

Winter School on Numerical Methods for Strongly Correlated Quantum Systems, February 19-23 2018, Marburg

Deep Learning and Quantum Many-Body Computation

Lei Wang (王磊) Institute of Physics, CAS <u>https://wangleiphy.github.io</u>

Fall School 2013 on Advanced Algorithms for Correlated Quantum Matter

L Fakher Assaad Announcement, Fall School 2013, Schools/Conferences 💆 April 9, 2013

No Comments »

Our first Fall school on

Advanced Algorithms for Correlated Quantum Matter

took place in Würzburg, during the week of September 30 to October 4.



Plan



Introduction



Deep learning theoretical minimum



Applications to quantum many-body physics and beyond



Hands on session (Jin-Guo Liu, Shuo-Hui Li)

Hands on https://github.com/GiggleLiu/marburg

Deep Learning and Quantum Many-Body Physics - Hands on Session

Table of Contents

We have prepaired four examples

- Computation Graphs and Back Propagation
- RealNVP network for sampling
- Restricted Boltzmann Machine for image restoration
- Deep Neural Network as a Quantum Wave Function Ansatz

They have been uploaded to both Google drive and Github repository. Have fun!

Preparations

You may use either local or online accesses to our python notebooks.

If you are not using an Nvidia GPU or its driver are not properly configured, online access is recommended, otherwise you may loss some fun in this session.

Lecture note http://wangleiphy.github.io/lectures/DL.pdf

Lecture Note on Deep Learning and Quantum Many-Body Computation

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February 14, 2018

Abstract

This note introduces deep learning from a computational quantum physicist's perspective. The focus is on deep learning's impacts to quantum many-body computation, and vice versa. The latest version of the note is at http://wangleiphy.github.io/. Please send comments, suggestions and corrections to the email address in below.

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exact diagonalization

quantum Monte Carlo





dynamical mean field theories





exact diagonalization

quantum Monte Carlo

tensor network

states



dynamical mean field theories

Algorithmic improvement in past 20 years outperformed Moore's law





exact diagonalization

quantum Monte Carlo



tensor network states



dynamical mean field theories







exact diagonalization

quantum Monte Carlo



tensor network states



dynamical mean field theories



Materials Discovery/Ab Initio/DFT

Microscopic Composition Data Generation

via laborious Computation/Experiments Macroscopic Properties

"Machine Learning in Materials Science: Recent Progress and Critical Next Steps" Rampi Ramprasad @ IPAM program on Understanding Many-Particle Systems with ML, 2016

Materials Discovery/Ab Initio/DFT



"Machine Learning in Materials Science: Recent Progress and Critical Next Steps" Rampi Ramprasad @ IPAM program on Understanding Many-Particle Systems with ML, 2016

Statistical Physics

Spin Glasses/Complex Networks

Soft Matter/Biophysics





Deep learning has its statistical physics gene

Quantum Information & Computation



Cai et al, PRL 114, 110504 (2015)

	¹³ C	<i>F</i> ₁	<i>F</i> ₂	F ₃
¹³ C	15479.9Hz			F_3
<i>F</i> ₁	-297.7Hz	-33130.1Hz	1	13C
<i>F</i> ₂	-275.7Hz	64.6Hz	-42681.4Hz	• • • • • • • • • • • • • • • • • • •
<i>F</i> ₃	39.1Hz	51.5Hz	-129.0Hz	-56443.5Hz
T_{2}^{*}	1.22s	0.66s	0.63s	0.61s
<i>T</i> ₂	7.9s	4.4s	6.8s	4.8s

Li et al, PRL 114, 140504 (2015)



Perdomo-Ortiz et al, 1708.09757



Rigetti Computing, 1712.05771

Review "Quantum machine learning", Biamonte, Wittek et al, Nature 2017







ALE ON

Al: Your New Brain



52 mins | N/R

Deep Learning is a radical and recent revolution from engineering. Deep learning allows computer systems to better analyse and interpret large volumes of data. By using deep neural networks, computers can analyse, understand and respond to complex situations as quickly as men. It is a decisive step in the way machines learn to represent the world as humans do. Deep learning brings back to the forefront the search for artificial intelligence.

Timeline of AI research



Timeline of AI research



Five schools of ML







Universal Function Approximator

Cybenko 1989 Hornik, Stinchcombe, White 1989





Q: Why does deep learning work?



Q: Why does deep learning work?

A: Law of physics: symmetry, locality, compositionality, renormalization group, and quantum entanglement.

Lin, Tegmark, Rolnick ,1608.08225 Mehta, Schwab, 1410.3831 Levine et al, 1704.01552 ...

1st edition 1969 expanded 1972 commented 1988







Perceptrons



Marvin L. Minsky Seymour A. Papert

Figure 0.1

0.3 Cybernetics and Romanticism

Our discussion will include some rather sharp criticisms of earlier work in this area. Perceptrons have been widely publicized as "pattern recognition" or "learning" machines and as such have been discussed in a large number of books, journal articles, and voluminous "reports." Most of this writing (some exceptions are mentioned in our bibliography) is without scientific value and we will not usually refer by name to the works we criticize. The sciences of computation and cybernetics began, and it seems quite rightly so, with a certain flourish of romanticism. They were laden with attractive and exciting new ideas which have already borne rich fruit. Heavy demands of rigor and caution could have held this development to a much slower pace; only the future could tell which directions were to be the best. We feel, in fact, that the solemn experts who most complained about the "exaggerated claims" of the cybernetic enthusiasts were, in the balance, much more in the wrong. But now the time has come for maturity, and this requires us to match our speculative enterprise with equally imaginative standards of criticism.

 $\psi_{\text{CIRCLE}}(X) = \begin{cases} 1 \text{ if the figure } X \text{ is a circle,} \\ 0 \text{ if the figure is not a circle;} \end{cases}$



 $\psi_{\text{CONVEX}}(X) = \begin{cases} 1 \text{ if } X \text{ is a convex figure,} \\ 0 \text{ if } X \text{ is not a convex figure;} \end{cases}$



 $\psi_{\text{CONNECTED}}(X) = \begin{cases} 1 \text{ if } X \text{ is a connected figure,} \\ 0 \text{ otherwise.} \end{cases}$





"Manifesto of Connectionism"

1988



"T-C Problem"

Contains many interesting experiments & theories on toy problems and foundational thoughts by the pioneers Copyrighted Material

David J. C. MacKay

Information Theory, Inference, and Learning Algorithms



Insightful, fun to read



Figure 29.2. A lake whose depth at $\mathbf{x} = (x, y)$ is $P^*(\mathbf{x})$.



Figure 29.3. A slice through a lake that includes some canyons.

Modern textbooks

1996

2006





Neural Networks for Pattern Recognition

Christopher M. Bishop







Figure 1.11: Since the introduction of hidden units, artificial neural networks have doubled in size roughly every 2.4 years. Biological neural network sizes from Wikipedia (2015).

- 1. Perceptron (Rosenblatt, 1958, 1962)
- 2. Adaptive linear element (Widrow and Hoff, 1960)
- 3. Neocognitron (Fukushima, 1980)
- 4. Early back-propagation network (Rumelhart et al., 1986b)
- 5. Recurrent neural network for speech recognition (Robinson and Fallsic
- 6. Multilayer perceptron for speech recognition (Bengio et al., 1991)
- 7. Mean field sigmoid belief network (Saul et al., 1996)
- 8. LeNet-5 (LeCun *et al.*, 1998b)
- 9. Echo state network (Jaeger and Haas, 2004)
- 10. Deep belief network (Hinton et al., 2006)

- 11. GPU-accelerated convolutional network (Chellapilla et al., 2006)
- 12. Deep Boltzmann machine (Salakhutdinov and Hinton, 2009a)
- 13. GPU-accelerated deep belief network (Raina et al., 2009)
- 14. Unsupervised convolutional network (Jarrett et al., 2009)
- 15. GPU-accelerated multilayer perceptron (Ciresan et al., 2010)
- 16. OMP-1 network (Coates and Ng, 2011)
- 17. Distributed autoencoder (Le et al., 2012)
- 18. Multi-GPU convolutional network (Krizhevsky et al., 2012)
- 19. COTS HPC unsupervised convolutional network (Coates et al., 2013)
- 20. GoogLeNet (Szegedy et al., 2014a)





write

read



I do not understand. To Why coust × Sort .PC Bethe Ansitz Prob. Why const × sort. Po Know how to solve every problem that has been solved Non Linear Openical Hype

"What I can not create, I do not understand"









To recognize shapes, first learn to generate images

Geoffrey E. Hinton 📥 🕅

Department of Computer Science, University of Toronto, 10 Kings College Road, Toronto, M5S 3G4 Canada
Generative Modeling



"Auto-Encoding Variational Bayes", Kingma and Welling, 1312.6114

Generative Modeling



"Auto-Encoding Variational Bayes", Kingma and Welling, 1312.6114

Latent space interpolation

arithmetics of the "smile vector"



White, 1609.04468

Probabilistic Generative Modeling $p(\mathbf{x})$

How to express, learn, and sample from a high dimensional probability distribution ?







"random" images

"natural" images

Prob

DEEP LEARNING

Ian Goodfellow, Yoshua Bengio, and Aaron Courville

How the high c

e from a oution ?

deling

Page 159

"... the images encountered in Al applications occupy a negligible proportion of the volume of image space."

"random

Probabilistic Generative Modeling $p(\mathbf{x})$

How to express, learn, and sample from a high dimensional probability distribution ?



https://blog.openai.com/generative-models/

Generative Modeling and Physics



"Boltzmann" Machines

$$p(\mathbf{x}) = \frac{e^{-E(\mathbf{x})}}{\mathcal{Z}}$$

statistical physics



"Born" Machines

$$p(\mathbf{x}) = \frac{|\Psi(\mathbf{x})|^2}{\mathcal{N}}$$

quantum physics

Generative Modeling and Physics



"Boltzmann" Machines



$$p(\mathbf{x}) = \frac{|\Psi(\mathbf{x})|^2}{\mathcal{N}}$$

quantum physics

$$p(\mathbf{x}) = \frac{e^{-E(\mathbf{x})}}{\mathcal{Z}}$$

statistical physics

Physicists' gifts to ML

Mean Field Theory



Tensor Networks



Monte Carlo Methods



Quantum Computing



Why machine learning for many-body physics ?

- Conceptual connections: a novel and natural way to think about (quantum) many-body systems
- Data driven approach: making scientific discovery based on big data
- Techniques: neural networks, kernel methods, pattern recognition, feature extraction, dimensional reduction, clustering analysis, probabilistic modeling, recommender systems, expectation maximization, variational inference, hardware acceleration, software frameworks...

Four Pillars of Machine Learning

Data







Cost function



Optimization

Switch to blackboard



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Deep Learning and Quantum Many-Body Computation

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+Tensor Network States



Lecture note http://wangleiphy.github.io/lectures/DL.pdf

Name	Training Cost	Data Space	Latent Space	Architecture	Sampling	Likelihood	Expressibility	Difficulty (Learn/Sample)
RBM	Log- likelihood	Arbitrary	Arbitrary	Bipartite	МСМС	Intractable partition function	*	<u>8</u> 8/888
DBM	ELBO	Arbitrary	Arbitrary	Bipartite	MCMC	Intractable partition function & posterior	***	<u>9</u> 9/999
Autoregressive Model	Log- likelihood	Arbitrary	None	Ordering	Sequential	Tractable	**	& / & &
Normalizing Flow	Log- likelihood	Continuous	Continuous, Same dimension as data	Bijector	Parallel	Tractable	**	<u>\$</u> / \$
VAE	ELBO	Arbitrary	Continuous	Arbitrary?	Parallel	Intractable posterior	***	X / X
MPS/TTN	Log- likelihood	Arbitrary?	None or tree tensor	No loop	Sequential	Tractable	***	<u>&</u>
GAN	Adversarial	Continuous	Arbitrary?	Arbitrary	Parallel	Implicit	****	<u>8</u> 8 8 8 7 8 8

Table 2: A summary of generative models and their salient features. Question marks mean generalizations are possible, but nontrivial.

WARNING

The following content may contain spoilers

They may spoil your fun of imagination & creation

Proceed with caution!!!

Material and Chemical Discovery

Material Discovery



Data Generation

via laborious Computation/Experiments Macroscopic Properties

"Machine Learning in Materials Science: Recent Progress and Critical Next Steps" Rampi Ramprasad @ IPAM program on Understanding Many-Particle Systems with ML, 2016

Material Discovery



"Machine Learning in Materials Science: Recent Progress and Critical Next Steps" Rampi Ramprasad @ IPAM program on Understanding Many-Particle Systems with ML, 2016

Chemical design using VAE



Density Functionals

Finding the density-functional

Table 1. Physical Review Articles with more than 1000 Citations Through June 2003							
Publication	# cites	Av. age	Title	Author(s)			
<i>PR</i> 140 , A1133 (1965)	3227	26.7	Self-Consistent Equations Including Exchange and Correlation Effects	W. Kohn, L. J. Sham			
<i>PR</i> 136 , B864 (1964)	2460	28.7	Inhomogeneous Electron Gas	P. Hohenberg, W. Kohn			
PRB 23, 5048 (1981)	2079	14.4	Self-Interaction Correction to Density-Functional Approximations for Many-Electron Systems	J. P. Perdew, A. Zunger			
PRL 45, 566 (1980)	1781	15.4	Ground State of the Electron Gas by a Stochastic Method	D. M. Ceperley, B. J. Alder			
PR 108, 1175 (1957)	1364	20.2	Theory of Superconductivity	J. Bardeen, L. N. Cooper, J. R. Schrieffer			
PRL 19, 1264 (1967)	1306	15.5	A Model of Leptons	S. Weinberg			
PRB 12, 3060 (1975)	1259	18.4	Linear Methods in Band Theory	O. K. Anderson			
<i>PR</i> 124 , 1866 (1961)	1178	28.0	Effects of Configuration Interaction of Intensities and Phase Shifts	U. Fano			
<i>RMP</i> 57 , 287 (1985)	1055	9.2	Disordered Electronic Systems	P. A. Lee, T. V. Ramakrishnan			
<i>RMP</i> 54 , 437 (1982)	1045	10.8	Electronic Properties of Two-Dimensional Systems	T. Ando, A. B. Fowler, F. Stern			
PRB 13, 5188 (1976)	1023	20.8	Special Points for Brillouin-Zone Integrations	H. J. Monkhorst, J. D. Pack			
PR, Physical Review; PRB, Physical Review B; PRL, Physical Review Letters; RMP, Reviews of Modern Physics.							

Top four most-cited PR papers are all DFT-foundational papers!

Finding the density-functional

1 = 1 = 1 2 = 3 = 1 3 = 1	4. arXiv:100710338 4. arXiv:100710338 5. arXiv:100710338 4. arXiv:100710338 5. arXiv:1007	1.18/27/0006381377 0.16896/7333119782 9.08969/1230317771 9.08969/1230317771 3.0229777831457916 3.0229777831457916 3.0229777831457916 3.022977831457916 3.0229727831457916 3.0229727831457916 3.0229728142015 3.022972814201571457 3.02491777831457916 3.024917778516 3.0249177120167 4.225514205571457 3.224595214711611 3.741424547875556 3.2451578277825101 1.015145448695551455 1.0177100506514595 3.245157877525101 1.015145448695551455 3.245157877525101 1.015145448695551455 3.245157877525101 1.01514548695551455 3.245157877525101 1.01514548695551455 3.245157877525101 1.01514548695551455 3.245157877525101 1.01514548695551455 3.245157877525101 3.245157877525101 3.245157877525101 3.245157877525101 3.2451578755556 3.2451578755556 3.2451578755556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.245157857556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515787556 3.24515775756 3.24515775757575756 3.245157757575757	0.07150.01007123796 005299522291643 0.0786530271468507 0.05354571663071468507 0.0535457166307146 0.05325216012004 0.053545716630771 0.0457123160126000771 0.045712314012004 0.055511440681493 0.05451154140681493 0.05451154140681493 0.05451154140681493 0.05451154140681493 0.05451154140681493 0.05451154140681493 0.05451154140681493 0.05451154140681493 0.05451154140681493 0.05451154141068141 0.0545511411411476851 0.06425113414176851 0.06425113414176851 0.0542511341476851	029994432094254 0562248643000414 056224864300051427 045704457130304 0457044457130354 0457044457130354 0457044457130354 045904457131256 0459044571320561005 052905720055005 052905712059054 052905720057057200 05290572007200591 05290572007200570 05290572007200591 05290572007200591 05290572007200591 05290572007200591 05290572007200591 05290572007200591 05290572007200591 05290572007200591 05290572007200591 0529057200592005972005920 052905720059200 0529057200597200597200597200597200597200597200597200597200597200597772005977720059777200597772005777200577720057777777777	$\begin{array}{c} 0.013210520884288\\ 8.304551.2015142\\ 3.911674577648888\\ 8.6730877015531\\ 3.541514636747033\\ 3.332712157375289\\ 7.1351520881538055\\ 8.885541922485173\\ 5.262085897610552\\ 4.469481708562284\\ 4.30489508434211428\\ 1.340024891088614\\ 4.408481708562280\\ 5.4723344579600375\\ 5.2550224857088171\\ 3.764107410086705\\ 5.550224857088171\\ 3.764107410086705\\ 5.55022485731608771\\ 3.764107410086705\\ 5.55022485731608771\\ 3.764107410086705\\ 5.5002285731608771\\ 3.766107510086705\\ 5.5002285731608771\\ 3.766307311086706\\ 5.5002285731602\\ 5.5002285731608\\ 5.5002285731602\\ 5.5002285731602\\ 5.5002285731602\\ 5.5002285731662\\ 5.5002285731662\\ 5.5002857557\\ 5.500285755\\ 5.500285755\\ 5.50028575\\ 5.50028575\\ 5.50028575\\ 5.50028575\\ 5.50028575\\ 5.50028575\\ 5.50028575\\ 5.50028575\\ 5.50028575\\ 5.50028575\\ 5.50028575\\ 5.50028575\\ 5.50028575\\ 5.5002857\\ 5.5002857\\ 5.5002857\\ 5.5002857\\ 5.5002857\\ 5.5002857\\ 5.5002857\\ 5.500285\\ 5.5002857\\ 5.500$	0.068914500213322 0.0755151820090127322 0.075515182009012732 0.0879292787020057 0.0859092787020057 0.0953090639956121 0.0975204593734856 0.0950439289593134 0.0621095289593134 0.062108632271975239 0.062209251975239 0.062209251575503 0.0622045251555503 0.0622045252858459 0.06521552051575503 0.0622045225858459 0.06521711863928584549	$\begin{array}{l} u_{2,3}(94431) (787675333)\\ u_{4,1}(812)(8152)(29265)\\ u_{4,1}(812)(815)(29295)\\ u_{4,1}(815)(1920)(1108)(200)\\ u_{4,1}(811)(1983)(200)(1106)\\ u_{4,1}(810)(1983)(200)(1106)\\ u_{4,1}(810)(1983)(200)\\ u_{4,1}(810)(190)(1983)(200)\\ u_{4,1}(810)(190)(1983)(200)\\ u_{4,1}(810)(190)(190)(190)\\ u_{4,1}(810)(190)(190)(190)\\ u_{4,1}(810)(190)(190)(110)\\ u_{4,1}(810)(190)(190)(110)\\ u_{4,1}(810)(190)(190)(110)\\ u_{4,1}(810)(190)(190)(110)\\ u_{4,1}(810)(190)(190)(110)\\ u_{4,1}(810)(190)(190)(190)(110)\\ u_{4,1}(810)(190)(190)(110)(190)(190)(190)(190)(1$	$\begin{array}{l}$	0.048538/2853/918 0.066594/00648079 0.0955970684502097 0.03515368077127609 0.0326461708973192 0.0326461708973192 0.03586518804821763 0.07250632775145438 0.0725032775145438 0.07970384658584057 0.09191615126472238 0.07970384658584057 0.039545110164542845	0.42203411507208 0.57110570944138 0.501205714957 0.40242203714957 0.58192448712604 0.43256425645331 0.54847898943487 0.56874811700886 0.56953590842875 0.40561480510430 0.58704170558277 0.40712756957590 0.49240438421889
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- - - - - - - -	5.78856/94330483 5.87525335721763 5.85725335721763 5.95725335721763 5.95957292050397 5.95957292050397 5.95957292050397 5.959572925845 11.061751747253 5.25513145514341 1.55955248921101 0.17034545504119 0.17034545550550	5.28680463616790 5.28680463616790 1.86611227494436 5.16612208143045 4.9300241516469 7.1054309027282 5.555534289006 7.855411776611835 6.396954341139937 2.5796560551447 2.5796560551447 2.5798560551447 2.5798560551447 2.5798560551447 2.5798560551447 2.5798560551447 2.579856055145 2.5902424701031 1.01515454960556 3.283098134816701 2.05073346025613 2.0370332205463 2.0370332205463 2.0370332205463	0.04773124501652048 0.0320089788648952 0.0993184090181399 0.06475078553307116 0.084318444680493 0.070780472466704 0.0707007731769758 0.066431890648578378 0.066431890447018 0.066431890447018 0.06628793144708318 0.0628793144708318 0.077726595705811765	0.45538099439149144 0.4501033283280557 0.569973329550055 0.4481376527388373 0.4223871321591302 0.583905823689045 0.583907873631762917 0.4135235776817701 0.43852545602048 0.433523576817701 0.43852545602048 0.5355291752108914 0.4335237008297072	$\begin{array}{c} 7.135152688153955\\ 5.88551922485173\\ 5.262683897610352\\ 3.62263291813646\\ 4.606936643431428\\ 1.340024891088614\\ 4.408481706528226\\ 5.472334579600375\\ 2.550224851908171\\ 3.764107410086705\\ 2.706093393731662\end{array}$	0.0956349249199585 0.06240932209593134 0.0972169632428748 0.0401865271978259 0.06326693058647106 0.0781592051575039 0.06298528328388489 0.06524771468342888459	$\begin{array}{c} 0.4408949440211174\\ 0.5618611754744713\\ 0.4726711603381638\\ 0.5253173968297499\\ 0.5381643193286885\\ 0.5383153095983426\\ 0.4611686076617371 \end{array}$	2.243825016881491 6.486450948532671 8.89032075863951 1.155756643175955 2.832289239384128 7.396341414064901 7.90542867326401	0.05865588304821763 0.07293633775145438 0.05632091198742537 0.0910615024672208 0.07970384658584057 0.05945110164542845 0.03887933278705098	$\begin{array}{c} 0.5687481170088\\ 0.5695359084287\\ 0.4056148051043\\ 0.5870317055827\\ 0.4171275695759\\ 0.4924043842188\end{array}$
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22 1 -2 2 2 2 1 -2 2 2 2 1 1 2 2 1 1 2 2 2 1 1 2 2 2 2 2 2 2 2	29.5667822500307 29.5678257845 1.6315276257845 1.6315276257845 1.6315276257845 1.63152472551 1.630525280103 1.5559524892101 0.17034845510611 1.5559524892101 0.17034845506119 0.17034845506119 0.1703484506119 2.2611972053223466 1.3695824221402 2.261197203522 2.60077613552304 1.646920867899 2.389711906113 2.389711906113 2.389711906113 2.389711906113 2.389711906113 2.38971191373367 1.9464555255550	8.45309228159469 7.105433090279282 8.53955034289036 7.85341779611835 6.3698431139937 4.228544205571447 2.57968606551495 1.107700596345898 8.74124547878586 4.545173787725101 1.01515454000506 3.283098134816701 1.01515454000506 3.283098134816701 2.066773486230531 2.06773358205483	0.06475078553307116 0.048318440680993 0.07284904722467074 0.07070077317679758 0.05730660608578378 0.0607189009977901 0.0664318905447018 0.04624199264776803 0.0462419224777803 0.0462419224777803 0.046241922477803	0.4481376527388373 0.4223871323591302 0.5839058233689045 0.5080787363762617 0.4964415398755241 0.4185235776817701 0.4888525450630048 0.5359207521608914 0.4236237608297072 0.4728106433106254	3.62263291813646 4.606936643431428 1.340024891088614 4.408481706562826 5.472334579600375 2.550224851908171 3.764107410086705 2.706093393731662	0.04018659271978259 0.06326693058647106 0.0781592051575039 0.06298528328388489 0.06570186368826426 0.06424771468342688	0.5253173968297499 0.5381643193286885 0.5383353695983426 0.4611686076617371	1.155756643175955 2.832289239384128 7.396341414064901 7.90542867326401	0.0910615024672208 0.07970384658584057 0.05945110164542845 0.03887933278705098	0.5870317055827 0.4171275695759 0.4924043842188
11 21 2 - 1 3 - 1 4 - 2 2 - 1 4 - 2 4 - 2	8-10080522848575 11.061751474531 4.40893290103 2.7315047923880 2.7315047923880 1.559524821101 0.170344855064119 -0.1201785547433 1.64622823185429 -0.1201785547433 1.64622823185429 -0.1201785547433 1.64622823185429 2.2614197703532 2.2614197703552 2.361421406413 2.369579113773367 1.9464558256554 1.9465582526559 1.9465582526559	7.105-438009279282 8.53955014289006 7.853417770611835 6.39698431139937 4.228544205571447 2.579686066551495 8.26435624701031 8.74124547878586 4.245173787725101 1.015154584908506 3.283098134816701 2.056773466230531 2.056773466230531 2.056773466230531	0.083118446680493 0.07284904722467074 0.072077317679758 0.05730660685578378 0.0607189009977901 0.0664318905447018 0.05955381913217193 0.04624196264776803 0.0628793144768381 0.03433189693421491 0.03728595708511765	0.4223871323591302 0.5839058233689045 0.5080787363762617 0.3964415398755241 0.4135235776817701 0.4888525450630048 0.3359207521608914 0.4236237608297072 0.4739106 (03196254)	$\begin{array}{c} 4.609336643431428\\ 1.340024891088614\\ 4.408481706562826\\ 5.472334579600375\\ 2.550224851908171\\ 3.764107410086705\\ 2.706093393731662 \end{array}$	0.06326693058647106 0.0781592051575039 0.06298528328388489 0.06570186368826426 0.06424771468342688	0.5381643193286885 0.5383353695983426 0.4611686076617371	2.832289239384128 7.396341414064901 7.90542867326401	0.07970384658584057 0.05945110164542845 0.03887933278705098	0.4171275695759 0.4924043842188
23 33 51 51 51 51 51 7 - 1 8 - 90 -1 -1 -2 2 - 12 -3	1.6312/7652578485 1.6312747351 4.44089329011033 2.731504789228804 12.35513145514341 13.5085248921101 0.1703484854064119 0.1703484854064119 1.646528551857891 3.668538242214002 2.2461977203532 2.3697314906413 2.3695791377387 1.94645582556659 1.965582792080	8.5.39550342289036 7.85341770611835 6.39698431139937 4.228544205571447 2.57958606551495 1.107700396345898 8.26435624701031 8.26435624701031 8.26435624701031 2.05773486230531 2.056773486230531 2.05703352205483 0.400475855881034	0.07284904722467074 0.07070077317679758 0.05730660668578378 0.06071899009977901 0.0664318905447018 0.05955381913217193 0.04624196264776803 0.0628793144768381 0.03433189693421491 0.03728595708511765	0.5839038253889045 0.5080787363762617 0.5964415398755241 0.4135235776817701 0.4888525450630048 0.5359207521608914 0.4336237608297072 0.4782106429206224	1.340024891088614 4.408481706562826 5.472334579600375 2.550224851908171 3.764107410086705 2.706093393731662	0.0781592051575039 0.06298528328388489 0.06570186368826426 0.06424771468342688	0.5383353695983426 0.4611686076617371	7.396341414064901 7.90542867326401	0.05945110164542845 0.03887933278705098	0.49240438421888
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7 1 8 9 1 2 1; 3 3 4 4 4 5 8 1 3 1 3 1 3 1 1 1 1 1	11.55095248921101 0.1703484854064119 0.1703484854064119 0.13017855474333 1.646528551854299 2.371179702223466 13.6638342214402 2.216419772035322 2.216419772035329 2.2897314506413 5.36579917377367 1.94645582566549 1.1055582792086	1.107700596345898 8.26435624701031 8.74124547878586 4.545173787725101 1.015154584908506 3.283098134816701 2.056773486230531 2.03703352205463 6.400475835681034	$\begin{array}{c} 0.05955381913217193\\ 0.04624196264776803\\ 0.0628793144768381\\ 0.03433189693421491\\ 0.07726595708511765 \end{array}$	0.5359207521608914 0.4236237608297072 0.4736106423106264	2.706093393731662	0.06576720199559433	0.5481686020053234	1.399253719979948	0.07540490302513119	0.46554569889653
8	0.1703484854064119 0.13017855474333 1.646528518554399 2.371179702223466 13.69383242214402 2.216419772035322 -6.00076435563004 8.16409108667899 22.3897314906413 5.595799113773367 1.94645582566549 1.10555827502006	8.26435624701031 8.74124547878586 4.545173787725101 1.015154584908506 3.283098134816701 2.056773486230531 2.03703352205463 6.400475885681034	$\begin{array}{c} 0.04624196264776803\\ 0.0628793144768381\\ 0.03433189693421491\\ 0.07726595708511765\end{array}$	0.4236237608297072		0.06561841006617781	0.4269114966922994	1.501048590877154	0.06352034496843162	0.4331821043592
9 - 0 0 - 1 1 - 2 1 - 2 2 - 2 1 - 2 2 - 2 1 - 2 2 - 2 2 - 2 1 - 2 2	-0.13017855474333 -1.646528531854399 -2.371179702223466 -2.371179702223466 -0.0076435533604 -8.16409108667899 -22.3897314906413 5.59579917377367 -1.96645582566549 -1.105558257832309	8.74124547878586 4.545173787725101 1.015154584908506 3.283098134816701 2.056773486230531 2.03703352205463 6.400475835681034	0.0628793144768381 0.03433189693421491 0.07726595708511765	0.4736106402106264	7.025290029097274	0.07980750197266955	0.4683927184025036	2.822503099972245	0.05222522416667061	0.48109985214310
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1 2 - 1; 3 4 5 - 3; 6 - 22; 7 - 3; 8 9; 0; 1; 2 - 10; 3; 4, 1; 2 - 2; 7 - 3; 1; 2 - 2; 1; 2 - 2; 1; 2 - 10; 3; 1; 2 - 10; 3; 1; 2 - 10; 3; 1; 2 - 10; 3; 1; 2 - 10; 3; 1 - ; 2 - 10; 3; 4 - ; 1 - ; 2 - 10; 3 - ; 4 - ; 4 - ; 4 - ; 4 - ; 5 - ; 5 - ; 5 - ; 5 - ; 1 - ; 2 - 10; 3 - ; 4 - ; 4 - ; 4 - ; 5 - ;	-2.371179702223466 13.69383242214402 -2.216419772035322 -6.00076435563604 8.16409108667899 22.3897314906413 5.595799173773367 1.9464558256549 -1.105558295233069	1.015154584908506 3.283098134816701 2.056773486230531 2.03703352205463 6.400475835681034	0.07726595708511765	0.4919021595234177	1.726935494533148	0.03135796595505673	0.580800322296872	2.502191185545461	0.0856788809687475	0.59096213316118
2 = 12 3 = -12 4 = -12 5 = -22 6 = -22 7 = 12 8 = 12 9 = -12 9 = -12 1 = -12 2 = -10 3 = -12 1 = -12 2 = -10 3 = -12 1	13.69383242214402 -2.216419772035322 -6.00076435563604 8.16409108667899 22.3897314906413 5.595799173773367 1.94645582566549 -1.1055582566549 -1.1055582566549	3.283098134816701 2.056773486230531 2.03703352205463 6.400475835681034		0.4008988537732911	6.688534202733123	0.0869544063742346	0.403293222827825	6.297133313147086	0.03345369328197418	0.5433070470097
3 - 3 4 - 4 5 - 2 6 - 2 7 - 3 8 - 3 8 - 3 9 - 3 0 - 3 1 - 3 2 - 10 3 - 3 4 - 10 5 - 3 - 3	-2.216419772053322 -6.00076435563604 8.16409108667899 22.3897314906413 5.595799173773367 1.94645582566549 -1.1055589295530669	2.03703352205463 6.400475835681034	0.06841617803957927	0.4304195496937475	5.887062834756559	0.05152399439496422	0.4321995606997443	3.207122477750064	0.07371808389404321	0.4967284534354
41 5 - 2 6 -2 7 - 3 8 - 2 7 - 3 8 - 2 - 3 - 3 - 3 - 3	-0.00076435363004 8.16409108667899 22.3897314906413 5.595799173773367 1.94645582566549 -1.1055582566549	2.03703352205463 6.400475835681034	0.0825699915945694	0.479224783903814	6.945590707033352	0.07408636456892297	0.4957750456547108	5.846222671659907	0.0836452454472081	0.4094720200825
	22.3897314906413 5.595799173773367 1.94645582566549	0.400410550051054	0.07605517542793995	0.4501291515683585	1.45256556478288	0.07433092379389013	0.4233969076404344	8.95059302019488 5.262078.46.4222.45	0.05703615620837187	0.4679023659842
7 8 9 1 210 3 4 10 5	5.595799173773367 1.94645582566549 -1.105559822532069	3 751807395744921	0.03423355943135343	0.334405381884868749	7 550337937177391	0.07282844500128038	0.4272330837180330	4 720884445482556	0.00780034100001002	0.5500503374710
8 9 - 1 - 2 -10 3 - 4 10 5 -1	1.94645582566549	4 522456026868127	0.03620201946841309	0.5050210060676815	1.885091277540955	0.03840505807570421 0.06521780385848891	0.4961601035955842	9.47421945496329	0.0556740133396159	0.3350505374710
9 - 0 - 1 - 2 -10 3 - 4 10 5 -1	1 105559822522069	2.751346713386582	0.0948195528516815	0.4901204212506473	7.863592227266858	0.0951797983951825	0.5196620049802691	9.51608680035275	0.07785377315463609	0.5806015592262
0 -: 1 -: 2 -10 3 -: 4 10 5 -:	- 1.100000000000000000000	5.725277193011525	0.03097303116261406	0.5511177785567803	7.988513342309234	0.0928323179868588	0.5146415116367569	1.101098863639624	0.0882939028519791	0.5265108634130
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	-3.886381532577754	4.95871172966177	0.06823254438777603	0.5645951313008806	9.08135225317634	0.04472856905840844	0.4299117124064201	8.24973637849809	0.08854431361856	0.54161936488610
2 -1 3 -1 4 10 5 -4	-1.341930696378109	6.451869235304859	0.05482804889270922	0.5694170176403242	4.416924333519995	0.04212208612720639	0.5897125000677342	8.86521100790565	0.0866581794842557	0.53117442302276
3 – 4 10 5 –	10.16467121571373	6.705508349541454	0.0934749698077619	0.4420693171728495	2.858371131410651	0.03722557506068529	0.4216580500297413	6.670274811535954	0.0977332470946321	0.53875608512918
4 10 5 -6	-1.107633246744663	7.390220519784453	0.07970661674181083	0.5081940602224835	3.815123656821275	0.04965529863397879	0.497023655525965	9.69945245311718	0.07039341131023045	0.4990744291774
a -1	10.39451871866851	1.478170300165134	0.03602109509210016	0.5799113381048154	2.105782960173057	0.0861928382367878	0.4812528298377607	7.010226383015251	0.03535327789989237	0.49699896645771
	-0.139925361351959	4.045190240200832	0.03579955552582782	0.3678362348598895	9.32386837735074	0.0858648976559044	0.5698752996855582	9.81895903799508	0.04704020956533079	0.5708692337579
0	3.000124569605117	4.944179742822627	0.0531916525333049	0.4834640277977335	9.3847979419491	0.0840810063497973	0.4090254720704045	3.573880603434117	0.07158934023489803	0.5598196803643
8 -	0.00734079112684 0.3011566691835799	2.588178201634472 8.7899620736435#	0.07482186947515447 0.04833452202772747	0.4950144569660614 0.45920393736037 [±]	9.93467757777872	0.03877152903045122 0.09739642020712e*	0.3780039568499292 0.4280349684452506	4.285706479098184 4.931948094146255	0.05940487550770145 0.0969410287755629	0.4544513368813
	0.3460178058324283	6 242957525364009	0.0000568314224112	0.4205662570527381	4 73983230004983	0.0450110225161678	0.559400017887981	9 11978947942194	0.06189826031162779	0.4931008194495
0 -3	-5 704905642148452	4 447521595114223	0.06770523205457797	0.5047965897298675	3 987888630073714	0.03595136615254331	0.5929011044925536	5 22121823715344	0.04029431905467698	0.5141294116814
1 0	0.1425795779687519	6.919606258393273	0.0821756368975312	0.5976799418614426	8.04099037018168	0.03129262110881438	0.4686530881925831	3.421695873368174	0.05166215779587051	0.4208560803818
2	0.6843702894502789	8.27200587323167	0.0547013388431661	0.4453254786423237	7.433883810628654	0.04612202343826998	0.5269730370279639	8.3641619521824	0.07996879390804805	0.5036755718396
3 -1	14.06571757369153	6.220712308892191	0.04765956545437692	0.4898959293071353	8.72249431241257	0.05059967705235588	0.4421274052875277	2.416276423317733	0.07373660930828208	0.54038506525357
4 2	8.32346109443768	9.29716067662943	0.0656810603414827	0.4960066859011466	6.796263459296078	0.04037116107097755	0.4389885737869158	2.206183147865627	0.0804910989081056	0.5806221323132
5 -1	-5.252317079780442	3.424683176707511	0.0867529985575643	0.4322548560407479	6.859255296971943	0.0955962752949951	0.517620399931194	5.826144942819697	0.0910408442631135	0.4167014408128
6 (6.18641388898792	3.789578783769164	0.07617326304382499	0.5418490045761073	1.363177133649232	0.03197249245240319	0.5284999992906743	4.9879001955338	0.04126125322920861	0.4895167206754
7 (0.4821906326173532	1.195769022526768	0.04928749082970199	0.5286859472378347	8.76714063033632	0.0870852412295278	0.5989638152903285	2.489565114307663	0.05568685410478115	0.5787056957942
8	5.707663438868804	4.058614230578957	0.04743875933294599	0.4981149890354436	1.015171237842736	0.085826684646538	0.5470349320774566	6.343764732282688	0.0878769436185823	0.5449452367497
9 -1	-0.1857958679022612	5.159763617905121	0.0850570422587659	0.5311491284465588	7.238990148015965	0.05867048711393652	0.5662410781222187	8.70600609334284	0.04088387548046445	0.5305143392409
0	2.321394443893878	3.319181325701307	0.05391080867981007	0.5914435434000773	9.11776045377491	0.03583354001918901	0.4069413088494417	6.117009330479202 5.505840206051121	0.04553014156422459	0.4131324263527
	2.451009994722774	4.005247740100538	0.07620861067494449	0.5759225433332955	0.143529918394192	0.0507347280360008	0.4980631985926895	5.505849300951131	0.0971440303580883	0.4517346772110
3 -10	10.67971490671366	4 728468083127391	0.06509200806253813	0.4959400801351127	9.81266481664175	0.0951346706530719	0.5047212015277842	3 180268423645401	0.06891913385037023	0.5758580789792
4	1.375998039323297	2.740626958875014	0.06438323836566841	0.5077158168564866	1.813952930718781	0.0845523320869031	0.407247659218711	1.054506345314588	0.0998274789144316	0.5956344420441
5 -	-4.330863793299111	3.209443235555092	0.05150806767094947	0.5932432195310449	4.682408324655706	0.03641376226612134	0.4491940043173043	9.57800470422746	0.089704223465467	0.4702887735348
6 /	6.961655278126058	3.013659237176324	0.0802684211883349	0.5733460791404235	7.441047648005995	0.0924462539370359	0.5216671466381739	8.15403131934562	0.05611934350568269	0.4910483719005
7 -1	-5.30540083281513	2.088882156026381	0.07464091227469428	0.4740072756248339	4.228694369663863	0.03993178348974601	0.4402946238148492	4.912298433960689	0.06528359492264517	0.4923580906843
8 :	3.395104400983763	7.9733680986292	0.0911843583955236	0.5314007871406556	6.375772536276909	0.0933026364108379	0.447244215655568	7.387561983870292	0.0977643384454912	0.4798245902933
9	1.330224789015745	5.105339790874075	0.06331718284342962	0.5503804706506275	9.5740821641842	0.07463500644132846	0.5814481952546582	5.810342341443878	0.03327635127803191	0.5550216356360
0 -1	-0.2920604955263079	0.773414983805557	0.07595819905259191	0.5210834626114553	4.229974804881476	0.03532177545633547	0.5725615130215063	8.88452823254966	0.0932985710685446	0.50463881248570
2 - 24	6.630303088825135	6.476325542442258	0.00240344040172004	0.4238523441420071	6.969363897694016	0.06506307327818108	0.4031443030007202	2.18540074180400	0.0000100000000000000000000000000000000	0.3174384304075
3	3.065748817927897	1 300093759156537	0.06741885075590173	0.4866345116967513	6.942052231590217	0.07107963920756023	0.4930672781311588	7 \$34\$70£2601402\$	0.06446115603870624	0.53672192182163
4 -	-1.743105697039855	3.145607697855832	0.0415292992761004	0.5859414343226601	5.945295724435049	0.07414379406386953	0.4548629476738681	1.062923665624632	0.07636214080338054	0.43302912543318
5 -	-1.631255302904965	3.121291975208031	0.03133561741752311	0.524510056949801	8.03118879837252	0.0987376029412809	0.5128559599511593	7.572783963151993	0.0936192481138518	0.4523240987335
6 - 9	-9.50982692642515	7.367027947839741	0.07398108515426552	0.4753257600466925	1.589160147317211	0.07398588942349949	0.4644105814910987	1.719981611302808	0.04986976063479617	0.5394709698394
7 -	-4.496736421068983	8.56498650586069	0.0870950155799119	0.4807004710871501	8.85815411069566	0.0936690521145114	0.4120764594786555	2.422694718173737	0.05651923264880363	0.48323515477488
8 -	-1.002977917543076	9.43121814362608	0.03689894383172801	0.4801850915018365	6.762463110315146	0.0977990134875495	0.5880377299069773	8.48288777357423	0.05983735955021298	0.4837560035001
9 -!	-9.23106545170694	8.47929696159459	0.05472141225455761	0.4949989702352598	4.776138672418544	0.03835162624659654	0.5785166211495689	4.459069855546714	0.06892772167363432	0.59085293118447
0 14	14.99926304831282	4.708917711658332	0.0907364284065382	0.4550033334959929	5.373320800648651	0.03739924536269347	0.4468132406615605	1.831662246071428	0.05825558914206748	0.56643419964278
1 4	4.189181104505013	7.583635162152007	0.0936829708421792	0.4110679099121856	6.09002215219153	0.05895044789139901	0.5451253692040614	6.851478307492325	0.04763840334231468	0.50106331608502
4 1 9 0	0.52837188138842	a.414315967033806	0.05054048464274665	0.3043307410524706	a.070996567281799 4.001176002002500	0.00908276328974509	0.5702069702356848	0.300783854112533 4.527748264214510	0.0388888383066967	0.37841554675662
a -2.	£ 604738077045653	1.020002400388586	0.04540230831054488	0.3420078576324179	4.091170923293506	0.03830885039652842	0.304879512949007	4.521148284314512	0.00373894102927981	0.40705085064968
5 10	15.27988423246628	6.229538426957454	0.0821521091215863	0.4118748449252315	2.377028497509498	0.0963110933106458	0.4746736556808109	5.398545541594487	0.0822574656780643	0.52589472331904
6	1.377130763885458	9.15176346333775	0.04818682488618507	0.574408949666749	2.366656226877287	0.05059199769749539	0.4731074949729489	4.34290365370739	0.07492904049493838	0.40386563758923
7 -6	-0.7756959351484244	8.1525112801581	0.0812975344211981	0.5112853751964107	4.530310672134927	0.06652912486134806	0.5946245231853162	1.568860626254933	0.04256882025605258	0.54910278010433
8 -	9.50432792804336	4.670517118870347	0.04398267799553492	0.4519472673718893	2.155276187476066	0.0489411436180854	0.5694756278652033	1.947130206816878	0.06321309041201674	0.4122312147733
9 /	3.754137123031758	6.801389212739803	0.07003309342623426	0.5129214842481318	9.92433910143913	0.0931392820982872	0.4104016495146404	5.23036608102518	0.0919529182014262	0.4465294974738
0	-4.499804654067136	4.406584351091798	0.0970211159011626	0.4772975938521527	2.270764431848441	0.0853562757122116	0.4669596920988839	4.42557413334857	0.0517800509473799	0.5645191809121
1 -13	13.9999061688152	8.30408622139241	0.0903948738093222	0.5053209583744364	2.454354187669313	0.0857681690400504	0.576877467653029	7.167289037979035	0.0831206320171505	0.42213396807927
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3 -8	-8.70611662690158	3.078380132262833	0.06327626752293522	0.4017988981679418	2.138629261588504	0.05374733302715019	0.5432443229891937	7.596013793576791	0.0999924467044729	0.51152456225763
4 3	3.578654662113496	4.294915349281119	0.0664706641817281	0.3566289165852036	3.387516420897519	0.06654228293431248	0.4304935498494862	8.43232828156106	0.06121769693920587	0.5527076848906
0 I 6	-6.387446031119122	5.003300003333494 5.05212364674403 F	0.00823903823041594 0.05306972452715127	0.3332353008476618 0.4657297418468141	1.2635942984150266	0.07730032999103362 0.05392235360604765	0.4274310541541941 0.4355571244074699	9.81884128475822	0.03350347733060968 0.0434164393614163	0.5091073130786
7 -1	3.029693711262450	1.767169254925799	0.0386273054880002	0.4174202422881019	9.99189882828504	0.0307220020094700	0.5316587974869799	4 79441120410622	0.04366392717108025	0.5202815575042
s	-0.791031105864576	8.38082427065573	0.0552127907704862	0.5821800194923650	3.864226559651998	0.05464216708052787	0.5051543239785165	4.445064096761642	0.03386907179361738	0.4659081177.469
9	2.97083681738158	9.22706363472046	0.06912140386549836	0.5630023378185795	2.929880196570098	0.07966659968684009	0.4992263633935188	6.920427033384797	0.03123407491202272	0.4077156601519
0 -	-7.110772604917624	3.106633667560681	0.04873990025387701	0.5697049535893381	8.30700777463754	0.05249501630989304	0.5669783762910612	1.13457393933062	0.07200760153994357	0.4446720724747
1 -	-7.162305080703513	5.387619660361665	0.04581500385875453	0.5197835066282974	8.22551991773337	0.0831226693907787	0.4274987667560087	6.828948529150043	0.05943349593138421	0.5115861497137
2	1.720368406482304	6.780548897314363	0.0870012111933092	0.5984908484842784	6.587571277412653	0.05694105237128053	0.5226697825342788	5.99005641944593	0.07837921322316456	0.4668236040752
3 P	0.1494884045649762	8.09818524171748	0.0976595255928496	0.4848535596042637	2.153483785757176	0.04734211110674212	0.4077222220507315	7.143110762448606	0.04682210332386052	0.5090846438323
4 -4	-0.962821097034532	7.260437643310942	0.05083396575279076	0.54745303715986	8.38162990306018	0.05791050943688269	0.5794395625497382	2.722302743095399	0.083744615781603	0.53954284172516
5 1	0.935122045036145	2.31788301454997	0.05976249487823031	0.5809204376238206	8.19172407354263	0.06806778195768599	0.5479374417815378	9.93990336225375	0.04266977230181523	0.5959901705863
6 0	0.4328277236540677	4.113414259206836	0.07988404513340022	0.5262079910925557	7.436994191324823	0.07641699196144898	0.4316282085515486	9.59671807016201	0.07198966517052108	0.4563024970288
7 (0.853043516035702	3.229317247568396	0.04664288308967379	0.4916641780174803	9.19533615142581	0.0944216012526871	0.5792638413577232	6.980966479991427	0.07647312161060935	0.5407763967437
8 -3	-3.516191871248886	9.20769534239692	0.07214599607965883	0.4111312070946356	7.568725646832963	0.0806902033322297	0.4952042950743076	8.94919747461644	0.04263443777290076	0.57352619608650
9 19 00	19.07243760549639	2.270663590855083	0.0971170179967765	0.4613017967987272	8.22480560472966	0.0536024772561282	0.4745303011865644	5.970009703387312	0.0982032349257953	0.5029128207513
N	1.944000514744405	4.017102041449901	0.04437090645089548	0.3073055615301741	3.124030679477685	0.07622772645899346	v.4308882837991222	9.350822342112657	0.07659119397629786	0.40362437639913

an 1000 Citations Through June 2003

	Author(s)
Including Exchange and Correlation Effects	W. Kohn, L. J. Sham
Gas	P. Hohenberg, W. Kohn
to Density-Functional Approximations for	J. P. Perdew, A. Zunger
ron Gas by a Stochastic Method	D. M. Ceperley, B. J. Alder
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	S. Weinberg
Theory	O. K. Anderson
nteraction of Intensities and Phase Shifts	U. Fano
stems	P. A. Lee, T. V. Ramakrishnan
wo-Dimensional Systems	T. Ando, A. B. Fowler, F. Stern
in-Zone Integrations	H. J. Monkhorst, J. D. Pack
iew Letters; RMP, Reviews of Modern Physics.	

ers are all DFT-foundational papers!

machine learned one dimensional kinetic-energy functional with O(10³) parameters

Snyder et al, PRL 108, 253002 (2012)

Recent Progresses





Avoiding Euler equation by directly learning n[v] map

Beockherde, Vogt, Li, Tuckerman, Burke, Meuller 1609.02815 Learning the xc-functional from DMRG calculation in 1D continuous space

Li, Baker, White, Burke, 1609.03705

"Phase" Recognition

Supervised Approach

Ising configurations



+ many more on quantum spins, fermions, disordered systems, topological models ...





















ferromagnetic



disordered



ferromagnetic







disordered

only data, no label









ferromagnetic

disordered

Different Schemes Nieuwenburg, Liu, Huber, 1610.02048 Liu, Nieuwenburg, 1706.08111 Broecker, Assaad, Trebst, 1707.00663 LW, 1606.00318 Discovering phase transition with dimensional reduction and clustering analysis



Extensions Wetzel, 1703.02435 Hu, Singh, Scalettar, 1704.00080 Wetzel, Scherzer, 1705.05582 Wang and Zhai, 1706.07977

Variational Ansatz

RBM as a variational ansatz

Carleo and Troyer, 1606.02318



- Exact construction for 1d SPT, 2d toric code state etc
- Related to tensor network, string-bond, correlator product states
- Killer app ? Long-range, volume law entanglement, chiral state, improved Jastrow

Deng, Li, Gao, Chen, Cheng, Xiang, LW, Clark, Glasser, Carl Budich, Imada...

Deep neural net as a variational ansatz



- Train the deep neural net ansatz using Backprop
- Feature discovery and abstraction power of the deep hierarchical structure
- Bottleneck appears to be the stochastic optimization (VMC)

Monte Carlo Update Proposals

A Video from Google DeepMind

http://www.nature.com/nature/journal/v518/n7540/fig_tab/nature14236_SV2.html


 Use Boltzmann Machines as recommender systems for Monte Carlo simulation of physical systems

Li Huang and LW, 1610.02746 Liu, Qi, Meng, Fu, 1610.03137

Proposals from Boltzmann Machine



 Use Boltzmann Machines as recommender systems for Monte Carlo simulation of physical systems

Li Huang and LW, 1610.02746 Liu, Qi, Meng, Fu, 1610.03137

Proposals from Boltzmann Machine



 Use Boltzmann Machines as recommender systems for Monte Carlo simulation of physical systems

Li Huang and LW, 1610.02746 Liu, Qi, Meng, Fu, 1610.03137

• Moreover, BM parametrizes Monte Carlo policies and explores novel algorithms! LW, 1702.08586

Local vs Cluster algorithms





Local vs Cluster algorithms







is slower than



Local vs Cluster algorithms





Algorithmic innovation outperforms Moore's law!

Deep learning the MC proposal

$$A(\mathbf{x} \to \mathbf{x}') = \min \left[1, \frac{q(\mathbf{x}' \to \mathbf{x})}{q(\mathbf{x} \to \mathbf{x}')} \cdot \frac{\pi(\mathbf{x}')}{\pi(\mathbf{x})} \right]$$

$$\uparrow$$
Policy Fixed by the Physics

- A-NICE-MC 1706.07561
- Generalize hybrid MC using neural networks 1711.09268
- Probabilistic programs as proposals 1801.03612



MPS for pattern recognition

$$\approx \begin{array}{c} \mathbf{\mathcal{C}} \mathbf{\mathcal{C$$

$$f(\mathbf{x}) = \sum_{\{s\}} W_{s_1 s_2 \cdots s_N} \phi^{s_1}(x_1) \otimes \phi^{s_2}(x_2) \otimes \cdots \phi^{s_N}(x_N)$$
$$\phi^{s_j}(x_j) = \left[\cos\left(\frac{\pi}{2} x_j\right), \ \sin\left(\frac{\pi}{2} x_j\right) \right]$$



%99.03 accuracy on MNIST dataset*

* bond dimension 120 images scaled to 14*14

 $\int f^{\circ}(\mathbf{X})$

cf Liu et al, 1710.04833 Novikov et al,1605.03795

Stoudenmire and Schwab, 1605.05775



Unsupervised petraining with a TTN





Comparable accuracy to ConvNets

Stoudenmire, 1801.00315











"Teach a quantum state to write digits"

Generative modeling using Matrix Product States



Connections to Boltzmann Machine, Chen, Cheng, Xie, LW, Xiang 1701.04831

Generative modeling using Matrix Product States





Q: How to quantify our prior knowledge on the data distribution ?





Q: How to quantify our prior knowledge on the data distribution ?





Q: How to quantify our prior knowledge on the data distribution ?



Q: How to quantify our prior knowledge on the data distribution ?



Quantum Perspective on De















Classical Mutual Information

$$I = -\left\langle \ln \left\langle \frac{p(\mathbf{x}, \mathbf{y}') p(\mathbf{x}', \mathbf{y})}{p(\mathbf{x}', \mathbf{y}') p(\mathbf{x}, \mathbf{y})} \right\rangle_{\mathbf{x}', \mathbf{y}'} \right\rangle_{\mathbf{x}, \mathbf{y}}$$

Quantum Renyi Entanglement Entropy

$$S = -\ln\left\langle \left\langle \frac{\Psi(\mathbf{x}, \mathbf{y}')\Psi(\mathbf{x}', \mathbf{y})}{\Psi(\mathbf{x}', \mathbf{y}')\Psi(\mathbf{x}, \mathbf{y})} \right\rangle_{\mathbf{x}', \mathbf{y}'} \right\rangle_{\mathbf{x}, \mathbf{y}}$$

Striking similarity implies common inductive bias

+Quantitative & interpretable approaches +Principled structure design & learning

Cheng, Chen, LW, 1712.04144

Deep Learning and Quantum Entanglement: Fundamental Connections with Implications to Network Design

Yoav Levine David Yakira Nadav Cohen Amnon Shashua The Hebrew University of Jerusalem

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Abstract

Deep convolutional networks have witnessed unprecedented success in various machine learning applications. Formal understanding on what makes these networks so successful is gradually unfolding, but for the most part there are still significant mysteries to unravel. The inductive bias, which reflects prior knowledge embedded in the network architecture, is one of them. In this work, we establish a fundamental connection between the fields of quantum physics and deep learning. We use this connection for asserting novel theoretical observations regarding the role that the number of channels in each layer of the convolutional network fulfills in the overall inductive bias. Specifically, we show an equivalence between the function realized by a deep convolutional arithmetic circuit (ConvAC) and a quantum many-body wave function, which relies on their common underlying tensorial structure. This facilitates the use of quantum entanglement measures as welldefined quantifiers of a deep network's expressive ability to model intricate correlation structures of its inputs. Most importantly, the construction of a deep convolutional arithmetic circuit in terms of a Tensor Network is made available. This description enables us to carry a graph-theoretic analysis of a convolutional network, tying its expressiveness to a min-cut in the graph which characterizes it. Thus, we demonstrate a direct control over the inductive bias of the designed deep convolutional network via its channel numbers, which we show to be related to the min-cut in the underlying graph. This result is relevant to any practitioner designing a convolutional network for a specific task. We theoretically analyze convolutional arithmetic circuits, and empirically validate our findings on more common convolutional networks which involve ReLU activations and max pooling. Beyond the results described above, the description of a deep convolutional network in well-defined graph-theoretic tools and the formal structural connection to quantum entanglement, are two interdisciplinary bridges that are brought forth by this work.

Deep Learning and Quantum Entanglement: Fundamental Connections with Implications to Network Design

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Quantum Machine Learning

- Search
- Sampling
- Clustering
- Optimization
- Linear system solver
- Support vector machines
- Principal component analysis



Cai et al, PRL 114, 110504 (2015)

	¹³ C	<i>F</i> ₁	F ₂	F ₃
¹³ C	15479.9Hz			F ₃
<i>F</i> ₁	-297.7Hz	-33130.1Hz	Ι	13C
<i>F</i> ₂	-275.7Hz	64.6Hz	-42681.4Hz	F ₁
<i>F</i> ₃	39.1Hz	51.5Hz	-129.0Hz	-56443.5Hz
T_2^*	1.22s	0.66s	0.63s	0.61s
<i>T</i> ₂	7.9s	4.4s	6.8s	4.8s

Li et al, PRL 114, 140504 (2015)

few qubits demo

"Use a quantum computer to speed up ML subroutines"

Review "Quantum machine learning", Biamonte et al, Nature 2017

Quantum Boltzmann Machines \$15 million "analog quantum device"



figure 1. This graph is built from unit cells containing Quarter dubits even Will BOach Unit cell She qubits and couplers realise a complete bipartite graph $K_{4,4}$ where

tions. The sizes we typically used in our numerical sim-

~2000 "qubits"

Born Machine in the Cloud



Collapse to a bit-string by measurement





Renormalization Group

Deep Neural Network and RG



Goodfellow, Bengio, Courville, <u>http://www.deeplearningbook.org/</u>

Page 6 Figure 1.2



Q

Venues / ICLR 2013 conference

Deep learning and the renormalization group

Cédric Bény

15 Jan 2013 ICLR 2013 conference submission readers: everyone

Decision: reject

Abstract: Renormalization group methods, which analyze the way in which the effective behavior of a system depends on the scale at which it is observed, are key to modern condensed-matter theory and particle physics. The aim of this paper is to compare and contrast the ideas behind the renormalization group (RG) on the one hand and deep machine learning on the other, where depth and scale play a similar role. In order to illustrate this connection, we review a recent numerical method based on the RG---the multiscale entanglement renormalization ansatz (MERA)---and show how it can be converted into a learning algorithm based on a generative hierarchical Bayesian network model. Under the assumption---common in physics----that the distribution to be learned is fully characterized by local correlations, this algorithm involves only explicit evaluation of probabilities, hence doing away with sampling.



arxiv:1301.3124

Q

Venues / ICLR 2013 conference

Deep learning and the renormalization group

Cédric Bény

15 Jan 2013 ICLR 2013 conference submission readers: everyone

Decision: reject

Yann LeCun

05 Apr 2013 ICLR 2013 submission review readers: everyone

Review: It seems to me like there could be an interesting connection between approximate inference in graphical models and the renormalization methods.

There is in fact a long history of interactions between condensed matter physics and graphical models. For example, it is well known that the loopy belief propagation algorithm for inference minimizes the Bethe free energy (an approximation of the free energy in which only pairwise interactions are taken into account and high-order interactions are ignored). More generally, variational methods inspired by statistical physics have been a very popular topic in graphical model inference.

The renormalization methods could be relevant to deep architectures in the sense that the grouping of random variable resulting from a change of scale could be be made analogous with the pooling and subsampling operations often used in deep models.

It's an interesting idea, but it will probably take more work (and more tutorial expositions of RG) to catch the attention of this community.

Q

Venues / ICLR 2013 conference

Deep learning and the renormalization group



ICLR 2013 conference submission 15 Jan 2013 readers: everyone

PDF

Decision: reject

Yann LeCun

ICLR 2013 submission review 05 Apr 2013 readers: everyone

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A Common Logic to Seeing Cats and Cosmos



Olena Shmahalo / Quanta Magazine

There may be a universal logic to how physicists, computers and brains tease out important features from among other irrelevant bits of data.

"An exact mapping between the Variational Renormalization Group and Deep Learning", Mehta and Schwab, 1410.3831
"Exact Mapping"



$$e^{-H(\boldsymbol{h})} = \sum_{\boldsymbol{x}} e^{T(\boldsymbol{x},\boldsymbol{h}) - H(\boldsymbol{x})}$$

RG Transformation

 $e^{-E(\boldsymbol{h})} = \sum_{\boldsymbol{x}} e^{-E(\boldsymbol{x},\boldsymbol{h})}$

Boltzmann Machine

Harsh comments below the Quanta Magazine article

Noah says: December 26, 2014 at 9:54 am

I just spend an hour reading Mehta-Schwab paper from the beginning to end. Let me say that "A Common Logic to Seeing Cats and Cosmos" is a sensationalist article about a trivial paper, which will have no impact whatsoever. The whole M-S paper is based on the fact that couplings of two systems appear in more than one context and that distributions can sometimes appear as marginal distributions on product spaces. There is no one-to-one mappings between renormalization group (RG) scheme of Kadanoff and Restricted Boltzmann Machines (RBM) in Deep Neural Networks (DNN) in their paper. What they show is that RBM can be represented as a RG scheme with a very specific choice of coupling function T in equation (18). Conveniently, this coupling function depends on the Hamiltonian of the spin system, which it normally should not. Equivalence in equations (8) and (9) is also not correct. Condition (9) of course implies that the scheme is exact, but not the other way around, unless the authors make some implicit assumptions about coupling function T not mentioned in the paper. The paper contains no nontrivial ideas, it does not "open up a door to something very exciting", and I will not hold my breath expecting new breakthroughs because of this connection.

Dictionary: RG vs Deep Learning

Property	Variational RG	Deep Belief Networks
How input distribution is defined	Hamiltonian defining P(v)	Data samples drawn from P(v)
How interactions are defined	T(v,h)	E(v,h)
Exact transformation	$Tr_{h}e^{T(\mathbf{v},\mathbf{h})} = 1$	KL divergence between P(v) and variational distribution is zero
Approximations	Minimize or bound free energy differences	Minimize the KL divergence
Method	Analytic (mostly)	Numerical
What happens under coarse-graining	Relevant operators grow/irrelevant shrink	New features emerge

From Schwab's talk at PI: <u>http://pirsa.org/displayFlash.php?id=16080006</u>

More on the DL-RG Connections

- "Why does deep and cheap learning work so well ", Lin, Tegmark, Rolnick, 1608.08225
- Comment on the above paper, Schwab and Mehta, 1609.03541
- PCA meets RG, Bradde and Bialek, 1610.09733
- Mutual information RG, Koch-Janusz and Ringel, 1704.06279
- Media coverage/blog posts/student term papers etc



Neural Network

Renormalization Group



Shuo-Hui Li and LW, 1802.02840



Neural Network





Renormalization Group



Shuo-Hui Li and LW, 1802.02840

Multi-Scale Entanglement Renormalization Ansatz



Vidal 2006

Multi-Scale Entanglement Renormalization Ansatz



Vidal 2006

MERA as a quantum circuit





Physical variables











Bijector Block

Bijective & Differentiable map, i.e., Diffeomorphism

Forward

$$\begin{cases} x_{<} = z_{<} \\ x_{>} = z_{>} \odot e^{s(z_{<})} + t(z_{<}) \end{cases}$$

Backward

$$\begin{cases} z_{<} = x_{<} \\ z_{>} = (x_{>} - t(x_{<})) \odot e^{-s(x_{<})} \end{cases}$$

Log-Det-Jacobian

$$\ln \left| \det \left(\frac{\partial x}{\partial z} \right) \right| = \sum_{i} [s(z_{<})]_{i}$$



Normalizing flow, Rezende et al, 1505.05770 Special case: Real NVP, Dinh et al, 1605.08803

Bijector Block

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Normalizing flow, Rezende et al, 1505.05770 Special case: Real NVP, Dinh et al, 1605.08803

Inference





Real NVP, Dinh et al, 1605.08803

Generate



Real NVP, Dinh et al, 1605.08803

Bijectors form a group

$$\begin{aligned} \mathbf{x} &= g(\mathbf{z}) \\ g &= \cdots \circ g_2 \circ g_1 \end{aligned} \qquad \ln \left| \det \left(\frac{\partial \mathbf{x}}{\partial \mathbf{z}} \right) \right| = \sum_i \ln \left| \det \left(\frac{\partial g_{i+1}}{\partial g_i} \right) \right| \end{aligned}$$



Modular design Flexible blocks and stacking

"Disentangler" only architecture



Correlation length ~ Network depth









Given a dataset, learn its probability density by minimizing the negative likelihood

$$NLL_{\theta} = -\sum_{x \in \text{dataset}} \ln q_{\theta}(x)$$

Network parameters

Equivalent to reduce the Kullback–Leibler divergence

$$\mathbb{KL}\left(\frac{\pi(\boldsymbol{x})}{Z} \| q_{\boldsymbol{\theta}}(\boldsymbol{x})\right)$$

However, typical Stat-Mech problem has access only to the energy function

$$\mathcal{L}_{\theta} = \int \mathrm{d} \boldsymbol{x} \, q_{\theta}(\boldsymbol{x}) \left[\ln q_{\theta}(\boldsymbol{x}) - \ln \pi(\boldsymbol{x}) \right]$$

$$\mathcal{L}_{\theta} = \int \mathrm{d}\boldsymbol{x} \, q_{\theta}(\boldsymbol{x}) \left[\ln q_{\theta}(\boldsymbol{x}) - \ln \pi(\boldsymbol{x}) \right]$$

$$\uparrow$$
Entropy

$$\mathcal{L}_{\theta} = \int d\mathbf{x} \, q_{\theta}(\mathbf{x}) \left[\ln q_{\theta}(\mathbf{x}) - \ln \pi(\mathbf{x}) \right]$$

$$\uparrow \qquad \uparrow$$
Entropy
Energy

Learn from the data generated by the network itself

$$Z = \int \mathrm{d}\boldsymbol{x} \, \boldsymbol{\pi}(\boldsymbol{x})$$

F

Partition function

Learn from the data generated by the network itself

$$\mathcal{L}_{\theta} + \ln Z = \mathbb{KL}\left(q_{\theta}(\boldsymbol{x}) \, \left\| \, \frac{\pi(\boldsymbol{x})}{Z} \right\} \ge 0$$

The loss function is lower bounded by the physical free energy (Gibbs-Bogoliubov-Feynman inequality)

"Reparametrization trick"

How to compute the gradient w.r.t random sampling ?



End-to-end training using **back-propagation**

Interlude: WaveNet Story



Given a parallel WaveNet student $p_S(x)$ and WaveNet teacher $p_T(x)$ which has been trained on a dataset of audio, we define the *Probability Density Distillation* loss as follows:

$$D_{\mathrm{KL}}\left(P_S||P_T\right) = H(P_S, P_T) - H(P_S) \tag{6}$$

DeepMind <u>https://deepmind.com/blog/wavenet-generative-model-raw-audio/</u> 1609.03499 <u>https://deepmind.com/blog/high-fidelity-speech-synthesis-wavenet/</u> 1711.10433

Demo: Ising model

$$\pi(\boldsymbol{s}) = \exp\left(\frac{1}{2}\boldsymbol{s}^T \boldsymbol{K} \boldsymbol{s}\right)$$

Demo: Ising model

$$\pi(s) = \exp\left(\frac{1}{2}s^T K s\right)$$
$$\propto \int d\mathbf{x} \exp\left(-\frac{1}{2}\mathbf{x}^T (K + \alpha I)^{-1} \mathbf{x} + s^T \mathbf{x}\right)$$

decouple
Demo: Ising model

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decouple

$$\pi(\boldsymbol{x}) = \exp\left(-\frac{1}{2}\boldsymbol{x}^T (K + \alpha I)^{-1} \boldsymbol{x}\right) \prod_i \cosh(x_i)$$

Demo: Ising model

 π

$$(s) = \exp\left(\frac{1}{2}s^{T}Ks\right)$$
$$\propto \int d\mathbf{x} \exp\left(-\frac{1}{2}\mathbf{x}^{T}(K+\alpha I)^{-1}\mathbf{x} + s^{T}\mathbf{x}\right)$$

decouple

$$\pi(\boldsymbol{x}) = \exp\left(-\frac{1}{2}\boldsymbol{x}^T (K + \alpha I)^{-1} \boldsymbol{x}\right) \prod_i \cosh(x_i)$$

trace out s

 $\pi(\mathbf{s}|\mathbf{x}) = \prod_{i} \left(1 + e^{-2s_i x_i}\right)^{-1}$ continuous dual of the Ising model

A = I"Gaussian-Bernoulli Boltzmann Machine"

Zhang, Sutton, Storkey, Ghahramani, NIPS 2012

Generated Samples



x's are continuous fields dual to Ising spins

Variational Loss



Loss can be further improved by using more expressive networks

Variational Loss



Loss can be further improved by using more expressive networks

Renormalized Collective Variables



Also know their effective couplings => renormalized energy function







Arithmetics of the "smile vector"



White, 1609.04468 implemented using the variational autoencoder by Kingma and Welling, 1312.6114

How is it useful?



Automatically identify collective variables (metadynamics molecular simulation)



Automatically derive effective field theory (free energy surface)



Monte Carlo update proposals

Sampling in the latent space

Change-of-variables in a learnable way

$$Z = \int dx \pi(x) = \int dz \pi(g(z)) \left| \det \left(\frac{\partial x}{\partial z} \right) \right|$$

Physical
Prob. Dist.

$$A = \int dz \pi(g(z)) \left| \det \left(\frac{\partial x}{\partial z} \right) \right|$$

Latent variable
Prob. Dist.

Latent space is less correlated, therefore, easier to sample

Metropolized Independent Sampler

Acceptance rate with detailed balance condition

$$A(\mathbf{x} \to \mathbf{x}') = \min \left[1, \frac{q(\mathbf{x})}{q(\mathbf{x}')} \cdot \frac{\pi(\mathbf{x}')}{\pi(\mathbf{x})} \right]$$

iased physics even for
erfect proposals
osals are independent Propose Physical
Ratio Probability

- Unb impe
- Proposals are independent

Trainable transition kernel:

Song, Zhao, Ermon, 1706.07561 Levy, Hoffman, Sohl-Dickstein, 1711.09268

Surrogate energy function:

Li Huang and LW, 1610.02746 Liu, Qi, Meng, Fu, 1610.03137

Remarks on TNS Connection

• What we had is a classical downgrade of MERA

(Bény 2013) Probability Density~ Quantum Wavefuntion Classical Mutual Information ~ Entanglement Entropy "Decorrelator" ~ Disentangler Decimator~Isometry Bijector~Unitary

- Deep Learning machinery provides structural flexibility, modular abstraction, end-to-end training
- We give back to DL understandings of what are they doing (and hopefully, how to do better)

Remarks on DL

Old Wisdoms

Pooling layer in ConvNets ~ Decimation

Hidden nodes in RBM/DBN ~ Renormalized Variables

New Insights

Dialed convolution + Factor out layers = Decimation

Kept latent variables = Renormalized Variables







Spherical chicken in vacuum

Animals in the wild





Here we are

Spherical chicken in vacuum

Animals in the wild





Simplified, but not oversimplified model with balanced interpretability and expressibility

Remarks on RG

- Conventionally, RG is a semi-group, not a group
- NeuralRG builds on bijectors, hence a group (coarse-graining due to the multiscale structure)
- Probabilistic (Jona-Lasinio 75') and Information Theory (Apenko 09') views on RG (same is true for neural & tensor networks)
- Diffeomorphism does not change topology of the manifolds, therefore, may be limited.

The Universe as a Generative Model

$$\mathcal{L} = \int dx \int -g \left[\frac{m_p^2}{z} R - \frac{1}{4} F_{AV}^{A} F_{A}^{AV} + 2 \overline{\psi}^i r^{\mu} \mathcal{D}_{\mu} \psi^i + \left(\overline{\psi}^i_{\lambda} \mathcal{U}_{ij} \Phi \psi^j_{\lambda} + h.c. \right) - \left[\mathcal{D}_{\mu} \Phi \right]^2 - V(\Phi) \right]$$

RG = Infer the Effective Field Theory



Thank you!

