271030 GMT Run/Event: 195099 / 137440354

Higgs Boson Discovery in 2012

#### Discovery to Precision...





Why are neutrinos massive?

#### What are the origins of the LHCb flavour anomaly?



#### What is the nature of dark matter & dark energy?



Why is there more matter than antimatter?

#### What are the details of cosmic inflation?

How can the Higgs boson be light when the mass receives large quantum corrections?

#### ... but no new physics so far



Selection of observed limits at 95% C.L. (theory uncertainties are not included). Probe up to the quoted mass limit for light LSPs unless stated otherwise. The quantities  $\Delta M$  and x represent the absolute mass difference between the primary sparticle and the LSP, and the difference between the intermediate sparticle and the LSP relative to  $\Delta M$ , respectively, unless indicated otherwise.

# Build better tools to identify known particles

### Heavy Resonance Tagging



- Hadronically decaying top/Higgs/W/Z
- Contained in one (large-R) jet
- How to distinguish from light quark/gluon jets (and from each other)
- For new physics searches (and SM studies)

Towards an Understanding of the Correlations in Jet Substructure D Adams et al (BOOST 2013 Participants), Eur.Phys.J. C75 Top Tagging, T Plehn, M Spannowksy, J.Phys. G39 (2012) 083001 Boosted Top Tagging Method Overview, GK, Proc.Top2017

#### Mass

Calculate using a grooming algorithm (eg mMDT/softdrop or pruning)

- Centers of hard radiation
   n-subjettiness or energy correlation
   functions
- Flavour
   b tagging of large-R jets or subjets

#### Combinations







- Measure particle energies in calorimeter
- Reconstruct jet from individual measurements
- Image preprocessing
  - center, rotate, mirror, pixelate, trim, normalise





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# Deep Learning

### Humans vs Machines

#### • 2015 Image Classification:

- K. He et al (Microsoft Research), Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification, 1502.01852
- 2016 **Go**:
  - Alpha Go (D. Silver et al, Mastering the game of Go with deep neural networks and tree search, Nature 529, pp484–489 and D.
     Silver et al Mastering the game of Go without human knowledge, Nature 550, pp354–359)

#### • 2016 Speech recognition:

- W. Xiong et al (Microsoft Research) Achieving Human Parity in Conversational Speech Recognition, 1610.05256
- 2017 **Poker** (heads-up no-limits Texas Hold'em):
  - N Brown and T Sandholm, Superhuman AI for heads-up no-limit poker: Libratus beats top professionals, Science 359, Issue 6374, pp418-424
- 2018 Translation (Chinese-English)
  - H H Awadalla et al (Microsoft AI & Research) Achieving Human Parity on Automatic Chinese to English News Translation
- 20?? Particle Physics



• to be seen



GT: horse cart 1: horse cart 2: minibus 3: oxcart 4: stretcher 5: half track



**GT: birdhouse** 1: birdhouse 2: sliding door 3: window screen 4: mailbox 5: pot



GT: forklift 1: forklift 2: garbage truck 3: tow truck 4: trailer truck 5: go-kart



**GT: coucal** 1: coucal 2: indigo bunting 3: lorikeet 4: walking stick 5: custard apple



GT: komondor 1: komondor 2: patio 3: llama 4: mobile home 5: Old English sheepdog



2: slug



1: yellow lady's slipper 3: hen-of-the-woods 4: stinkhorn 5: coral fungus



GT: torch 1: stage 2: spotlight 3: torch 4: microphone 5: feather boa



GT: mountain tent 1: sleeping bag 2: mountain tent 3: parachute 4: ski 5: flagpole



1: acoustic guitar 2: shoji 3: bow tie 4: cowboy hat 5: banjo



**GT:** geyser 1: geyser 2: volcano 3: sandbar 4: breakwater 5: leatherback turtle



#### GT: go-kart

1: go-kart 2: crash helmet 3: racer 4: sports car 5: motor scooter



16

GT: microwave 1: microwave 2: washer 3: toaster 4: stove 5: dishwasher

### ImageNet



#### **14M** labelled images

- 20k categories
- http://image-net.org

# A Very Simple Network



$$y = f(f(x_1)w_1 + f(x_2)w_2)$$
$$f(x) = \Theta(x) \cdot x$$



- Backpropagation + Gradient descent
  - Pass input  $(x_1, x_2)$  to ANN
  - Calculate output (y) and difference to true value  $\hat{y}$  ) This is the loss function L
  - Find gradient of loss function with respect to weights
  - Use gradient to find new weights

**Regression loss function:** 

$$L(y, \hat{y}) = (y - \hat{y})^2$$
$$w'_i = w_i + \alpha \cdot \frac{\partial I}{\partial u}$$

#### Problem: Classification

Distinguish a pair of classes (binary) or several (multi-class).

#### Cat vs Dog



### Classification

$$H(p,q) = -\sum p_i \ln q_i = H(p) + D_{KL}(p||q)$$

 Minimizing cross entropy: For fixed p - minimise difference (KL-divergence) between q and p

$$\frac{1}{N}\ln\Pi_i q_i^{Np_i} = \sum_i p_i \ln q_i = -H(p,q)$$

 Minimizing cross entropy: Equivalent to maximising the likelihood





### Complexity

ResNet-50

 $7 \times 7, 64$ , stride 2

 $3 \times 3$  max pool, stride 2

 $\times 3$ 

 $\times 4$ 

×6

 $\times 3$ 

1×1,64

3×3, 64

1×1,256

1×1, 128 3×3, 128

1×1, 512 1×1,256

3×3,256

1×1, 1024

1×1, 512

3×3, 512

1×1, 2048

global average pool

1000-d fc, softmax

 $25.5 \times 10^{6}$ 

 $4.1 \times 10^{9}$ 

output

56×56

 $28 \times 28$ 

14×14

7×7

 $1 \times 1$ 

ResNeXt-50  $(32 \times 4d)$ 

 $7 \times 7$ , 64, stride 2

 $3 \times 3$  max pool, stride 2

3×3, 128, *C*=32

3×3, 256, *C*=32

3×3, 512, *C*=32

3×3, 1024, *C*=32

global average pool

1000-d fc, softmax

 $25.0 \times 10^6$ 

**4.2**×10<sup>9</sup>

 $\times 3$ 

 $\times 4$ 

 $\times 6$ 

 $\times 3$ 

1×1, 128

1×1,256

1×1,256

1×1, 512

1×1,512

1×1, 1024

1×1, 1024

1×1, 2048

### Convolution





Efficient use of weights and natural encoding of translational symmetry.

### Convolution network



#### How to build a convolution network?

- Multiple parallel and successive convolutions
- Pooling
- Simple network in the end





### **Comparison Studies**

- That's A LOT of different approaches
- How do they compare?
- Many aspects let's start with a very simple problem
  - Top Jets vs QCD jets
  - Only use four-vectors
  - Ignore detector effects, pile-up and, uncertainties
- Available at:
  - <u>http://tinyurl.com/yxq8q3uk</u>

#### Dataset

- Comparison study of different top tagging algorithms on common sample.
- Pythia + Delphes, AntiKt (R=0.8) top jets with pT in [550,650] GeV vs QCD
- I.2M training events, 400k each for validation and testing
- Up to 200 constituent 4-vectors per jet



#### The Machine Learning Landscape of Top Taggers

G. Kasieczka (ed)<sup>1</sup>, T. Plehn (ed)<sup>2</sup>, A. Butter<sup>2</sup>, K. Cranmer<sup>3</sup> D. Debnath<sup>4</sup>,
M. Fairbairn<sup>5</sup>, W. Fedorko<sup>6</sup>, C. Gay<sup>6</sup>, L. Gouskos<sup>7</sup>, P. T. Komiske<sup>8</sup>, S. Leiss<sup>1</sup>, A. Lister<sup>6</sup>,
S. Macaluso<sup>3,4</sup>, E. M. Metodiev<sup>8</sup>, L. Moore<sup>9</sup>, B. Nachman,<sup>10,11</sup>, K. Nordström<sup>12,13</sup>,
J. Pearkes<sup>6</sup>, H. Qu<sup>7</sup>, Y. Rath<sup>14</sup>, M. Rieger<sup>14</sup>, D. Shih<sup>4</sup>, J. M. Thompson<sup>2</sup>, and S. Varma<sup>5</sup>

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arXiv: 1902.09914

### Overview



	AUC	Accuracy	$1/\epsilon_{P}(\epsilon)$	q = 0.3	#Parameters
		licearcej	mean	median	
CNN [16]	0.981	0.930	$995{\pm}15$	$966{\pm}18$	610k
$\operatorname{ResNeXt}$ [30]	0.984	0.936	$1246{\pm}28$	$1286{\pm}31$	1.46M
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GoaT (see text)	0.985	0.939	1440		25k

# Images

#### Pulling Out All the Tops with Computer Vision and Deep Learning, S Macaluso, D Shih, 1803.00107

stage	output	ResNet-50		<b>ResNeXt-50</b> (32×4d)		
conv1	112×112	7×7, 64, stride 2		7×7, 64, stride 2		
		$3 \times 3$ max pool, stride	2	$3 \times 3$ max pool, stride 2		
conv?	56~56	[ 1×1, 64 ]		[ 1×1, 128		
01172	20×20	3×3, 64 ×3		3×3, 128, <i>C</i> =32 ×3		
		1×1, 256		1×1,256		
		[ 1×1, 128 ]		[ 1×1, 256 ]		
conv3	28×28	3×3, 128 ×4	.	3×3, 256, <i>C</i> =32 ×4		
		1×1, 512		1×1,512		
		[ 1×1, 256 ]		[ 1×1, 512 ]		
conv4	14×14	3×3,256 ×	5	3×3, 512, <i>C</i> =32 ×6		
		[ 1×1, 1024 ]		1×1,1024		
		[ 1×1, 512 ]		[ 1×1, 1024 ]		
conv5	7×7	3×3, 512 ×3	3	3×3, 1024, <i>C</i> =32 ×3		
		1×1, 2048		1×1, 2048		
	1 \sc 1	global average pool		global average pool		
	1 X 1	1000-d fc, softmax		1000-d fc, softmax		
# pa	arams.	<b>25.5</b> ×10 <sup>6</sup>		<b>25.0</b> ×10 <sup>6</sup>		
FI	LOPs	<b>4.1</b> ×10 <sup>9</sup>		<b>4.2</b> ×10 <sup>9</sup>		

Feature

Conv

kernel

4x4

64@36x36

maps

Feature

64@18x18

Max-pool

2x2

kernel

maps

Feature

Conv

kernel

4x4

maps

Feature

Conv

kernel

4x4

128@37x37

maps

Inputs

4@37x37

	AUC	Accuracy	$\begin{vmatrix} 1/\epsilon_B \ (\epsilon_S = 0.3) \\ mean median \end{vmatrix}$		#Parameters
$\begin{array}{c} \text{CNN} \ \boxed{16} \\ \text{ResNeXt} \ \boxed{30} \end{array}$	$0.981 \\ 0.984$	0.930 0.936	995 $\pm 15$ 1246 $\pm 28$	$966{\pm}18$ $1286{\pm}31$	$\begin{array}{c} 610 \mathrm{k} \\ 1.46 \mathrm{M} \end{array}$
TopoDNN [18] Multi-body <i>N</i> -subjettiness 6 [24] Multi-body <i>N</i> -subjettiness 8 [24] TreeNiN [43] P-CNN ParticleNet [47]	$\begin{array}{c} 0.972 \\ 0.979 \\ 0.981 \\ 0.982 \\ 0.980 \\ 0.985 \end{array}$	$\begin{array}{c} 0.916 \\ 0.922 \\ 0.929 \\ 0.933 \\ 0.930 \\ 0.938 \end{array}$	$ \begin{vmatrix} 378 \pm 5 \\ 802 \pm 12 \\ 926 \pm 20 \\ 1209 \pm 23 \\ 838 \pm 13 \\ 1383 \pm 45 \end{vmatrix} $	$391 \pm 8$ $783\pm13$ $886\pm18$ $1167\pm24$ $841\pm14$ $1374\pm41$	59k 57k 58k 34k 348k 498k
LBN [19] LoLa [22] Energy Flow Polynomials [21] Energy Flow Network [23] Particle Flow Network [23]	0.981 0.980 0.980 0.979 0.982	0.931 0.929 0.932 0.927 0.932	$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	$971\pm 20$ $751\pm 11$ $729\pm 11$ $1005\pm 29$	705k 127k 1k 82k 82k
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### Basis

How Much Information is in a Jet? K Datta, A Larkoski, 1704.08249 Reports of My Demise Are Greatly Exaggerated: N-subjettiness Taggers Take On Jet Images, L Moore et al 1807.04769 Energy flow polynomials: A complete linear basis for jet substructure,

PT Komiske, ER Metodiev, J Thaler, 1712.07124

<b>N-Subjettiness:</b>	particle 1 $/^{z_1}$
particle 1	particle 2
θ	$\theta_{12}$ $z_2$ $\theta_{23}$
	$\theta_{13}$
particle 2	particle 3

$$\tau_N^{(\beta)} = \frac{1}{p_{TJ}} \sum_{i \in \text{Jet}} p_{Ti} \min\left\{R_{1i}^\beta, R_{2i}^\beta, \dots, R_{Ni}^\beta\right\}$$

2-body:	$ au_1^{(1)},  au_1^{(2)}$	$-\!\!\!<$	$=\sum_{m}\sum_{m}\sum_{m}\sum_{m}\sum_{m}\sum_{m}\sum_{m}\sum_{m}$
3-body:	$ au_1^{(0.5)},  au_1^{(1)},  au_1^{(2)},  au_2^{(1)},  au_2^{(2)}$		$i_1 = 1$ $i_2 = 1$ $i_3 = 1$ $i_4 = 1$
4-body:	$\tau_1^{(0.5)}, \tau_1^{(1)}, \tau_1^{(2)}, \tau_2^{(0.5)}, \tau_2^{(1)}, \tau_2^{(2)}, \tau_3^{(1)}, \tau_3^{(2)}$		1000 graphs use
5-body:	$\tau_1^{(0.5)}, \tau_1^{(1)}, \tau_1^{(2)}, \tau_2^{(0.5)}, \tau_2^{(1)}, \tau_2^{(2)}, \tau_3^{(0.5)}, \tau_3^{(1)}, \tau_3^{(2)}, \tau_4^{(1)}, \tau_4^{(2)}, \tau_4^{(1)}, \tau_4^{(2)}, \tau_4^{(1)}, \tau_4^{(2)}, \tau_4^{(1)}, \tau_4^{(2)}, \tau_4$	2)	
6-body:	$\tau_1^{(0.5)}, \tau_1^{(1)}, \tau_1^{(2)}, \tau_2^{(0.5)}, \tau_2^{(1)}, \tau_2^{(2)}, \tau_3^{(0.5)}, \tau_3^{(1)}, \tau_3^{(2)}, \tau_4^{(0.5)}, \tau_$	$\tau_4^{(1)}, \tau_4^{(2)},$	$ au_5^{(1)}, au_5^{(2)}$

	AUC	Accuracy	$1/\epsilon_B \ (\epsilon_B \ \mathrm{mean})$	S = 0.3) median	#Parameters
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 $ullet_{j} \iff \sum_{i_{j}=1} z_{i_{j}}$ 

#### **Energy Flow Polynomials:**

# $= \sum_{i_1=1}^{M} \sum_{i_2=1}^{M} \sum_{i_3=1}^{M} \sum_{i_4=1}^{M} \sum_{i_4=1}^{M} z_{i_1} z_{i_2} z_{i_3} z_{i_4} \theta_{i_1 i_2} \theta_{i_2 i_3} \theta_{i_2 i_4}^2 \theta_{i_3 i_4}$

*k* \_\_\_\_\_

1000 graphs used in linear model

 $\ell \iff heta_{i_k i_\ell}$ 

#### Lorentz Layer and Lorentz Boost Network

Deep-learning Top Taggers & No End to QCD A Butter, GK, T Plehn, M Russell 1707.08966 Lorentz Boost Networks: Autonomous Physics-Inspired Feature Engineering M. Erdmann, E. Geiser, Y. Rath, and M. Rieger 1812.09722

Input is a pT sorted list of Lorentz four-vectors: (calo towers or particle flow objects)

Combination Layer (**CoLa**): create linear combinations:  $k_{\mu,i} \stackrel{\text{CoLa}}{\longrightarrow} \widetilde{k}_{\mu,j} = k_{\mu,i} C_{ij}$ 

 $k_{\mu,i} = \begin{pmatrix} E_0 & E_1 & \dots & E_N \\ p_{x,0} & p_{x,1} & \dots & p_{x,N} \\ p_{y,0} & p_{y,1} & \dots & p_{y,N} \\ p_{y,0} & p_{y,1} & \dots & p_{y,N} \end{pmatrix}$ 

Lorentz Layer (**LoLa**): Use resulting matrix to extract physics features. Main assumption is the Minkowski metric

Fully connected layers for final output

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#### Lorentz Boost Network





# Deep Sets

Energy Flow Networks: Deep Sets for Particle Jets, PT Komiske, EM Metodiev, J Thaler, 1810.05165

PFN: 
$$F\left(\sum_{i=1}^{M} \Phi(p_i)\right)$$

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Translated Azimuthal Angle  $\phi$ 

Particles

Observable





Translated Rapidity y

# N-Vectors

Jet Constituents for Deep Neural Network Based Top Quark Tagging, J Pearkes et al, 1704.02124 QCD-Aware Recursive Neural Networks for Jet Physics, G Louppe et al, 1702.00748 ParticleNet: Jet Tagging via Particle Clouds, H Qu, L Gouskos, 1902.08570

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			mean	median	
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LoLa [22]	0.980	0.929	$768 {\pm} 11$	$751{\pm}11$	127k
Energy Flow Polynomials [21]	0.980	0.932	380		l 1k
Energy Flow Network [23]	0.979	0.927	$734{\pm}13$	$729{\pm}11$	82k
Particle Flow Network [23]	0.982	0.932	$1005 \pm 21$	$1005 \pm 29$	82k
GoaT (see text)	0.985	0.939	1440		25k

#### Fully connected



#### I D Convolution











#### **Rediscovered Ensembling!**

# Transfer Learning

- There exist very powerful architectures for image classification
  - InceptionResNetV2 weights available (55M weights, 572 layers)
  - Trained on 1000 classes of "real" photographs
  - Why not just apply it to jet images?
  - Preprocessing



Image class "ice cream" identifies QCD jets

% training sample used

10

transfer trained

images

15

20

### Systematic Uncertainties



- Simulate systematic differences between training MC and collision data
- Test network response under
  - rescaling of 4-vector inputs (mimic jet energy scale)
  - adding Pile-Up
- Test mitigation with data augmentation/ adversarial training

Plot by Sven Bollweg (BSc thesis), work with Heidelberg (Blehn),

# Data Augmentation

- Test network response under global rescaling of all 4-vector inputs (simimilar to jet energy scale)
- Re-train network using shifted samples as well.
  - So the network sees multiple (shifted) copies of the event = data augmentation
- Trade off performance and stability
- Now looking into multiple simultaenous uncertainties
  - resolution
  - pile up
  - lost particles
  - . . .
- Can adversarial training help further?



# Bayesian Networks

1.3

H<sub>3</sub>

1



0.8

0.0 -

-0.4 -

0.0

1.2

- So far discussed handling uncertainties on the inputs
- How can we with training data not fully covering the phase space?
- Sampling over Gaussian distribution for weights

C Blundell et al, ICML Proc's 2015

04

0.0

0.0

-0.4

Weigh

0.8

1.2

0.4

### Bayesian' Cont'd

- learn classification output and uncertainty
- $(60 \pm 30)\%$  top is very different from  $(60 \pm 1)\%$  top
- tagger calibration part of the network training
- for instance: effect of MC statistics



Plehn - Aspen 2019 Bollweg, Haussmann, GK, Luchmann, Pehn, Thompson: Upcomimg

### Preview

- First look at impact of Jet Energy Scale uncertainty
- Only rescale leading subset



Bollweg, Haussmann, GK, Luchmann, Pehn, Thompson: Upcomimg

# Look for unknown signatures

# Can we look for new physics, without knowing what to look for?

# Can we avoid systematic uncertainties in searches?



### Autoencoder



$$L = (\hat{y} - g(f(x)))^2$$

- Self-supervised learning
- Latent space/bottleneck with compressed representation
- Dimension reduction
- Denoising

kvfrans <u>deeplearningbook.org</u>

### Autoencoder for Physics



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- Can we find new physics without knowing what to look for?
- Train on pure QCD light quark/gluon jets and apply to top tagging
- Top quarks/ new physics identified as anomaly

#### QCD or What?

T Heimel, GK, T Plehn, JM Thompson, 1808.08979 Searching for New Physics with Deep Autoencoders M Farina, Y Nakai, D Shih, 1808.08992



# **Combined Setup**

- Autoencoder alone will also learn mass distribution
- Counteract with adversary:



### Mass Sculpting

• Tune mass dependency with Lagrange multiplier:

$$L = L_{\text{auto}} - \lambda L_{\text{adv}}(M)$$



# Signal contamination

- Procedure works also when signal is present in training data
- We now have a versatile tool to search for new physics (anomalies) in a purely data driven and unsupervised way
  - Apply to LHC collision data!
  - Potential trigger!



### Variational Autoencoder



- We want to sample from latent space
- Split into mean and standard deviation
- Add penalty term (Kullback-Leibler divergence) so mean/std are close to unit Gaussian

kvfrans towardsdatascience.com

#### Concrete



#### Variational Autoencoder



**Reconstruction Loss Only** 

KL Loss Only

 $\sum_{i=1}^{n} \sigma_i^2 + \mu_i^2 - \log(\sigma_i) - 1$ 

i=1

**Combined Loss** 

$$L = (\hat{y} - g(f(x)))^2$$

kvfrans towardsdatascience.com



Latent Constraints: Learning to Generate Conditionally from Unconditional Generative Models, J Engel, M Hoffman, A Roberts, 1711.05772

### Extend to event tagging



- Variational auto encoder
- Train on SM event cocktail
- Test sensitivity to different BSM models

• Opportunity for future trigger?

Variational Autoencoders for New Physics Mining at the Large Hadron Collider O. Cerri et al, 1811.10276

#### Alternative: CWoLa



# Alternative: CWola Hunting



• Assume signal is resonant in one variable

54

- Define signal region and sidebands
- Train classifier and look for excess

Anomaly Detection for Resonant New Physics with Machine Learning JH Collins, K Howe, B Nachman 1805.02664

# Spectrum of MC Reliance



#### Dependence on Simulation

Assumes a classifier trained on MC will be correct on data as well Assume MC gets the fractions of different classes right on average Assume that we can tune the adversarial setup such that an anomaly based on data is credible.

Assume simulation is good. Do not depend on specific model (but still limited by which models are in the mix)

Assume interpolation between phases spaces in data.

### What else?

- Autoencoding is an exciting new tool in our box
- What else can we do?
  - Better understand what's going on in the latent space?
  - Event level?
  - Other things than searches?
  - ...

# LHC Olympics 2020



https://indico.cern.ch/event/809820/page/16782-Ihcolympics2020

#### LHC Olympics 2020 Dataset

- Challenge to find new physics in simulated events
- Whatever approach you like BUT we will not tell what the signal is
- Warm up phase: now until ~1.1.2020
  - IM QCD events + Signal (labelled) available, single jet 1.3 TeV trigger
  - Use to develop methods to find new physics.
- Challenge Phase: ~1.1.2017 ~15.1.2017:
  - Find new physics (yes/no, mass, x-sec) in the dataset
  - No labels provided
- At ML4Jets (15.1.-17.1.2020):
  - Identify winners, discuss strategies and write-up

#### Get the data here:

https://zenodo.org/record/2629073#.XKyG0-szbh9

# Conclusions

- Deep learning and its applications to physics is a lively and exciting research area
- Images are a powerful tool to represent physics/detector/other information (although they are not perfect)
- Potential for new physics searches from:
  - Better reconstruction of known particles
  - Detection techniques for long-lived objects
  - New model-independent searches

# Thank you!