HOUSTON

DEPARTMENT OF PHYSICS



SMU UH ? X-ray Simulation CTEQ ATLAS Medipix 01 02 03 05 04 2006 2013 2015 SMU UH Xerry Morte Parton Distribution-Lesion detection Function Machine Learning MEKS(GPU)

Child prod.

About me

About me

ATLAS	CTEQ	Medical/Image Physics	Machine Learning	
GEANT4 ROOT COOL PANDA	MEKS: a program computes differential cross-section for single-inclusive jets and di-jet pairs at NLO accuracy in pQCD	A c++ code to simulate x ray attenuation/phase contrast image	A Model Observer using Histogram of Gradients(HOG), Support Vector Machine(SVM), and Density-based spatial clustering of applications with	A Lung lesion detector with CNN.
QT4	that runs on GPU.	Experiment with Medipix3,	noise (DBSCAN) methods.	
Python	1.3 0 0 0 0 0 0 0 0 0 0 0 0 0	a photon courting detector.		
01	6 02 2012	03 2013	04 2014	05 2015



2/ (Un-)Supervised Learning

3 Practical Tools

Outline

4 Deep Learning in HEP

Learning Methods



Unsupervised

ML Applications



Text and Language



Speech and Audio



Gene Expression



Product Recommendation







Climate Change



Geology



Traditional Recognition Approach

Low-level sensing



feature extraction & selection (hand-crafted)



Object detection / classification



Low-level vision features (edges, SIFT, HOG, etc.)

Learning Algorithm (e.g., SVM)

- Most critical for accuracy
- Account for most of the computation for testing
- Most time-consuming in development cycle
- Often hand-craft in practice

Computer vision features



and many others: SURF, MSER, LBP, Color-SIFT, Color histogram, GLOH,

Learning Feature Hierarchy

Feature representation



3rd layer Objects

0	E	1A	0		0	-	14
1	5	8	D		(0	1	1
1	0		1	15			2
	12		10		1	7	0
	10	1	-			0	1

2nd layer Objects

1st layer Edges

Learn hierarchy

- All the way from pixels ——> classifier
- One layer extracts features from output of previous layer
- Learn useful higher-level features from images
- Fill in representation gap in recognition





Pixels

Convolution Neural Networks (CNNs): 1989



Input Image

LeNet: a layered model composed of convolution and subsampling operations followed by a holistic representation and ultimately a classifier for handwritten digits.

Convolution Neural Networks (CNNs): 1989



The input is converted into a convolution layer Cx via the convolution process. Then, Cx is treated as the input data, converted to a set of smallerdimension feature maps Sx+1 via the subsampling process



An entire procedure of using CNNs to compute a output. We can see that after each layer, the dimensions of the feature maps are decreased, which makes CNNs a useful model to reduce the number of parameters that must be learned and thus improves upon general feed-forward back-propogation training.

Convolutional Nets: 2012



AlexNet: a layered model composed of convolution, subsampling, and further operations followed by a holistic representation and all-in-all a landmark classifier on ILSVRC12

- + data
- + gpu
- + non-saturating nonlinearity
- + regularization (DropOut)

7 hidden layers, 60 M parameters, Trained on 2 GPUs for a week



Top detection:

person 2.467470 swimming trunks -1.263134 puck -1.296530

Second-best detection:

mushroom 0.015308 helmet -0.656349 bathing cap -0.736946

Third-best detection:

mushroom -0.210073 helmet -0.268050



Top detection:

person	3.855254
bow	-1.046176
chair	-1.302708

Second-best detection:

screwdrive	-0.177056
vacuum	-0.951643
spatula	-0.971048

Third-best detection:

stove -0.325801 snowplow -0.580681 toaster -0.746113



Top detection:

person	1.812851
snowplow	-1.222213
bow	-1.271971

Second-best detection:

table	-0.782973
dishwasher	-1.269662
golf ball	-1.279250

Third-best detection:

sofa	-0.951138
bench	-1.278376
spatula	-1.534883



Top detection:

person	1.227990
purse	-1.180718
flower pot	-1.322483

Second-best detection:

helmet	-0.383887
person	-1.007048
bicycle	-1.079069

Third-best detection:

-0.849368
-1.121394
-1.203280



Top detection:

person	2.105693
purse	-1.266800
binder	-1.387294

Second-best detection:

diaper -0.342870 plastic bag -0.784050 backpack -1.197001

Third-best detection:

miniskirt	-
band aid	
syringe	-

-0.354545 -1.249658 -1.321468

ILSVRC12

Team name	Error (5 guesses)	Description	Krizbovsky et al 16.4%
SuperVision	0.15315	AlexNet	error (top-5)
ISI	0.26172	Weighted sum of scores from each classifier with SIFT+FV, LBP+FV, GIST+FV, and CSIFT+FV, respectively.	Next best (non-convnet) – 26.2% error
OXFORD_VGG	0.26979	Mixed selection from High-Level SVM scores and Baseline Scores	

The ImageNet Large Scale Visual Recognition Challenge (ILSVRC) evaluates algorithms for object detection and image classification at large scale. ImageNet is an image database with 14,197,122 labeled images, 20k classes



.

Dog, domestic dog, Canis familiaris

A member of the genus Canis (probably descended from the common wolf) that has been domesticated by man since prehistoric times; occurs in many breeds; "the dog barked all night"

1603

pictures

88.15%

Popularity

Percentile

Wordnet IDs

Numbers in brackets: (the number of synsets in the subtree).	Treemap Visualization	Images of the Synset	Downloads	
ImageNet 2011 Fall Release (32326)	🖌 🔪 ImageNet 2011 Fall R	elease $ angle$ / $ angle$ Domestic anima	al, domesticated animal	Dog, domestic dog, Canis familiaris
- plant, flora, plant life (4486)	Hunting	Wo	rking	
e- geological formation, formation (1)				
natural object (1112)				
- sport, athletics (176)				i 🔤 📰 🌠 📑 🚺 🚮
- artifact, artefact (10504)	8 8 4 14 3		- CARLES IN COMPANY	
- fungus (308)				· 🗶 😰 🐺 🍋 🚮 🔙
- person, individual, someone, some		S 37 10 10		
🔶 🕂 animal, animate being, beast, brut				A Star And A Star
invertebrate (766)				
- homeotherm, homoiotherm, ho				
work animal (4)				
- darter (0)		Toy	Great	Cur Pug
survivor (0)				
- range animal (0)			» 🔛 💽 🖉	
- creepy-crawly (0)				
 domestic animal, domesticated 			Dalmatian	Basenji Mexican
il- domestic cat, house cat, Fel				
🔶 dog, domestic dog, Canis fa	ALA			
- pooch, doggie, doggy, b				
F- hunting dog (101)		Poo	ch Lapdog	Poodle
🖻 dalmatian, coach dog, ci				
i⊧- cur, mongrel, mutt (2)				
i⊷ corgi, Welsh corgi (2)		A line and		Griffon Cor
- Mexican hairless (U)			Noufound	Spitz
- lapdog (U)	Martin Martin 1			
- Newfoundland, Newfour	and the second s			
I⊧ poodle, poodle dog (4)		· · · · ·		
- basenji (0)	HAVE DECK			

ImageNet category of Dog, domestic dog, Canis familiaris

ImageNet



ImageNet category of Particles....

Convolutional Nets: 2014



ILSVRC14 Winners: ~6.6% Top-5 error

- GoogLeNet: composition of multi-scale dimensionreduced modules (pictured)
- VGG: 16 layers of 3x3 convolution interleaved with max pooling + 3 fully-connected layers
- + depth
- + data
- + dimensionality reduction

Unsupervised Learning





- Model distribution of input data
- Can use unlabeled data (unlimited)
- Can be refined with standard supervised techniques (e.g. backprop)
- Useful when the amount of labels is small

Models

- Basic: PCA, KMeans
- Denoising auto-encoders
- Sparse auto-encoders
- Restricted Boltzmann machines
- Sparse coding
- Independent Component Analysis
- •

...

Deep Learning Libraries

Caffe

- Berkeley Vision and Learning Center (BVLC)
- Pure C++ / CUDA architecture with CuDNN acceleration
- Seamless switch between CPU and GPU

Theano/Pylearn2

- U. Montreal
- scientific computing framework in Python
- symbolic computation and automatic differentiation

Torch7

- NYU
- scientific computing framework in Lua
- supported by Facebook

All express deep models All are nicely open-source All include scripting for hacking and prototyping • Speed with Krizhevsky's 2012 model:

- K40 / Titan: 2 ms / image, K20: 2.6ms
- Caffe + cuDNN: **1.17ms / image** on K40
- 60 million images / day
- 8-core CPU: ~20 ms/image
- ~ 9K lines of C/C++ code
 - with unit tests ~20k

Caffe offers the model definitions optimization settings pre-trained weights so we can start right away.

The BVLC models are licensed for unrestricted use.

C++ 84.2%

Caffe

Python 10.5%

Cuda 3.9%

Other 1.4%

NVIDIA cuDNN is a GPU-accelerated library of primitives for deep neural networks.

Caffe/CuDNN roadmap



A 3D lesion detector







A 3-D lesion detector for Lung tumor is developed based on caffe.

Adopted CNN network but works on CT images(3D, gray color)

Trained on Lung Image Database Consortium (LIDC) dataset. (1012 cases, each case is a 512*512*(200-400) image.

Rank 4/14 on SPIE Lung Nodule Classification Challenge with training on only 100 labeled cases. (would be better if we have more labeled cases, or have pre-trained with unsupervised learning then fine-tune with labeled data)

Higgs Boson Machine Learning Challenge



Completed • \$13,000 • 1,785 teams

Higgs Boson Machine Learning Challenge

Mon 12 May 2014 - Mon 15 Sep 2014 (5 months ago)

Dashboard	
Home	÷
Data	8
Make a submission	Ľ
Information	0
Description	
Evaluation	
Rules	
Prizes	
About the Sponsors	
Timeline	
Winners	
Forum	ø
Leaderboard	100
Public	
Private	

Leaderboard

- 1. Gábor Melis
- 2. Tim Salimans
- 4. ChoKo Team
- 5 chang chan
- 6. quantify
- 7. Stanislav Semenov & Co (HSE

Use the ATLAS experiment to identify the Higgs boson

Competition Details » Get the Data » Make a submission



Winning submission:

Bag of 70 dropout (50%) deep neural networks (600,600,600), channel-out activation function, l1=5e-6 and l2=5e-5 (for first weight matrix only). Each input neurons is connected to only 10 input values (sampled with replacement before training).

Higgs: Binary Classification Problem



Machine Learning Repository Center for Machine Learning and Intelligent Systems

HIGGS Data Set

Download: Data Folder, Data Set Description

Abstract: This is a classification problem to distinguish between a signal process which produces Higgs bosons and a background process which does not.

Data Set Characteristics:	N/A	Number of Instances:	11000000	Area:	Physical
Attribute Characteristics:	Real	Number of Attributes:	28	Date Donated	2014-02-12
Associated Tasks:	Classification	Missing Values?	N/A	Number of Web Hits:	17738

HIGGS UCI Dataset: 21 low-level features AND 7 high-level derived features Train: 10M rows, Test: 500k rows



Searching for exotic particles in high-energy physics with deep learning

P. Baldi, P. Sadowski & D. Whiteson

Affiliations | Contributions | Corresponding authors

Nature Communications 5, Article number: 4308 | doi:10.1038/ncomms5308 Received 19 February 2014 | Accepted 04 June 2014 | Published 02 July 2014





Higgs: Binary Classification Problem

AUC				
Technique	Low-level	Low-level	Complete	
BDT	0.73	0.78	0.81	
NN	0:733	0.777	0.816	
DN	0.880	0.800	0.855	





(a)



Can we benefit from this deep learning revolution?

Traditional computer vision task processing







Examine signal and background properties, set "cuts"



Result

HEP



Big Data



LHC: 25 petabytes

Youtube: One hour video are uploaded per second... =3600*24*365*1GB=31 petabytes?

Logistic Regression

The Model

Classification is done by projecting an input vector onto a set

$$P(Y = i | x, W, b) = softmax_i(Wx + b)$$
$$= \frac{e^{W_i x + b_i}}{\sum_j e^{W_j x + b_j}}$$

Loss Function

Learning optimal model parameters involves minimizing a loss function.

$$\mathcal{L}(\theta = \{W, b\}, \mathcal{D}) = \sum_{i=0}^{|\mathcal{D}|} \log(P(Y = y^{(i)} | x^{(i)}, W, b))$$
$$\ell(\theta = \{W, b\}, \mathcal{D}) = -\mathcal{L}(\theta = \{W, b\}, \mathcal{D})$$

$$y_{pred} = \operatorname{argmax}_i P(Y = i | x, W, b)$$

Caffe net plot

Multilayer Perceptron

The Model

Classification is done by projecting an input vector onto a set

$$f(x) = G(b^{(2)} + W^{(2)}(s(b^{(1)} + W^{(1)}x))),$$

$$y_{pred} = \operatorname{argmax}_i P(Y = i | x, W, b)$$

Loss Function

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$$\ell(\theta = \{W, b\}, \mathcal{D}) = -\mathcal{L}(\theta = \{W, b\}, \mathcal{D})$$



Restricted Boltzmann Machines

Energy-Based Model

Energy-Based Model associate a scalar energy to each configuration of the variables of interest.

The energy of the joint configuration is:

$$\begin{split} E(\mathbf{v},\mathbf{h};\theta) &= -\sum_{ij} W_{ij} v_i h_j - \sum_i b_i v_i - \sum_j a_j h_j \\ \theta &= \{W,a,b\} \text{ model parameters.} \end{split}$$

Probability of the joint configuration is given by the Boltzmann distribution:

$$P_{\theta}(\mathbf{v}, \mathbf{h}) = \frac{1}{\mathcal{Z}(\theta)} \exp\left(-E(\mathbf{v}, \mathbf{h}; \theta)\right) = \frac{1}{\mathcal{Z}(\theta)} \prod_{ij} e^{W_{ij}v_ih_j} \prod_i e^{b_iv_i} \prod_j e^{a_jh_j} \mathcal{Z}(\theta) = \sum_{\mathbf{h}, \mathbf{v}} \exp\left(-E(\mathbf{v}, \mathbf{h}; \theta)\right) \qquad \text{partition function} \qquad \text{potential functions}$$

Restricted: No interaction between hidden variables.



Auto-Encoder



Auto-Encoder



Stacked Auto-Encoders

Auto-Encoder



Auto-Encoder



Stacked Auto-Encoders

Convolutional Neural Networks

The Model

Classification is done by projecting an input vector onto a set

$$f(x) = G(b^{(2)} + W^{(2)}(s(b^{(1)} + W^{(1)}x))),$$

$$y_{pred} = \operatorname{argmax}_i P(Y = i | x, W, b)$$

Loss Function

Learning optimal model parameters involves minimizing a loss function.

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$$\ell(\theta = \{W, b\}, \mathcal{D}) = -\mathcal{L}(\theta = \{W, b\}, \mathcal{D})$$



cuDNN Performance Acceleration





Baseline Caffe compared to Caffe accelerated by cuDNN on K40

Baseline Caffe compared to Caffe accelerated by cuDNN on TitanZ

All comparisons are against a 12-core Intel E5-2679v2 CPU @ 2.4GHz running Caffe with Intel MKL 11.1.3.