Identifying QCD transition using Deep Learning

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arXiv:1612.04262

Outline

Introduction to Deep Learning

Simple example of DL and application in Physics

QCD EoS-meter in HIC using DL

Summary and outlook

What is deep learning?

Artificial Intelligence (AI)

Machine Learning (ML)

Deep Learning (DL)

Booming in theory and applications!

- 1. Big Data
- 2. GPU parallel
- 3. New architecture

2006

Geoffrey Hinton

Supervised learning---most commen DL

RL

Reinforcement Learning (or Deep Q-learning)

Playing Games

RNN/LSTM/GRU

Recurrent Neural Network Long Short Term Memory Gated Recurrent Unit

Natural Language processing

CNN

Convolution Neural Network

Image recognition/ classification

Fancy applications (RL)

AlphaGo (by Google DeepMind) beat human master



Self-driving cars Robot control Playing Games like flappybird, Starcraft

RNN/LSTM for natural language generation

Chinese Poetry Generation with Planning based Neural Network

Zhe Wang[†], Wei He[‡], Hua Wu[‡], Haiyang Wu[‡], Wei Li[‡], Haifeng Wang[‡], Enhong Chen[†]

[†]University of Science and Technology of China, Hefei, China

[‡]Baidu Inc., Beijing, China

秋夕湖上

By a Lake at Autumn Sunset 一夜秋凉雨湿衣,

A cold autumn rain wetted my clothes last night, 西窗独坐对夕晖。

And I sit alone by the window and enjoy the sunset. 湖波荡漾千山色,

With mountain scenery mirrored on the rippling lake, 山鸟徘徊万籁微。

A silence prevails over all except the hovering birds.

秋夕湖上

By a Lake at Autumn Sunset 荻花风里桂花浮,

The wind blows reeds with osmanthus flying, 恨竹生云翠欲流。

And the bamboos under clouds are so green as if to flow down. 谁拂半湖新镜面,

The misty rain ripples the smooth surface of lake, 飞来烟雨暮天愁。

And I feel blue at sunset.

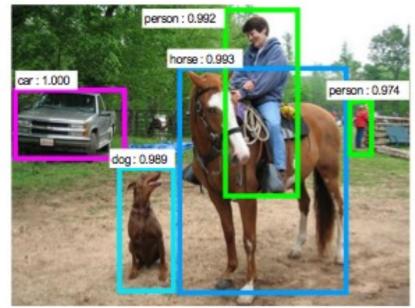
Table 6: A pair of poems selected from the blind test. The left one is a machine-generated poem, and the right one is written by Shaoti Ge, a poet lived in the Song Dynasty.

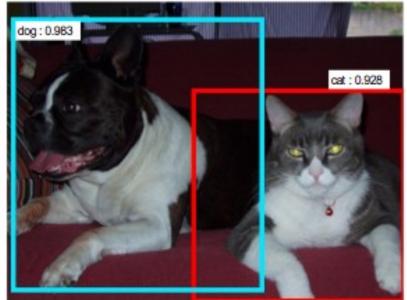
arXiv: 1610.09889v1

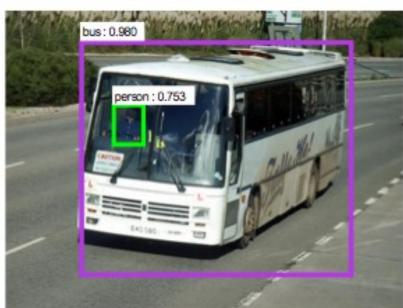
Object detection using CNN

Example detection results of Faster R-CNN









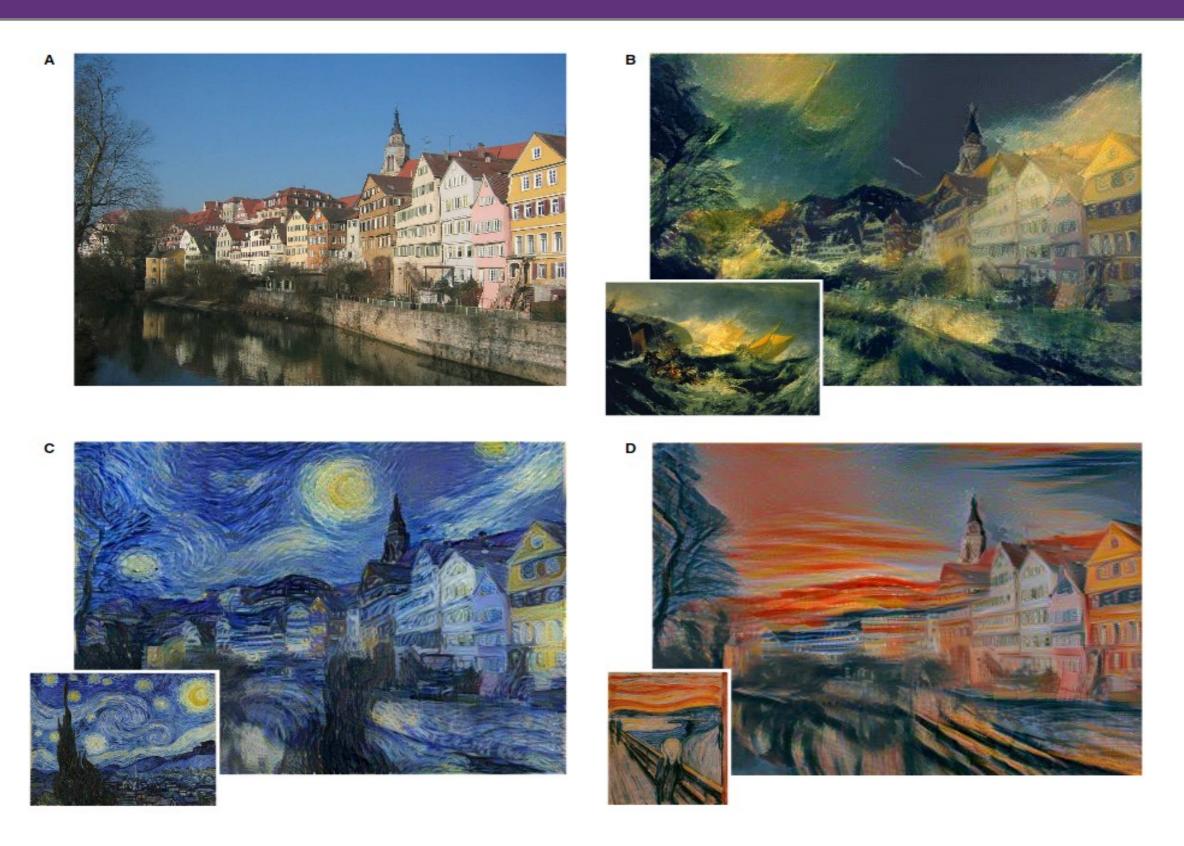




Shaoqing Ren, Kaiming He, Ross Girshick, & Jian Sun. "Faster R-CNN: Towards Real-Time Object Detection with Region Proposal Networks". NIPS 2015.

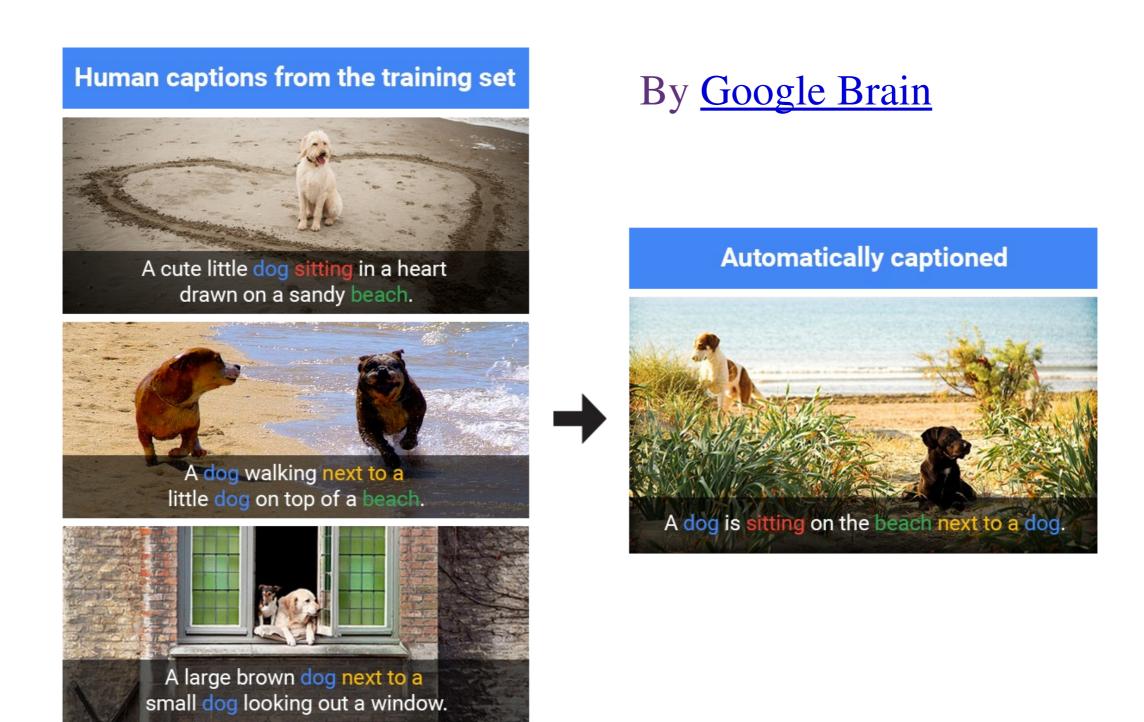
Slides from KaiMing, He's recent talk

Artistic style transfer using CNN



arXiv:1508.06576 style can be modelled and transferred!

Hybrid CNN + LSTM for image captioning

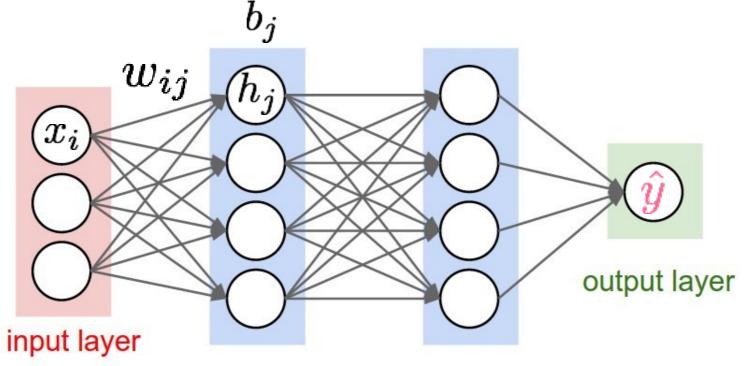


Using concepts learned from similar scenes in the training set.

An example of DL structure:

Fig from CS231N, Stanford

1, Feed-Forward



hidden layer 1 hidden layer 2

$$z_j = \sum_{i=1}^N x_i w_{ij} + b_j$$

Linear operations:rotating, boosting,...

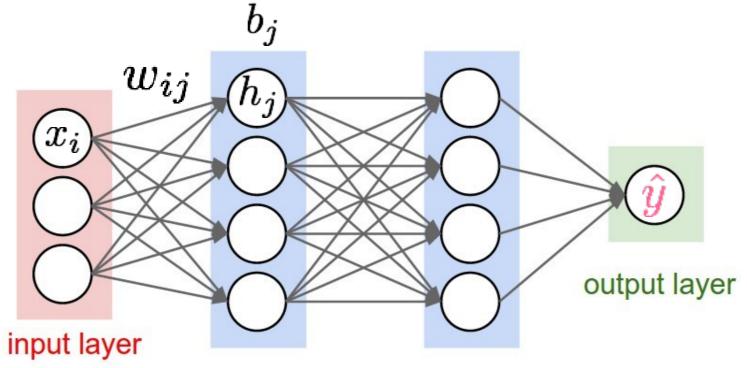
increasing or decreasing dimensions

$$h_j = \sigma(z_j)$$

non-linear activation function: correlation/links

Fig from CS231N, Stanford

1, Feed-Forward



hidden layer 1 hidden layer 2

$$z_j = \sum_{i=1}^N x_i w_{ij} + b_j$$

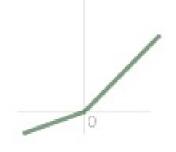
(a) Sigmoid

(b) ReLU $\sigma(z) = \frac{1}{1 + \exp(-z)} \qquad \sigma(z) = \left\{ \begin{array}{ll} z, & z > 0 \\ 0, & z \le 0 \end{array} \right. \qquad \sigma(z) = \left\{ \begin{array}{ll} z, & z > 0 \\ az, & z \le 0 \end{array} \right.$

(c) PReLU



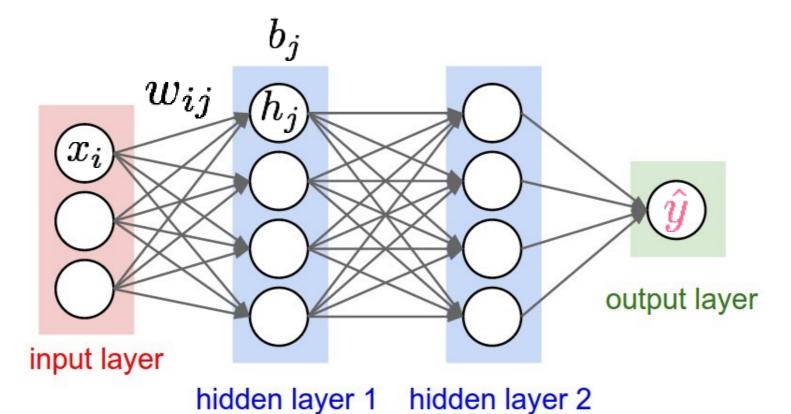




increasing or decreasing dimensions

Fig from CS231N, Stanford

1, Feed-Forward



Transformation of feature space:

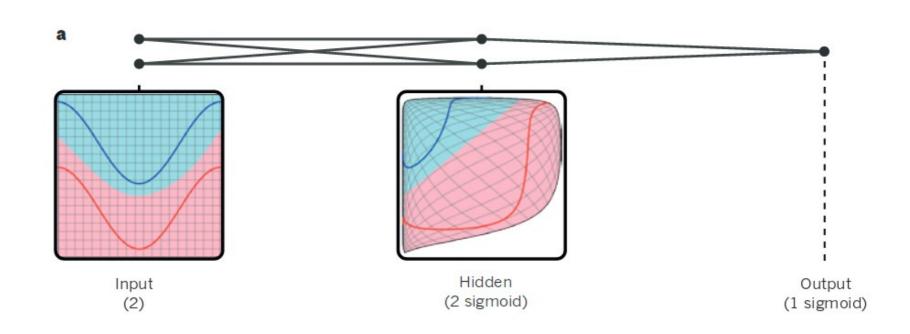
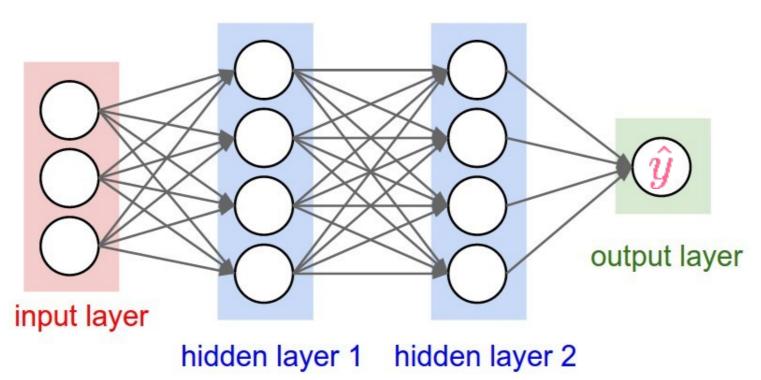


Fig from CS231N, Stanford

2, Back Propagation



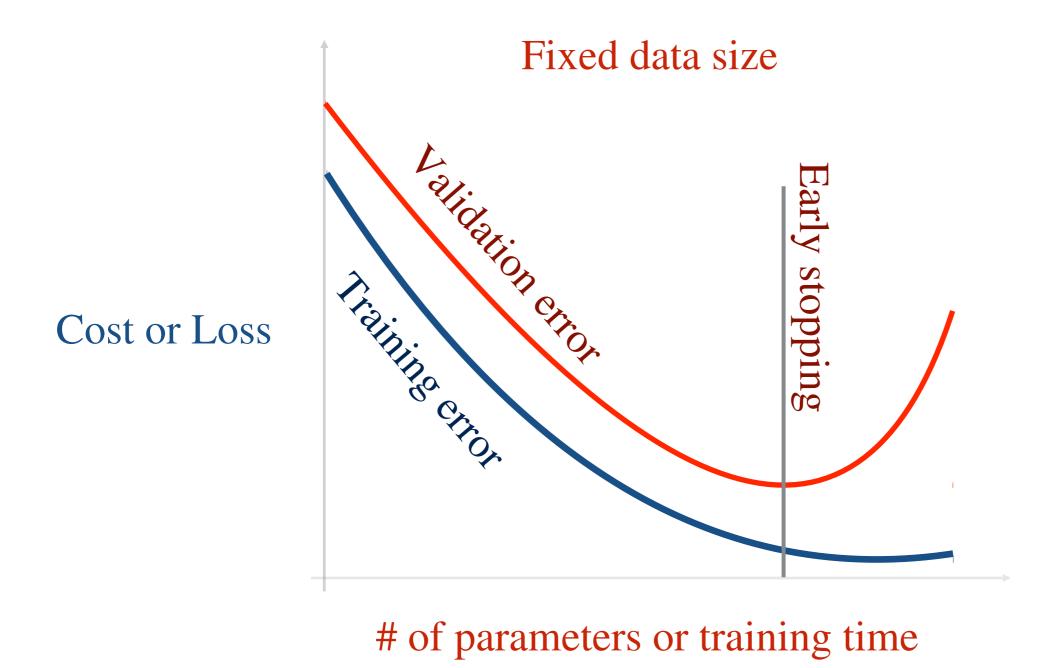
$$l(\theta) = \sum_{i} (\hat{y}_i - y_i)^2$$

Mean square error (simplest loss function) with \hat{y}_i the predicted value and y_i true value $\theta = \text{set of all the trainable parameters}$

$$\theta' = \theta - \epsilon \frac{\partial l(\theta)}{\partial \theta}$$

SGD for parameterupdate to minimize loss function

Overfitting problem in fully connected network



Too many parameters may easily over-fit to training dataset

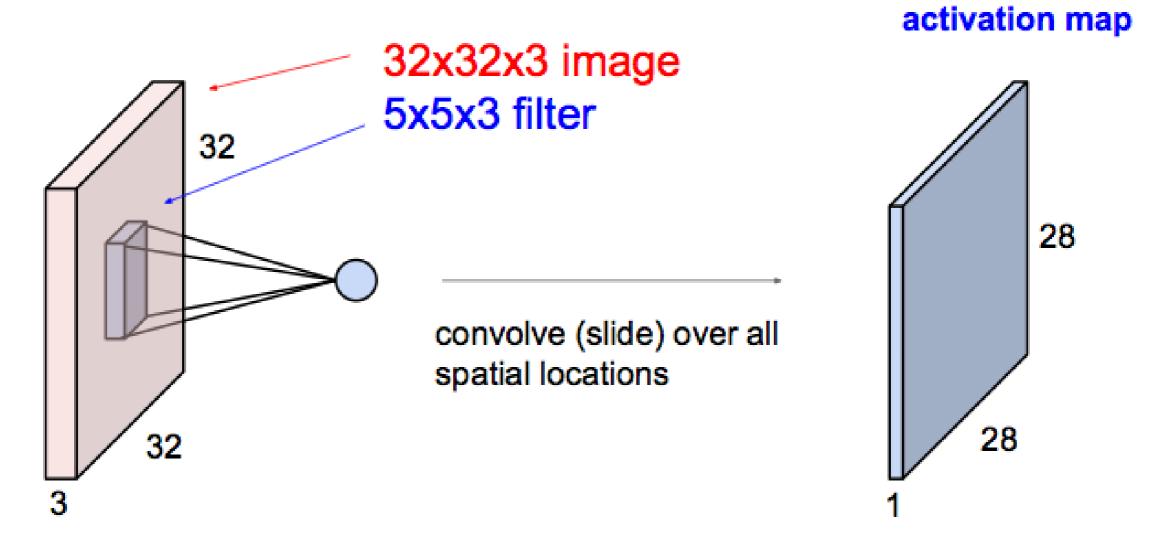
Ways to reduce overfitting

- 1. Early stopping
- 2.Increase training dataset by
 - a.preparing more data.
 - b.data augmentation (crop, scale, rotate, flip ...).
- 3. Reduce number of parameters
 - a.Dropout: randomly discarding neurons.
 - b.Drop connection: randomly discarding connections.
 - c.CNN: locally connected to a small chunk of neurons in the previous layer.
 - d.Go deeper.
- 4. Regularization, weight decay ...

Convolution neural network

Fig from CS231N, Stanford

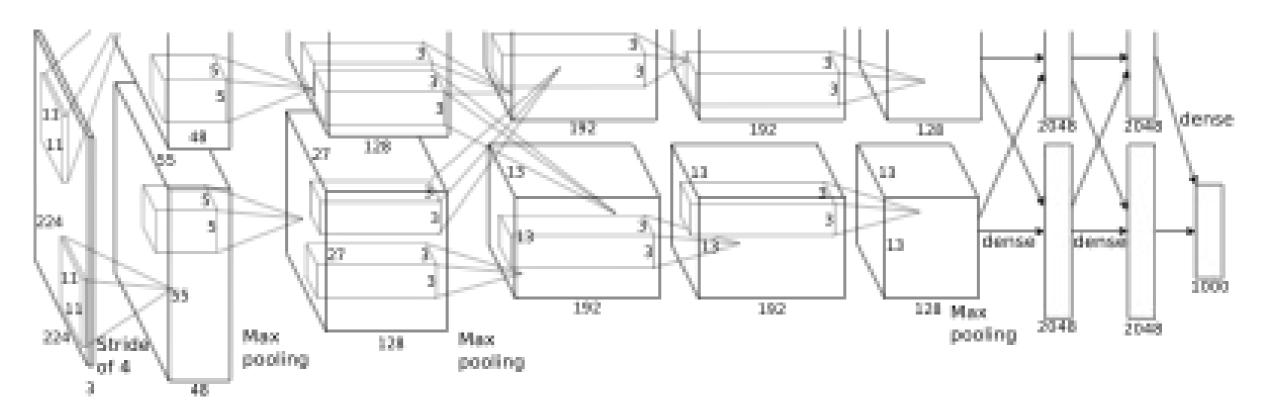
Convolution Layer



Advantage: scaling, rotating, translation invariant features can be learned since only subregion is connected to the filter/kernel which scan the whole input to feel the <u>2-d structure</u> and <u>local statistics</u>, and <u>Weight shared</u>.

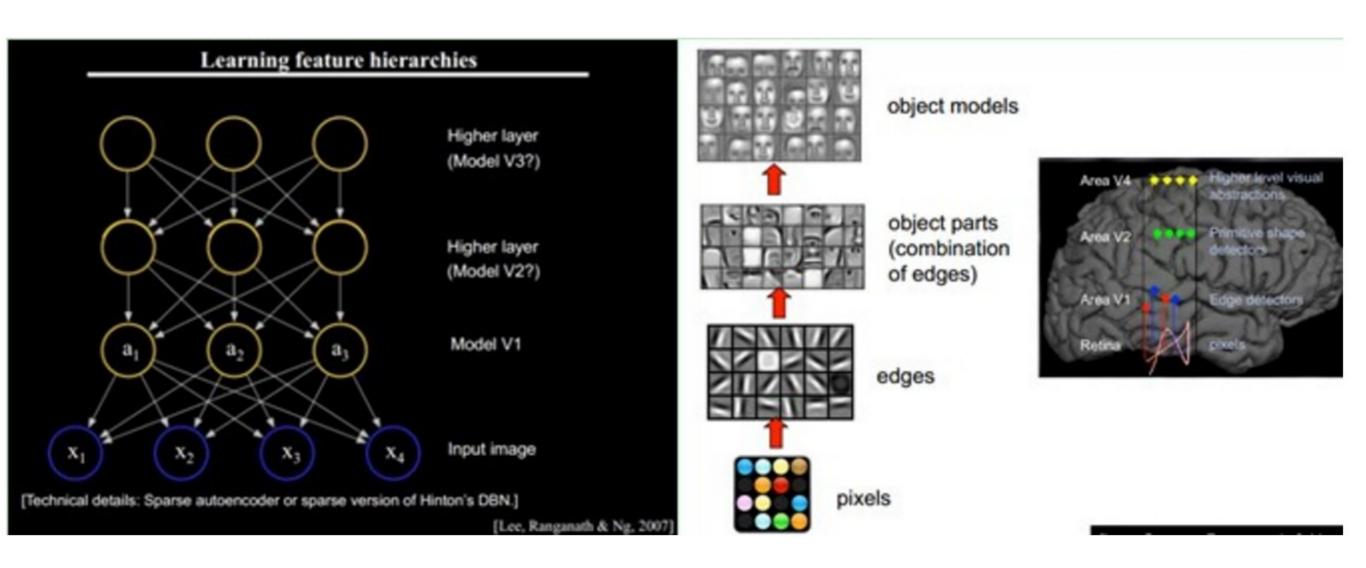
An example for CNN structure

AlexNet, Krizhevsky et al. 2012



- 8 layers, 60 million parameters
- Data augmentation and Dropout are used to reduce overfitting, first use ReLU
- Removing any hidden layer results in 2% loss.

What CNN did after the training?



Distributed representations are learned!

Open Source Libraries



Keras + TensorFlow in the present study

Keras is a high level neural network library, written in Python and capable of running on top of either TensorFlow or Theano.

```
# Build one fully connected neural network (100->64->10 neurons) in Keras
from keras.models import Sequential
from keras.layers import Dense, Activation

model = Sequential()
model.add(Dense(output_dim=64, input_dim=100))
model.add(Activation("relu"))
model.add(Dense(output_dim=10))
model.add(Activation("softmax"))
model.compile(loss='categorical_crossentropy', optimizer='sgd',
metrics=['accuracy'])
```

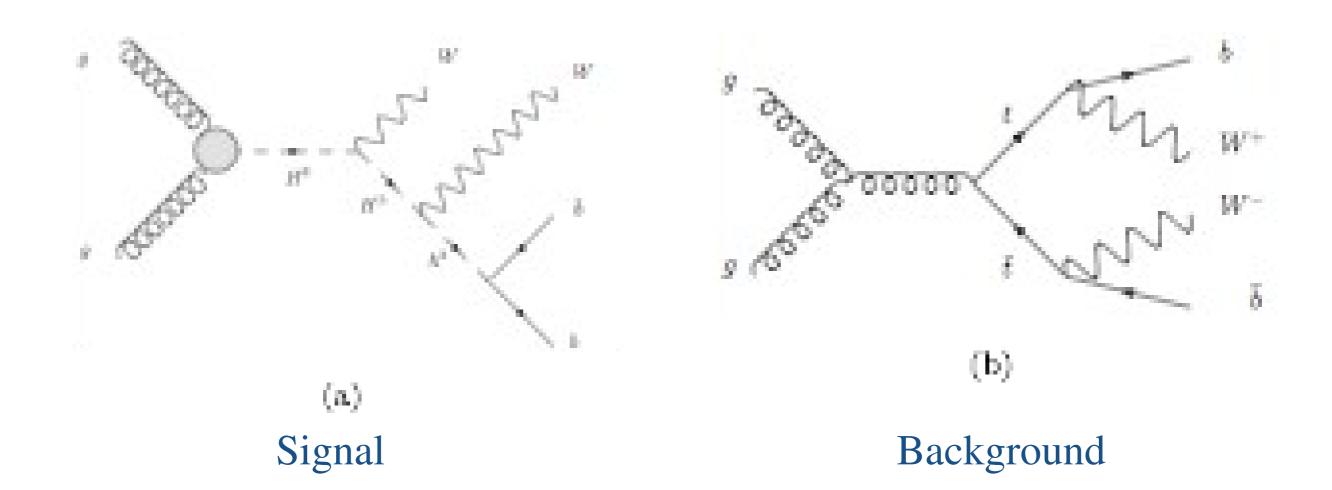
Deep learning in Physics (Particle Physics)

Searching for Exotic Particles in High-Energy Physics with Deep Learning

P. Baldi, P. Sadowski, and D. Whiteson

Nature Communications

Higgs benchmark



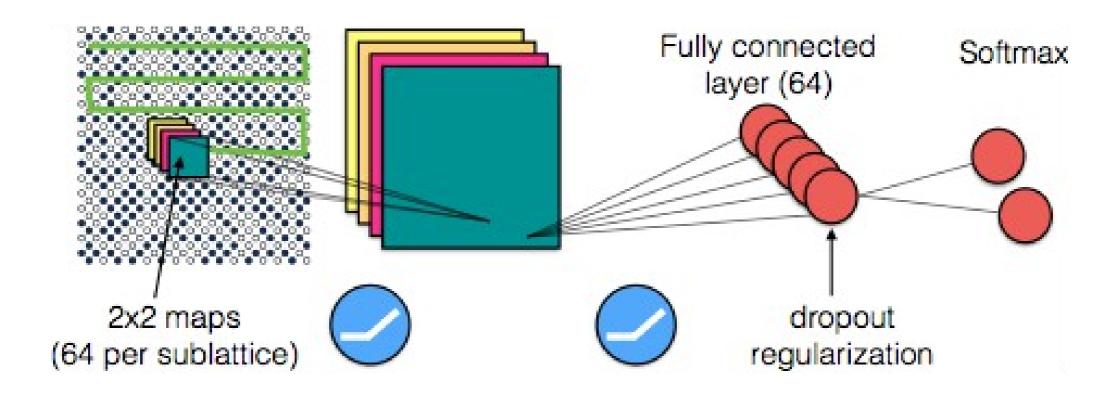
Deep learning in Physics (Heavylon Jet)

- P. Baldi, K. Bauer, C. Eng, P. Sadowski, and D. Whiteson, Jet Substructure Classification in High-Energy Physics with Deep Neural Networks, Phys. Rev. D93 (2016), no. 9 094034, [arXiv:1603.09349].
- D. Guest, J. Collado, P. Baldi, S.-C. Hsu, G. Urban, and D. Whiteson, Jet Flavor Classification in High-Energy Physics with Deep Neural Networks, arXiv:1607.08633.
- J. S. Conway, R. Bhaskar, R. D. Erbacher, and J. Pilot, Identification of High-Momentum Top Quarks, Higgs Bosons, and W and Z Bosons Using Boosted Event Shapes, arXiv: 1606.06859.
- J. Barnard, E. N. Dawe, M. J. Dolan, and N. Rajcic, Parton Shower Uncertainties in Jet Substructure Analyses with Deep Neural Networks, arXiv:1609.00607.

Deep learning in Physics (Cond-Mat Ising)

Machine learning phases of matter

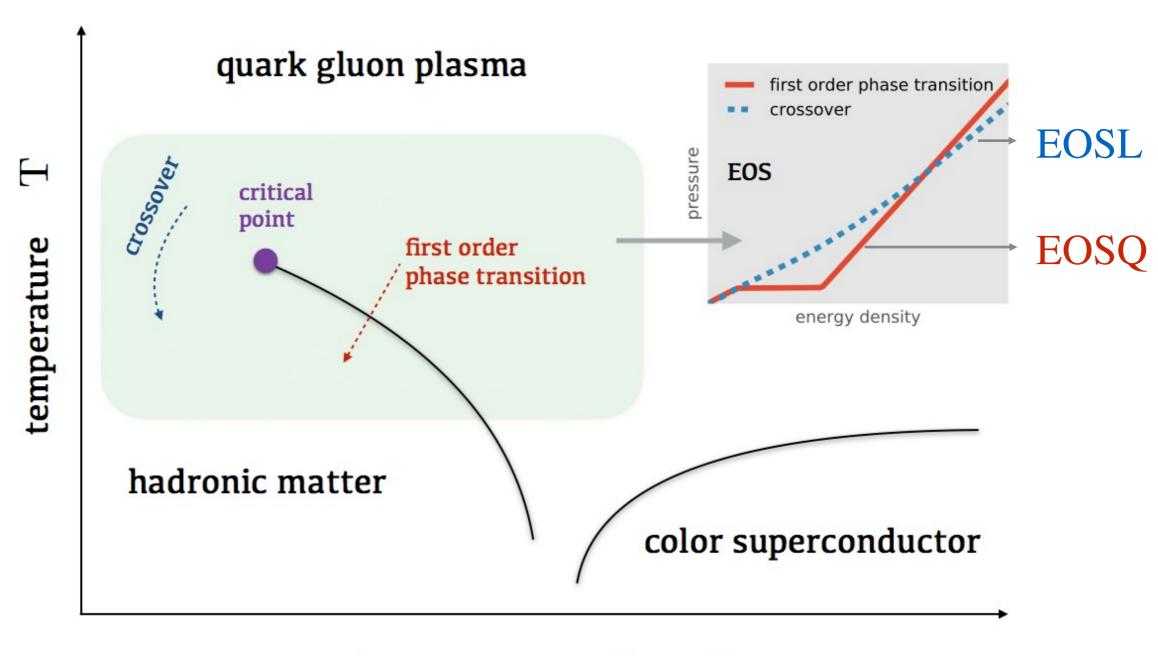
Juan Carrasquilla¹ and Roger G. Melko^{2,1}



Extract order parameter from the spin configurations, can encode phases and discriminate Phase Transition for spin, Coulomb and even topological phases.

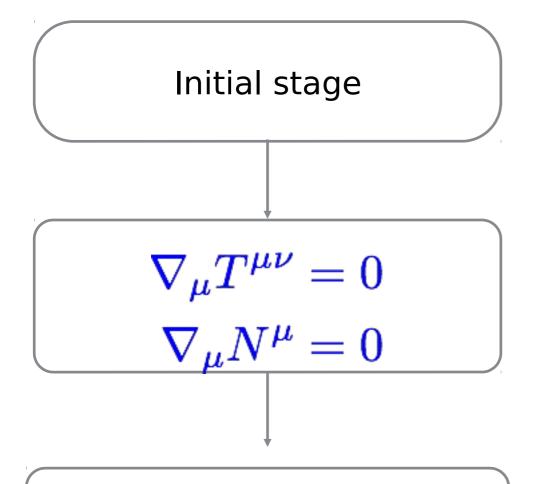
Identifying QCD transition in HIC using DL

QCD transition: 1st order or crossover?



baryon chemical potential μ_B

Uncertainties in the simulation of HIC



Pre-Equilibrium dynamics?
Fast thermalization/tau0?
Initial entropy deposition?
Baryon stopping?
Initial state fluctuations and flow?

EoS and transport coefficients (shear viscosity, bulk viscosity)

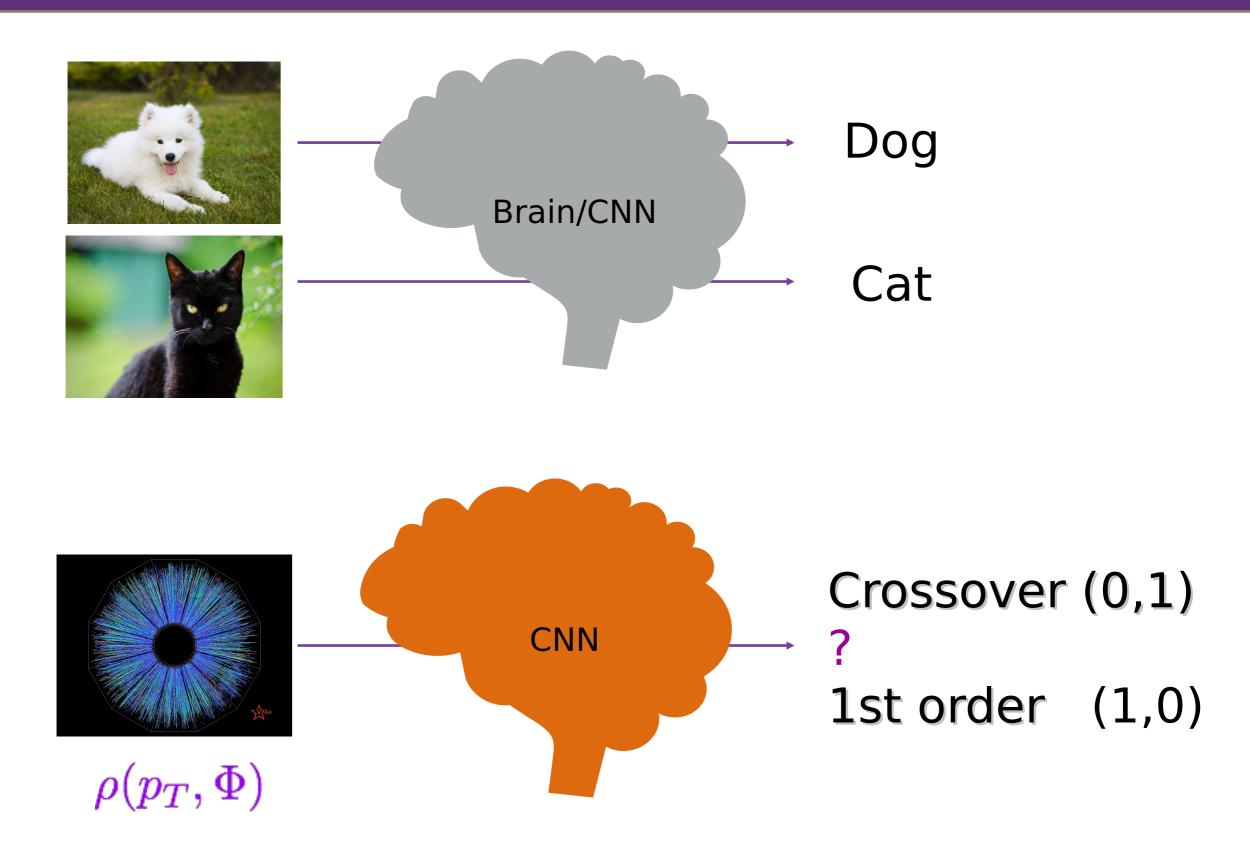
$$p^{\mu}\partial_{\mu}f + F \cdot \partial_{p}f = C$$

some unfixed scattering cross sections

Particle momentum distribution

Big uncertainty when comparing with Exp. data

New perspective --- Deep Learning



Key idea for our prototype study

Supervised learning using deep convolution neural network with huge amount of labeled training data (spectra, EoS type) from event-by-event relativistic hydrodynamic simulations.

Training dataset

$$\rho(p_T, \Phi)$$
 for charged pions at mid-rapidity $\rho(p_T, \Phi) \equiv \frac{dN_i}{dY p_T dp_T d\Phi} = g_i \int_{\sigma} p^{\mu} d\sigma_{\mu} f_i$

TRAINING	η/s	= 0	$\eta/s = 0.08$		
DATASET	EOSL	EOSQ	EOSL	EOSQ	
Au-Au $\sqrt{s_{NN}} = 200 \mathrm{GeV}$	7435	5328	500	500	
Pb-Pb $\sqrt{s_{NN}} = 2.76 \mathrm{TeV}$	4967	2828	500	500	

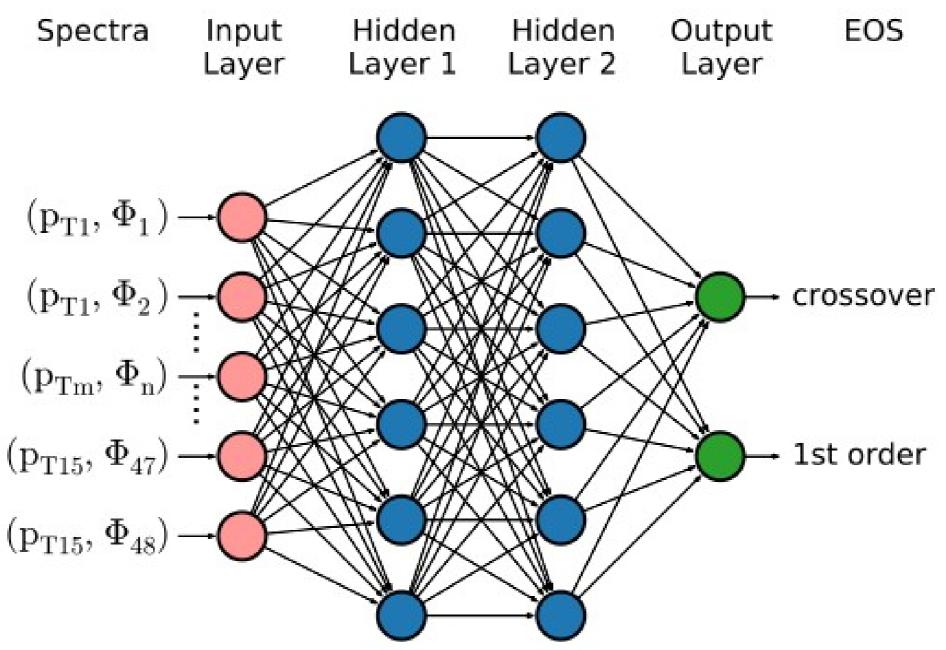
- CLVisc: (3+1D viscous hydrodynamic program parallelized on GPU using OpenCL) with AMPT initial condition (~22000 events, doubled by left-right flipping, 10% for validation).
- To is 0.4 fm for Au+Au and 0.2 fm for Pb+Pb collisions
- T_dec=0.137 GeV

Testing dataset

TESTING DATASET GROUP 1 : iEBE-VISHNU + MC-Glauber								
Centrality:	$\eta/s = 0$		$\eta/s = 0.08$		$\eta/s = 0.16$			
10-60%	EOSL	EOSQ	EOSL	EOSQ	EOSL	EOSQ		
$Au-Au \sqrt{s_{NN}} = 200 \mathrm{GeV}$	300	250	250	150	200	250		
Pb-Pb $\sqrt{s_{NN}} = 2.76 \mathrm{TeV}$	500	650	200	195	350	400		
TESTING DATASET GROUP 2 : CLVisc + IP-Glasma								
Au-Au $\sqrt{s_{NN}} = 200 \mathrm{GeV}$	EOSL			EOSQ				
b $\lesssim 8 \text{ fm } \& \eta/s = 0$	4165			4752				

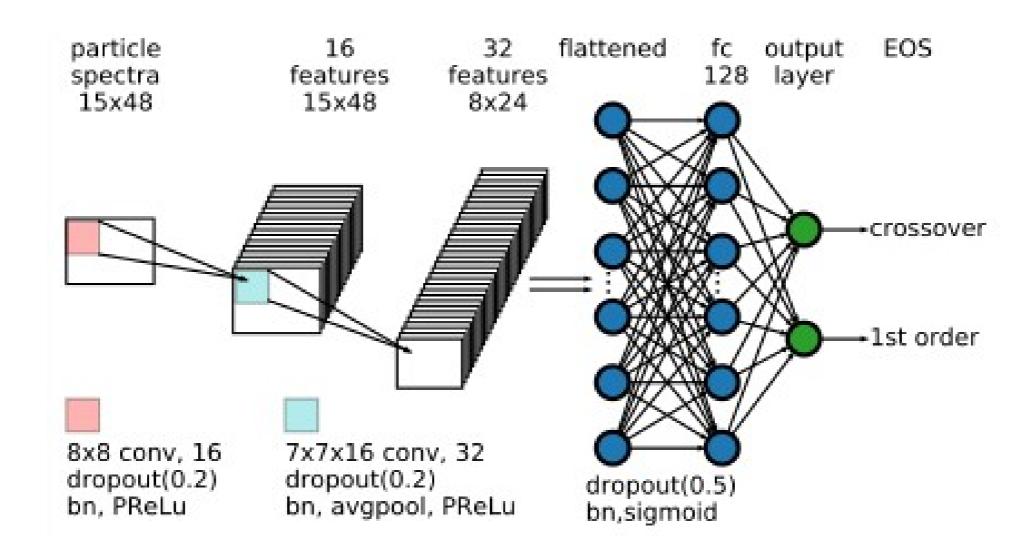
- iEBE-VISHNU: another viscous hydro package with different numerical solver for the partial differential equations and with different initial conditions, eta/s.
- τ_0 is 0.6 fm for all the testing dataset.
- T_dec in [0.115GeV, 0.142GeV] for iEBE-VISHNU

First try with fully connected neural network



Overfit to the training dataset! Does not work for testing dataset. ----- no generalization.

CNN architecture for EoS-meter



Batch normalization, Dropout, L2 Rregularization, PreLU are used to prevent the overfitting.

Train 500 epochs, in mini-batch with size=64 Learning rate: 0.0001, decay with rate: 1.0E-6

Results

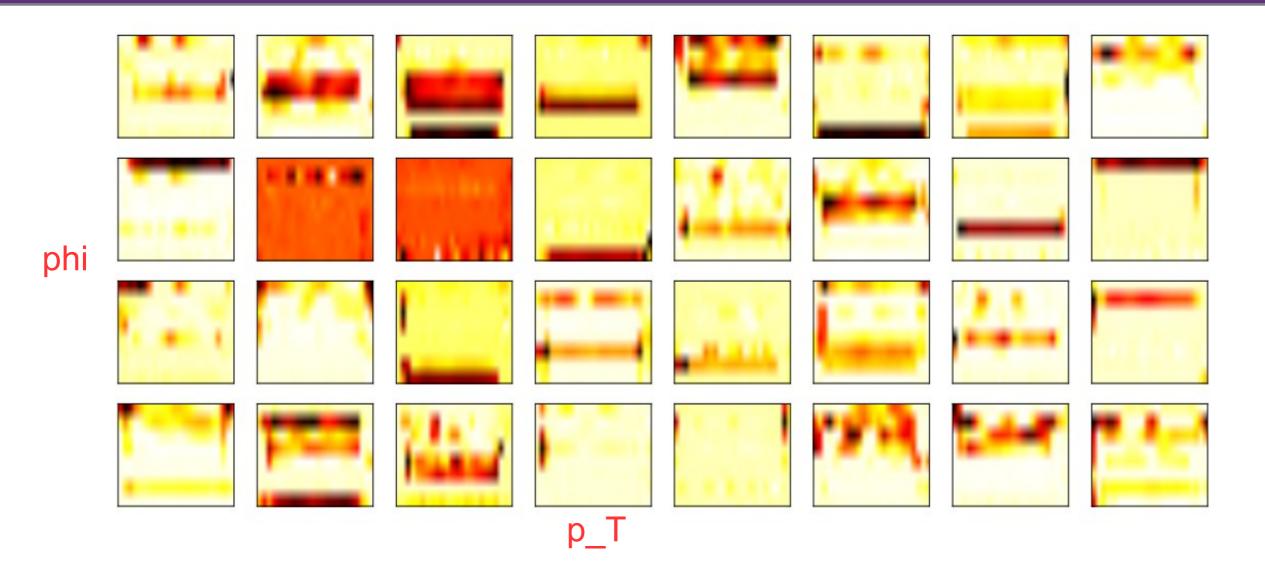
TESTING	GROUP 1		GROUP 2	
ACCURACIES	EOSL	EOSQ	EOSL	EOSQ
Number of events	1800	1895	4164	4752
Accuracy	95.1%	95.8%	96.4%	96.4%

~95% prediction accuracy on avg. in independent testing dataset solely from the raw spectra

The performance is **robust against**: <u>initial conditions/fluctuations</u>, tao 0, eta/s, T_dec

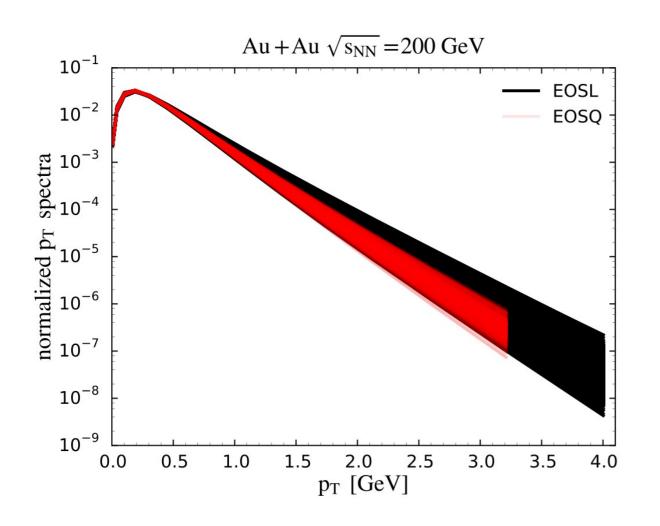
---- model independent (general rule is learned)

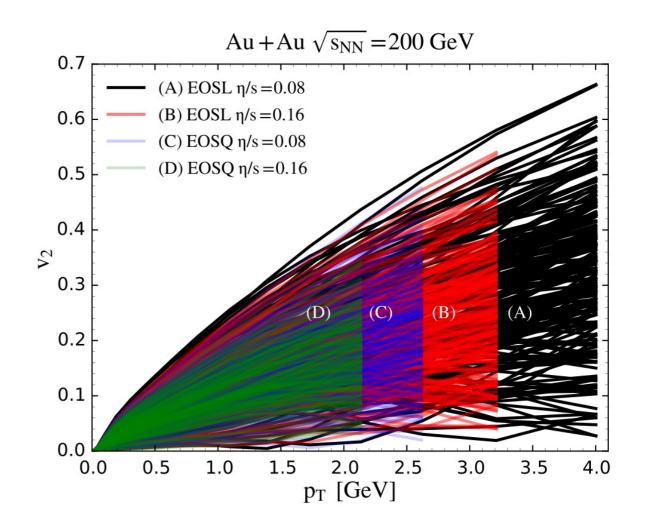
EoS-meter from CNN



- Each hotspot represents correlations in a small phase space (32 features in the 2nd convolution layer)!
- Correlation of these features from the next fully connected layer

Conventional observables





 Strongly depends on initial stage fluctuations and other parameters

CNN provides novel perspective in connecting QCD theory with HIC directly:

 There do exist 'mapping/Encoders/projection' from QCD transition onto the final state raw spectra, although they are not intuitive to conventional interpretation yet.

---They are clean (robust to other uncertainties and parameters)

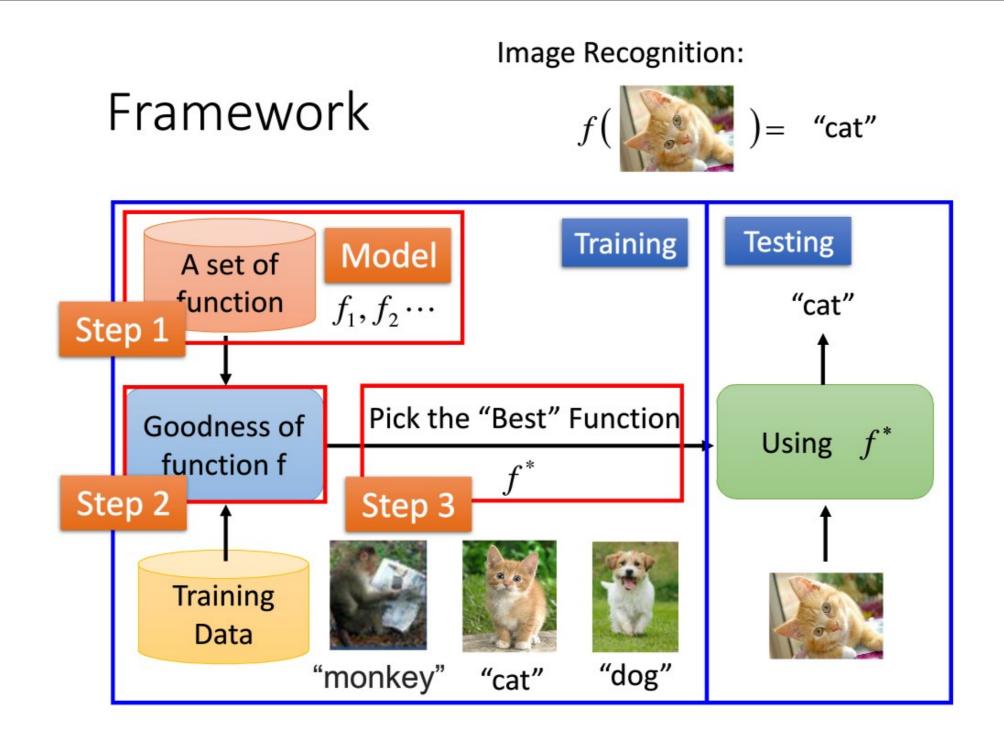
• The deep CNN can provide a powerful and efficient 'Decoder' for the above Encoder/mapping

-----the high-level representations act as 'EoS-meter'

Outlook

- Try to find out the underlying mechanism (guided back-propagation)
- Extend the model to work with real Exp. data
- Extract other dynamical parameters like eta/s.

What DL is doing?



Slides by Long-gang