# Deep Learning and Computer Vision in High Energy Physics

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SLAC

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# Aspects of Machine Learning (ML) in HEP

#### <u>Optimization</u>

- Bottom line is performance
- But can we build new better (simple?) features?

#### • <u>Teaching the learning</u>

- Guide and boost performance of ML algorithms using physics knowledge (i.e. domain specific knowledge)
- We don't want ML to relearn special relativity

#### • Learning from Learning ...(if we can)

- Can we extract information about what the ML is learning?
- Can we use this information to design new variables?
- Often visualization is a key component



Coefficient

# Machine Learning Applied Widely in HEP

#### • In analysis:

- Classifying signal from background, especially in complex final states
- Reconstructing heavy particles and improving the energy / mass resolution

#### • In reconstruction:

- Improving detector level inputs to reconstruction
- Particle identification tasks
- Energy / direction calibration
- In the trigger:
  - Quickly identifying complex final states

#### • In computing:

 Estimating dataset popularity, and determining needed number and location of dataset replicas



#### **Neural Networks and Deep Learning**

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## **Neural Networks**



- "Typical" neural network circa 2005
- Typical questions of optimization
  - Which variables to choose as inputs? How correlated are they?
  - How many nodes in the hidden layer?

## **Neural Networks**





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# **Training a Neural Network**

 Define a loss function that depends on predictions f(x;w) and targets y

$$L_{MSE} = \frac{1}{N} \sum_{i=1}^{N_{examples}} (y_i - f(x_i))^2$$
$$L_{BCE} = \frac{1}{N} \sum_{i=1}^{N_{examples}} -y_i \log f(x_i) - (1 - y_i) \log(1 - f(x_i))$$



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• Add **regularization** to control the model complexity and reduce overfitting

$$L' = L + \frac{1}{2} \sum_{j} w_j^2$$



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 $W_2$ 

• Add **regularization** to control the model complexity and reduce overfitting

$$L' = L + \frac{1}{2} \sum_{j} w_j^2$$

- Minimize the loss function using backpropagation
  - Fancy word for chain rule
  - Compute average gradient on training set
- Update weights with gradient descent

$$w_j \leftarrow w_j - \alpha \nabla_{w_j} L$$

–  $\alpha$  is called the learning rate

$$\nabla_{w_j} L = \frac{\partial L}{\partial f} \frac{\partial f}{\partial g_n} \frac{\partial g_n}{\partial g_{n-1}} \dots \frac{\partial g_{k+1}}{\partial g_k} \frac{\partial g_k}{\partial w_j}$$

## **Deep Neural Networks**



- As data complexity grows, need exponentially large number of neurons in a single-hidden-layer network to capture all the structure in the data
- Deep neural networks have many hidden layers
  - Factorize the learning of structure in the data across many layers
- Difficult to train, only recently has this become possible...

# Why did it take so long to train DNN's?

- Big Data: Large datasets vital for training (hundreds of) millions of parameters
- GPU's: Dramatically increased speed of training
- Improved optimization algorithms
- New regularization techniques: dropout, batch normalization, etc.
- New activation functions, like Rectified Linear Units



![](_page_10_Figure_7.jpeg)

![](_page_10_Figure_8.jpeg)

![](_page_10_Figure_9.jpeg)

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# **Deep NNs in HEP analysis**

- Compare dense Deep NN against BDT's and shallow NN's
- Deep NN found to outperform shallow NN and BDT's
  - small but statistically significant gain over simpler ML algorithms
- Physicists are good at doing physics!
  - Typical physics variables are high performing (e.g. invariant mass, Razor, etc.)
  - But Deep NN's can learn well from only 4-vector inputs

![](_page_11_Figure_7.jpeg)

Nature Communications 5, 4308 (2014)

BSM Higgs benchmark				
		AUC		
Technique	Low-level	High-level	Complete	
BDT	0.73(0.01)	0.78(0.01)	0.81 (0.01)	
NN	0.733(0.007)	$0.777 \ (0.001)$	0.816 (0.004)	
DN	0.880(0.001)	$0.800 \ (< 0.001)$	0.885(0.002)	
	Discovery significance			
Technique	Low-level	High-level	Complete	
NN	$2.5\sigma$	$3.1\sigma$	$3.7\sigma$	
DN	$4.9\sigma$	$3.6\sigma$	$5.0\sigma$	

- Hierarchical learning of representations
- Use **low level inputs** in smart ways
  - e.g. Feed in image pixels, rather than pre-computed features
  - Learn the structure in the data, rather than engineer it
  - No explicit need for feature engineering... unless you want to
- What deep learning is **<u>NOT</u>**:
  - A silver bullet
  - Replacement for thinking + domain knowledge
  - Always better than BDT, SVM, ...
  - Just feedforward neural networks!

## **Higher Level Representations**

 Successive layers build upon information learned in lower layers to construct progressively higher level representations of data

![](_page_13_Figure_2.jpeg)

## **NOT Simple Feedforward Neural Networks**

- NN's as a **complex graph** 
  - Nodes of graph are the layers
  - Edges of graph are data flow
  - Layers added to achieve a specific task, e.g. regularization
- Better to ask:
  - What does each layer / module do?
  - How is it connected to the previous and next layer?

GoogLeNet ILSVRC 2014 Winner 4M parameters

MaxPool 3x3+2(S) 7x7+2(S)

![](_page_14_Figure_9.jpeg)

Filter Concatenation

3×3 Convolution

1×1 Convolution

Previous Layer

1×1 Convolution

5×5 Convolution

1×1 Convolution

1×1 Convolution

3×3 Pooling

#### The Tip of the Iceberg

![](_page_15_Picture_1.jpeg)

#### **Convolution in 2D**

![](_page_16_Figure_1.jpeg)

![](_page_16_Figure_2.jpeg)

#### **Convolutions in 2D**

![](_page_17_Figure_1.jpeg)

Input image

Convolved image

• Scan the filters over the 2D image, producing the convolved images

![](_page_18_Figure_1.jpeg)

![](_page_18_Figure_2.jpeg)

![](_page_18_Figure_3.jpeg)

![](_page_18_Figure_4.jpeg)

through

![](_page_18_Picture_5.jpeg)

= 6	.6
-----	----

 $\blacksquare$  $\bigstar$  $\bigstar$  $\blacksquare$  $\blacksquare$ =-7.8 $\bigstar$  $\blacksquare$  $\blacksquare$  $\blacksquare$  $\blacksquare$  $\blacksquare$  $\blacksquare$  $\blacksquare$ **filter** $\blacksquare$ 1.0 - really want $\blacksquare$ 0.2 - sort of want

![](_page_18_Figure_8.jpeg)

![](_page_18_Figure_9.jpeg)

![](_page_18_Figure_10.jpeg)

![](_page_19_Figure_0.jpeg)

- Runner up, 2014 ILSVRC image recognition challenge
  - 140M parameters

![](_page_19_Figure_3.jpeg)

### **Representation Learning**

![](_page_20_Picture_1.jpeg)

![](_page_20_Picture_2.jpeg)

#### Filter

Layer 1

#### Matching images

L. Monier, G. Renard, <u>https://github.com/holbertonschool/deep-learning</u>

### **Representation Learning**

![](_page_21_Figure_1.jpeg)

#### **Representation Learning**

![](_page_22_Picture_1.jpeg)

![](_page_22_Picture_2.jpeg)

L. Monier, G. Renard, <u>https://github.com/holbertonschool/deep-learning</u>

#### **Deep Learning for Image Recognition**

![](_page_23_Figure_1.jpeg)

• Deep Convolutional Networks now have *super-human* performance in image recognition (ILSVRC Challenge)

#### **Deep learning and High Energy Physics**

## **Deep learning and High Energy Physics**

• How can we make use of high-performance deep learning algorithms in HEP?

- Can deep learning find interesting and useful high-level representations of physics data?
  - Can they teach us something new?
- Think about our low-level data in news ways that are amenable to deep learning
  - Can we frame HEP questions as if they were image recognition tasks?

### Neutrino Identification at NOvA

![](_page_26_Figure_1.jpeg)

![](_page_26_Figure_2.jpeg)

- Two 2D projections of the interactions
- Goal: discriminate between different neutrino interactions / backgrounds

![](_page_26_Figure_5.jpeg)

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## Neutrino Identification at NOvA

![](_page_27_Figure_1.jpeg)

![](_page_27_Figure_2.jpeg)

- Treat 2D projections as images
  - Convolutional Neural network for imaging tasks
- Make use of GoogLeNet
  - Use first layers with useful representations for structures in NOvA detector (e.g. edges, ...)
  - Train with two image inputs, one for each view

![](_page_27_Figure_8.jpeg)

#### Neutrino Identification at NOvA

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![](_page_28_Figure_2.jpeg)

- Convolution filters and outputs show interesting features about how the NN is providing discrimination
- Major gains over current algorithms in  $v_e$ -CC discrimination: 35%  $\rightarrow$  49% signal efficiency for the same background rejection

#### Jets at the LHC

![](_page_29_Picture_1.jpeg)

CMS

## Machine Learning and Jet Physics

• Can we use in internal structure of a jet (i.e. the individual energy depositions) to classify different kinds of jets?

![](_page_30_Figure_2.jpeg)

- Subfield of jet-substructure tries to answer this question using physics motivated features
- Can we learn the important information for discrimination directly from the data? And understand what we learned?

# Jet tagging using jet substructure

- **Typical approach:** Use physics inspired variables to provide signal / background discrimination
- Typical physics inspired variables exploit differences in:
  - Jet mass –
  - N-prong structure:
    - o 1-prong (QCD)
    - $\circ$  2-prong (W,Z,H)
    - o 3-prong (top)
  - Radiation pattern:
    - Soft gluon emission
    - Color flow
- Motivated data compressions, inspired by understanding of what should be discriminating...
  - We are likely losing information!

![](_page_31_Figure_13.jpeg)

## The Jet-Image

- Treat the detector as a camera: The Jet-Image

   Calorimeter towers as pixels
  - Energy depositions as intensity
- Use all available information for jet classification

![](_page_32_Figure_4.jpeg)

### **Image pre-processing**

![](_page_33_Figure_1.jpeg)

## **Pre-processing and space-time symmetries**

#### Pre-processing steps may not be Lorentz Invariant

- Translations in η are Lorentz boosts along z-axis
  - Do not preserve the pixel energies
  - Use transverse energy rather than energy as pixel intensity
- Jet mass is not invariant under Image normalization

Pythia 8,  $\sqrt{s} = 13 \text{ TeV}$ 

 $240 < p_T/GeV < 260 GeV, 65 < mass/GeV < 95$ 

![](_page_34_Figure_8.jpeg)

#### **Pre-processing and space-time symmetries**

![](_page_35_Picture_1.jpeg)

![](_page_35_Picture_2.jpeg)

In both pictures the total intensity of Einstein's face is about the same. However, **the image mass is different**!

#### http://mentalfloss.com/article/49222/11-unserious-photos-albert-einstein
#### **Pre-processing and space-time symmetries**

bright side



Standard computer vision tasks would likely not want to be sensitive to this!

In jet-tagging, these differences can have physical meaning

Need physics-domain knowledge input for how to pre-process

isity of ne.

However, the image mass is different!

#### http://mentalfloss.com/article/49222/11-unserious-photos-albert-einstein

dark

side

## **Discriminating Signal and Background**

- In the past, explored linear classification techniques applied to Jet-Images
  - Similar / improved performance over physicsinspired variables
  - Image paradigm allows excellent insight into the "physics" governing discrimination through visualization



- Linear methods can be limited
  - All the physics inside of a jet is not linear

#### Deep Jets – Convolutional Neural Networks



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#### **Performance with Deep Neural Networks**



#### **Combining Deep NN's with Substructure Variables**



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#### **Conditional Correlations with Network Output**



# Looking "into" the network to better see what it is learning

#### **Convolved representations**



First layer 11x11 convolutional filters



#### Convolved jet image differences

$$X_{sig}^{*}w - X_{bkg}^{*}w$$

## Average Most Activating Jet Images



# **Physics in deep representations**



Pearson Correlation Coefficient of the pixels intensity with the network output: <u>how discriminating information is contained within the network</u>

# **Physics in deep representations**



Pearson Correlation Coefficient of the pixels intensity with the network output: <u>how discriminating information is contained within the network</u>

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## Learning About Learning

Restricted Phase Space: 79 < m < 81 GeV and 0.19 <  $\tau_{21}$  < 0.21



Learning something beyond mass and  $\tau_{_{21}}\ldots$ 

**Spatial information indicative of radiation pattern for W and QCD:** New information learned by the network potentially related to colorflow

# Where is DL in HEP going next?

- Computer vision and imaging techniques may have broad applicability...
  - Calorimeter shower classification?
  - Energy calibration regression?
  - Pileup reduction?
  - Tracking?



- Sequential learning techniques (not discussed in this talk) may be useful in tasks with variable length data
  - Typical neural networks and BDT's require a fixed input size
  - But not all discrimination tasks in HEP have a fixed size data representation, e.g. jets with variable numbers of constituents, variable number of jets in an events, ...
- New network training paradigms may help with statistical inference, fast simulations, or reduce systematic uncertainties...

#### **Dealing with Systematic Uncertainties**

- Systematic uncertainties encapsulate our incomplete knowledge of physical processes and detectors
  Systematic uncertainty encoded as nuisance parameters, Z
- Can we teach a classifier to be robust to these kinds of uncertainties?



#### **Adversarial Networks**

- Adversarial training: a mini-max game
  - Train one neural network (f) to perform the classification task
  - Train a second network (r) to predict the nuisance parameter Z from f
- The loss encodes the performance of both classifiers, but is penalized when **r** does well

$$\hat{\theta}_f, \hat{\theta}_r = \arg\min_{\theta_f} \max_{\theta_r} E(\theta_f, \theta_r).$$

arXiv:1611.01046

G. Louppe, M. K., K. Cranmer,

$$E_{\lambda}(\theta_f, \theta_r) = \mathcal{L}_f(\theta_f) - \lambda \mathcal{L}_r(\theta_f, \theta_r),$$





# Learning to Pivot: Toy Example

G. Louppe, M. K., K. Cranmer, arXiv:1611.01046

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0.84

0.72

0.60

0.48

0.36

0.24

0.12

2.0

• 2D example

$$\begin{aligned} x &\sim \mathcal{N}\left((0,0), \begin{bmatrix} 1 & -0.5\\ -0.5 & 1 \end{bmatrix}\right) & \text{ when } Y = 0, \\ x &\sim \mathcal{N}\left((1,1+Z), \begin{bmatrix} 1 & 0\\ 0 & 1 \end{bmatrix}\right) & \text{ when } Y = 1. \end{aligned}$$

- Without adversary (top) large variations in network output with nuisance parameter
- With adversary (bottom) performance is independent!







# **Learning to Pivot: Physics Example**

- Tune the classification vs robustness in training to maximize significance, even beyond standard approaches
- Example:
  - W-tagging vs QCD
  - Physics inspired variables as inputs
  - Systematic: noise from additional "pileup" interactions in collision
  - Count events passing minimum network output threshold
    → compute significance including uncertainty (AMS)



#### Conclusion

- Machine learning already used widely in HEP
- Deep learning is a new and powerful paradigm for machine learning in certain contexts
- Framing HEP data in the new ways can allow us to benefit from deep learning
- Already seen performance improvements and new insights when using deep learning in HEP
- Large potential for new image recognition and deep learning applications in HEP

# Backup

# **Useful Python ML software**

- An aconda / Conda  $\rightarrow$  easy to setup python ML / scientific computing environments
  - <u>https://www.continuum.io/downloads</u>
  - <u>http://conda.pydata.org/docs/get-started.html</u>
- Integrating ROOT / PyROOT into conda
  - <u>https://nlesc.gitbooks.io/cern-root-conda-recipes/content/index.html</u>
  - <u>https://conda.anaconda.org/NLeSC</u>
- Converting ROOT trees to python numpy arrays / panda dataframes
  - <u>https://pypi.python.org/pypi/root\_numpy/</u>
  - <u>https://github.com/ibab/root\_pandas</u>
- Scikit-learn  $\rightarrow$  general ML library
  - <u>http://scikit-learn.org/stable/</u>
- Deep learning frameworks / auto-differentiation packages
  - <u>https://www.tensorflow.org/</u>
  - http://deeplearning.net/software/theano/
- High level deep learning package build on top of Theano / Tensorflow
  - <u>https://keras.io/</u>

## **Machine Learning**

# What is Machine Learning?

- Giving computers the ability to learn without explicitly programming them (Arthur Samuel, 1959)
- Statistics + Algorithms
- Computer Science + Probability + Optimization Techniques
- Fitting data with complex functions
- Pattern recognition: identifying patterns and regularities in data

## What do we use ML for?

#### <u>Supervised Learning</u>

- Given data with variables / features  $\{x_i \in X\}$  and  $\textbf{targets} \; \{y_i \in Y\},$  learn the function mapping f(X)=Y
- Classification: Y is a finite set of labels
- **Regression**:  $Y \in \text{Real Numbers}$
- Unsupervised Learning

- Given some data  $D = \{x_i \in X\}$ , but no labels, find structure in the data

- Clustering: partition the data into groups  $D = \{D_1 \cup D_2 \cup D_3 \dots \cup D_k\}$
- Dimensionality reduction: find a low dimensional (less complex) representation of the data with a mapping Z=h(X)

#### <u>Reinforcement learning</u>

 Learn to make the best sequence of decisions to achieve a given goal when feedback is delayed until you reach the goal

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Main focus today on supervised learning in HEP

#### - Given some data $D = \{x_i \in X\}$ , but no labels, find structure in the data

Unsupervised Learning

- Clustering: partition the data into groups

Won't Discuss this today... But there are existing and future applications in HEP
Dimensionality reduction: find a low dimensional (less complex)
Tepresentation of the data with a mapping Z=h(X)

#### Reinforcement learning

- Learn to make the best sequence of decisions to achieve a given goal when feedback is delayed until you reach the goal

Won't Discuss this at all today... Not yet clear how it will be used in HEP

#### **Supervised Learning**





• Estimate final performance on *test-set* 



#### Classification



- Learn a function to separate different classes of data
- Avoid over-fitting: -
  - Learning too fined details about your training sample that will not generalize to unseen data



# **Machine Learning in High Energy Physics**

- Many recent application of ML in HEP rely on Ensembles of decision trees, such as **Boosted Decision Trees** and Random Forests
- Powerful algorithms that are relatively simple, easy to train, and tend not to overfit (especially Random Forests)
- They are very popular in general:
  - Test 179 classifiers (no deep neural networks) on 121 datasets <a href="http://jmlr.csail.mit.edu/papers/volume15/delgado14a/delgado14a.pdf">http://jmlr.csail.mit.edu/papers/volume15/delgado14a/delgado14a.pdf</a>
  - The classifiers most likely to be the bests are the random forest (RF) versions, the best of which (...) achieves 94.1% of the maximum accuracy overcoming 90% in the 84.3% of the data sets
- But, **Deep Neural Networks** have outperformed such algorithms in certain domains, like Object Recognition in images



#### **Decision Trees**

# **Optimizing a Decision Tree**

- Building an optimal decision tree is an NP-complete problem
  - Hard to find a global optimization for all splittings at the same time
- Greedy optimization  $\rightarrow$  optimize one split at a time
  - Start with one leaf
  - Split leaf in two
  - Repeat as needed

# **Optimizing a Decision Tree**

- When to split? Minimize impurity =  $\Sigma_{\text{leaf}}$  Impurity(leaf)\*size(leaf)
  - Typical leaf impurity functions:
  - Gini =  $p^{*}(1-p)$
  - Entropy = -p\*log(p) (1-p)\*log(1-p)
    - Where p is the fraction of signal events in leaf, and size is the number of events falling into that leaf
  - Mean Square Error (regression): (1/n\_i)  $\Sigma_{i \ in \ leaf} \ (y_i m)^2$ 
    - Where  $y_i$  is the true value, and m is the average y of events in the leaf
- When to stop splitting? Many criteria
  - Fixed tree depth
  - Information gain is not enough
  - Fix minimum samples needed in leaf
  - Fix minimum number of samples needed to split leaf

#### Overfitting



- Single decision trees can quickly overfit
- Especially when increasing the depth of the tree

- Combine many decision trees, use the ensemble for prediction
- Averaging:  $D(x) = \frac{1}{N_{tree}} \sum_{i=1}^{N_{tree}} d_i(x)$ 
  - Random Forest, averaging combined with:
    - **Bagging:** Only use a subset of events for each tree training
    - Feature subsets: Only use a subset of features for each tree
- Boosting (weighted voting):  $D(x) = \sum_{i=1}^{N_{tree}} \alpha_i d_i(x)$ 
  - Weight computed such that events in current tree have higher weight misclassified in previous trees
  - Several boosting algorithms
    - AdaBoost
    - Gradient Boosting
    - XGBoost

#### **Ensembles of Trees**

- Ensembles of trees tend to work very well
  - Relatively simple
  - Relatively easy to train
  - Tend not to overfit (especially random forests)
  - Work with different feature types: continuous, categorical, etc.







#### optimal boundary





2000 trees

# CMS h→γγ (8 TeV)



#### **Neural Networks**

#### **Non-Linear Activations**

- The activation function in the NN must be a non-linear function – If all the activations were linear, the network would be linear:  $f(X) = W_n(W_{n-1}(...W_1|X)) = UX$ , where  $U = \Pi_i W_i$
- Linear functions can only correctly classify linearly separable data!
- For complex datasets, need nonlinearities to properly learn data structure


### Neural Networks and Local Minima



- Large NN's difficult to train...trapping in local minimum?
- Not in large neural networks <u>https://arxiv.org/abs/1412.0233</u>
  - Most local minima equivalent, and resonable
  - Global minima may represent overtraining
  - Most bad (high error) critical points are saddle points (different than small NN's)

Weight Initializations and Training Procedures

- Used to set weights to some small initial value
  - Creates an almost linear classifier
- Now initialize such that node outputs are normally distributed
- Pre-training with auto-encoder
  - Network reproduces the inputs
  - Hidden layer is a non-linear dimensionality reduction
  - Learn important features of the input
  - Not as common anymore, except in certain circumstances...
- Adversarial training, invented 2014

   Will potential HEP applications later



MaxOut





### **ReLU Networks**





http://www.jmlr.org/proceedings/papers/v15/glorot11a/glorot11a.pdf

- Sparse propagation of activations and gradients in a network of rectifier units. The input selects a subset of active neurons and computation is linear in this subset.
- Model is "linear-by-parts", and can thus be seen as an exponential number of linear models that share parameters
- Non-linearity in model comes from path selection

### **Convolutions in 2D**



Input image

Convolved image

• Scan the filters over the 2D image, producing the convolved images

### **Max Pooling**



Layer N



- Down-sample the input by taking MAX or average over a region of inputs
  - Keep only the most useful information



## Daya Bay Neutrino Experiment

- Aim to reconstruct inverse  $\beta$ -decay interactions from scintillation light recorded in 8x24 PMT's
- Study discrimination power using CNN's
  - Supervised learning  $\rightarrow$  observed excellent performance (97% accuracy)
  - Unsupervised learning: ML learns itself what is interesting!



arXiv:1601.07621

## **Jet-Images**

# Jet tagging using jet substructure

- **Typical approach:** Use physics inspired variables to provide signal / background discrimination
- Typical physics inspired variables exploit differences in:
  - Jet mass
  - N-prong structure:
    - 1-prong (QCD)
    - 2-prong (W,Z,H)
    - $\circ$  3-prong (top)
  - Radiation pattern:
    - Soft gluon emission
    - $\circ$  Color flow



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### **Pre-processing and space-time symmetries**

#### Pre-processing steps may not be Lorentz Invariant

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  - Do not preserve the pixel energies
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Pythia 8,  $\sqrt{s} = 13 \text{ TeV}$ 

 $240 < p_T/GeV < 260 GeV, 65 < mass/GeV < 95$ 



### **Restricted phase space**



Restrict the phase space in very small mass and  $\tau_{21}$  bins: Improvement in discrimination from new, unique, information learned by the network

### **Deep correlation jet images**



**Spatial information indicative of radiation pattern for W and QCD:** where in the image the network is looking for discriminating features

#### **Typical Neural Network Hidden Layer**



<u>Hidden layer</u> Different Colors represent different weights W\*x

### **Local Connectivity**



<u>Hidden layer</u> Different Colors represent different weights W\*x

Local connectivity: each neuron has a small "field of view" of a few inputs



Shared weights: each neuron uses the same weights...

Effect  $\rightarrow$  the neuron is scanned over different fields of view  $\rightarrow$  **Convolution** 

### **Convolutional Layer**



Add more neurons which scans the field of view
Each neuron is a *Filter* being convolved with the input
Convolutional Layer with 4 filters production 4x4 output vector size

## Why did it take so long to train DNN's?



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- Big Data
  - (Hundreds of) Millions of parameters  $\rightarrow$  large dataset vital for training
- GPU's
  - NN's require a lot of matrix multiplications... perfect for GPU's
  - Dramatically increased the speed of training
- But these aren't the only reasons...

## **Training Improvements**

- Gradient descent is computationally costly (since we compute gradient over full training set)
- Stochastic gradient descent \_\_\_\_\_
  - Compute gradient on one event at a time (in practice a small batch)
  - Noisy estimates average out
  - Stochastic behavior can allow "jumping" out of bad critical points
  - Scales well with dataset and model size
  - But can have some convergence difficulties
  - Improvements include:
     Momentum, RMSprop, AdaGrad, ...



### **Better Activation Functions**



#### Vanishing gradient problem

- Derivative of sigmoid:

$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)(1 - \sigma(x))$$

- Nearly 0 when x is far from 0!
- Gradient descent impossible!

- Rectified Linear Unit (ReLU)
  - $\operatorname{ReLU}(x) = \max\{0, x\}$
  - Derivative is constant!

 $\frac{\partial \operatorname{Re} LU(x)}{\partial x} = \begin{cases} 1 & \text{when } x > 0\\ 0 & \text{otherwise} \end{cases}$ 

ReLU gradient doesn't vanish

#### **Better Regularization Inside the Network**



(a) Standard Neural Net



(b) After applying dropout.

- Dropout
  - Randomly remove nodes during training
  - Avoid co-adaptation of nodes
  - Essentially a large model averaging procedure

#### New way to train networks... Potential for HEP?

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- Train two networks "against" each other
  - One to generates an image
  - Second one to distinguish real / fake images
  - Potential applications for fast simulation?



Domain adaptation: train with one dataset (MC) and apply on a slightly different one (data)

- Minimize use of information not in both domains
- Potential to reduce data/MC differences and systematic uncertainties during training?



http://arxiv.org/abs/1409.7495