深度学习的数学与物理







deep learning A random sample, and some thoughts



A research story

Monge-Ampère Flow for Generative Modeling











鄂维南

arXiv:1809.10188 https://github.com/wangleiphy/MongeAmpereFlow



林峰的主业:机器学习分子势能





原子种类、坐标...

Zhang, Han, Wang, Car, E, PRL '18 Zhang, Han, Wang, Saidi, Car, E, NIPS '18

-4 -2 0 2 4

林峰的主业:机器学习分子势能



-4 -2 0 2 4

Zhang, Han, Wang, Car, E, PRL '18 Zhang, Han, Wang, Saidi, Car, E, NIPS '18





"判别型"学习 $y = f(\mathbf{x})$ or $p(y | \mathbf{x})$

深度学习不仅是函数拟合



"生成型"学习

 $p(\mathbf{x}, \mathbf{y})$





I do not understand. TOWEARN; Why const × Sort. PO Bethe Ansitz Prob. Know how to solve every problem that has been solved Kand 2-D Hall accel. Temp Non Linear Dessical Hyper

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







https://www.christies.com/Features/A-collaboration-between-two-artists-one-human-one-a-machine-9332-1.aspx

\$432,500 佳士得纽约 2018.10.25







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\$432,500 佳士得纽约 2018.10.25









生成模型 背后的数学 "概率变换"

简单分布





生成

推断



Sanchez-Lengeling & Aspuru-Guzik, Science 2018



Probability transformation in picture



motion



Coupled harmonic oscillator

A Toy problem: Harmonic oscillator

Relative Center-of-mass motion





四个月后...

19:57 /		••• 4G 🔲 '
く WeC	hat (1) Lingfeng Zhang	•••
	anyway, the idea of optimal transport suddenly came to me Not sure what I said makes sense or not.	¢.
	Jul 12, 2018 00:51	
	Key is to learn a map from z to scalar u, and let x be \partial{u}/\partial{z}.	а
	Jul 12, 2018 01:52	
	突然有了无数种可能: phi4应该可以这么做,这时候u有什么物: 意义会很有趣; 当z和x分布接近时,定义u为z^2/2+v(z)然后学来 v应该会是很不错的选择,相应 x就是z加偏v比上偏z,而这本身 又是可以是一个从z到z1、z2 直到x的map,是一个像resnet- 样的flow。。。最后,像波色子 这样的对称性应该可以保证	₹ 理 Î J H H H H H H H H H H H H H H H H H H
	Jul 12, 2018 08:39	

四个月后...



📲 4G 🔳)

...

老顾谈几何

最优传输映射 自映射 $T: \Omega \to \Omega$ 的传输代价

(Transportation Cost) 定义为

$$\frac{1}{2} \int_{\Omega} |x - T(x)|^2 d\mu(x)$$

在所有保持测度的自映射中,传输代价最小者被称为 是最优传输映射(Optimal Mass Transportation

$$T^* = argmin_{T^*\mu=\nu} E(T)$$

最优传输映射的传输代价被称为是概率测度µ和概率 测度 ν 之间的Wasserstein距离,记为 $d_W(\mu,\nu)_{o}$ 。

在这种情形下,Brenier证明存在一个凸函数

$$T: x \mapsto \nabla u(x)$$

就是唯一的最优传输映射。这个凸函数被称为是Brenier势能函数(Brenier potential)。

由Jacobian方程,我们得到Brenier势满足蒙日-安培 方程,梯度映射的雅克比矩阵是Brenier势能函数的 海森矩阵(Hessian Matrix),

$$\left(\frac{\partial u}{\partial x_j}\right)(\mathbf{x}) = \frac{\mu(\mathbf{x})}{\nu \circ \nabla(\mathbf{x})},$$

蒙日-安培方程解的存在性、唯一性等价于经典的凸 几何中的亚历山大定理(Alexandrov Theorem)。

Lei, Su, Cui, Yau, Gu 1710.05488



菲尔兹奖青睐的领域:最优传输和蒙 日-安培方程

最优传输理论是数学历史上美学价值和实用价值 相结合的一个典范! 它在工程和医疗领域得到广 泛应用,例如图形学中的参数化、视觉中的曲面 注册、大数据中的几何分类、网络中的特征提 取。特别是最优传输理论为深度学习的生成模型 奠定了坚实的理论基础。



在宇宙中不易被风吹散

清华计算机系理论组的老一辈师长虽然已经退 休何旦州们传播的知道由并之们传承州们对



Monge problem (1781): How to transport earth with optimal cost?













Brenier

Otto

McCann

Villani

Figalli



Fields Metal '18

from Cuturi, Solomon NISP 2017 tutorial



Monge problem (1781): How to transport earth with optimal cost?













Brenier

Otto

McCann

Villani

Figalli

Fields Metal '10

Fields Metal '18

from Cuturi, Solomon NISP 2017 tutorial



Brenier theorem (1991)

Monge problem (1781): How to transport earth with optimal cost?

Under reasonable conditions the optimal map is

 $z \mapsto x = \nabla u(z)$

Simply impose symmtry in the scalar generating potential 一林峰的主业!





Monge-Ampère Equation

Monge problem (1781): How to transport earth with optimal cost ?

Under reasonable conditions the optimal map is $z \mapsto x = \nabla u(z)$ $\left(\frac{p(z)}{q(\nabla u(z))} = \det\left(\frac{\partial^2 u}{\partial z_i \partial z_j}\right)\right)$







Fields Metal '82

Made contributions in differential equations, also to the Calabi conjecture in algebraic geometry, to the positive mass conjecture of general relativity theory, and to real and complex Monge-Ampère equation

Brenier theorem (1991)

Monge-Ampère Equation

Transport Theory

How to transport earth with optimal cost ?



Under reasonable conditions the optimal map is $z \mapsto x = \nabla u(z)$ $\frac{p(z)}{q(\nabla u(z))} = \det\left(\frac{\partial^2 u}{\partial z_i \partial z_j}\right)$







Fields Metal '82

Made contributions in differential equations, also to the Calabi conjecture in algebraic geometry, to the positive mass conjecture of general relativity theory, and to real and complex Monge-Ampère equation

Brenier theorem (1991)

Monge-Ampère Equation

letters to nature

A reconstruction of the initial conditions of the Universe by optimal mass transportation

Uriel Frisch*, Sabino Matarrese†, Roya Mohayaee‡* & Andrei Sobolevski§*



viscosity (discovered by Maxwell) does not operate, so that a noncollisional mechanism involving a small-scale gravitational instability must be invoked.

Our reconstruction hypothesis implies that the initial positions can be obtained from the present ones by another gradient map: $\mathbf{q} = \nabla_{\mathbf{x}} \Theta(\mathbf{x})$, where Θ is a convex potential related to Φ by a Legendre–Fenchel transform (see Methods). We denote by ρ_0 the initial mass density (which can be treated as uniform) and by $\rho(\mathbf{x})$ the final one. Mass conservation implies $\rho_0 d^3 q = \rho(\mathbf{x}) d^3 x$. Thus, the ratio of final to initial density is the jacobian of the inverse lagrangian map. This can be written as the following Monge– Ampère equation²⁰ for the unknown potential Θ :

$$\det(\nabla_{x_i}\nabla_{x_i}\Theta(\mathbf{x})) = \rho(\mathbf{x})/\rho_0$$

where 'det' stands for determinant.

We emphasize that no information about the dynamics of matter other than the reconstruction hypothesis is needed for our method, whose degree of success depends crucially on how well this hypothesis is satisfied. Exact reconstruction is obtained, for example, for the Zel'dovich approximation (before particle trajectories cross) and for adhesion-model dynamics (at arbitrary times).

We note that our Monge–Ampère equation for self-gravitating matter may be viewed as a nonlinear generalization of a Poisson equation (used for reconstruction in ref. 4), to which it reduces if particles have moved very little from their initial positions.

It has been discovered recently that the map generated by the solution to the Monge–Ampère equation (1) is the (unique) solution to an optimization problem²¹ (see also refs 22 and 23).

Under reasonable conditions the optimal map is







The physics behind: fluid control

 $\frac{p(z)}{q(\nabla u(z))} = \det\left(\frac{\partial^2 u}{\partial z_i \partial z_j}\right) \qquad \xrightarrow{\text{OODERECT}} u(z) = |z|^2/2 + \epsilon \varphi(z)$ $\epsilon \to 0$

Monge-Ampère Equation



Simple density

$$\frac{\partial p(\boldsymbol{x},t)}{\partial t} + \nabla \cdot \left[p(\boldsymbol{x},t) \nabla \varphi \right]$$

Liouville Equation (Continuity equation of compressible fluids)

Complex density

With Linfeng Zhang, Weinan E 1809.10188





The physics behind: fluid control

 $\frac{p(z)}{q(\nabla u(z))} = \det\left(\frac{\partial^2 u}{\partial z_i \partial z_j}\right)$

 $u(z) = |z|^2/2 + \epsilon \varphi(z)$ $\epsilon \rightarrow 0$

Monge-Ampère Equation



Simple density

Continuous-time limit

$$\frac{\partial p(\boldsymbol{x},t)}{\partial t} + \nabla \cdot \left[p(\boldsymbol{x},t) \nabla \varphi \right]$$

Liouville Equation (Continuity equation of compressible fluids)





Complex density

With Linfeng Zhang, Weinan E 1809.10188





Neural Ordinary Differential Equations

Residual network



Chen et al, 1806.07366 NIPS '18 Best paper award



$$d\boldsymbol{x}/dt = f(\boldsymbol{x})$$

cf Harbor el al 1705.03341 Lu et al 1710.10121, E 17'...

Density estimation of hand-written digits

A standard benchmark for generative models, lower is better



data space

latent space







Variational study of Sherrington-Kirkpatrick spin glasses



Better variational energy than previous network structure





3

Direct sample magnetic domains respecting physical symmetry





Importance of a symmetric flow





With symmetry

Without symmetry

"mode collapse"



Neural Canonical Transformations







Incompressible symplectic flow in phase space

Identifying mutually independent collective modes for molecular simulations (MD, PIMD), and effective field theory

Neural Canonical Transformations

Incompressible symplectic flow in phase space



Identifying mutually independent collective modes for molecular simulations (MD, PIMD), and effective field theory



Fluid Mechanics





Tensor Networks

Quantum Circuits

Holographic RG



Dynamical System







But, this is not the first time we feel excited

8

Lecture Notes in Physics	
John W. Clark Thomas Lindenau Manfred L. Ristig (Eds.)	
Scientific Applications of Neural Nets	
Proceedings, Bad Honnel, Germany 1998	
Springer	

Doing Science With Neural Nets: Pride and Prejudice

When neural networks re-emerged on the scene in the mid-80s as a new and glamorous computational paradigm, the initial reaction in some sectors of the scientific community was perhaps too enthusiastic and not sufficiently critical. There was a tendency on the part of practitioners to oversell the powers of neural-network or "connectionist" solutions relative to conventional techniques – where conventional techniques can include both traditional theory-rich modeling and established statistical methods. The last five years have seen a correction phase, as some of the practical limitations of neural-network approaches have become apparent, and as scientists have become better acquainted with the wide array of advanced statistical tools that are currently available.

Why now, but not 20 years ago? What has changed ? What has not?



深度学习的秘诀究竟是什么?











深度学习的秘诀究竟是什么?















核心思想: 表示学习

关键技术: 微分编程

Representation Leanring



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

Page 6 Figure 1.2



Magic of learning representation

Neural style transfer



Gatys et al, 1508.06576

Latent space interpolation

Glow 1807.03039 https://blog.openai.com/glow/

Learning representation for science



Automatic chemical design, Gomez-Bombarelli et al, 1610.02415





Deep Learning and Renormalization Group



Bény, 1301.3124



Koch-Janusz and Ringel, 1704.06279



Mehta and Schwab, 1410.3831



You, Yang, Qi, 1709.01223 and more...



Deep Learning and Renormalization Group



 $+.007 \times$



Panda 58% confidence

Vulnerability of deep learning, Kenway, 1803.06111 & 1803.10995





Gibbon Goodfellow et al, 2014 99% confidence



and more...



Wavelet transformation for Lena and Ising





Guy, Wavelets & RG1999+ White, Evenbly, Qi, Wavelets, MERA, and holographic mapping 2013+

Wavelet transformation for Lena and Ising





Guy, Wavelets & RG1999+ White, Evenbly, Qi, Wavelets, MERA, and holographic mapping 2013+

Wavelet transformation for Lena and Ising





Guy, Wavelets & RG1999+ White, Evenbly, Qi, Wavelets, MERA, and holographic mapping 2013+



Neural Renormalization Group Flow Normalizing flow with multiscale network structures



Nonlinear & adaptive generalizations of wavelets And, a fresh approach to holographic duality

Swingle 0905.1317, Qi 1309.6282 and more



With Shuo-Hui Li 1802.02840



Differentiable Programming







Andrej Karpathy

Director of AI at Tesla. Previously Research Scientist at OpenAI and PhD student at Stanford. I like to train deep neural nets on large datasets.

https://medium.com/@karpathy/software-2-0-a64152b37c35

A new paradigm for programming computers

Software 2.0

Benefits compared to 1.0

- Computationally homogeneous
- Simple to bake into silicon
- Constant running time
- Constant memory usage
- Highly portable & agile
- Modules can meld into an optimal whole
- Better than humans

Writing software 2.0 by searching in the program space



Andrej Karpathy

Director of AI at Tesla. Previously Research Scientist at OpenAI and PhD student at Stanford. I like to train deep neural nets on large datasets.

https://medium.com/@karpathy/software-2-0-a64152b37c35



Differentiable Scientific Programming

- Most linear algebra operations (Eigen, SVD!) are <u>differentiable</u>
- Loop/Condition/Sort/Permutations are also differentiable
- ODE integrators are differentiable with O(1) memory
- Differentiable ray tracer and Differentiable fluid simulations
- Differentiable Monte Carlo/Tensor Network/Functional RG/ Dynamical Mean Field Theory/Density Functional Theory...

Differentiable programming is more than training neural networks





Differentiable Eigensolver $H\Psi = \Psi \Lambda$

What happen if H = H + dH? **Forward mode:**

Reverse mode: How should I change H given

Perturbation theory

Inverse perturbation theory! $\partial \mathscr{L}/\partial \Psi$ and $\partial \mathscr{L}/\partial \Lambda$?

Hamiltonian engineering via differentiable programming

https://github.com/wangleiphy/DL4CSRC/tree/master/2-ising see also Fujita et al, 1705.05372







Differentiable Quantum Programming With Liu, Zeng, Wu, Hu ×d 1804.04168, 1808.03425 0 0) measure θ_{I}^{α} θ_d^{α} 0 outcomes 0 two-sample test $\Delta \theta$ loss & gradient classical optimizer classical data





Train the quantum circuit as a probabilistic generative model Quantum sampling complexity underlines the "quantum supremacy"







- Variational quantum eigensovler (VQE)
- Quantum approximate optimization algorithm (QAOA)
- Quantum pattern recognition

. . .

• Quantum circuit Born machine (QCBM)

Quantum circuit classifier Born machine experiment TNS inspired circuit architecture Quantum generative model Quantum adversarial training

Farhi, Neven, 1802.06002 Havlicek et al, 1804.11326 Benedetti, Garcia-Pintos, Nam, Perdomo-Ortiz, 1801.07686 Huggins, Patel, Whaley, Stoudenmire, 1803.11537 Gao, Zhang, Duan, 1711.02038 Dallaire-Demers, Lloyd, Benedetti 1804.08641,1804.09139, 1806.00463





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It is a paradigm beyond quantum-classical hybrid





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It is a paradigm beyond quantum-classical hybrid

Short term:

What can we do with circuits of limited depth?

Long term:

Are we really good at programing quantum computers?





It is a paradigm beyond quantum-classical hybrid

- Variational quantum eigensovler (VQE)
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Quantum code







- Variational quantum eigensovler (VQE)
- Quantum approximate optimization algorithm (QAOA)
- Quantum pattern recognition
- Quantum circuit Born machine (QCBM)

Quantum circuit Born machine e> TNS inspired circ Quantum genera Quantum advers

. . .

It is a paradigm beyond quantum-classical hybrid

Quantum code







Summary

Neural Networks Tensor Networks



Quantum Circuits



1. Function Approximation

Probabilistic Transformation

3. Information Processing Device

Try it yourself!



https://github.com/wangleiphy/TRG https://github.com/li012589/NeuralRG https://github.com/wangleiphy/MongeAmpereFlow



https://github.com/GiggleLiu/QuantumCircuitBornMachine



https://github.com/QuantumBFS/Yao.jl/

Thank You!

Pan Zhang Shuo-Hui Li

Refs <u>1802.02840 1804.04168</u> <u>1808.03425</u> <u>1809.10188</u>

Jin-Guo Liu Song Cheng Weinan E Xiu-Zhe Luo Jinfeng Zeng Linfeng Zhang





Lecture Note on Deep Learning and Quantum Many-Body Computation

Institute of Physics, Chinese Academy of Sciences Beijing 100190, China

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.

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



* wanglei@iphy.ac.cn

Jin-Guo Liu, Shuo-Hui Li, and Lei Wang*

February 14, 2018

Abstract

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To catch up with the latest updates



Machine Learning for Quantum Many-Body Physics

Coordinators: Roger Melko, Amnon Shashua, Miles Stoudenmire, and Matthias Troyer Scientific Advisors: Juan Carrasquilla, Pankaj Mehta, Lei Wang, and Lenka Zdeborova

This KITP program will bring together experts from both physics and computer science to discuss the uses of machine learning in theoretical and experimental many-body physics. Machine learning will be explored as a complementary method to current computational techniques, including Monte Carlo and tensor networks, as well as a method to analyze "big data" generated in experiment. The program will include applications in the design of quantum computers and devices, such as the use of neural networks for the purposes of decoding, quantum error correction, and tomography. Theoretical connections between deep learning, the renormalization group, and tensor networks, will be examined in detail. Foundational questions in machine learning will be addressed, such as the formal concepts on information, intelligence, and interpretability. Finally, the theoretical possibility of a quantum





Jan 28, 2019 - Mar 22, 2019 INFORMATION Apply

KITP, Santa Barbara Program ML for Quantum Many-Body Physics Jan 28-Mar 22, 2019



APS March meeting focus session ML in Condensed Matter Physics Boston, Mar 4-8, 2019

