# Deep Learning for high energy nuclear physics

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Yann LeCun

Deep learning is constructing networks of parameterized functional modules & training them from examples using gradient-based optimization



#### DL: Neural Network with multi hidden layers









#### Loss functions





### NLL loss in flow model



Normalizing flow:

#### **NLL loss:**

$$egin{aligned} \mathbf{z}_{i-1} &\sim p_{i-1}\left(\mathbf{z}_{i-1}
ight) \ \mathbf{z}_{i} &= f_{i}\left(\mathbf{z}_{i-1}
ight), \mathbf{z}_{i-1} = f_{i}^{-1}\left(\mathbf{z}_{i}
ight) \ p_{i}\left(\mathbf{z}_{i}
ight) &= p_{i-1}\left(f_{i}^{-1}\left(\mathbf{z}_{i}
ight)
ight) \left|\detrac{df_{i}^{-1}}{d\mathbf{z}_{i}}
ight| \ & ext{Loss} &= -\log p(x) \end{aligned}$$



#### NLL loss in RL

 $S_t$ 

 $r_t$ 

Agent

**Environment** 





 $a_t$ 



$$heta = heta - lpha rac{1}{m} \sum_{i=1}^m 
abla_ heta l_i$$

**Example:**  $L( heta)= heta^2$  , simple 1D gradient descent , heta= heta-lpha imes2 heta ,





#### How to escape local minimum



- **1. Yann Lecun:**  $P(minimum) = 0.5^n$ , more saddle points
- 2. SGD introduces disturbance
- 3. Momentum helps to escape local minimum or saddle point



#### Momentum





### Adaptively chaning learning rate



$$egin{aligned} g_t &= 
abla_ heta l, \quad G &= \sum_t g_t^2, \ heta &= heta - rac{lpha}{\sqrt{G+\epsilon}} \cdot g_t. \end{aligned}$$



- Apply smaller Ir to the big  $\partial_{\theta_i} l$  direction
- SGD + Momentum + Adaptive LR  $\rightarrow$  Adam



### Auto Differentiation

#### • Forward Mode

Introduce dual numbers:  $x \rightarrow x + \dot{x} \mathbf{d}$ where  $\mathbf{d}^2 = 0$ 

$$(x + \dot{x}\mathbf{d}) + (y + \dot{y}\mathbf{d}) = x + y + (\dot{x} + \dot{y})\mathbf{d}$$
  

$$(x + \dot{x}\mathbf{d}) - (y + \dot{y}\mathbf{d}) = x - y + (\dot{x} - \dot{y})\mathbf{d}$$
  

$$(x + \dot{x}\mathbf{d}) * (y + \dot{y}\mathbf{d}) = xy + (x\dot{y} + \dot{x}y)\mathbf{d}$$
  

$$\frac{1}{x + \dot{x}\mathbf{d}} = \frac{1}{x} - \frac{\dot{x}}{x^2}\mathbf{d} \qquad (x \neq 0)$$

Forward mode for  $\ R^1 o R^n$ 

Reverse mode for  $\ R^n o R^1$ 

#### • Reverse Mode



$$egin{aligned} ext{step 2}: ar{w} = ar{w} + ar{b} rac{\partial b}{\partial w} \ ext{step 3}: ar{w} = ar{w} + ar{c} rac{\partial c}{\partial w} \end{aligned}$$



### Tools for AutoDiff

**O** PyTorch







... training deep models is a sufficiently difficult task that most algorithms are strongly affected by the choice of initialization. The initial point can determine whether the algorithm converges at all, with some initial points being so unstable that the algorithm encounters numerical difficulties and fails altogether.

Deep Learning, 2016



### Initialization methods

For Tanh activation function, the Xavier (Glorot) initialization is widely used.

For Sigmoid activation, one may use normalized Xavier initialization,

weights  $\sim N[0,\sigma]$ 

where  $\sigma = \sqrt{6/(n+m)}$ , where n is the number of input neurons and m is the number of output neurons of that layer.

For **ReLU** activation function, one should use **He** initialization, e.g., in tensorflow,

$$ext{weights} \sim ext{U}\left[-\sqrt{rac{6}{n}},\sqrt{rac{6}{m}}
ight],$$

where U stands for uniform distribution,



#### What has been learned (Global interpretation)



Olah, et al., "Feature Visualization", Distill, 2017.

shallow layers

deep layers



#### Local interpretation



- Ablation studies: LIME or Prediction Difference Analysis. M. Tulio Ribeiro, et. al. "Why should I trust you?"
- Class activation map: map the deep layers to the input image, look for the most important region for decision making. BoLei Zhou, et. al. "Learning Deep Features for discriminative localization"
- Layer-wise relevance propagation: set the relavance of the output layer to 1, propagate the relevance to the input data, to look for the most important region for decision making.



### DL nuclear physics across energy scales



- Deep generative models (such as normalizing flow and the diffusion model) have been used to sample Field Configureations in Lattice QCD
- Deep learning is widely used to solve inverse problems of HIC to study the EoS of hot QCD matter, the phase transition, the transport coefficients eta/s, ...
- Deep neural network is used to represent the manybody wave function of nucleus, to solve variational problems in ab initio calculations
- Deep learning is used to solve inverse problems of HIC to study the nuclear structure, for instance, the nuclear deformation, neutron skin, alpha cluster and short range correlation
- > DL for nuclear liquid droplet model...



#### Generativive models: MC sampling



Similar to Box Muller algorithm



Flow-based generative models for Markov chain Monte Carlo in lattice field theory Albergo, Kanwar, Shanahan 1904.1207



#### Reviews

Collo	quium: Ma	achine learning in nuclear physics	High energy nuclear physics meets
Amber B Morten H	oehnlein, Markus Ijorth-Jensen, Ta	s Diefenthaler, Nobuo Sato, Malachi Schram, Veronique Ziegler, Cristiano nja Horn, Michelle P. Kuchera, Dean Lee, Witold Nazarewicz, Peter Ostro	Fanel Machine Learning
Orginos, Rev. Moc	Alan Poon, Xin-F d. Phys. <b>94</b> , 0310	Nian Wang, Alexander Scheinker, Michael S. Smith, and Long-Gang Pang 03 – Published 8 September 2022	Wan-Bing He (Fudan U., Shanghai and Fudan U.), Yu-Gang Ma (Fudan U., Shanghai and Fudan U.), Long-Gang Pang, Huichao Song (CCNU, Wuhan, Inst. Part. Phys. and Hua-Zhong Normal U., LQLP and Peking U.), Kai Zhou (Frankfurt U., FIAS) (Mar 12, 2023)
Article	References No Citing Articles PDF HTML Export Citation	e-Print: 2303.06752 [hep-ph]	
			HEPML-LivingReview
>	1 DOTT		A Living Review of Machine Learning for Particle Physics
	ABST	RACT	Modern machine learning techniques, including deep learning, is rapidly being applied, adapted, and developed for high energy physics. The
	Advances in machine learning methods provide tools that have broad applicability in scientific reso These techniques are being applied across the diversity of nuclear physics research topics, leading		goal of this accument is to provide a hearly comprehensive list of citations for those aeveloping and applying these approaches to experimental, phenomenological, or theoretical analyses. As a living document, it will be updated as often as possible to incorporate the latest developments. A list of proper (unchanging) reviews can be found within. Papers are grouped into a small set of topics to be as useful as
Explor	ing QCD r	matter in extreme conditions with Machine	possible. Suggestions are most welcome. download review
Learning			The purpose of this note is to collect references for modern machine learning as applied to particle physics. A minimal number of
Kai Zhou	(Frankfurt II Fl	AS) Lingviao Wang (Frankfurt II, FIAS) Long-Gang Pang (CCNIL)	paper is listed in this document does not endorse or validate its content - that is for the community (and for peer-review) to decide.
Inst. Part.	Phys.), Shuzhe	Shi (Stony Brook U.)	should be included, (b) a paper has been misclassified, or (c) a citation for a paper is not correct or if the journal information is now available. In order to be as useful as possible, this document will continue to evolve so please check back before you write your next paper.
Mar 27, 2023			If you find this review helpful, please consider citing it using \cite{hepmllivingreview} in HEPML.bib. <ul> <li>Reviews</li> </ul>
1/6 page	c		<ul> <li>Modern reviews</li> </ul>
e-Print: 23	303.15136 [hep	-ph]	<ul> <li>Jet Substructure at the Large Hadron Collider: A Review of Recent Advances in Theory and Machine Learning [DOI]</li> <li>Deep Learning and its Application to LHC Physics [DOI]</li> </ul>







#### Pb speed~99.9999% c

Au speed  $\sim$ 99.99% c





### Explore QCD phase structure using HIC





#### Inverse problems in HIC





## Theoretical model: relativistic hydro



#### Name of CLVisc:

CCNU-LBNL Viscous Hydro, CCNU = Central China Normal University
 A 3+1D viscous hydro parallized on GPU using OpenCL

**Purpose:** Describe the non-equilibrium space-time evolution of hot QCD matter **Feature: 100 times faster** than using a single core CPU.

L.G. Pang, Q. Wang and X. N. Wang, PRC 86 (2012) 024911 L.G. Pang, B.W. Xiao, Y. Hatta, X.N.Wang, PRD 2015 L.G. Pang, H.Petersen, XN Wang, PRC97(2018)no.6,064918



### CLVisc for different EoS



eta/s = 0 Lattice QCD EoS (smooth cross over)

eta/s = 0 First order phase transition

eta/s = 0.08 Lattice QCD EoS

eta/s = 0.08 First order phase transition eta/s: shear viscosity / entropy density

Will the effect of EoS survive the dynamical evolution and exist in the final state hadrons?



#### statistical hadronization of (u,d,s) hadrons

A. Andronic, P. Braun-Munzinger, K. Redlich, J. Stachel, Nature 561 (2018) 321



$$n_i = (2s_i + 1) 4 \pi \int p^2 \left[ e^{\left(\sqrt{p^2 + m_i^2} - \mu_i 
ight)/T} \pm 1 
ight]^{-1} dp$$

 At LHC, equal amounts of matter and anti-matter are produced
 At BES region, more protons than anti protons



#### CLVisc vs experimental data

#### Longitudinal momentum distribution





0.5

0.0

1.0

1.5

p<sub>T</sub> [GeV]

2.0

2.5

3.0

p<sub>T</sub> [GeV]



# Challenges

Fig from S. Bass QM2017 (Bayesian method)

#### **Model Parameter:**



(1) Multiple parameters entangle with multiple observables

(2) Different parameter combinations describe the same data



### Bayesian analysis QCD EoS

The  $c_s^2$  is parameterized as a function of energy density in the following,

$$c_s^2(\epsilon) = c_s^2(\epsilon_h) + \left(\frac{1}{3} - c_s^2(\epsilon_h)\right) \frac{X_0 x + x^2}{X_0 x + x^2 + X'^2}$$
(2.12)

where  $X_0 = \sqrt{12}RX'c_s(\epsilon_h)$ ,  $x \equiv \ln \frac{\epsilon}{\epsilon_h}$ ,  $\epsilon_h$  is the energy density at T = 165 MeV, R and X' are the two parameters in the EoS to be determined. Randomly choosing R and X' from the range -0.9 < R < 2 and 0.5 < X' < 5 generate the unconstrained EoS that varies in a large region between  $c_s^2 = 0.05$  and  $c_s^2 = 0.33$ , as shown in Fig. 2.4-a. This corresponds to the a priori distribution of  $c_s^2$  parameters together with other 12 parameters in the model  $P(\theta)$ .

Likelihood:

$$P(D|\theta) = \prod_i \exp\left(-(z_i(\theta) - z_{i,\exp})^2/2\right)$$

Posterior:  $P(\theta \mid D) \propto P(D \mid \theta)P(\theta)$ 



S. Pratt, E. Sangaline, P. Sorensen, H. Wang, PRL. 114 (2015) 202301.







#### EoS for different phase transition types



baryon chemical potential  $\mu_B$ 



#### Determine nuclear phase transitions



Nature Communications 2018, LG. Pang, K.Zhou, N.Su, H.Petersen, H. Stoecker, XN. Wang.









#### Determining nuclear deformation





L.-G. Pang, K. Zhou and X.-N. Wang, arXiv:1906.06429



#### Data representation





#### Spinodal vs Maxwell 1st order phase transition



J. Steinheimer, L.G. Pang, K. Zhou, V. Koch and J. Randrup, JHEP 12 (2019) 122



#### Capture more local correlations

#### **Dynamical Edge Convolution Network**



Fig. 2. Left: Computing an edge feature,  $e_{ij}$  (top), from a point pair,  $x_i$  and  $x_j$  (bottom). In this example,  $h_{\Theta}$ () is instantiated using a fully connected layer, and the learnable parameters are its associated weights. **Right**: The EdgeConv operation. The output of EdgeConv is calculated by aggregating the edge features associated with all the edges emanating from each connected vertex.



#### Looking for self similarity in momentum space



Self similarity, scaling invariance



PLB 827(2022) 137001, Y.-G. Huang, L.-G. Pang, X.F. Luo and X.-N. Wang





off-diagonal = misclassified



Protons, Predicted labels

PLB 822 (2021) 136669, Y.J Wang, F.P. Li, Q.F. Li, H.L. L<sup>"</sup>u, and K. Zhou



#### Auto Encoder for order parameter

#### PHYSICAL REVIEW RESEARCH 2, 043202 (2020)

#### Nuclear liquid-gas phase transition with machine learning

Rui Wang<sup>1,2,\*</sup> Yu-Gang Ma,<sup>1,2,†</sup> R. Wada,<sup>3</sup> Lie-Wen Chen<sup>9,4</sup> Wan-Bing He,<sup>1</sup> Huan-Ling Liu,<sup>2</sup> and Kai-Jia Sun<sup>3,5</sup>





#### $(\mu_{BC}, \alpha_{\text{diff}}, w, \rho) \mapsto P(T, \mu_B) \mapsto \{\text{acceptable, unstable, acausal}\}.$

4 parameters from 3D Ising model Q

QCD EoS

Lables for classification



D. Mroczek, M. Hjorth-Jensen, J. Noronha-Hostler, P. Parotto, C. Ratti, and R. Vilalta, PRC 107, 054911



### Active learning procedure



D. Mroczek, M. Hjorth-Jensen, J. Noronha-Hostler, P. Parotto, C. Ratti, and R. Vilalta, PRC 107, 054911



# Quasi particle picture of QCD EoS





screened, dressed, regularized, quasi particle



# **DL For Quasi Particle Mass**

FuPeng Li, HL Lu, LG Pang, GY Qin, PLB 2023

$$\ln Z(T) = \ln Z_g(T) + \ln Z_{u,d}(T) + \ln Z_s(T),$$

Fermi-Dirac distributions,

$$\ln Z_g(T) = -\frac{16V}{2\pi^2} \int_0^\infty p^2 dp$$
  

$$\ln \left[ 1 - \exp\left(-\frac{1}{T}\sqrt{p^2 + m_g^2(T)}\right) \right], \quad (2)$$
  

$$\ln Z_{q_i}(T) = +\frac{12V}{2\pi^2} \int_0^\infty p^2 dp$$
  

$$\ln \left[ 1 + \exp\left(-\frac{1}{T}\sqrt{p^2 + m_{q_i}^2(T)}\right) \right], \quad (3)$$



quarks,  $m_s(T, \theta_2)$  for strange quark and  $m_g(T, \theta_3)$  for gluons, where  $\theta_1$ ,  $\theta_2$  and  $\theta_3$  are the parameters in DNN shown in Fig. 1.

The resulting pressure and energy density are computed using the following statistical formulae,

$$P(T) = T\left(\frac{\partial \ln Z(T)}{\partial V}\right)_T,\tag{5}$$

$$\epsilon(T) = \frac{T^2}{V} \left(\frac{\partial \ln Z(T)}{\partial T}\right)_V,\tag{6}$$





FuPeng Li, HL Lu, LG Pang, GY Qin, PLB 2023





Yuki Fujimoto, Kenji Fukushima, and Koichi Murase, PRD 98 (2018) 2, 023019





S. Soma, L. Wang, S. Shi, H. Stöcker, K. Zhou, PRD 107, (2023) 083028



# DL for numerical relativity

#### Solving Einstein equations using deep learning

Zhi-Han Li<sup>1</sup>, Chen-Qi Li<sup>1</sup>, Long-Gang Pang<sup>1a</sup> <sup>1</sup>Key Laboratory of Quark & Lepton Physics (MOE) and Institute of Particle Physics, Central China Normal University, Wuhan 430079, China

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R = \kappa T_{\mu\nu}$$

$$L(\theta) = \frac{1}{N} \sum_{i=0}^{N} \left( R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R - \kappa T_{\mu\nu} \right)^{2}$$







Y.L. Yang, P.W. Zhao, PRC 2023



# Using PINN





# Auto-Diff for parton fragmentation function



BW Zhang, HZ Zhang, in preparation



#### Jet quecnhing

Can Being Underwater Protect You From Bullets?



**1** If the bullet is shot from an angle of 30 Degrees, then being underwater in the range of 3-5 feet (0.9-1.5 meters) can ensure safety from most guns.



Jet quenching in hot QGP





Nuclear EoS: 
$$c_s^2 = \frac{dP}{d\epsilon} = \sin^2 \theta$$

Shear Viscosity: width of the shock wave



- Random production locations and propagating directions relative to collective flow
- Tilted by different path length and collective flow



L.M. Satarov, H. Stoecker, I.N. Mishustin, PLB 627 (2005) 64-70



# If it is possible to locate the initial jets





# DL assisted jet tomography (gamma-jet)



Z Yang, YY He, W Chen, WY Ke, LG Pang, XN Wang, EPJC 83 (2023) 7, 652



### Training data: CoLBT(LBT + CLVisc)

$$p\partial f(p) = -C(p) \quad (p \cdot u > p_{cut}^0)$$
$$\partial_{\mu} T^{\mu\nu}(x) = j^{\nu}(x)$$
$$j^{\nu} = \sum_{i} p_{i}^{\nu} \delta^{(4)}(x - x_{i}) \theta(p_{cut}^0 - p \cdot u)$$

LBT: YY He, T Luo, XN Wang, Y Zhu, PRC 91 (2015) 054908, PRC 97 (2018) 1, 019902

CLVisc:

LG Pang, Q Wang, XN Wang, PRC 86 (2012) 024911

**LG Pang, H Petersen, XN Wang,** PRC 97 (2018) 6, 064918

XY Wu, GY Qin, LG Pang, XN Wang, PRC 105 (2022) 3, 034909



CoLBT:

W Chen, T Luo, SS Cao, LG Pang, XN Wang, PLB 777 (2018) 86-90



$$p_{1}\partial f_{1} = -\int dp_{2}dp_{3}dp_{4}(f_{1}f_{2} - f_{3}f_{4}) |M_{12\rightarrow 34}|^{2} (2\pi)^{4} \delta^{4}(\sum_{i} p^{i}) + inelastic$$
Medium-induced gluon(HT):  

$$\frac{dN_{g}}{dzd^{2}k_{\perp}dt} \approx \frac{2C_{A}\alpha_{s}}{\pi k_{\perp}^{4}} P(z)\hat{q}(\hat{p} \cdot u)sin^{2}\frac{k_{\perp}^{2}(t-t_{0})}{4z(1-z)E}$$
Tracked partons:  
Jet shower partons  
Thermal recoil partons  
Radiated gluons  
Negative partons(Back reaction induced by energy-momentum conservation)

YY He, T Luo, XN Wang, Y Zhu, PRC 91 (2015) 054908, PRC 97 (2018) 1, 019902



### DL assisted jet tomography



#### **Network predictions**

#### **True locations**

Jet hadron correlation for selected events whose locations are constrained to specific regions using DL assisted jet tomography

Z Yang, YY He, W Chen, WY Ke, LG Pang, XN Wang, EPJC 83 (2023) 7, 652



#### Enhance the Diffusion Wake signal



Z Yang, YY He, W Chen, WY Ke, LG Pang, XN Wang, EPJC 83 (2023) 7, 652 Z Yang, T Luo, W Chen, LG Pang, XN Wang, PRL 130 (2023) 5, 052301



- Studying physics using HIC is a typical inverse problem
- DL builds nonlinear maps between final state observations and physical properties of nuclear matter
- Deep neural networks are widely used as varational functions that are learned through training
- The derivatives of the varational function can be computed with machine precision using auto-diff