Born Machines

A fresh approach to quantum machine learning

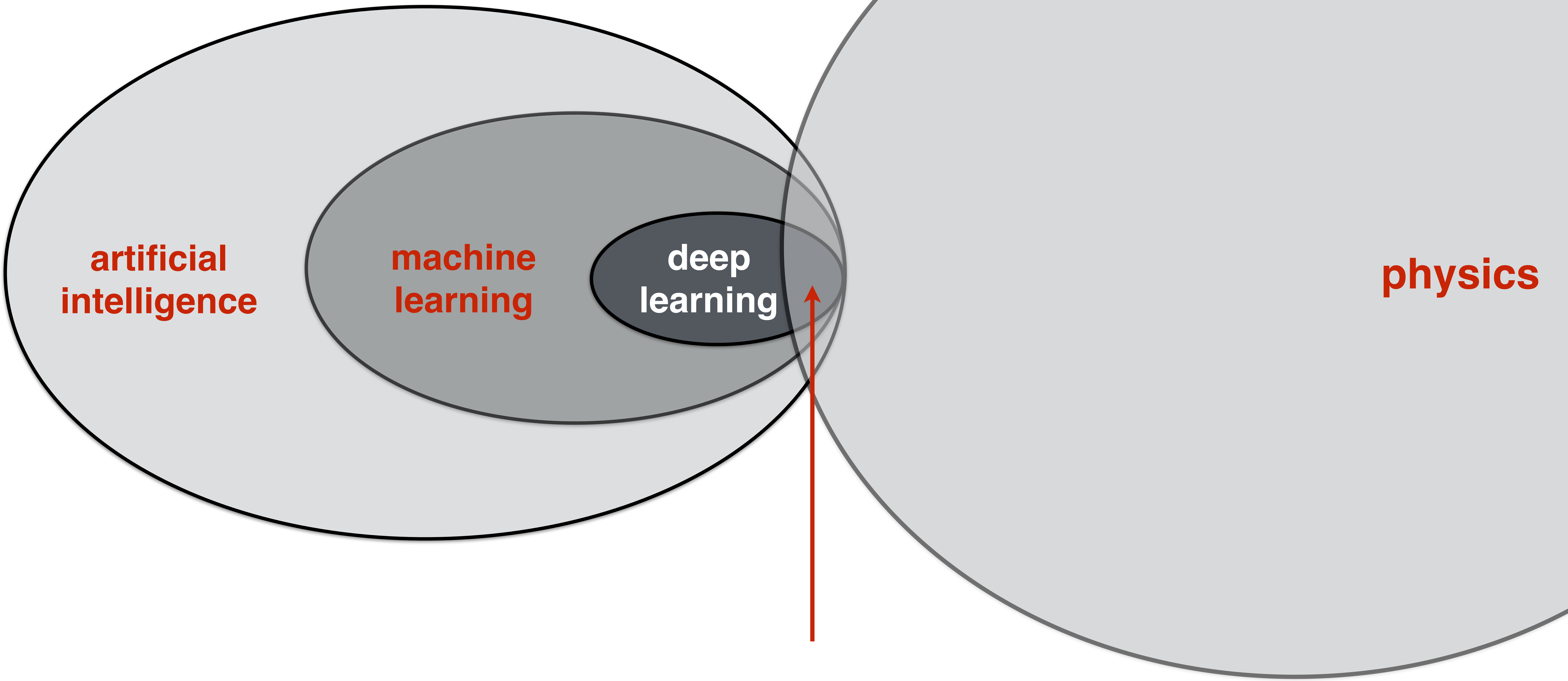
Lei Wang (王磊)

https://wangleiphy.github.io

Institute of Physics, Beijing

Chinese Academy of Sciences

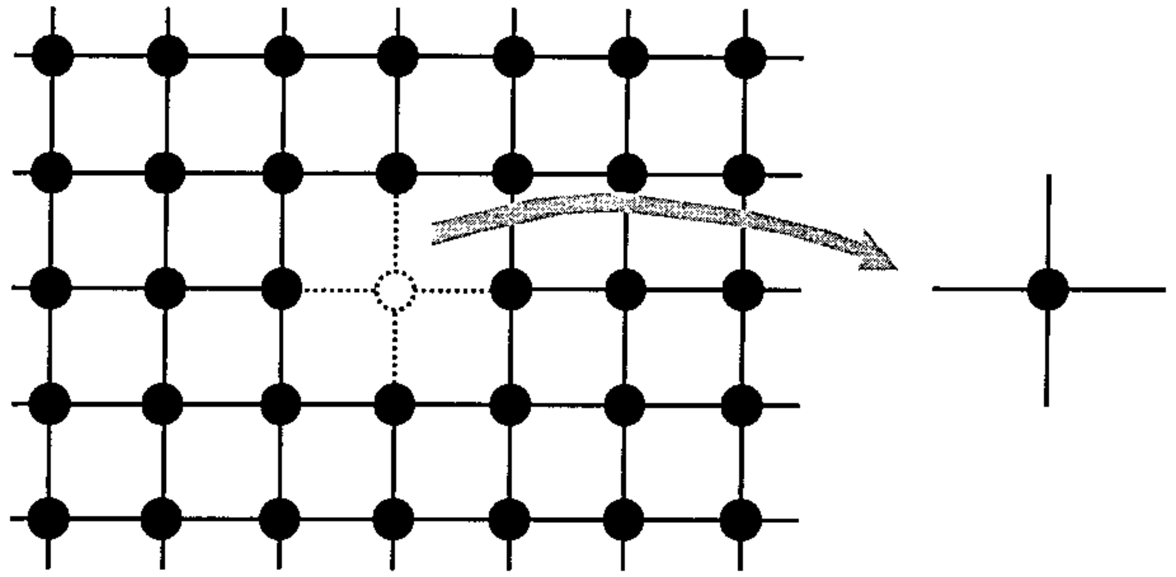
Liu, LW, PRA '18
Cheng, Chen, LW, Entropy '18
Han, Wang, Fan, LW, Zhang, PRX '18



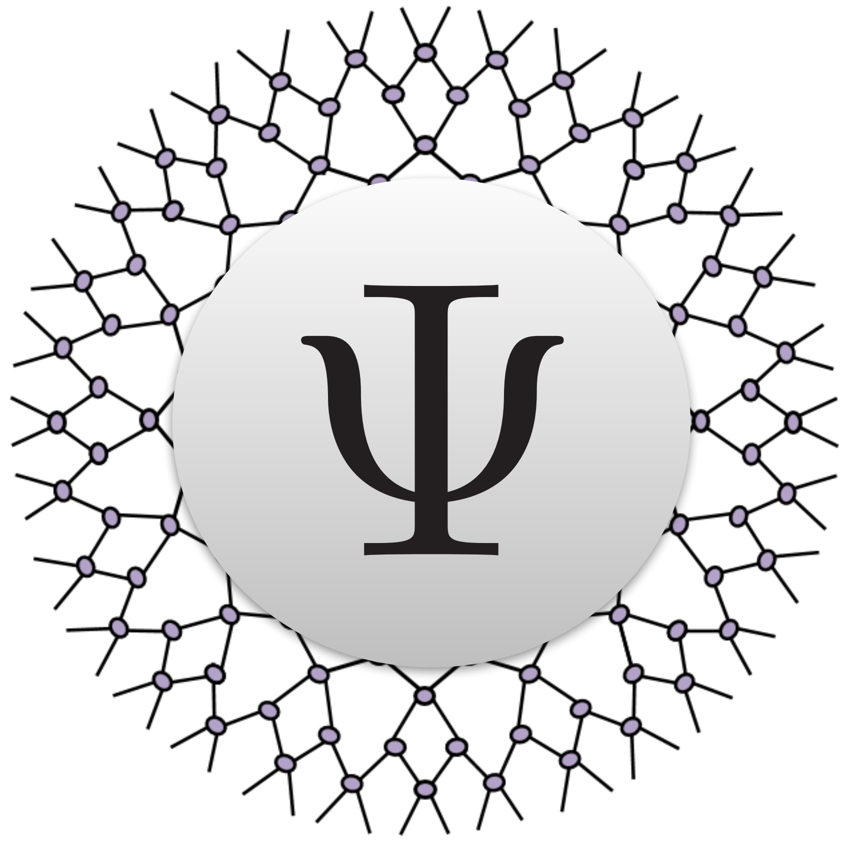
This talk: quantum physics
for machine learning

Physicists' gifts to Machine Learning

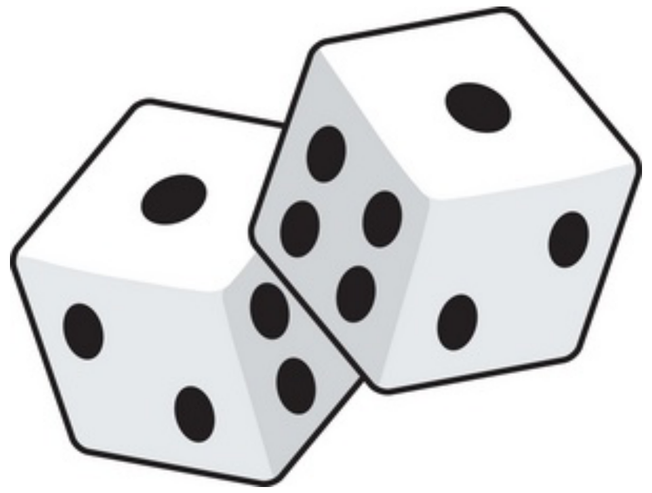
Mean Field Theory



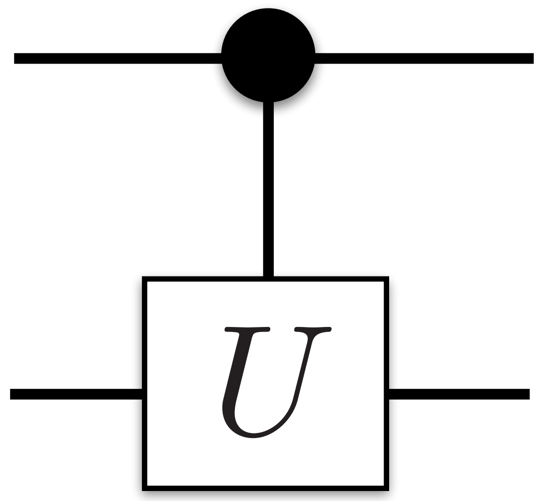
Tensor Networks



Monte Carlo Methods



Quantum Computing



Learning is more than function fitting

Discriminative

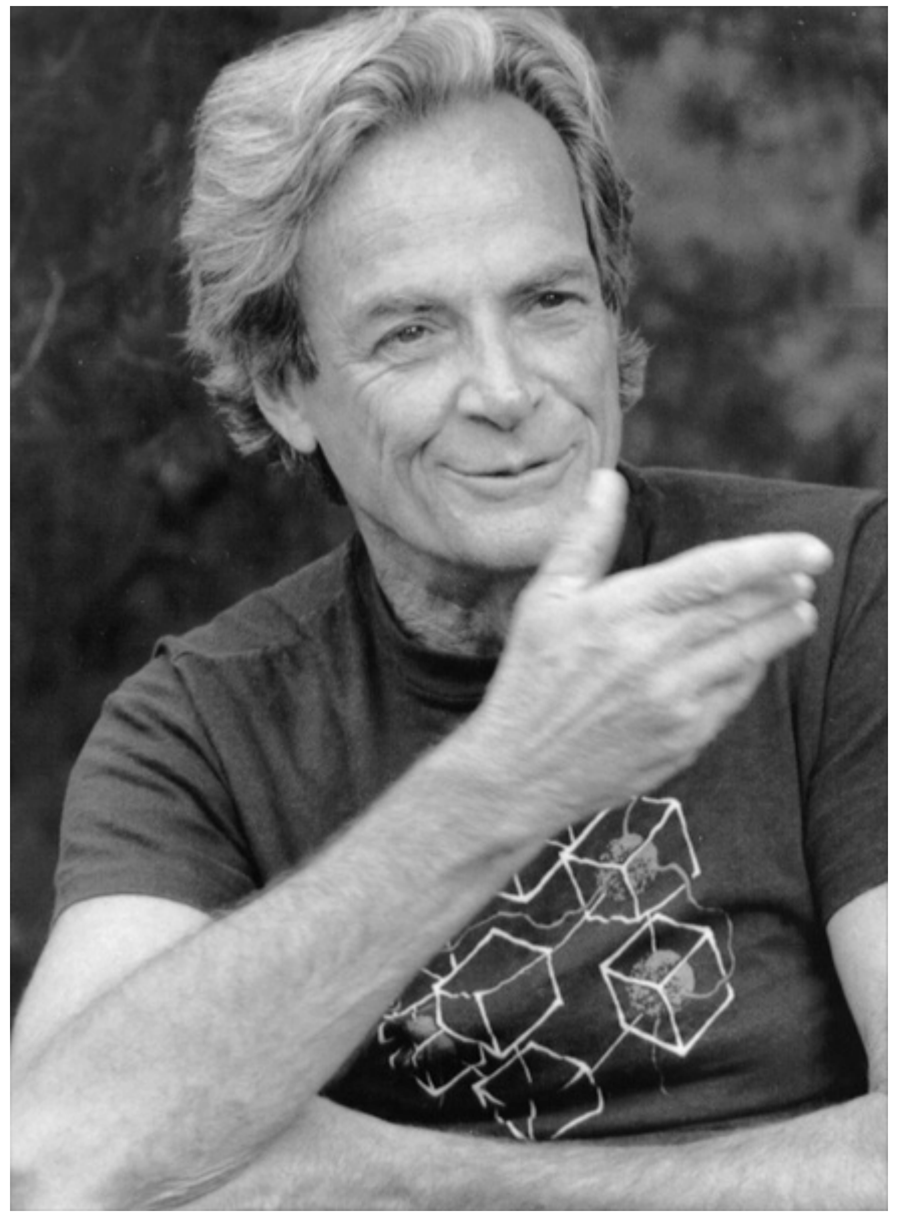
$$y = f(\boldsymbol{x})$$

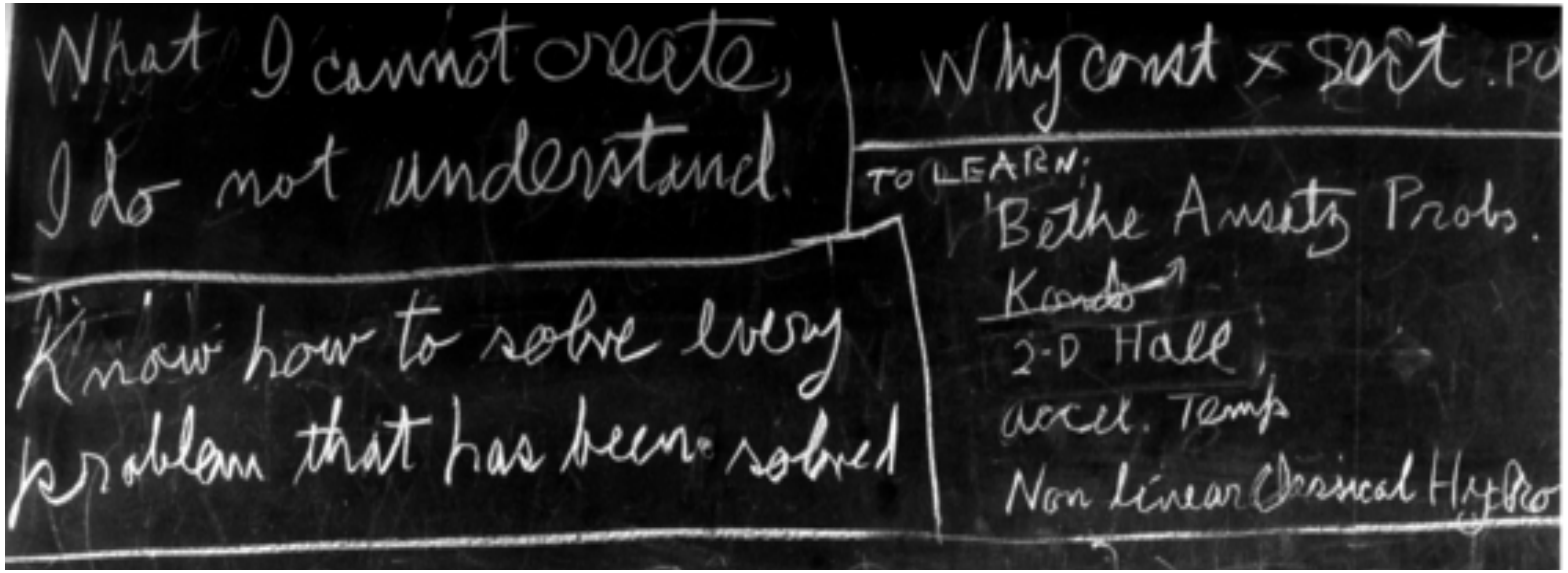
or $p(y \mid \boldsymbol{x})$

Generative

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

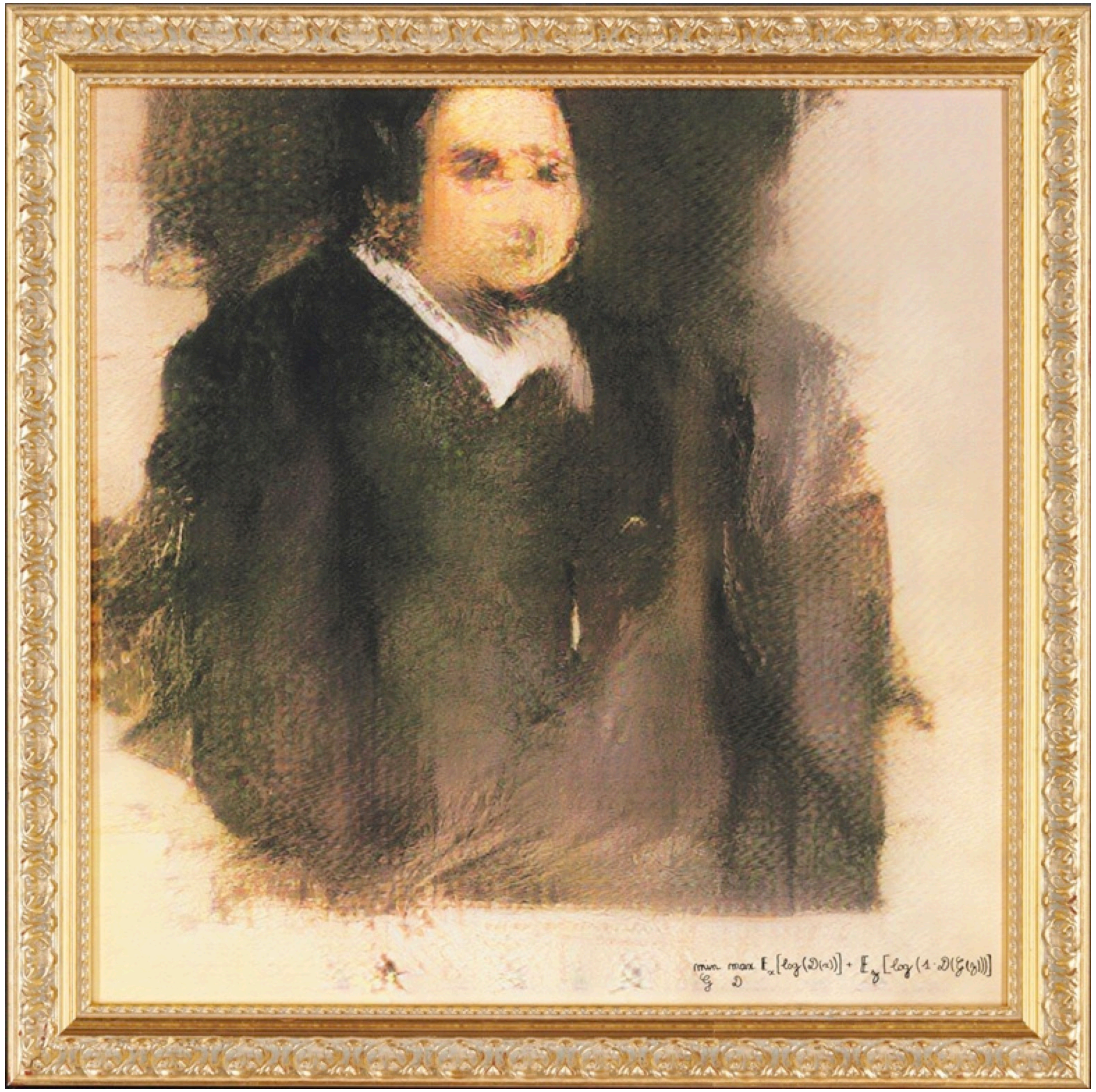
Learning is more than function fitting





“What I can not create, I do not understand”

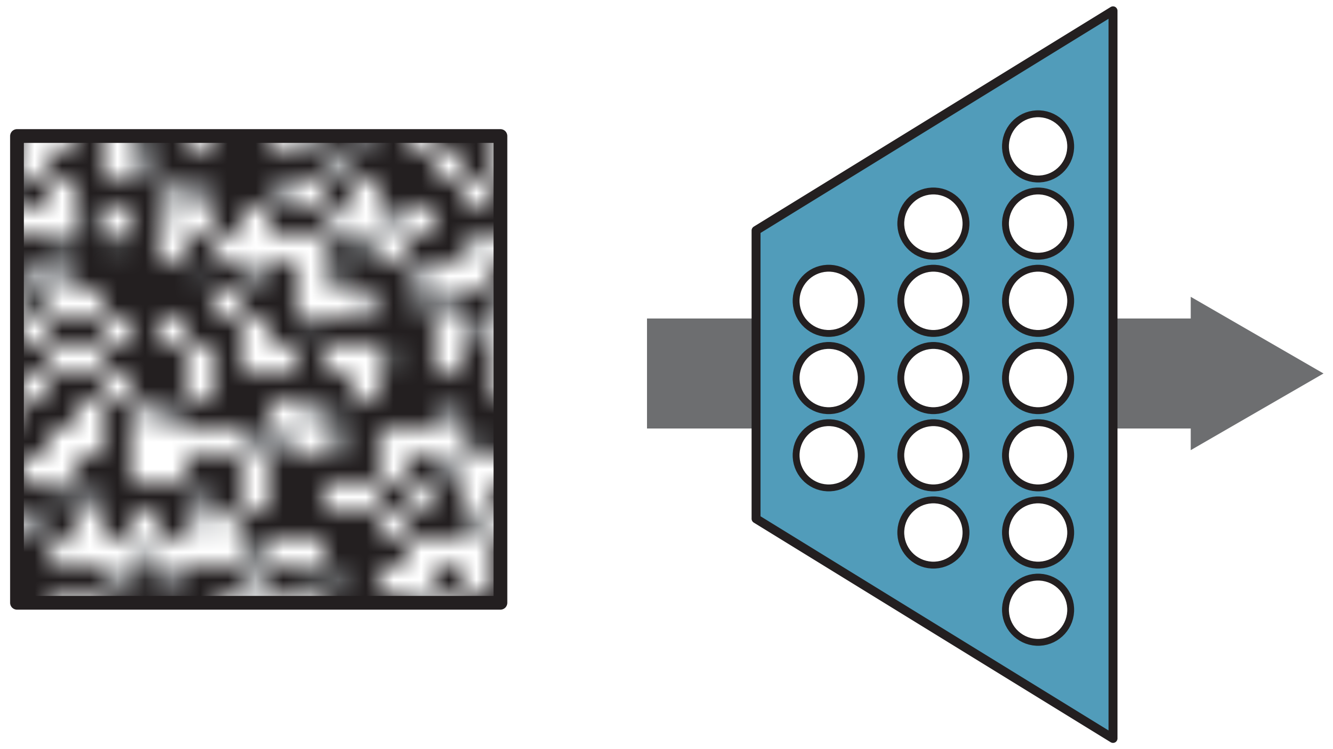
Generated Arts



$432,500
25 October 2018
Christie’s New York

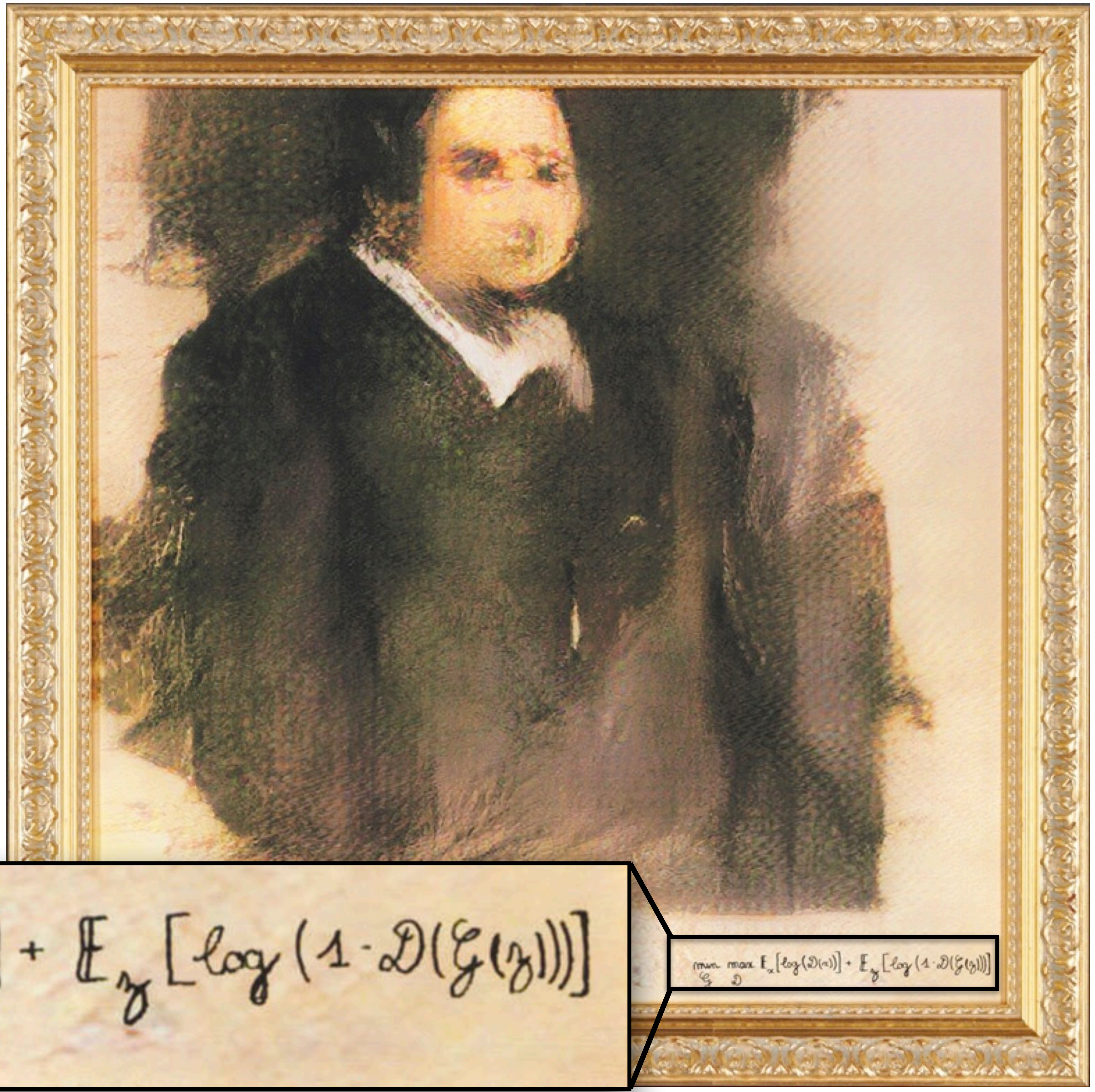
https://www.christies.com/Features/A-collaboration-between-two-artists-one-human-one-a-machine-9332-1.aspx

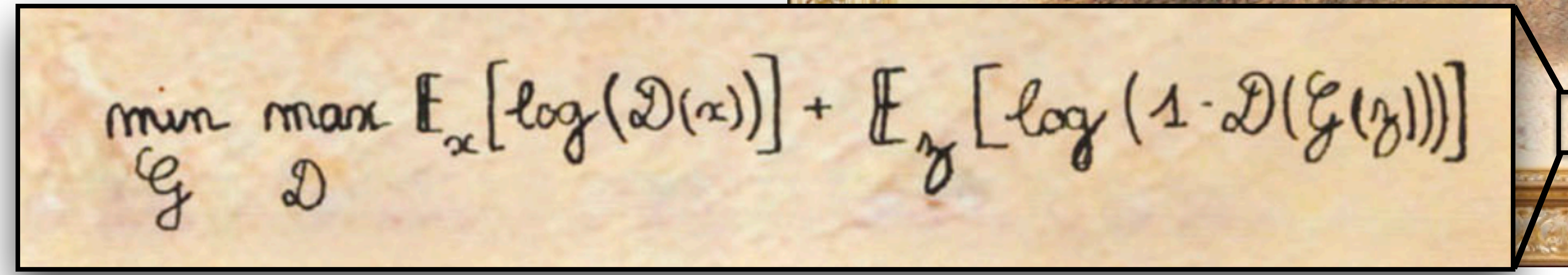
Generated Arts



Gaussian Noise

Generative Network





$432,500

25 October 2018

Christie's New York

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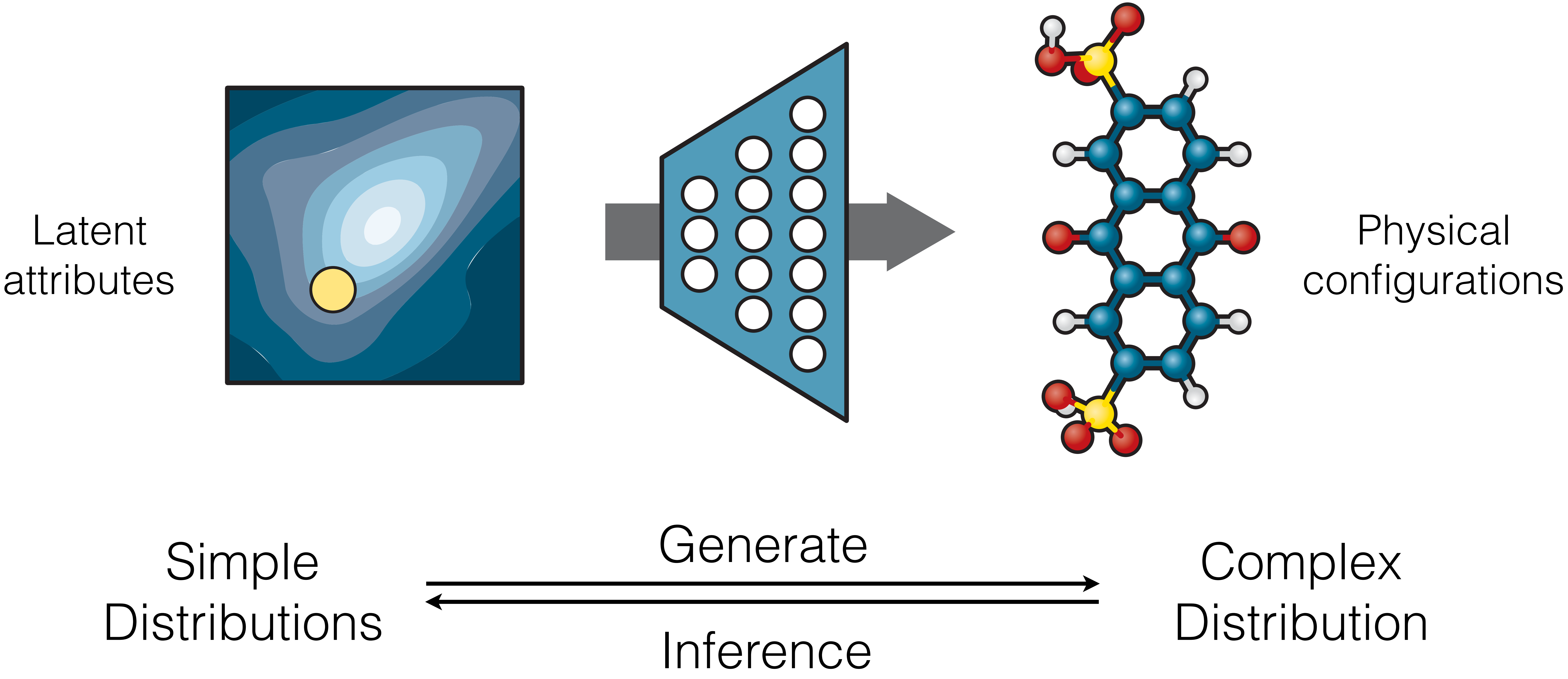
Generate Molecules

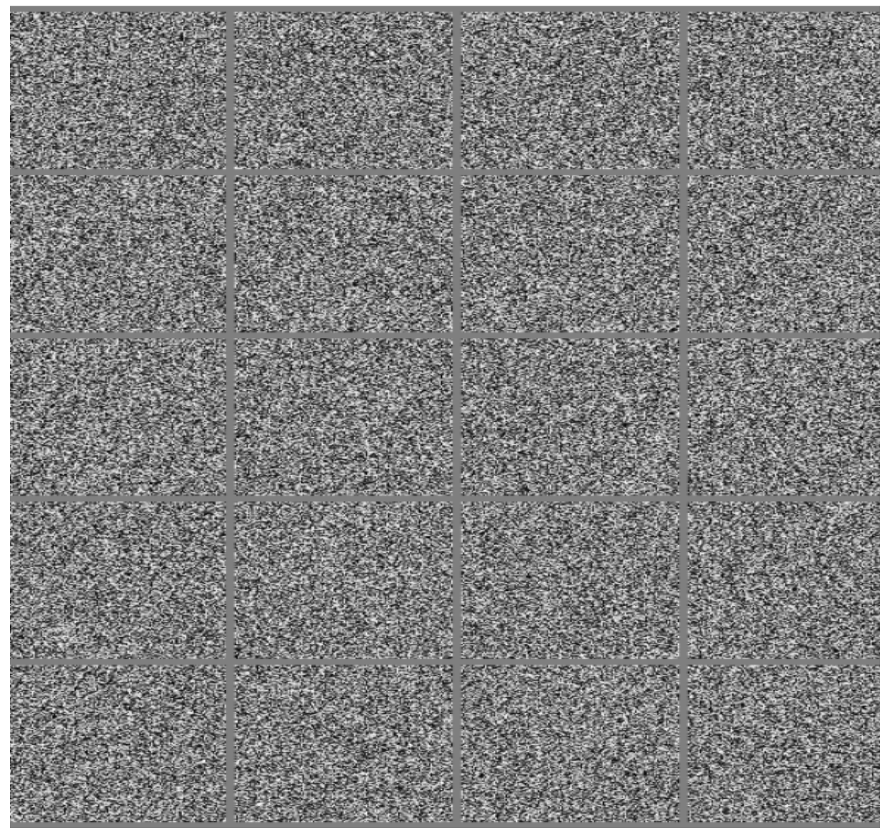


Sanchez-Lengeling & Aspuru-Guzik, Science 2018

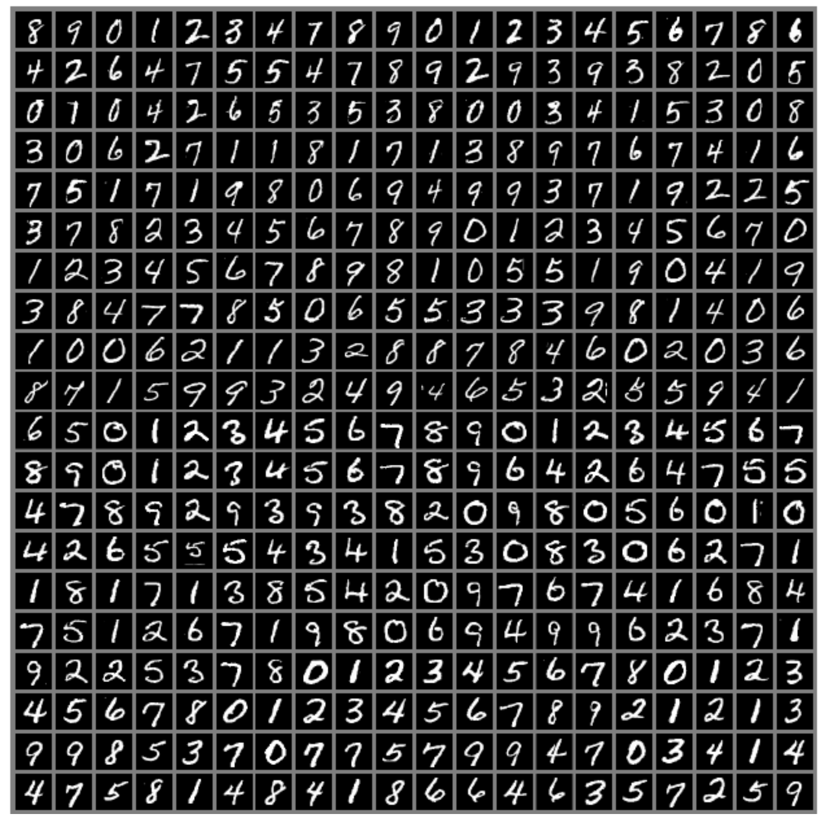
Probabilistic Generative Modeling

$$p(\boldsymbol{x})$$

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



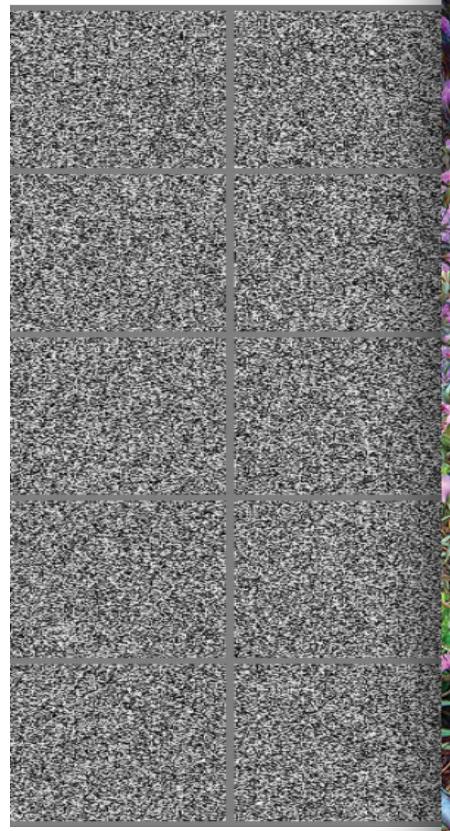
“random” images

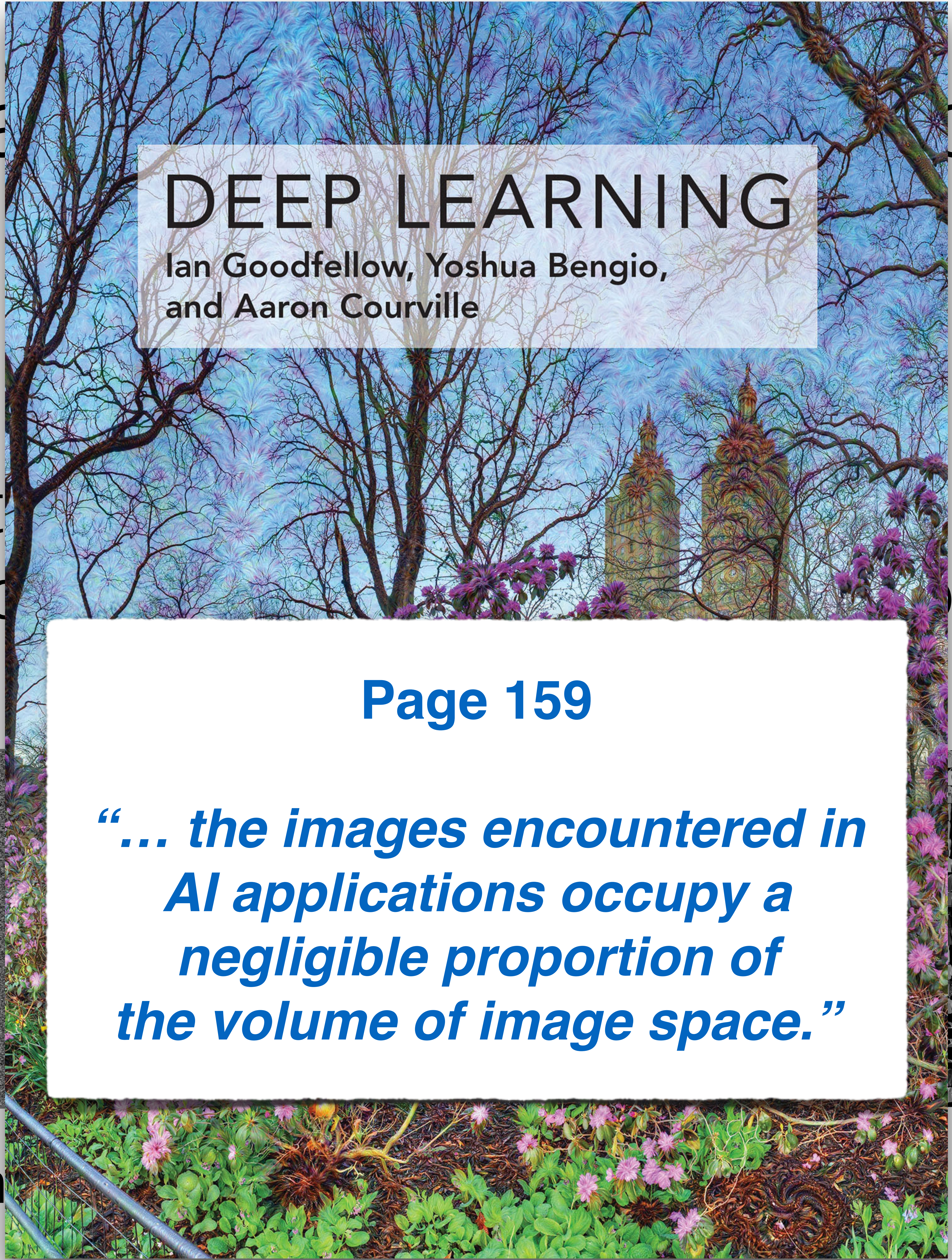


“natural” images

Proba odeling

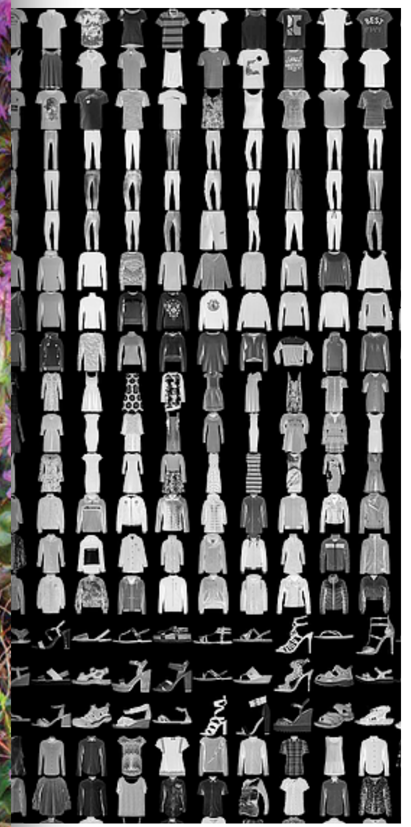
How t from a
high- ution ?





Page 159

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



"random

Probabilistic Generative Modeling

$$p(\boldsymbol{x})$$

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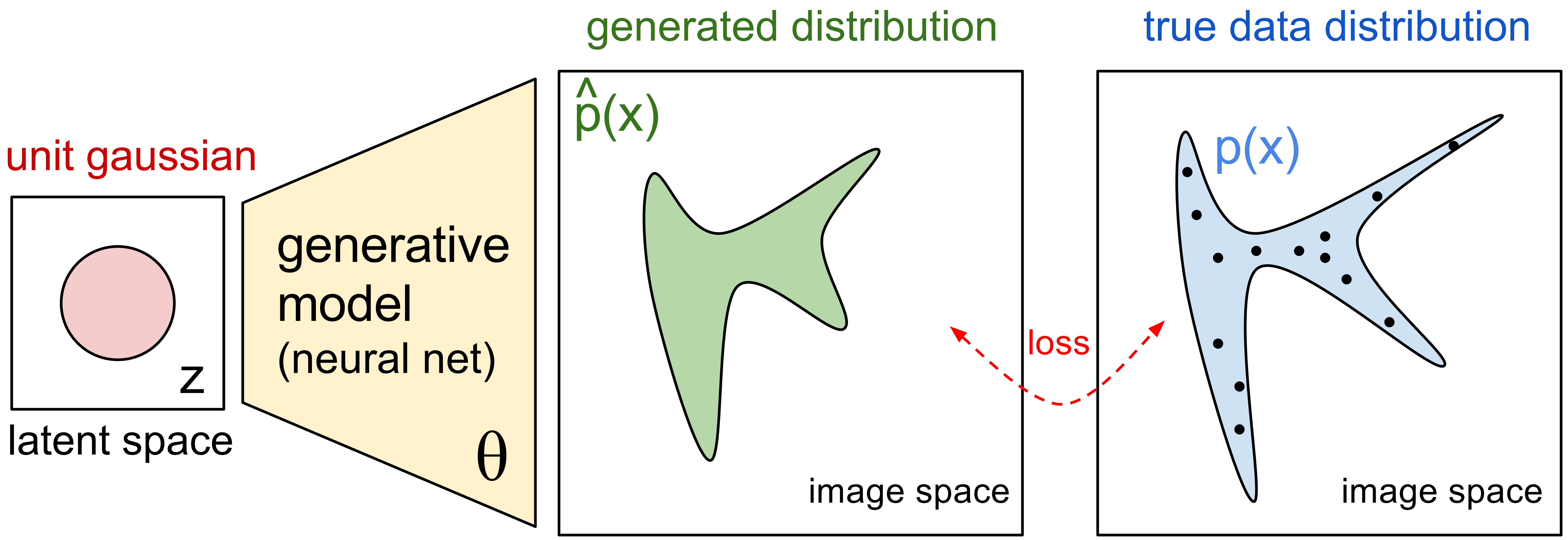
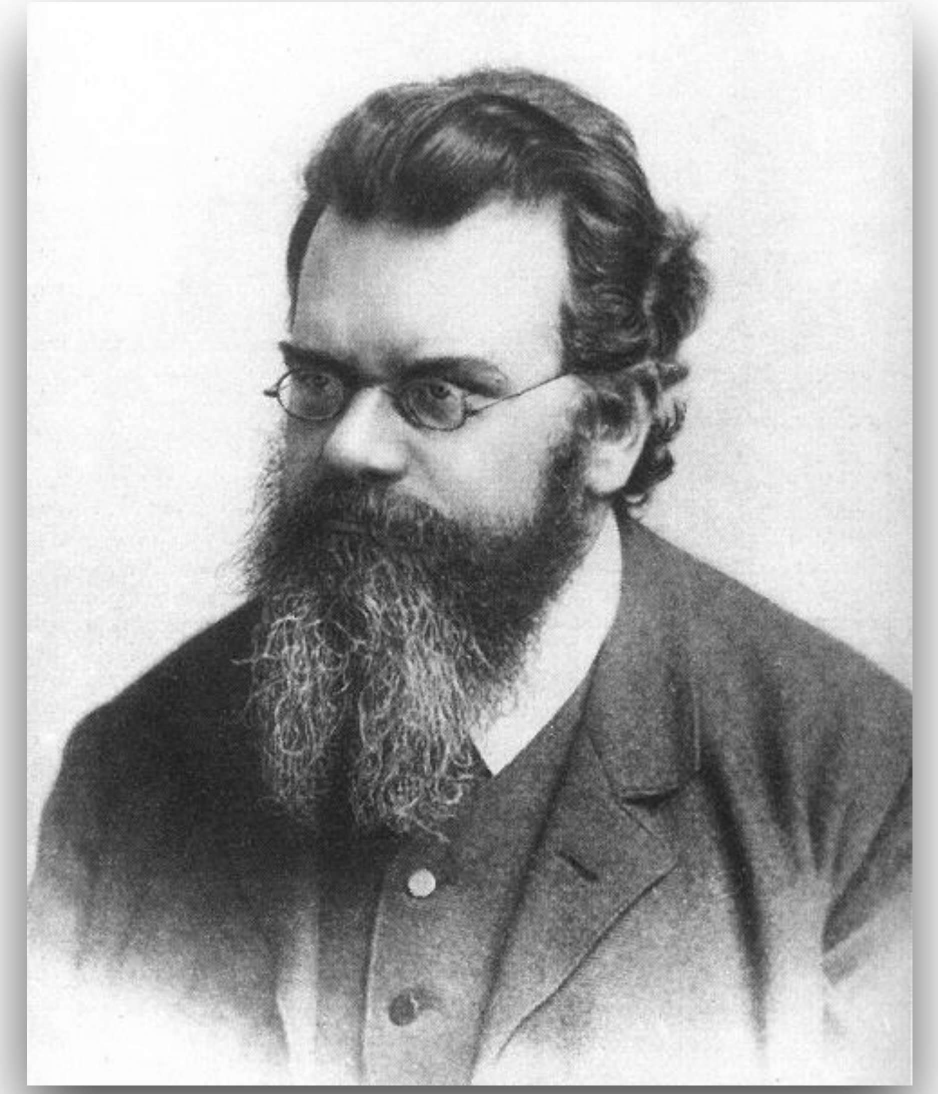


https://blog.openai.com/generative-models/



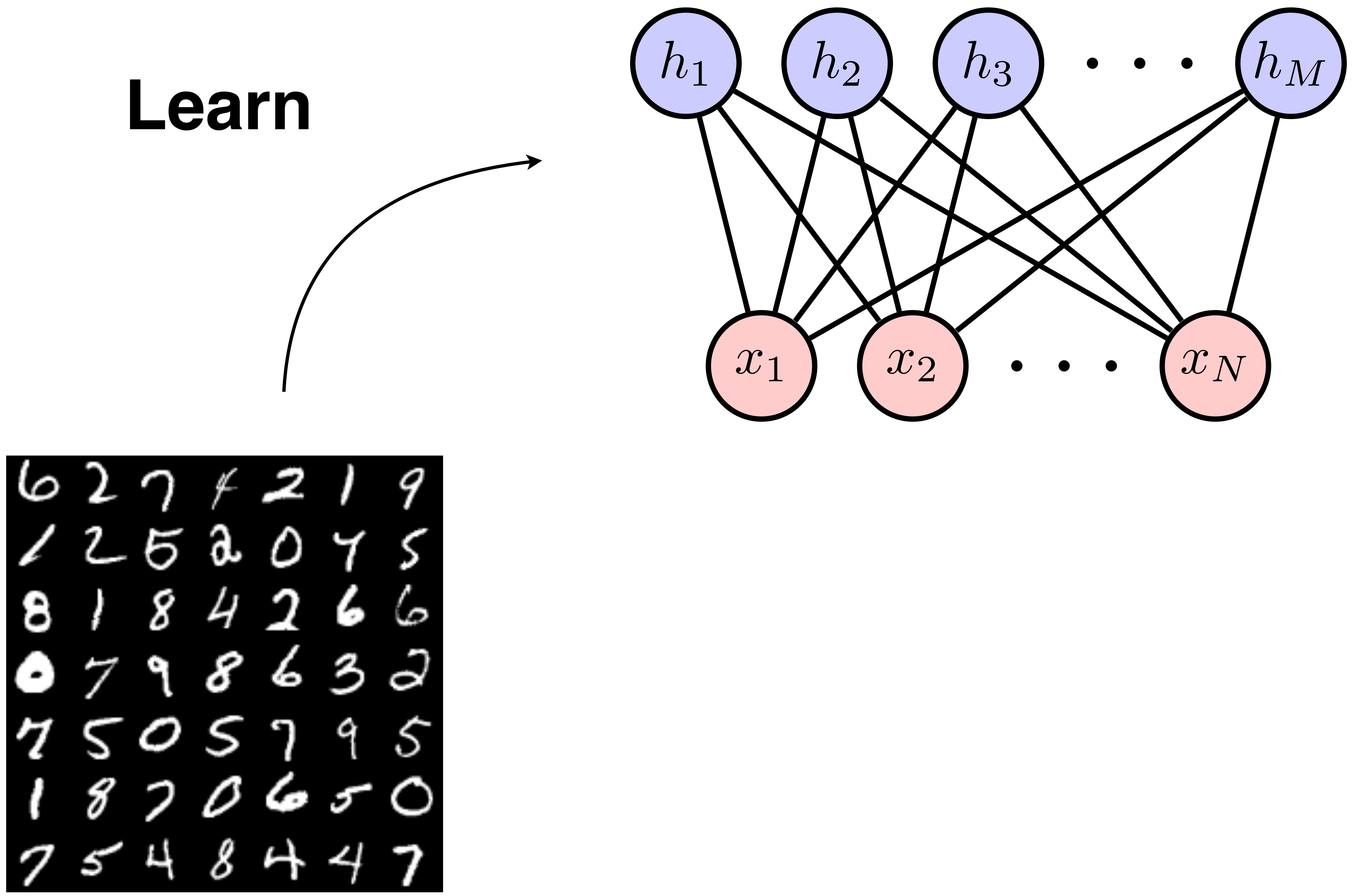
Boltzmann Machines

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

statistical physics

Generative Modeling using Boltzmann Machines

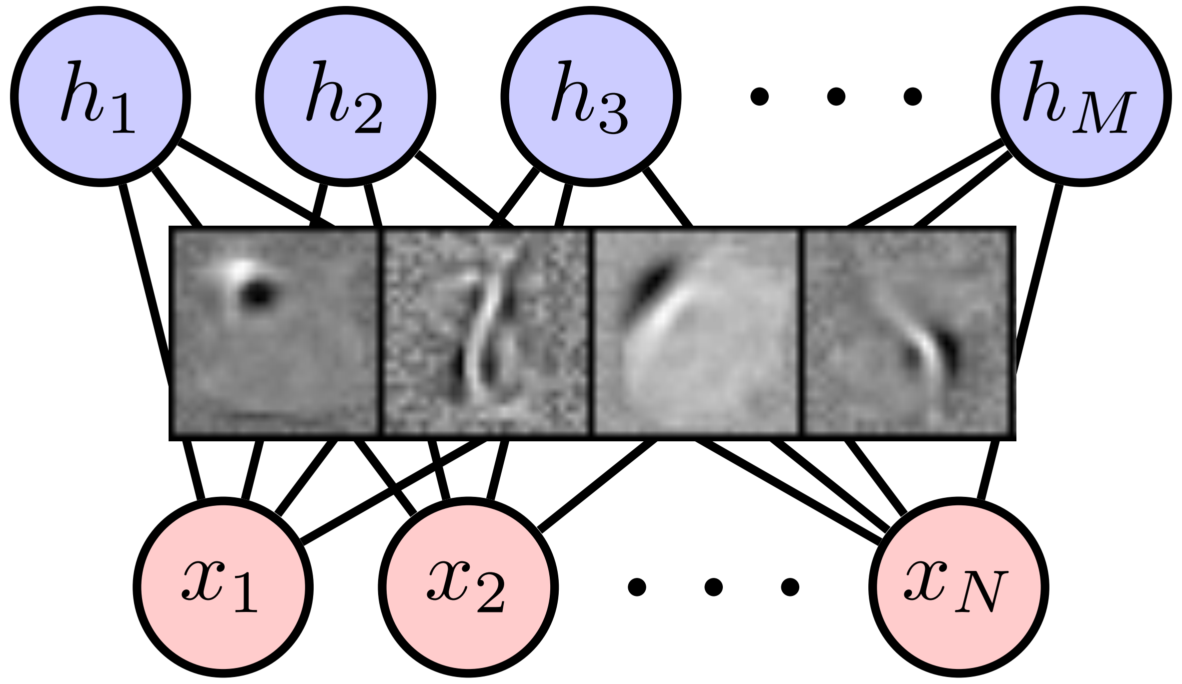
Negative log-likelihood loss $\mathscr{L} = -\frac{1}{|\mathscr{D}|}\sum_{\boldsymbol{x}\in\mathscr{D}} \ln p(\boldsymbol{x})$



Generative Modeling using Boltzmann Machines

Negative log-likelihood loss $\mathscr{L} = -\frac{1}{|\mathscr{D}|}\sum_{\boldsymbol{x}\in\mathscr{D}} \ln p(\boldsymbol{x})$

Learn



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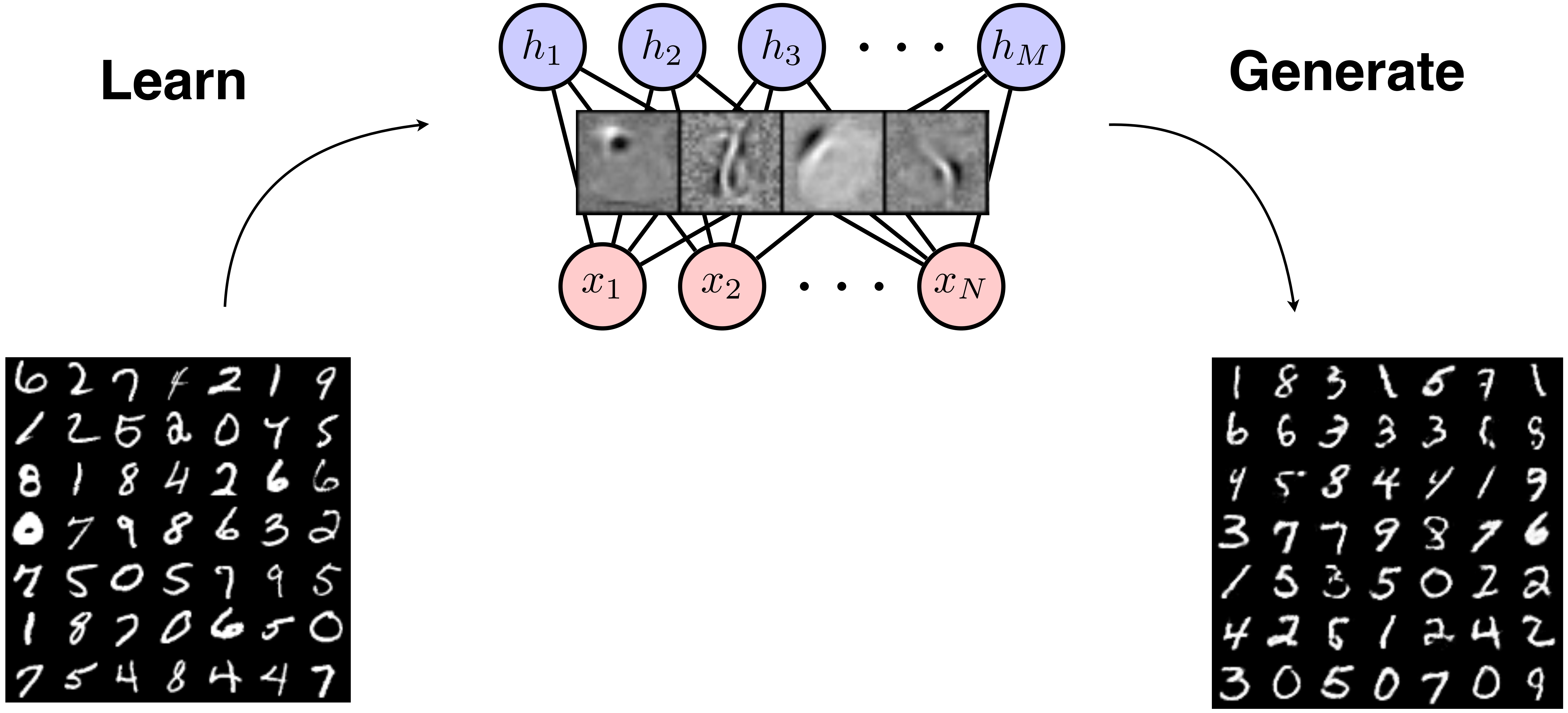
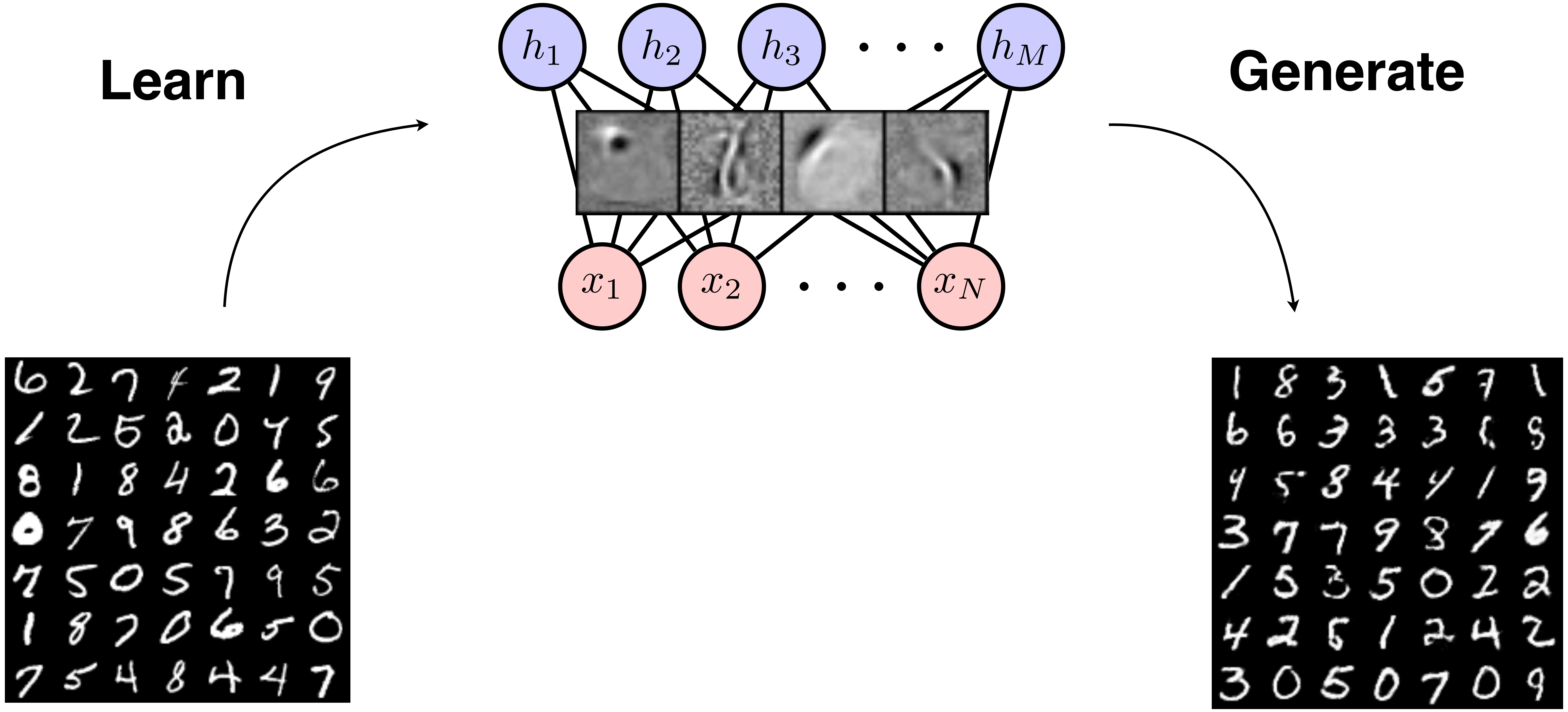
Negative log-likelihood loss $\mathscr{L} = -\frac{1}{|\mathscr{D}|}\sum_{\boldsymbol{x}\in\mathscr{D}} \ln p(\boldsymbol{x})$



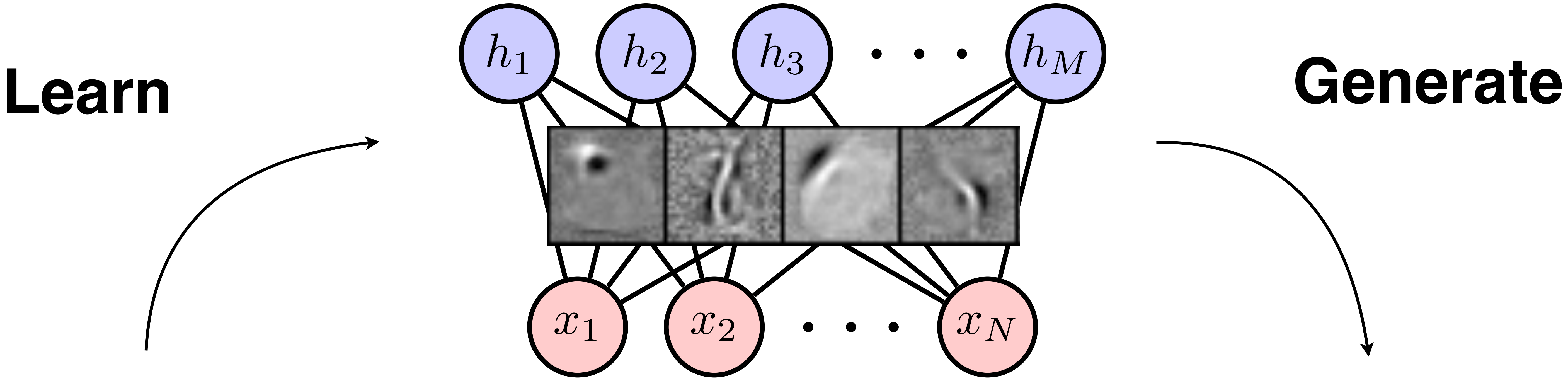
Generative Modeling using Boltzmann Machines

Negative log-likelihood loss $\mathscr{L} = -\frac{1}{|\mathscr{D}|}\sum_{\boldsymbol{x}\in\mathscr{D}} \ln p(\boldsymbol{x}) = \langle E(\boldsymbol{x})\rangle_{\boldsymbol{x}\sim\mathscr{D}} + \ln Z$



Generative Modeling using Boltzmann Machines

Negative log-likelihood loss $\mathscr{L} = -\dfrac{1}{|\mathscr{D}|} \sum_{\boldsymbol{x} \in \mathscr{D}} \ln p(\boldsymbol{x}) = \langle E(\boldsymbol{x}) \rangle_{\boldsymbol{x} \sim \mathscr{D}} + \ln Z$

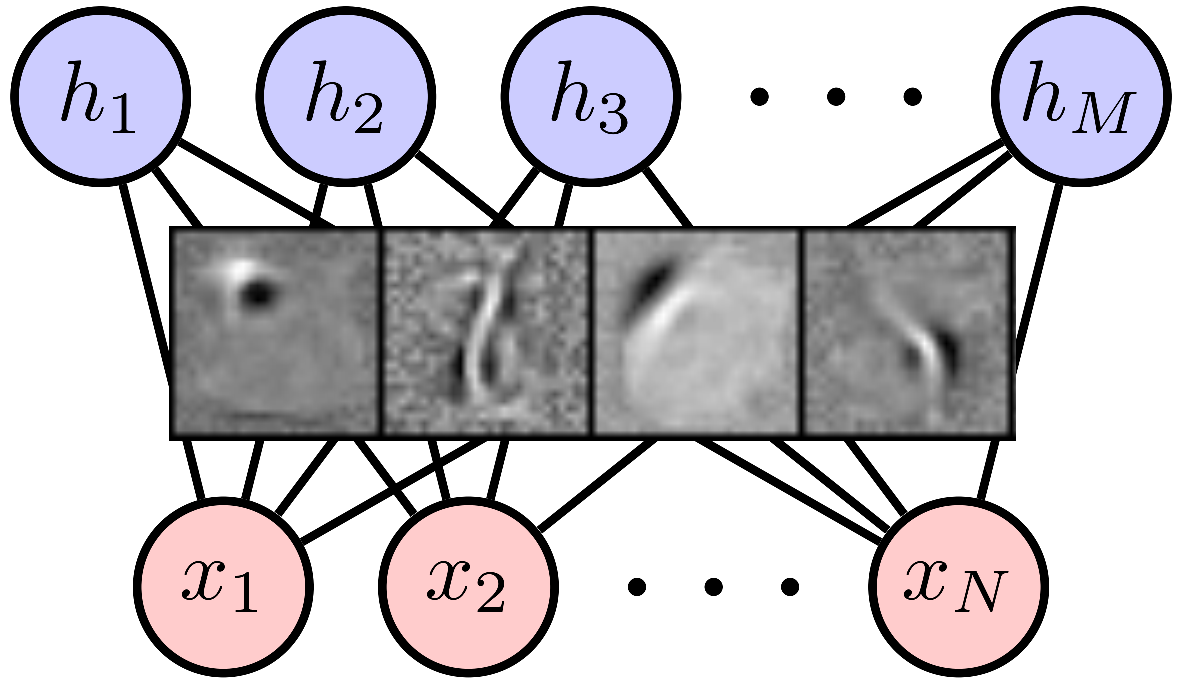


$$\nabla \mathscr{L} = \langle \nabla E \rangle_{\boldsymbol{x} \sim \mathscr{D}} - \langle \nabla E \rangle_{\boldsymbol{x} \sim p(\boldsymbol{x})}$$

Generative Modeling using Boltzmann Machines

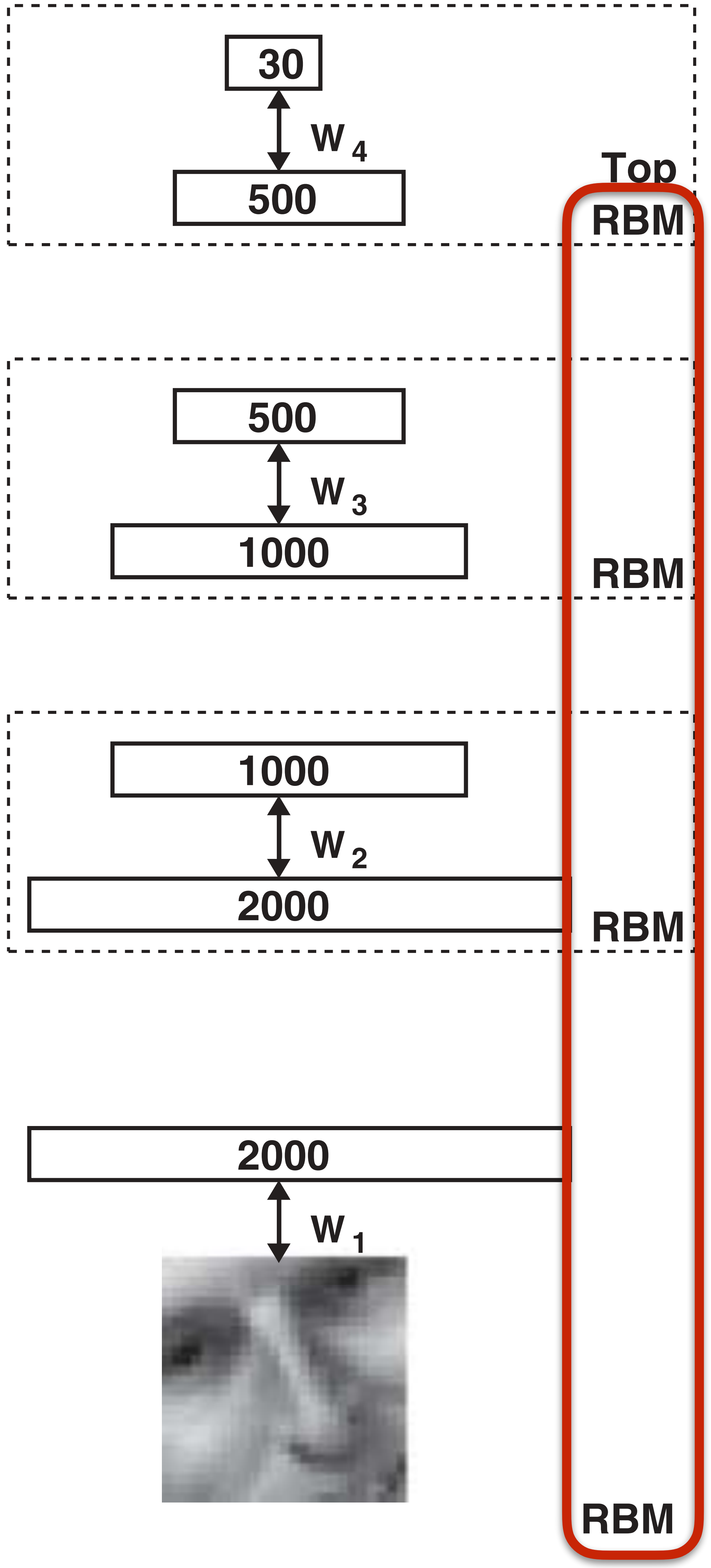
Negative log-likelihood loss $\mathscr{L} = -\frac{1}{|\mathscr{D}|}\sum_{\boldsymbol{x}\in\mathscr{D}} \ln p(\boldsymbol{x}) = \langle E(\boldsymbol{x})\rangle_{\boldsymbol{x}\sim\mathscr{D}} + \ln Z$

Learn



Generate

$$\nabla\mathscr{L} = \langle \nabla E\rangle_{\boldsymbol{x}\sim\mathscr{D}} - \langle \nabla E\rangle_{\boldsymbol{x}\sim p(\boldsymbol{x})}$$



Pretraining

Reducing the Dimensionality of Data with Neural Networks

G. E. Hinton* and R. R. Salakhutdinov

High-dimensional data can be converted to low-dimensional codes by training a multilayer neural network with a small central layer to reconstruct high-dimensional input vectors. Gradient descent can be used for fine-tuning the weights in such "autoencoder" networks, but this works well only if the initial weights are close to a good solution. We describe an effective way of initializing the weights that allows deep autoencoder networks to learn low-dimensional codes that work much better than principal components analysis as a tool to reduce the dimensionality of data.

Dimensionality reduction facilitates the classification, visualization, communication, and storage of high-dimensional data. A simple and widely used method is principal components analysis (PCA), which finds the directions of greatest variance in the data set and represents each data point by its coordinates along each of these directions. We describe a nonlinear generalization of PCA that uses an adaptive, multilayer "encoder" network

2006 VOL 313 SCIENCE www.sciencemag.org

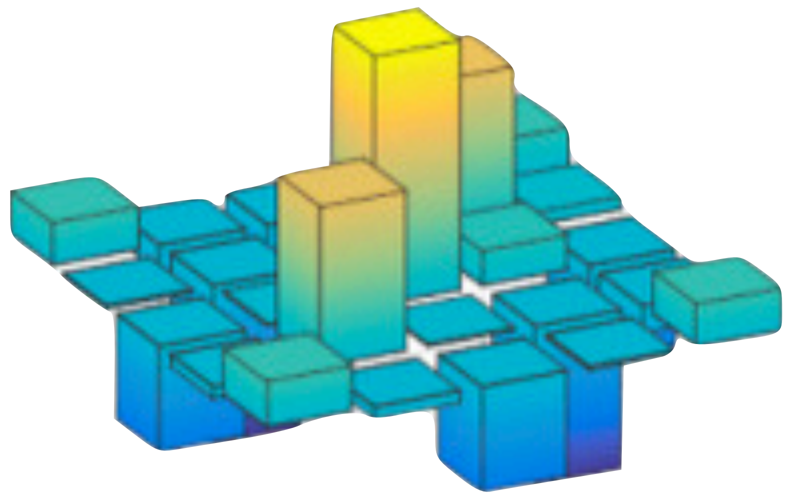
Renaissance of deep learning

Feedback to Physics

$$\Psi$$

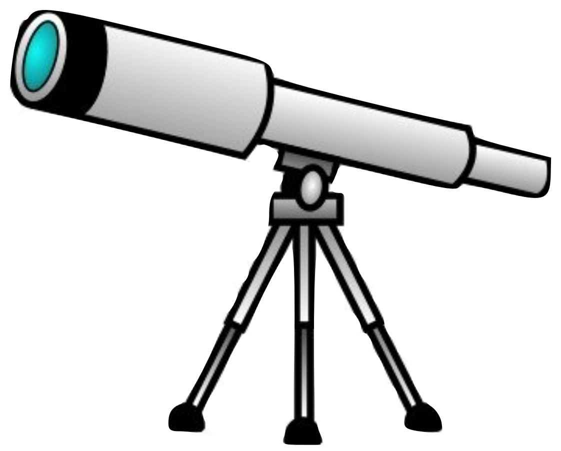
Wavefunctions ansatz

Carleo, Troyer…



Quantum tomography

Torlai, Melko, Carrasquilla…



Renormalization group

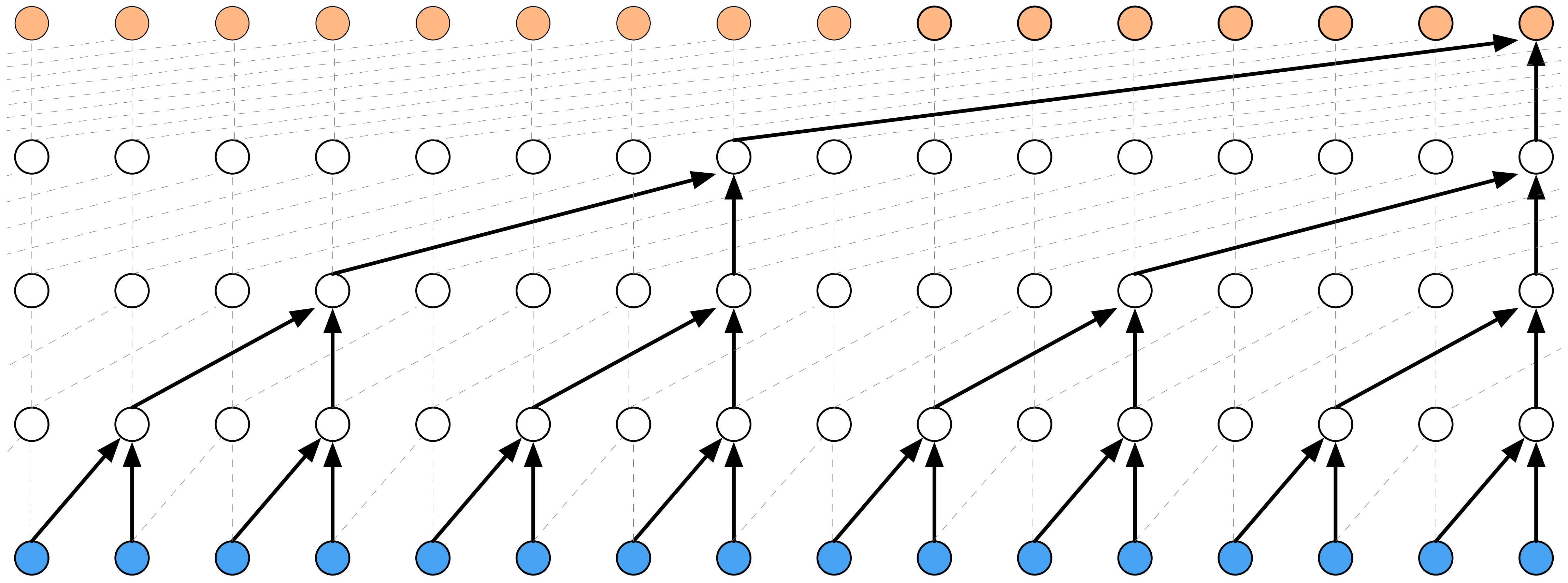
Beny, Metha, Schwab, …

Monte Carlo update

Huang, Liu, …

State-of-the-Art: Autoregressive Models

$$p(\boldsymbol{x}) = \prod_i p(x_i \,|\, \boldsymbol{x}_{<i})$$



Speech data

WaveNet 1609.03499,1711.10433

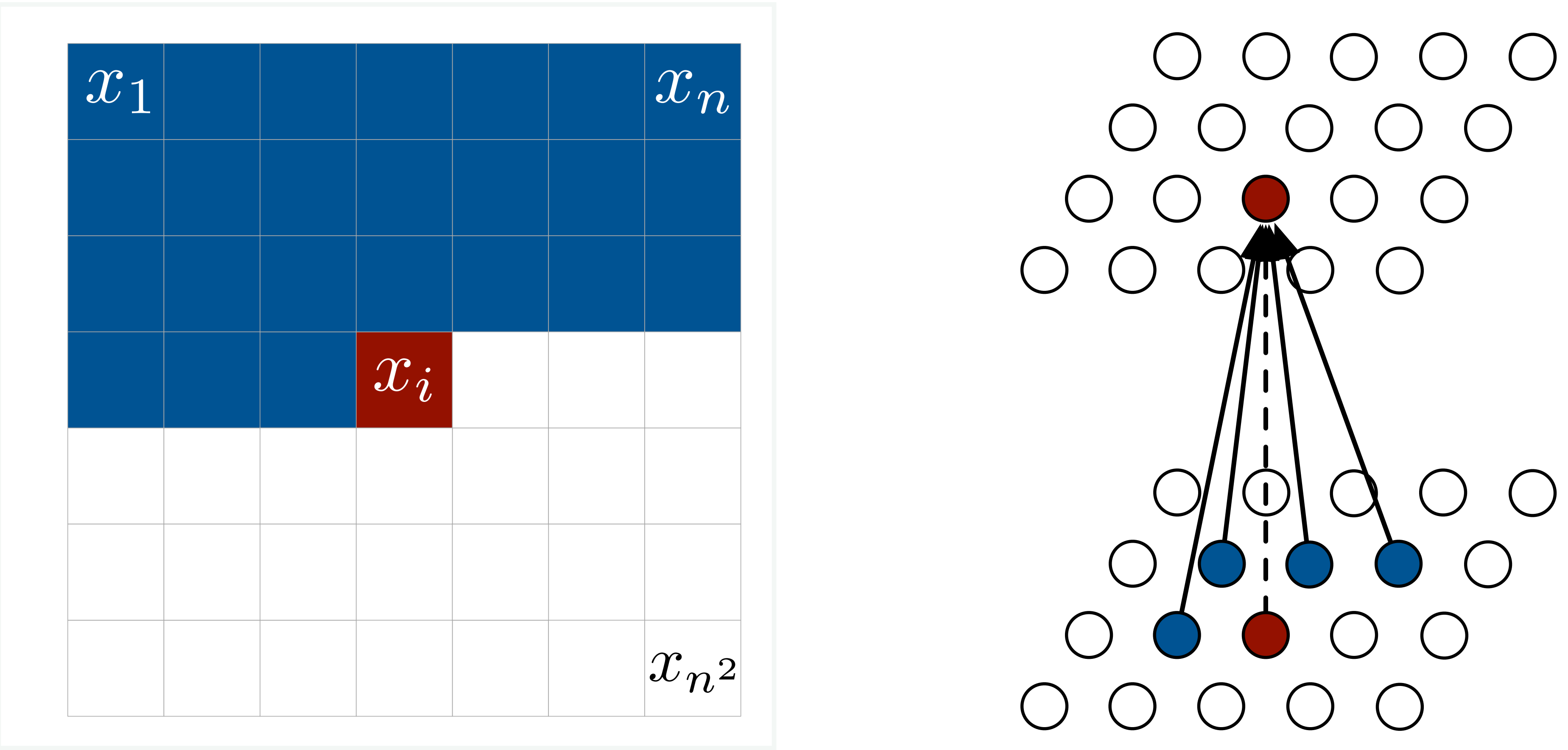
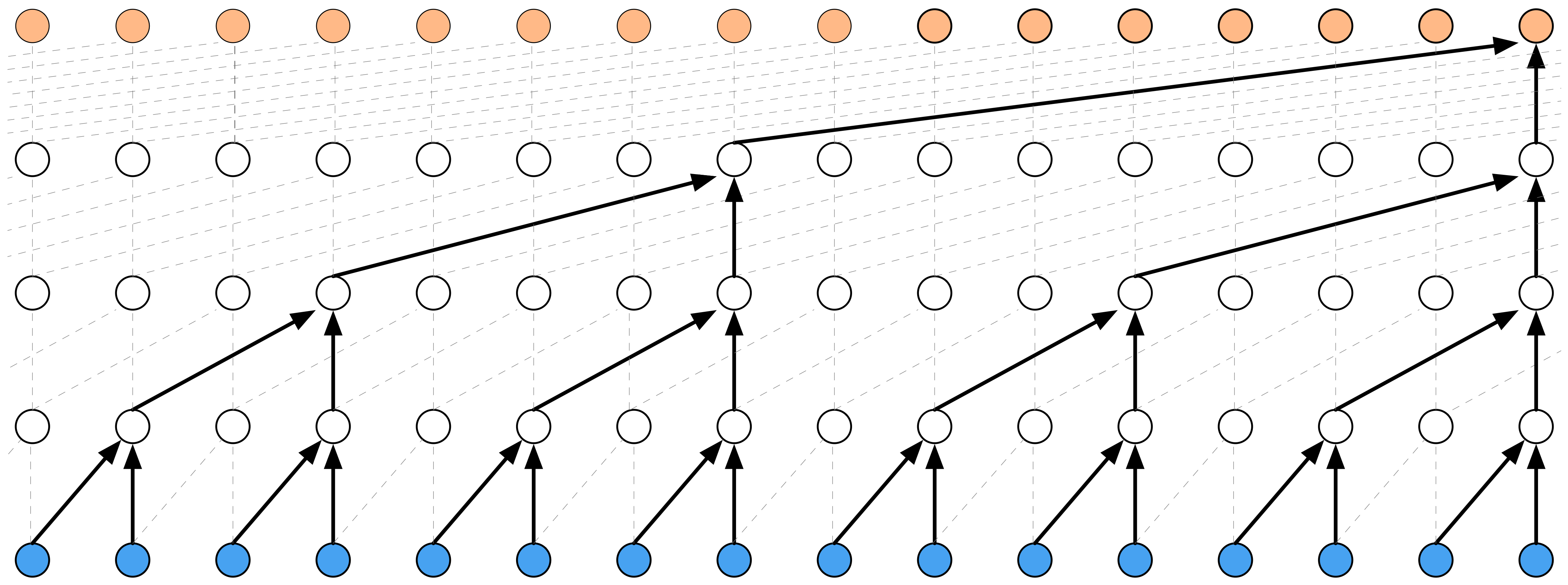


Image data

PixelCNN 1601.06759, 1606.05328

State-of-the-Art: Autoregressive Models

$$p(\boldsymbol{x}) = \prod_i p(x_i \mid \boldsymbol{x}_{<i})$$
$$= p(x_1)p(x_2 \mid x_1)p(x_3 \mid x_1, x_2)\cdots$$



Speech data

WaveNet 1609.03499,1711.10433

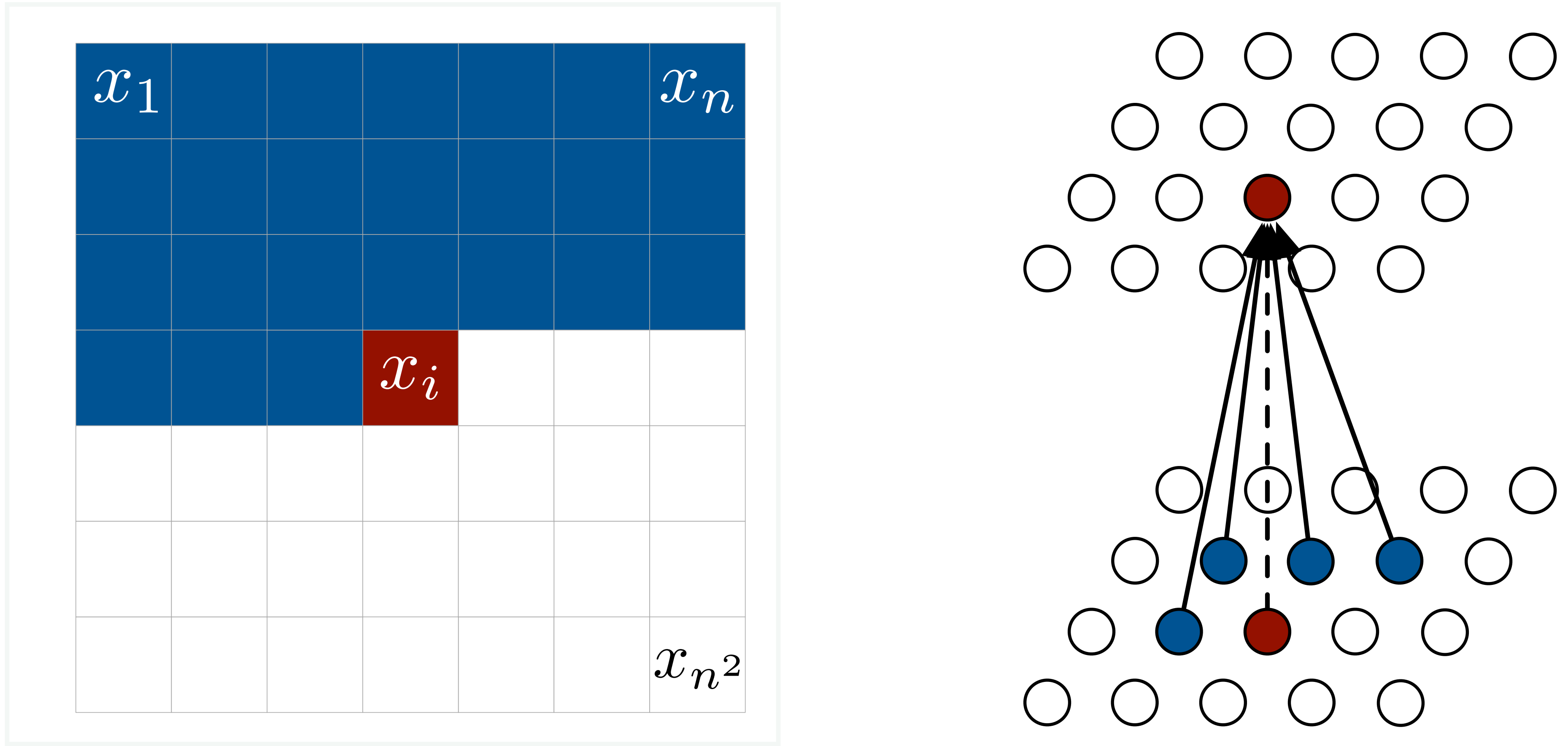


Image data

PixelCNN 1601.06759, 1606.05328

WaveNet in the Real World

2018 Google I/O

https://deepmind.com/blog/wavenet-generative-model-raw-audio/
https://deepmind.com/blog/high-fidelity-speech-synthesis-wavenet/
https://deepmind.com/blog/wavenet-launches-google-assistant/

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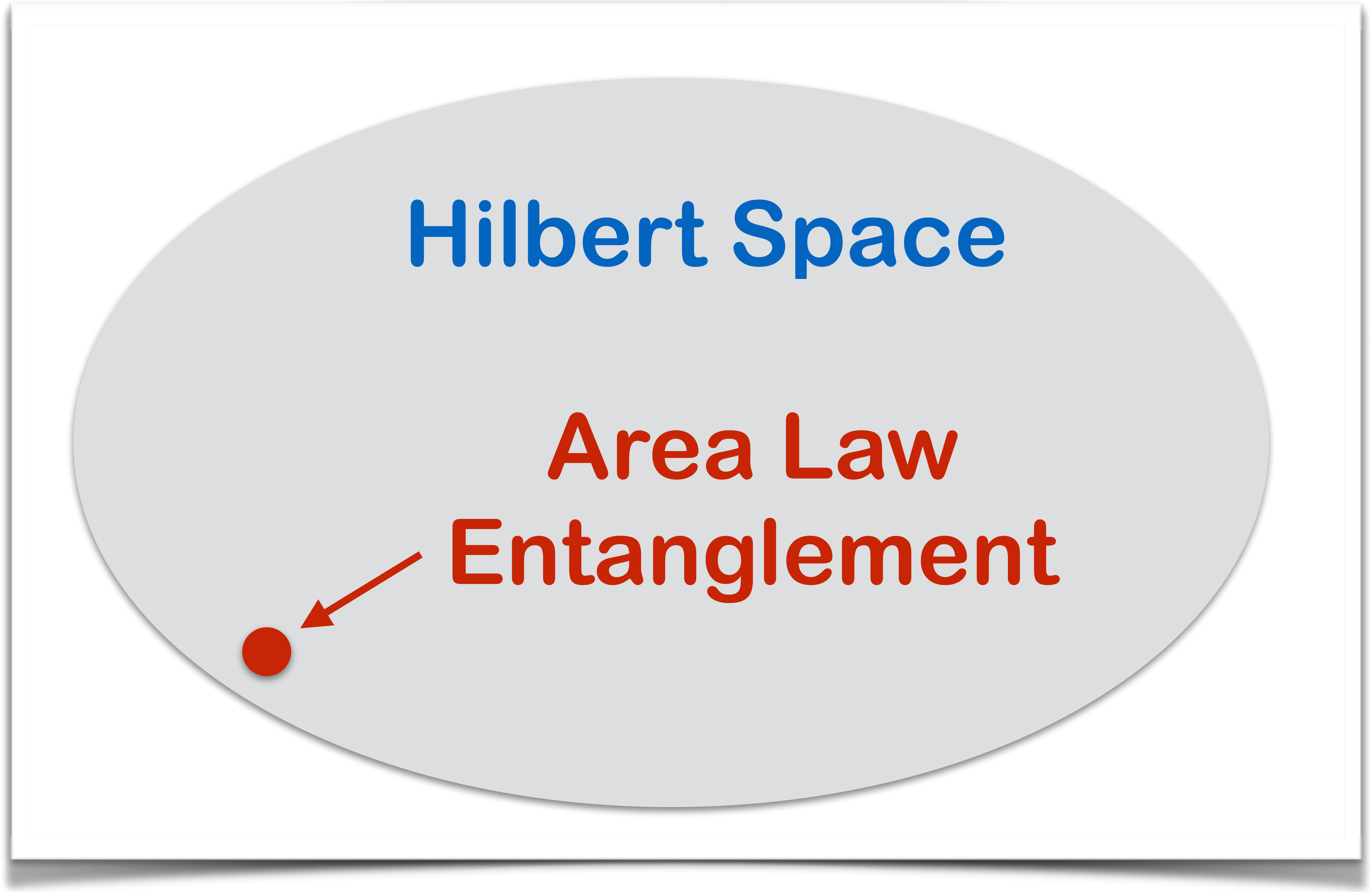
Born Machines

$$p(\boldsymbol{x}) = \frac{|\Psi(\boldsymbol{x})|^2}{Z}$$

quantum physics

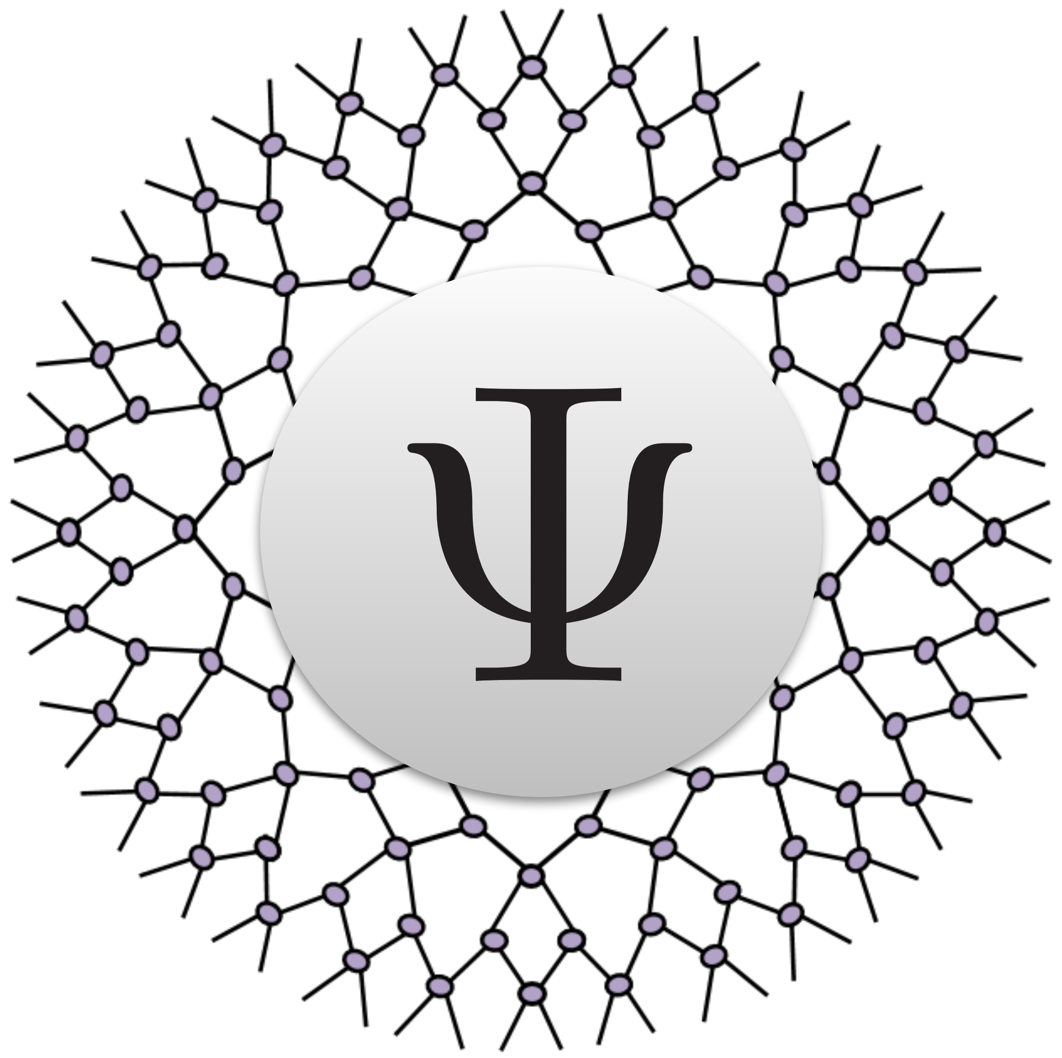


Born Machines

$$p(\boldsymbol{x}) = \frac{|\Psi(\boldsymbol{x})|^2}{Z}$$

quantum physics

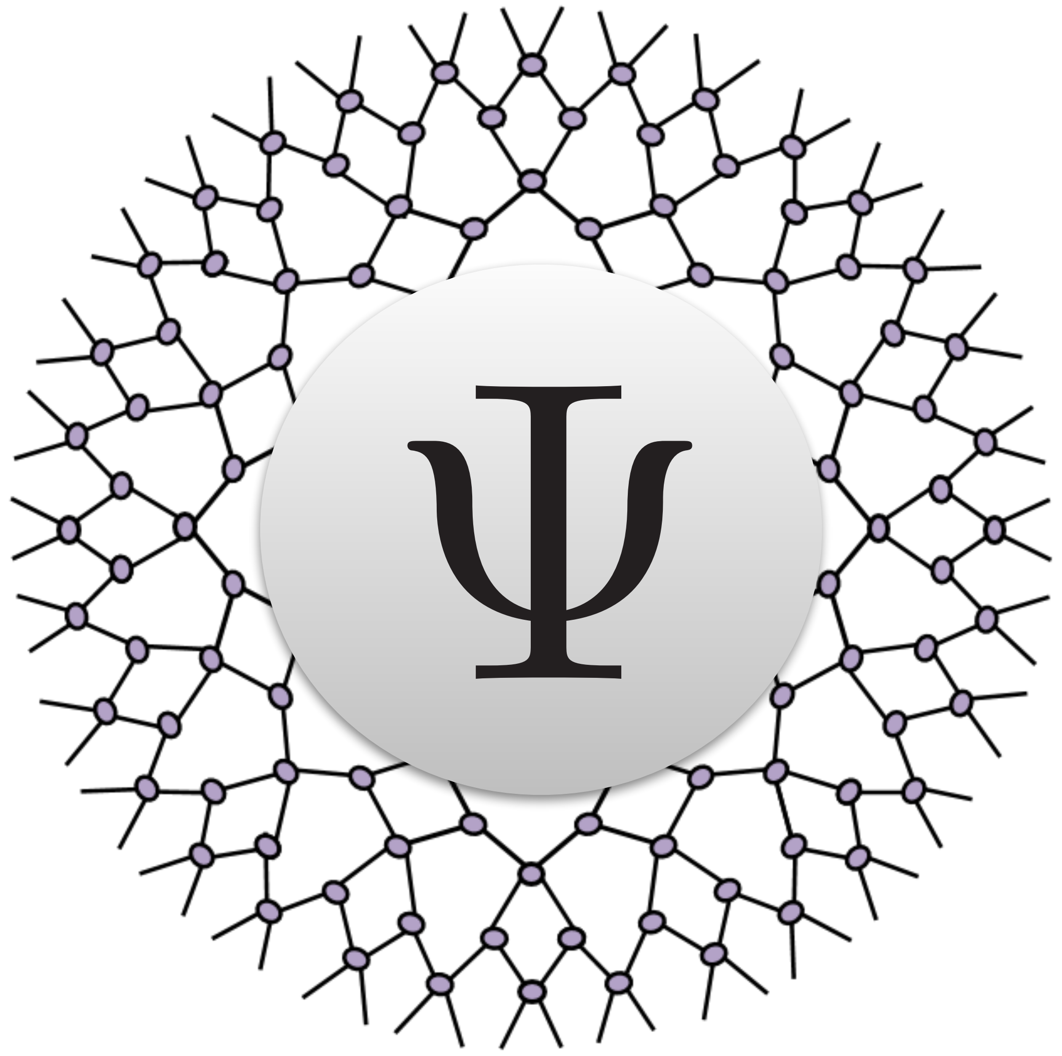
Quantum inspired generative modeling

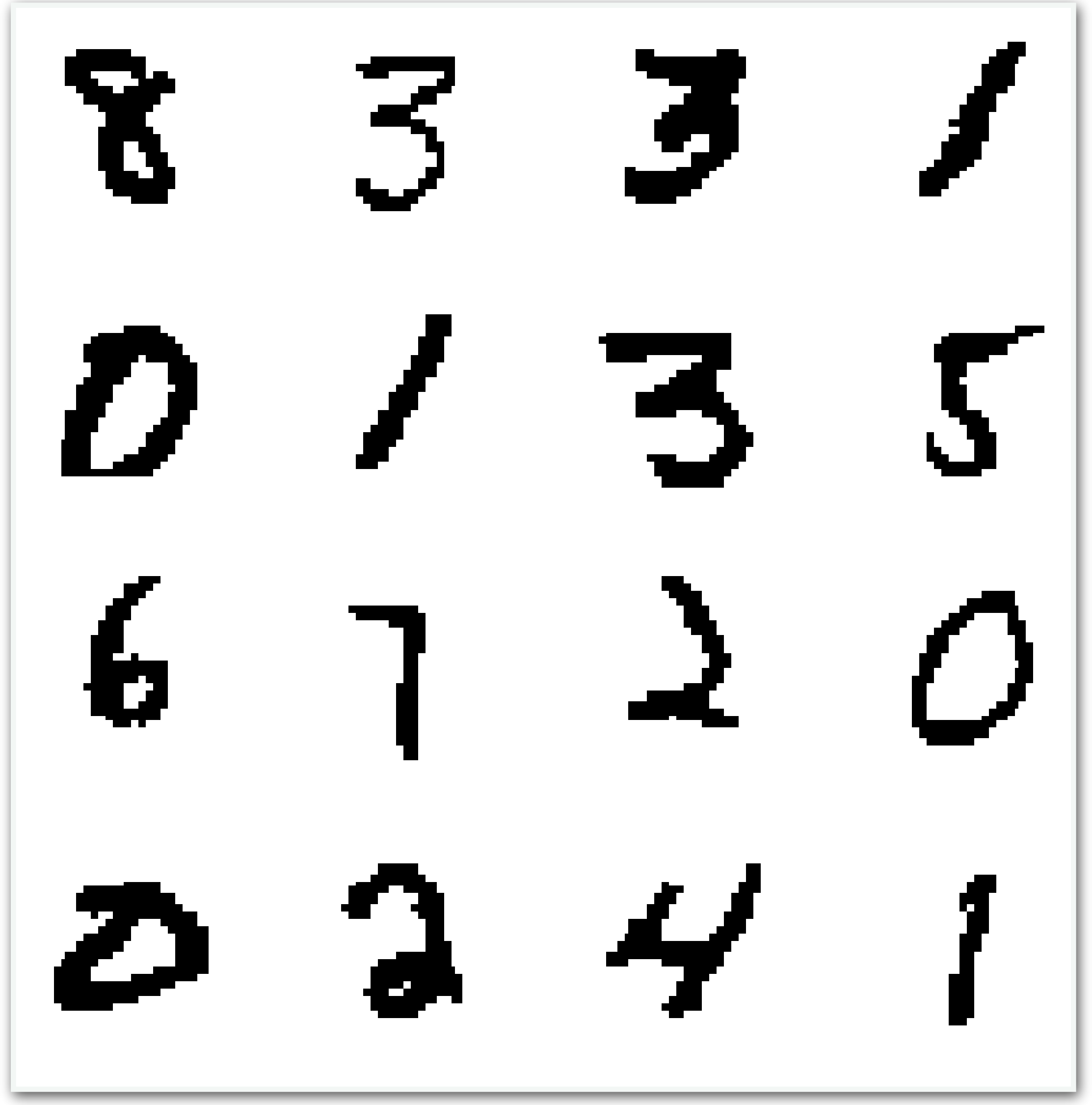


With Han, Wang, Fan, Zhang, 1709.01662, PRX '18

Quantum inspired generative modeling

Learn





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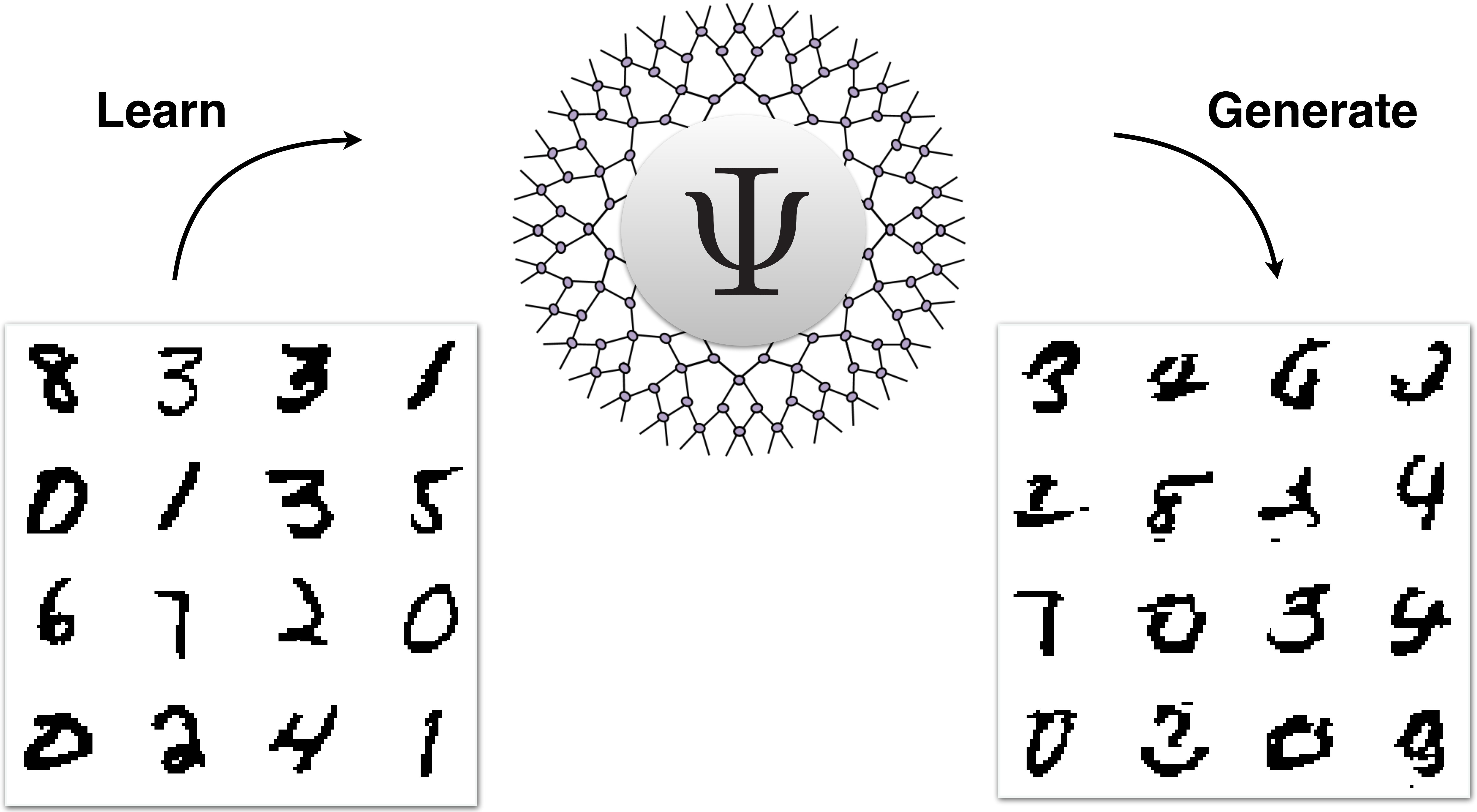
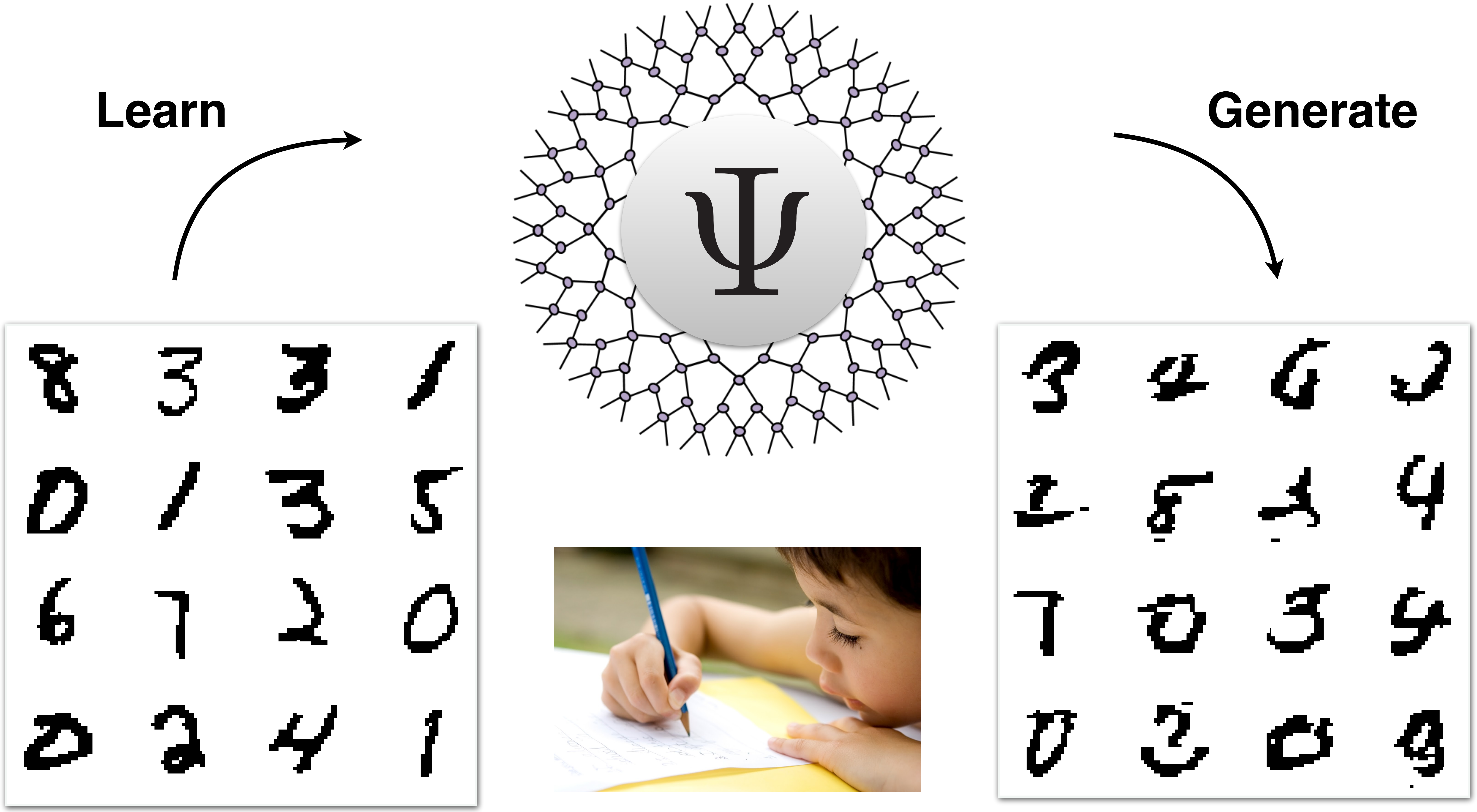


With Han, Wang, Fan, Zhang, 1709.01662, PRX '18

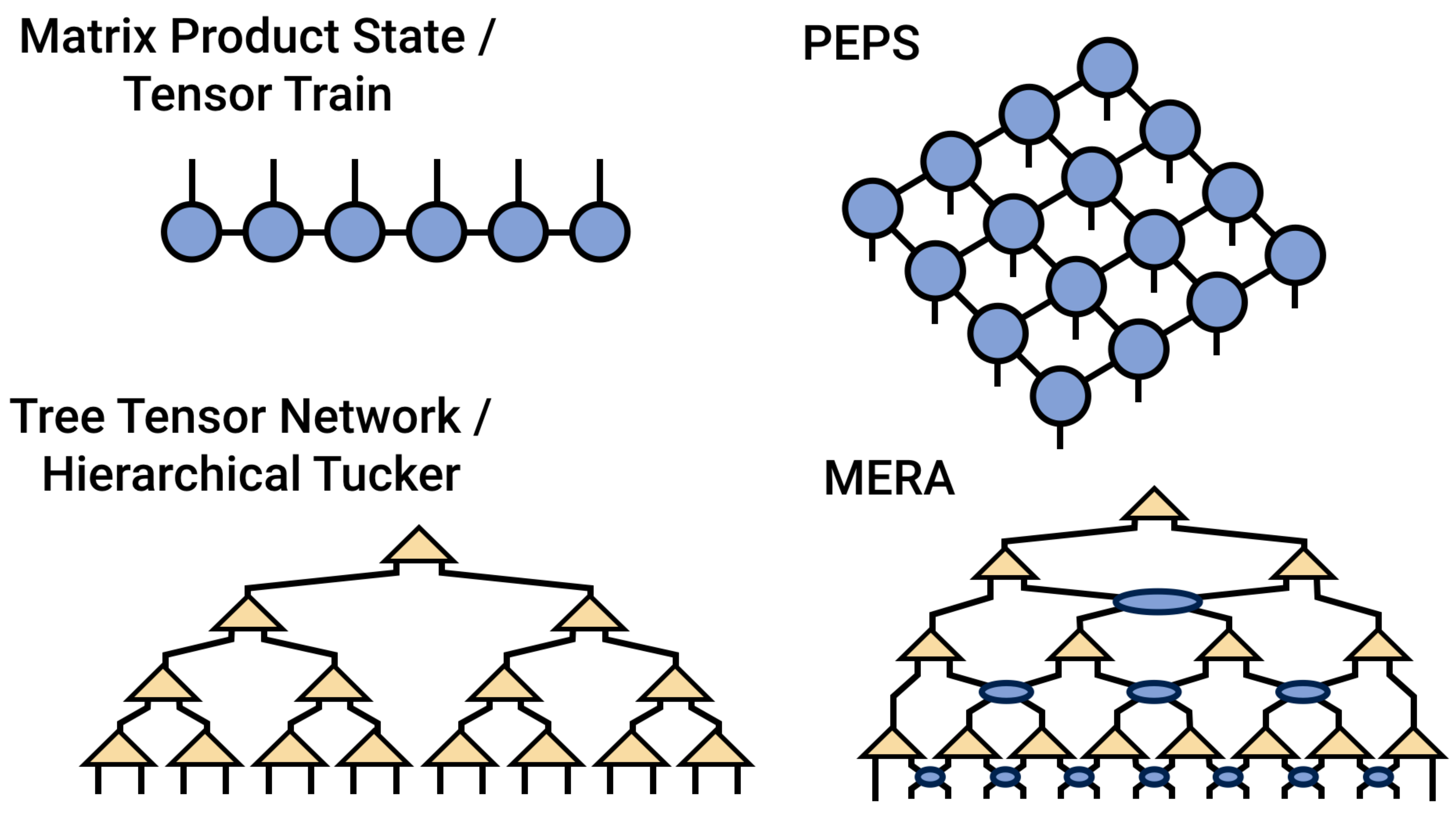
Quantum inspired generative modeling



"Teach a quantum state to write digits"

With Han, Wang, Fan, Zhang, 1709.01662, PRX '18

Generative modeling using Tensor Network States

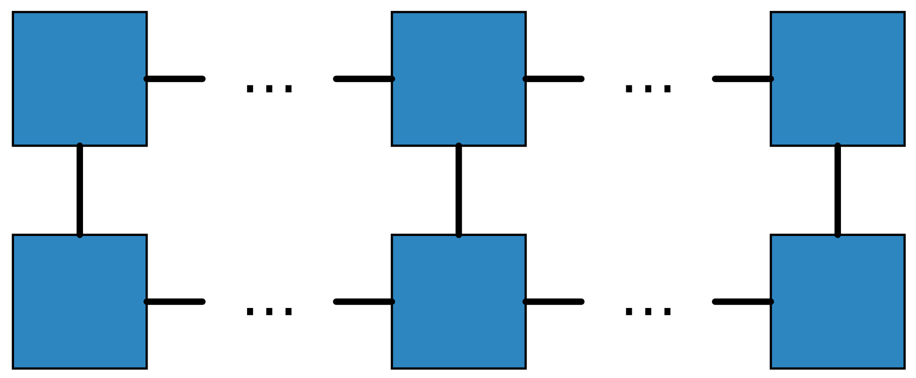


Tensor Network Machine Learning

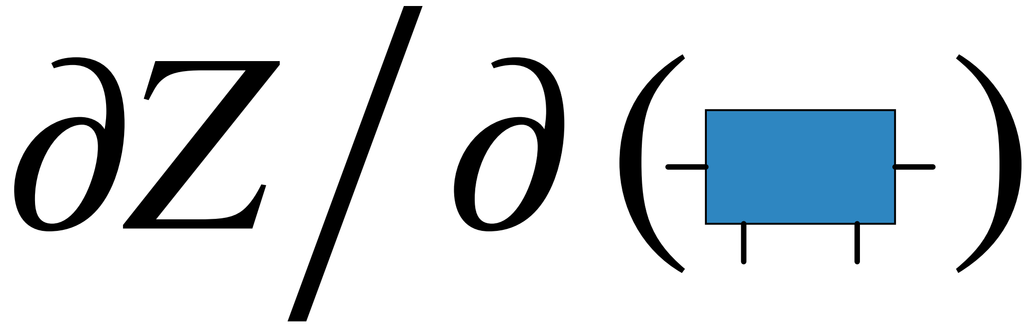
Cichocki et al 1604.05271,1609.00893,1708.09165…
Stoudenmire, Schwab NIPS 2016
Stoudenmire Q. Sci. Tech. 2018
Liu et al 1710.04833
Liu et al 1803.09111
Novikov et al 1509.06569
Hallam et al 1711.03357
Glasser et al 1806.05964
Kossaifi et al 1707.08308
Gallego, Orus 1708.01525
Pestun et al 1711.01416…

Nice features of MPS Born Machines

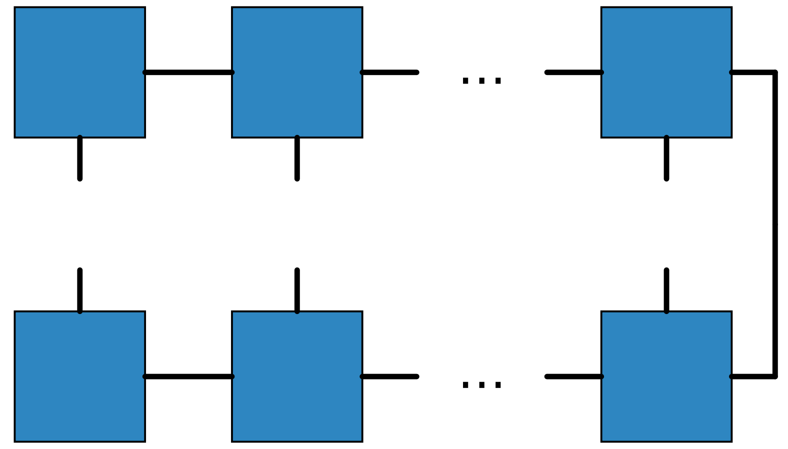
Han, Wang, Fan, LW, Zhang, 1709.01662, PRX ‘18

$Z =$ 

Tractable partition function via MPS contraction



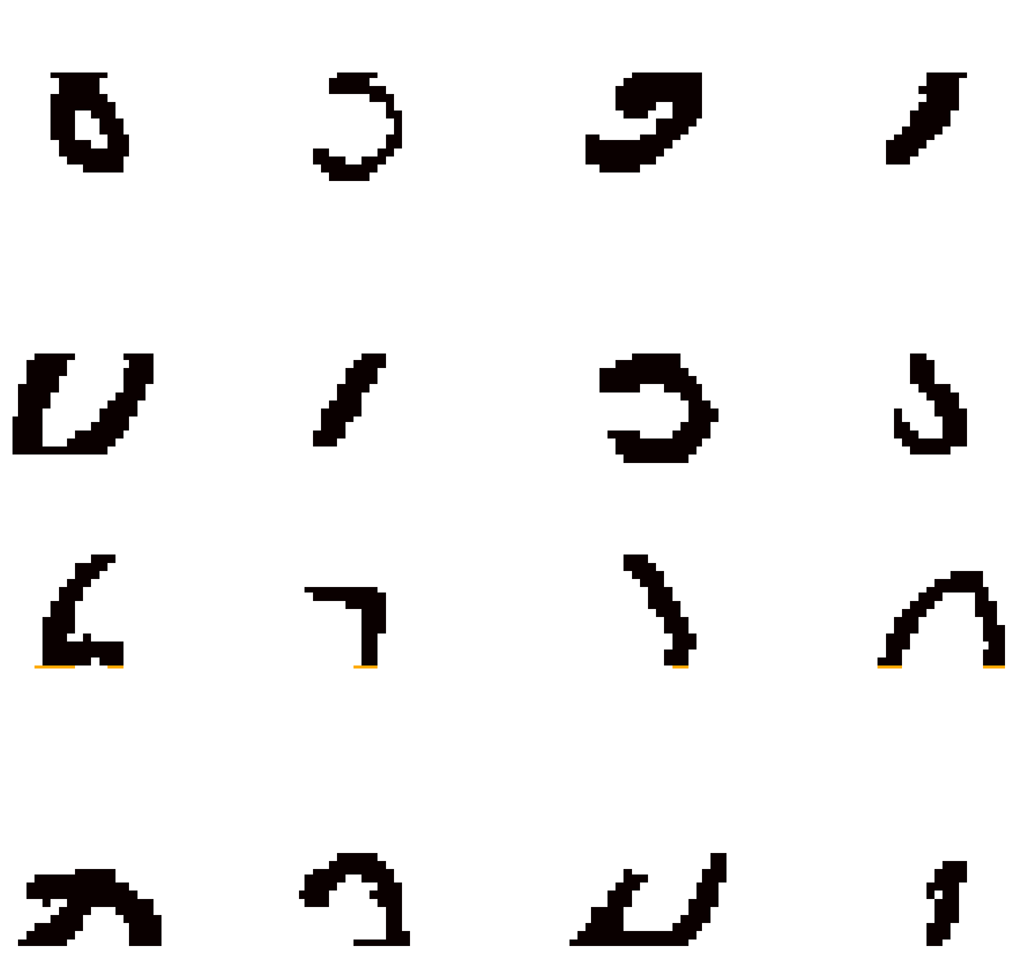
Efficient and adaptive learning via DMRG

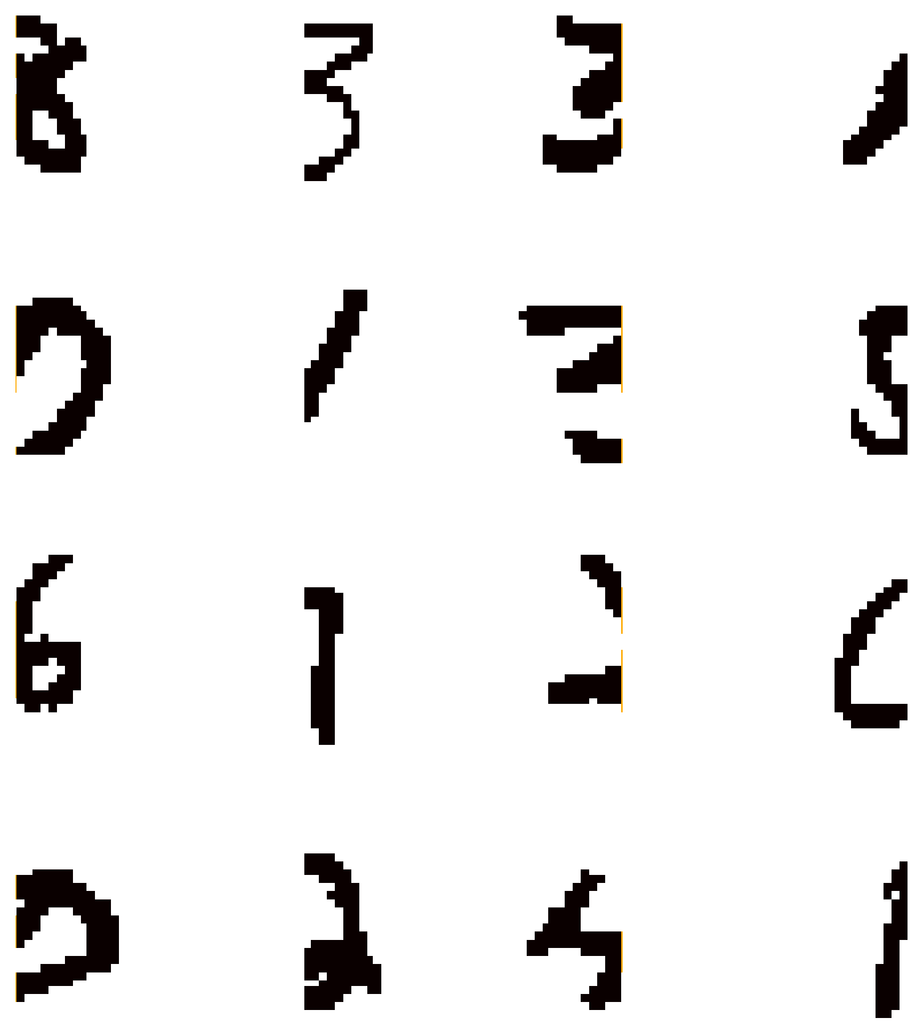


Direct sampling using “Zipper”

Image Restoration

With Han, Wang, Fan, Zhang, 1709.01662, PRX '18





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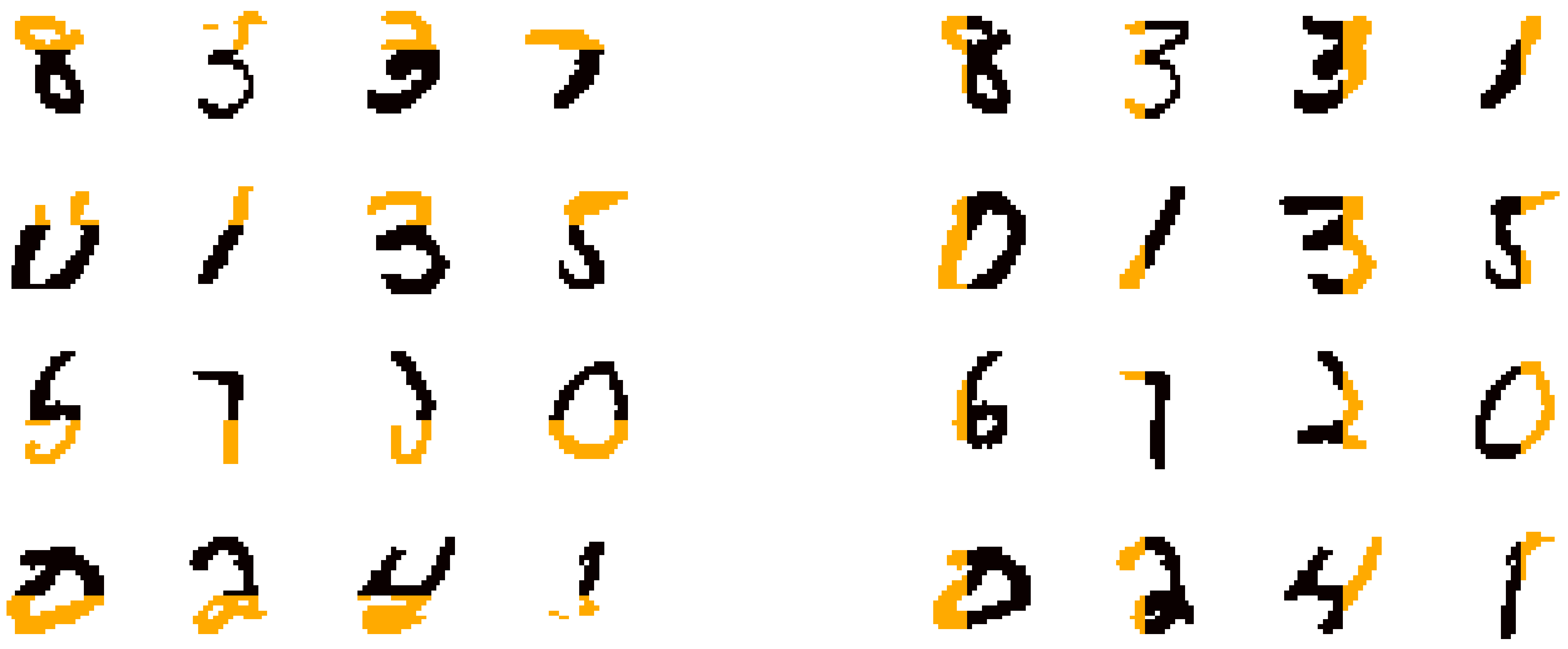
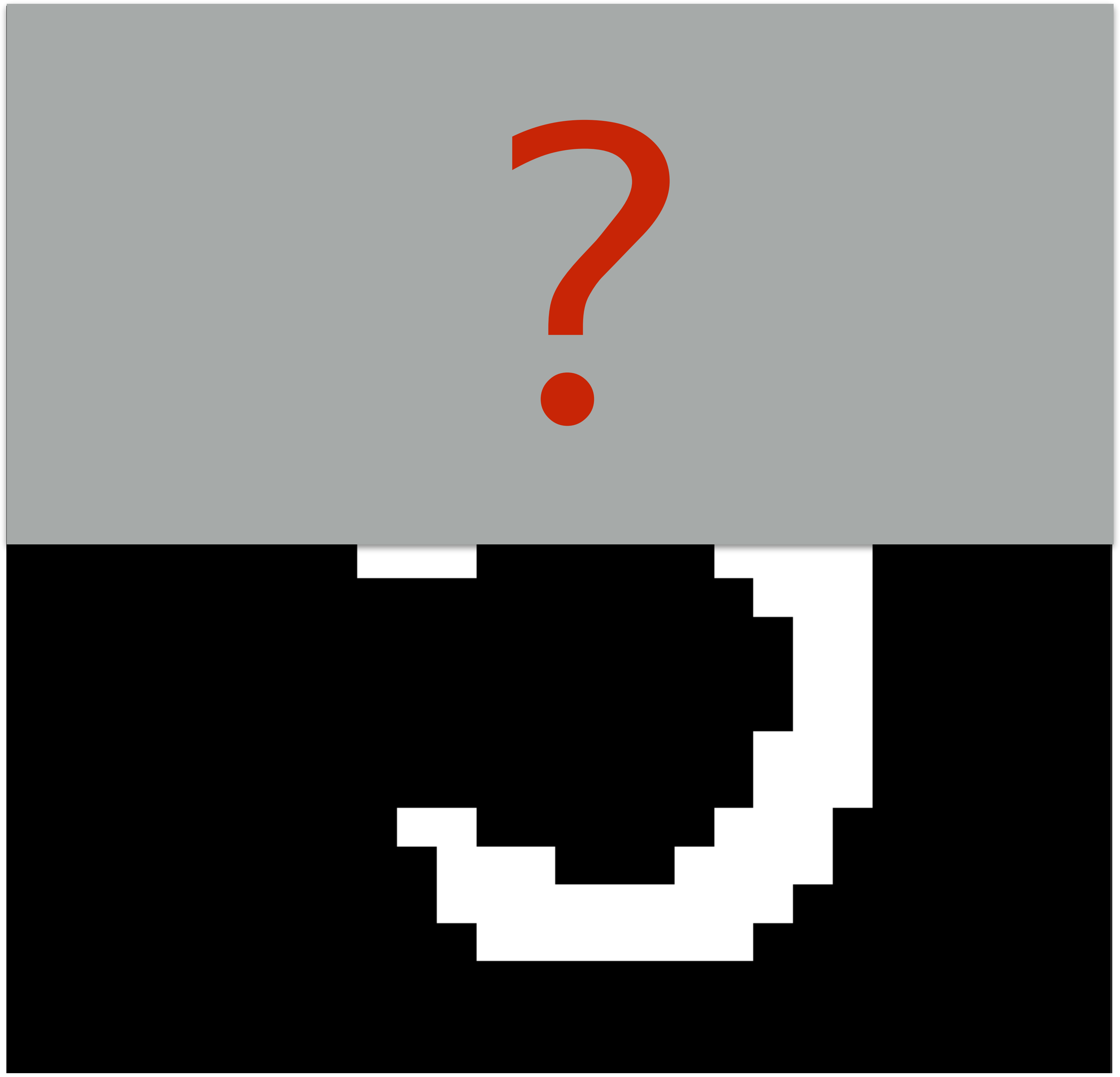


Arbitrary order, in contrast to autoregressive models

PixelCNN

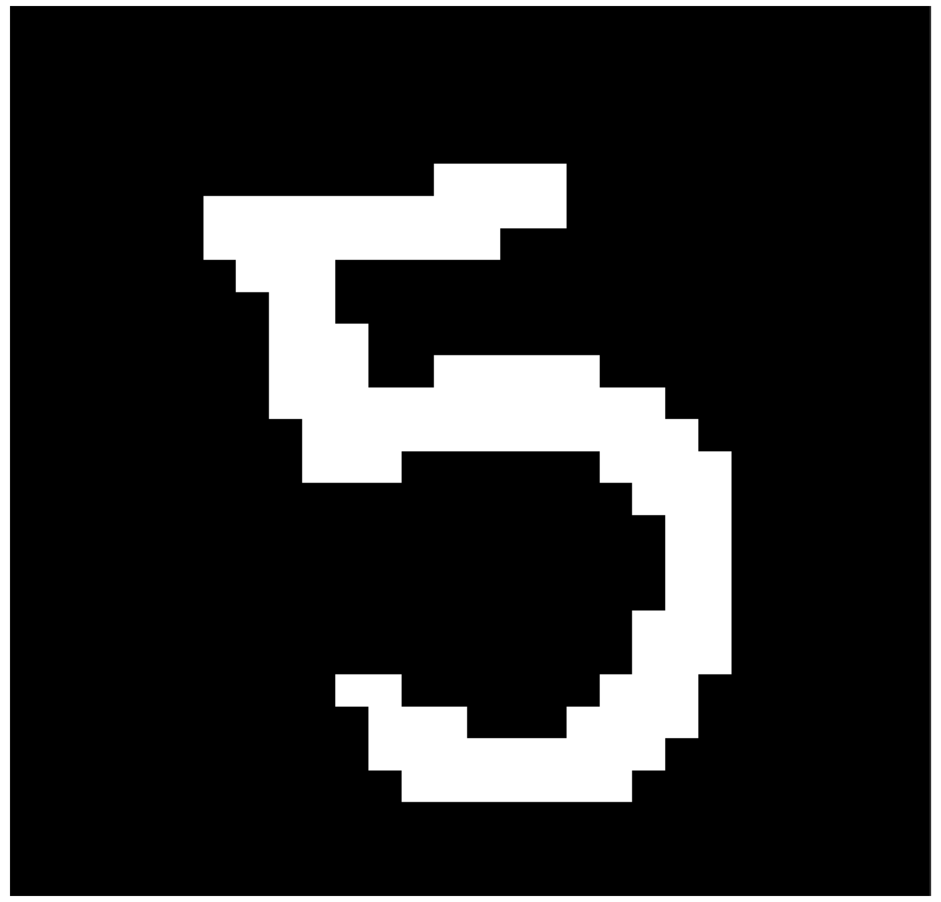
Quantum Perspective on Deep Learning

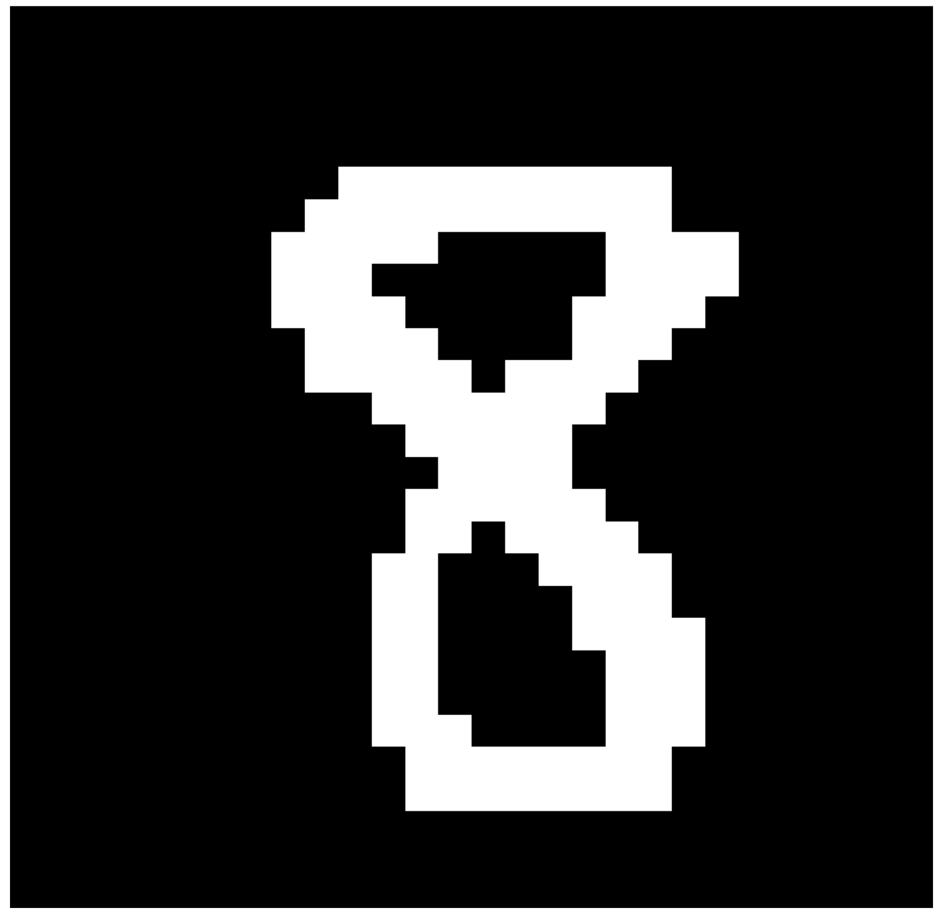


Quantum Perspective on Deep Learning

Q: How to quantify our inductive biases ?

A: Information pattern of probability distributions





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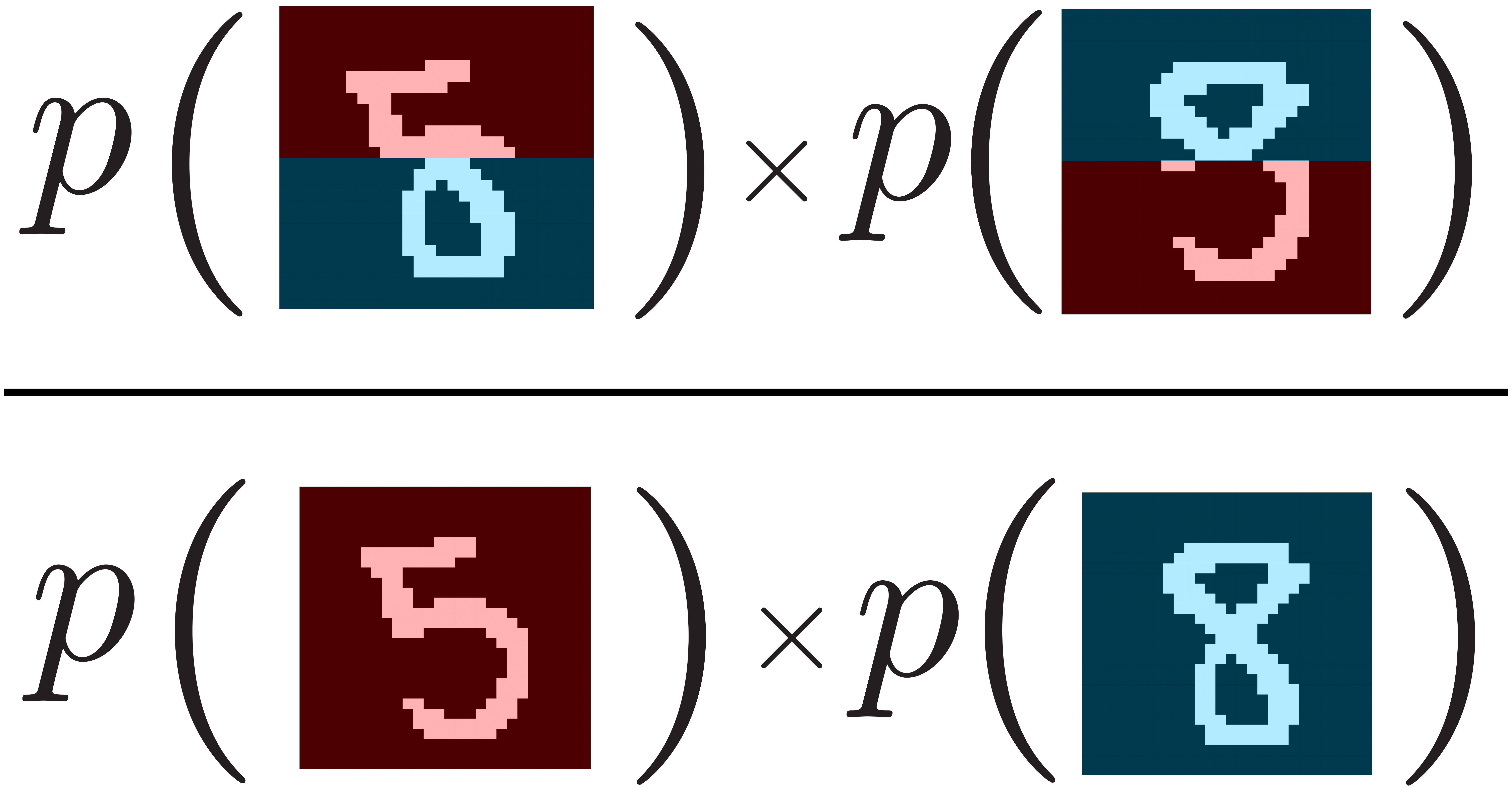


Quantum Perspective on Deep Learning

Classical mutual information

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

Quantum Renyi entanglement entropy

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

Striking similarity implies common inductive bias

+Quantitative & interpretable approaches
+Principled structure design & learning

Cheng, Chen, LW,
1712.04144, Entropy '18

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
{yoavlevine,davidyakira,cohennadav,shashua}@cs.huji.ac.il

ABSTRACT

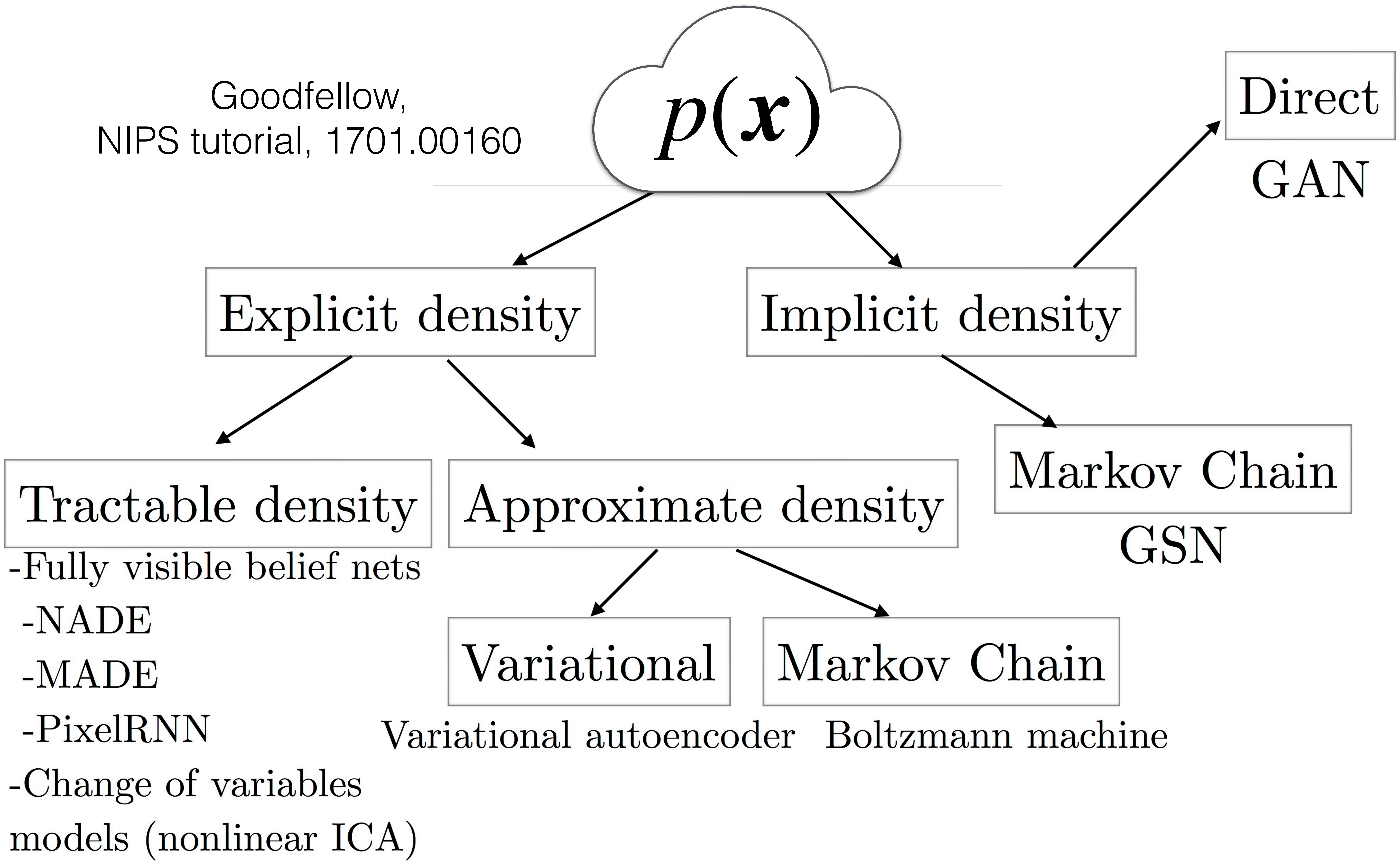
Formal understanding of the inductive bias behind deep convolutional networks, i.e. the relation between the network's architectural features and the functions it is able to model, is limited. In this work, we establish a fundamental connection between the fields of quantum physics and deep learning, and use it for obtaining novel theoretical observations regarding the inductive bias of convolutional networks. Specifically, we show a structural equivalence between the function realized by a convolutional arithmetic circuit (ConvAC) and a quantum many-body wave function, which facilitates the use of quantum entanglement measures as quantifiers of a deep network's expressive ability to model correlations. Furthermore, the construction of a deep ConvAC in terms of a quantum Tensor Network is enabled. This allows us to perform a graph-theoretic analysis of a convolutional network, tying its expressiveness to a min-cut in its underlying graph. We demonstrate a practical outcome in the form of a direct control over the inductive bias via the number of channels (width) of each layer. We empirically validate our findings on standard convolutional networks which involve ReLU activations and max pooling. The description of a deep convolutional network in well-defined graph-theoretic tools and the 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

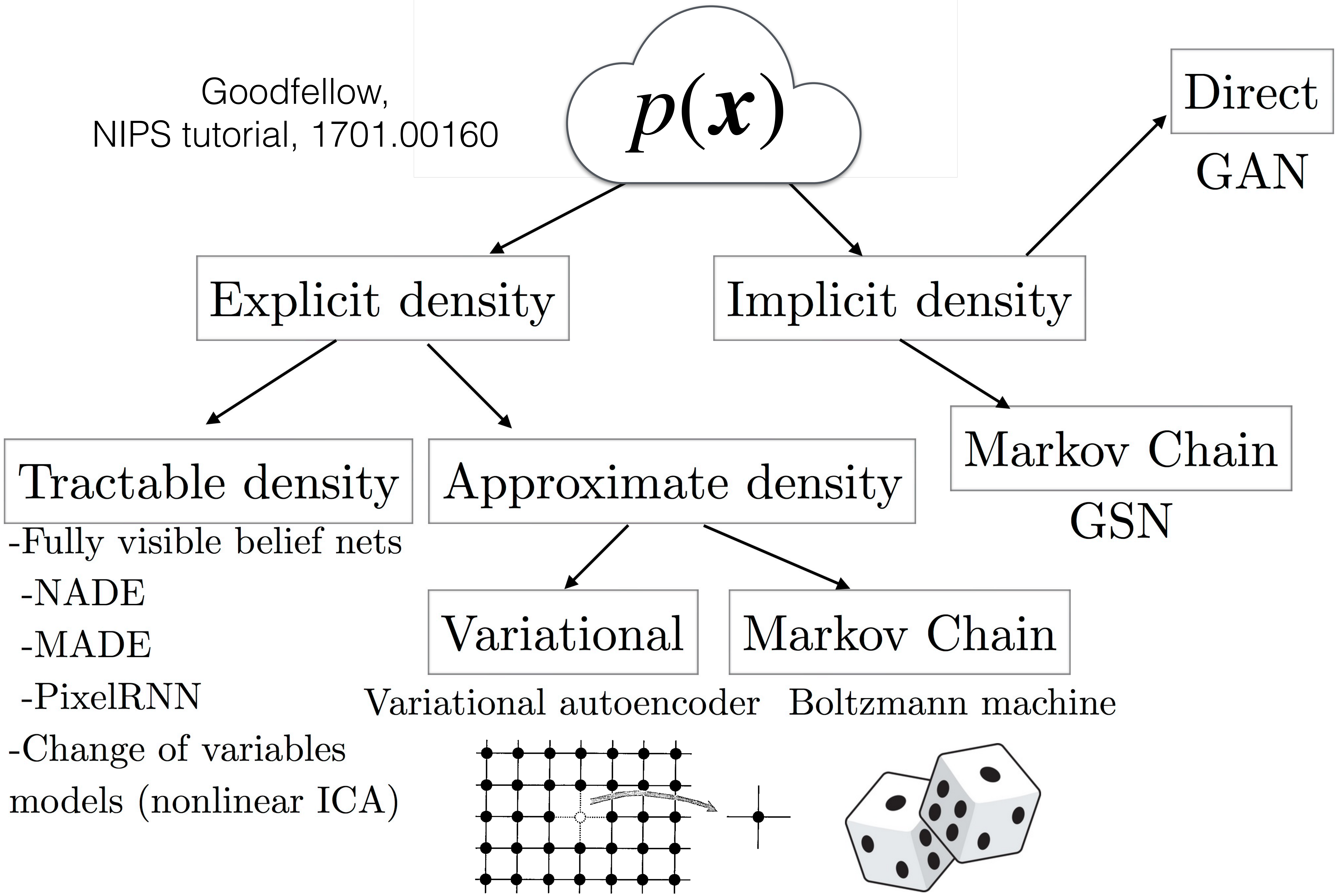
Yoav Levine, David Yakira, Nadav Cohen & Amnon Shashua
The Hebrew University of Jerusalem

Physics genes of generative models

Goodfellow,
NIPS tutorial, 1701.00160



Physics genes of generative models



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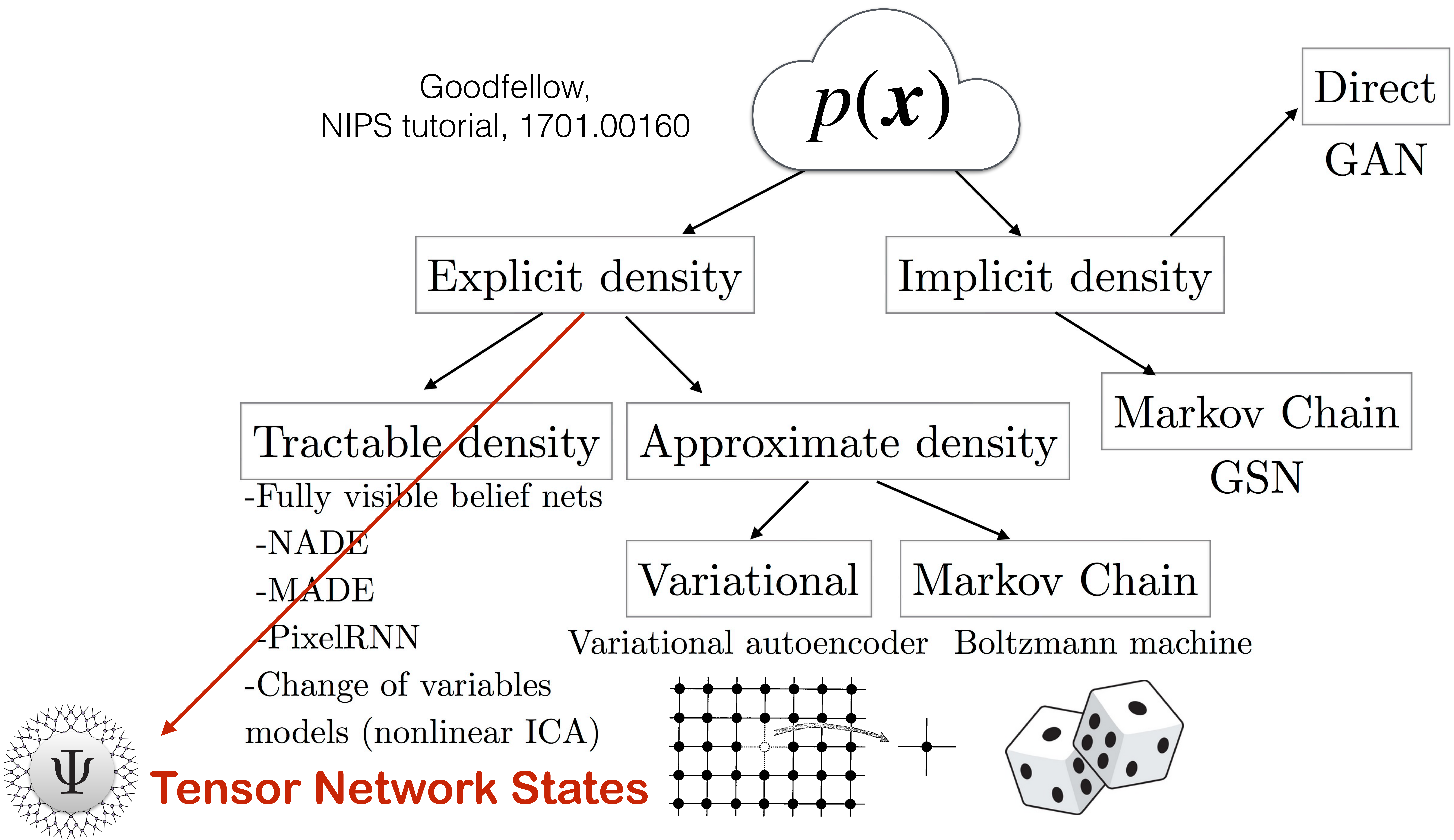
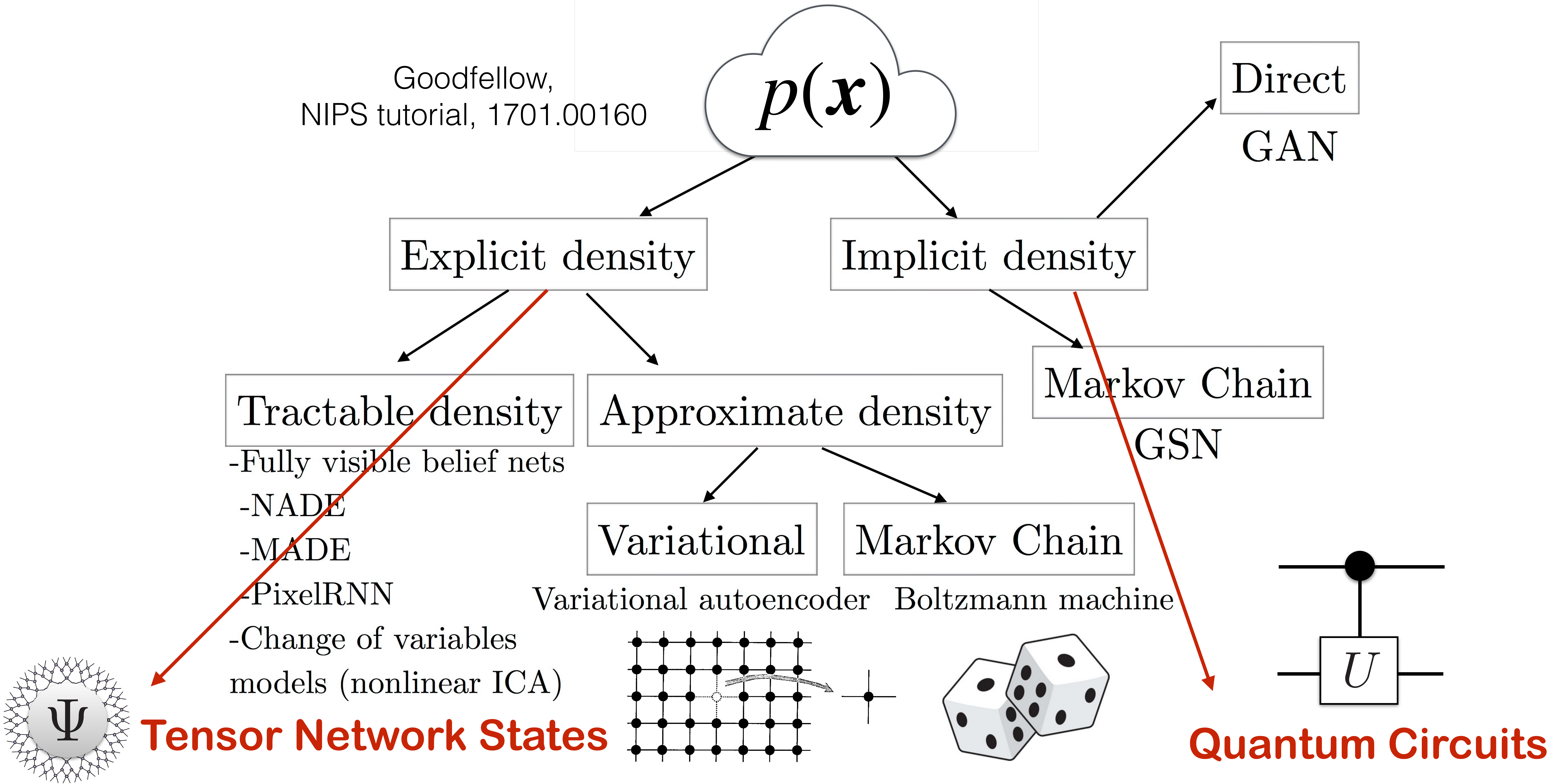
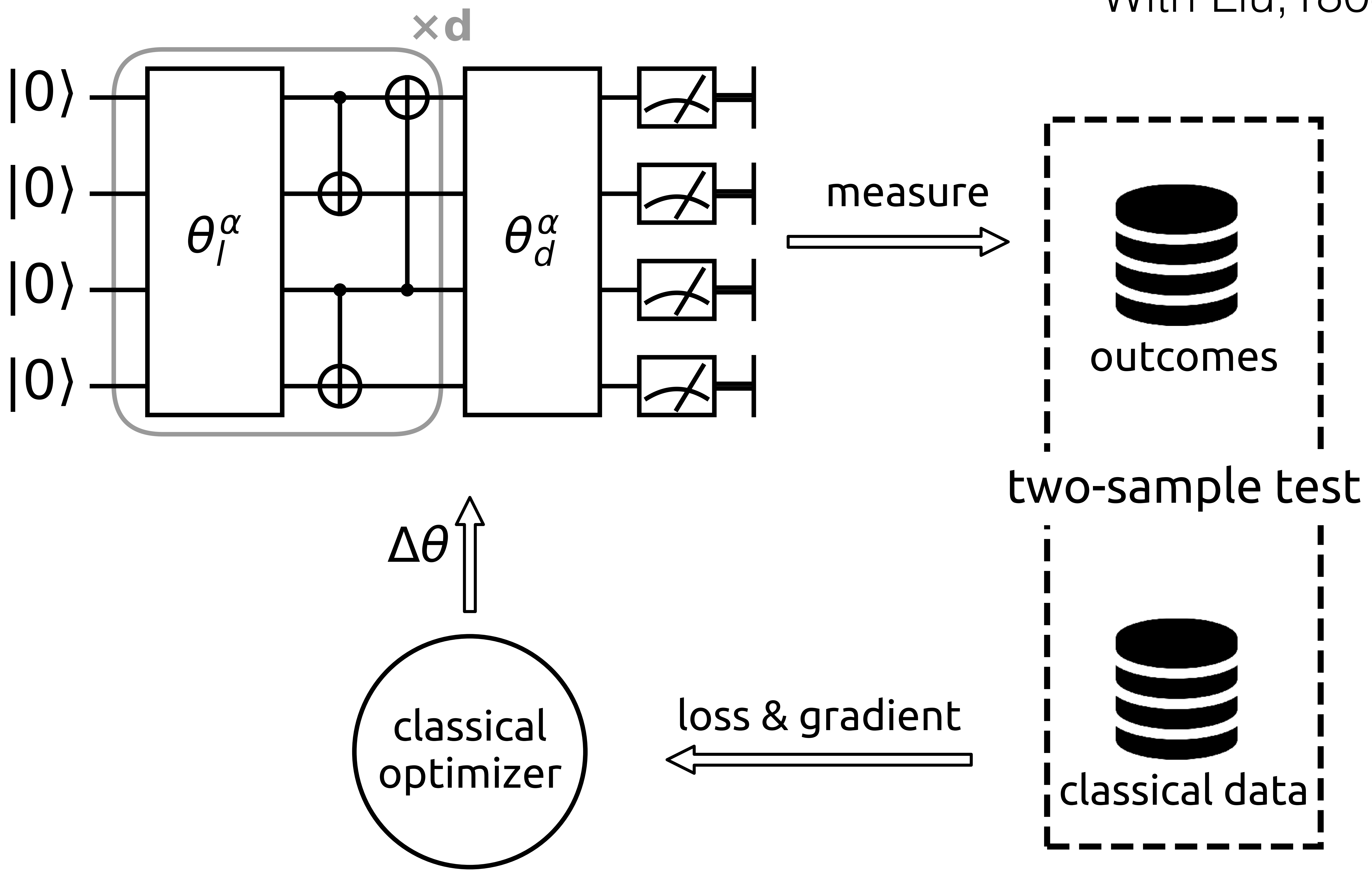


Physics genes of generative models



Quantum Circuit Born Machine

With Liu, 1804.04168, PRA '18

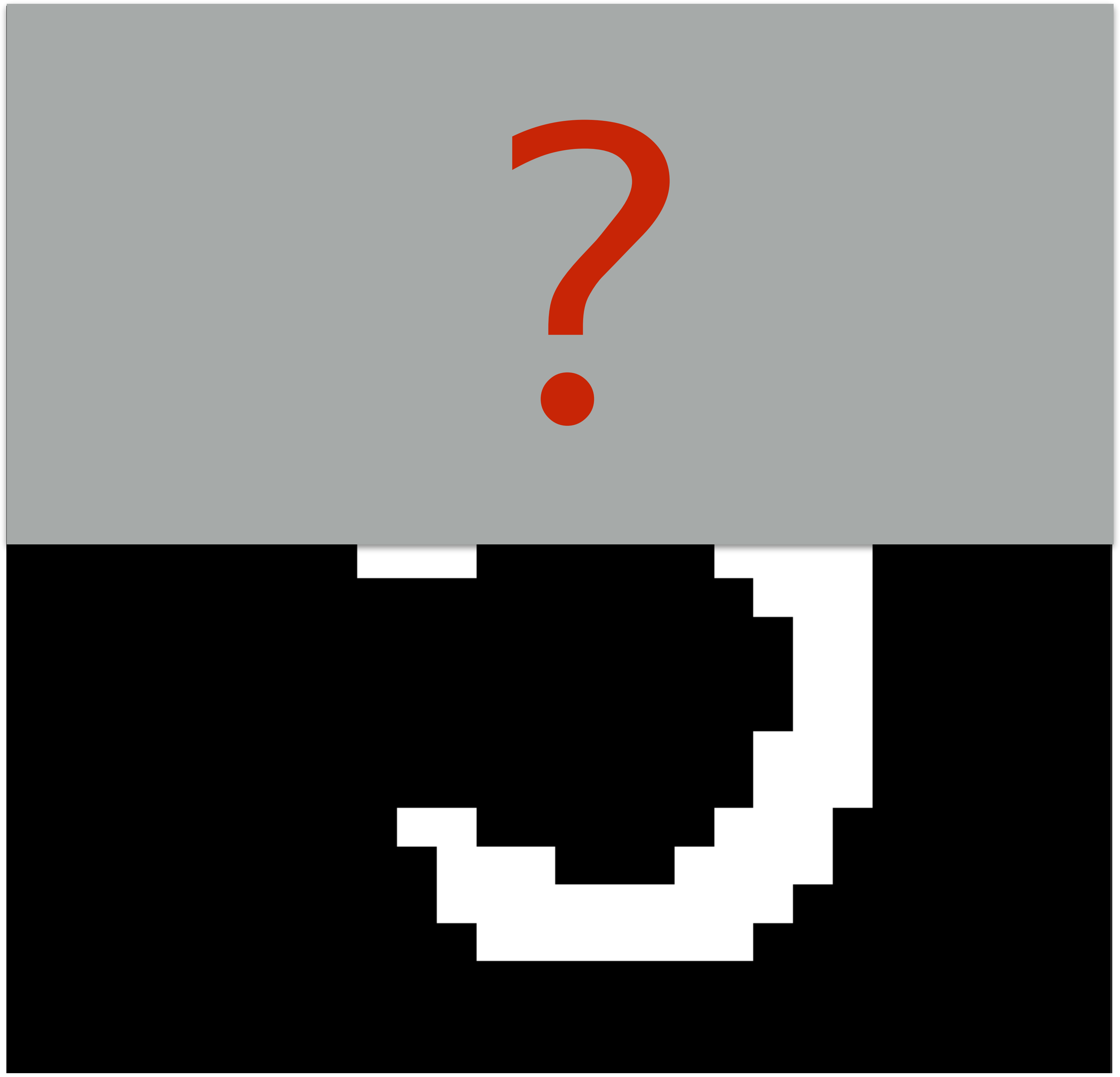


Train the quantum circuit as a probabilistic generative model

Quantum sampling complexity underlines the "quantum supremacy"

Quantum Inference

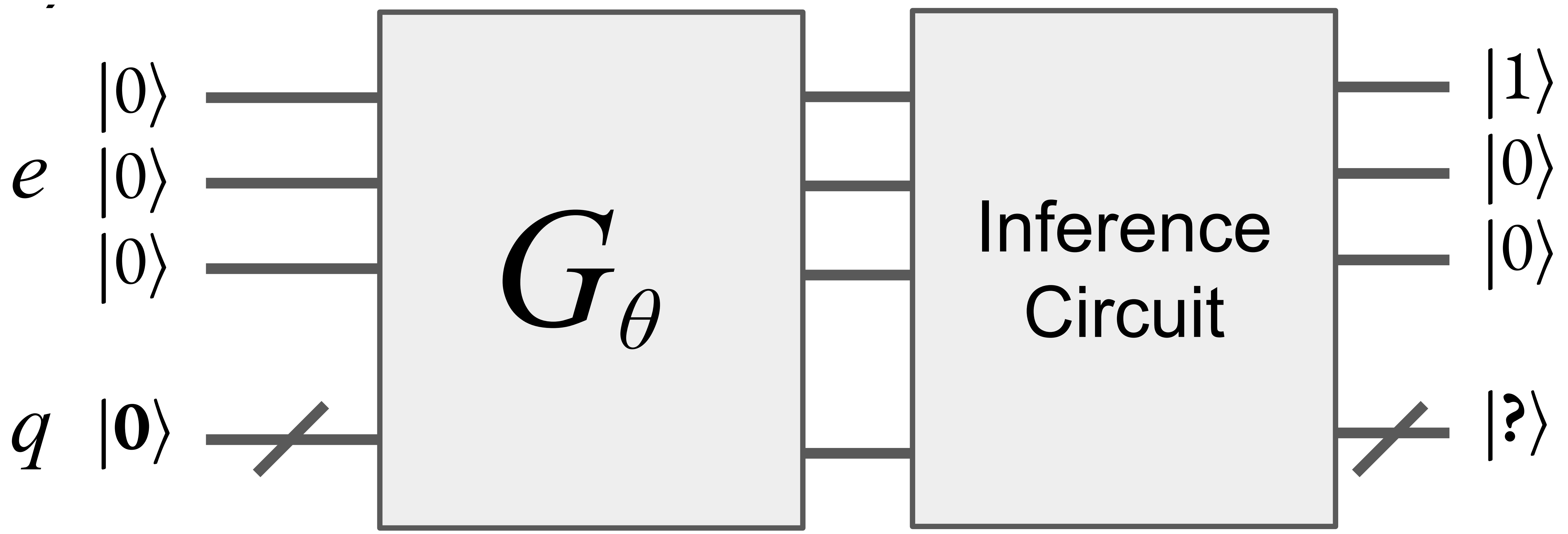
p(upper | lower)

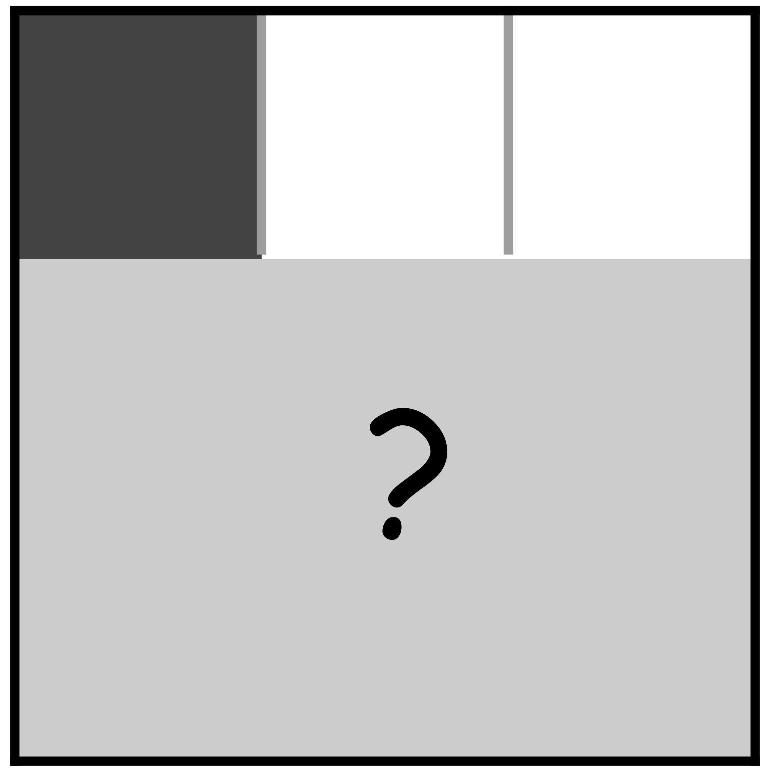


Quantum Inference

With Zeng, Wu, Liu, Hu, 1808.03425

Cf Low and Chuang, PRA '14



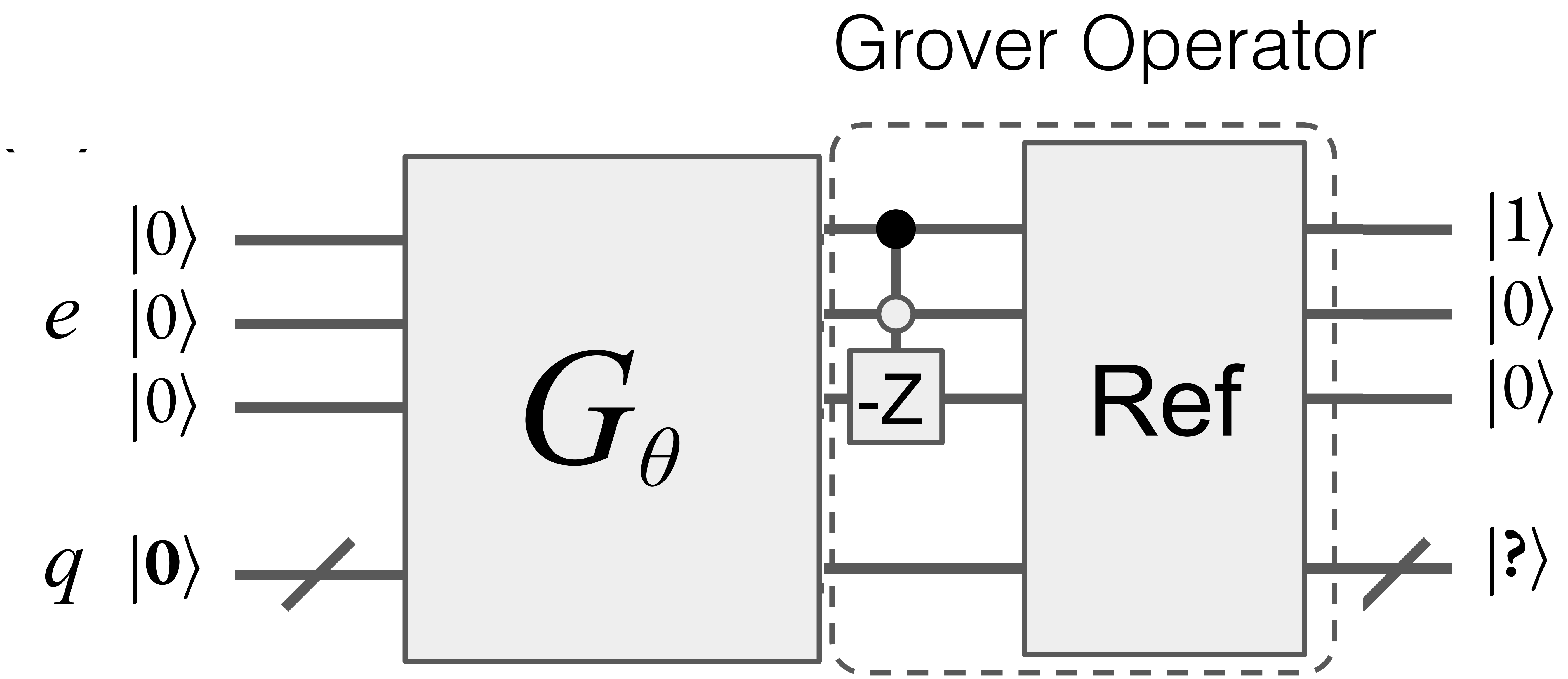


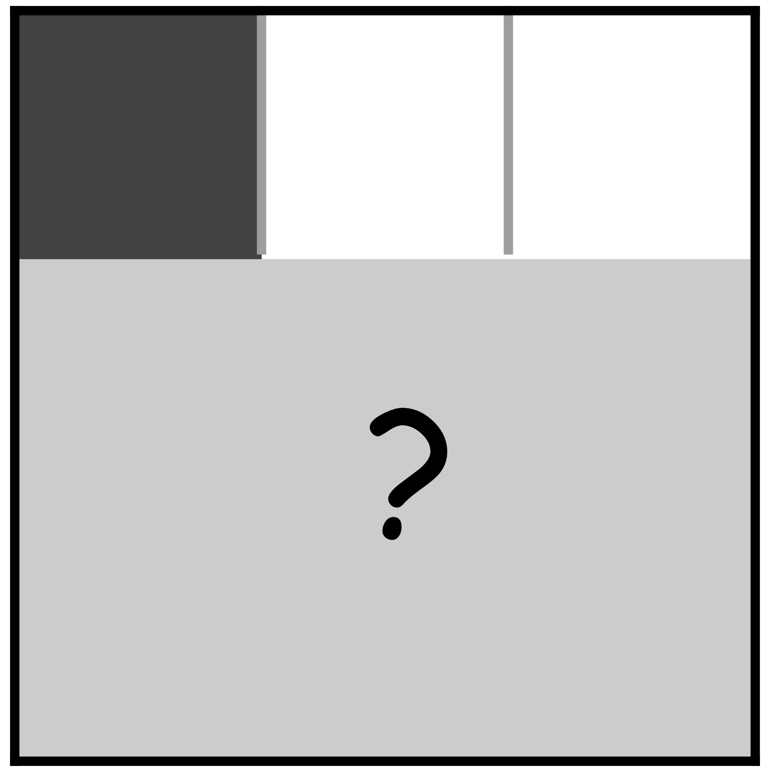
Accelerated quantum inference via Grover search

Quantum Inference

With Zeng, Wu, Liu, Hu, 1808.03425

Cf Low and Chuang, PRA ‘14

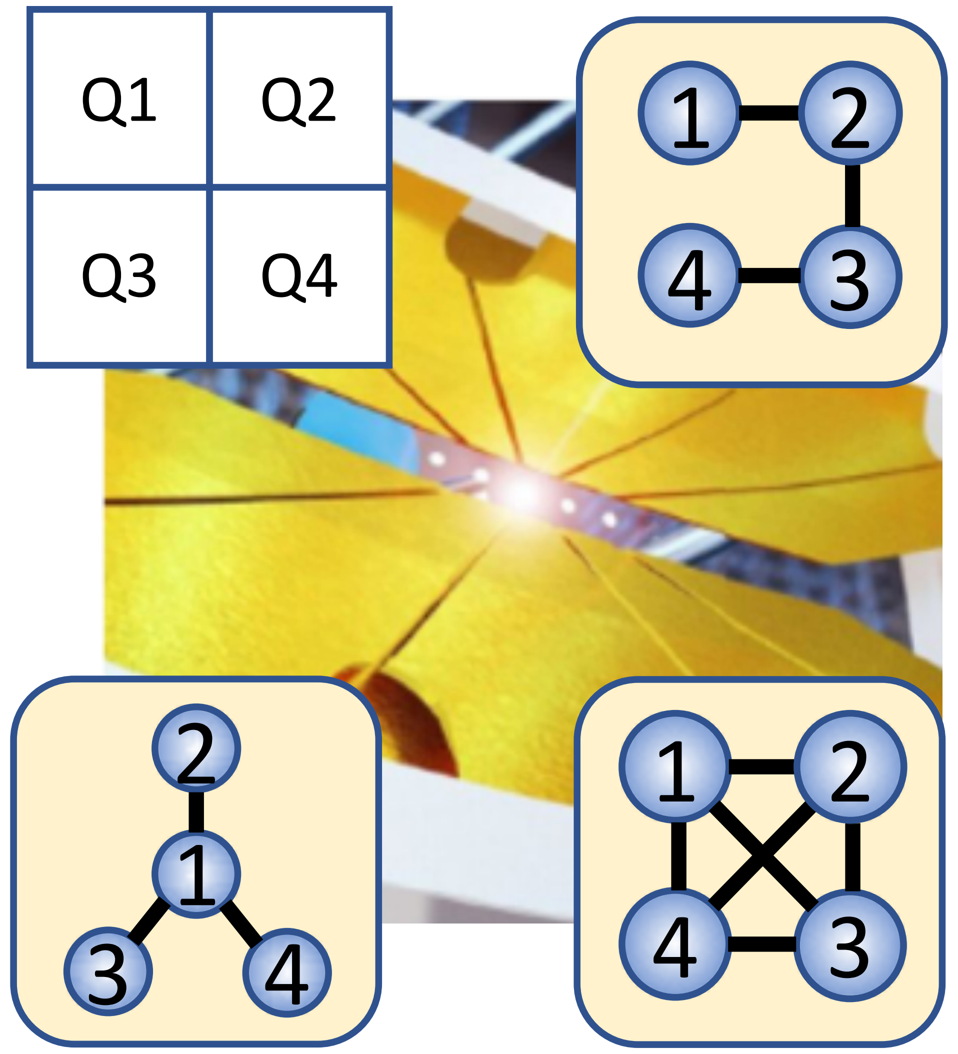


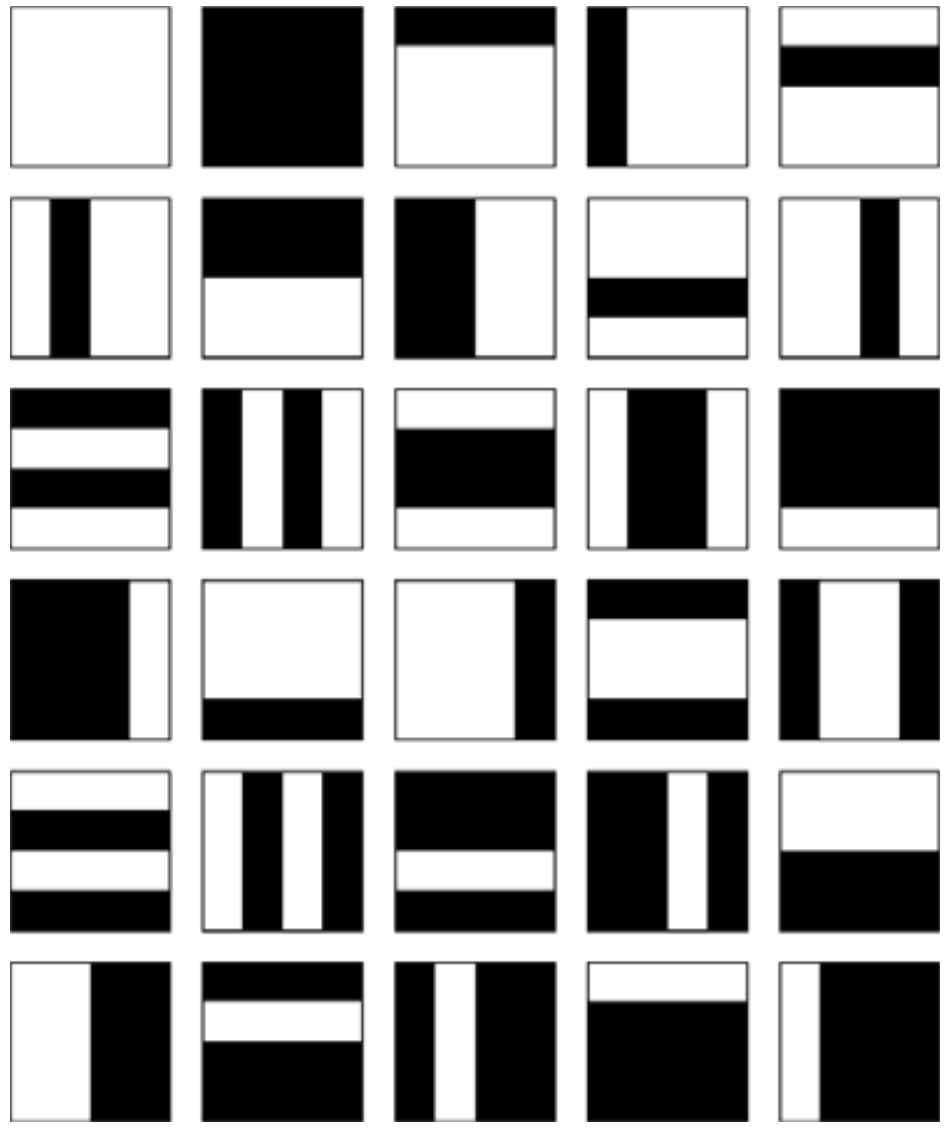


Accelerated quantum inference via Grover search

QCBM Experiments

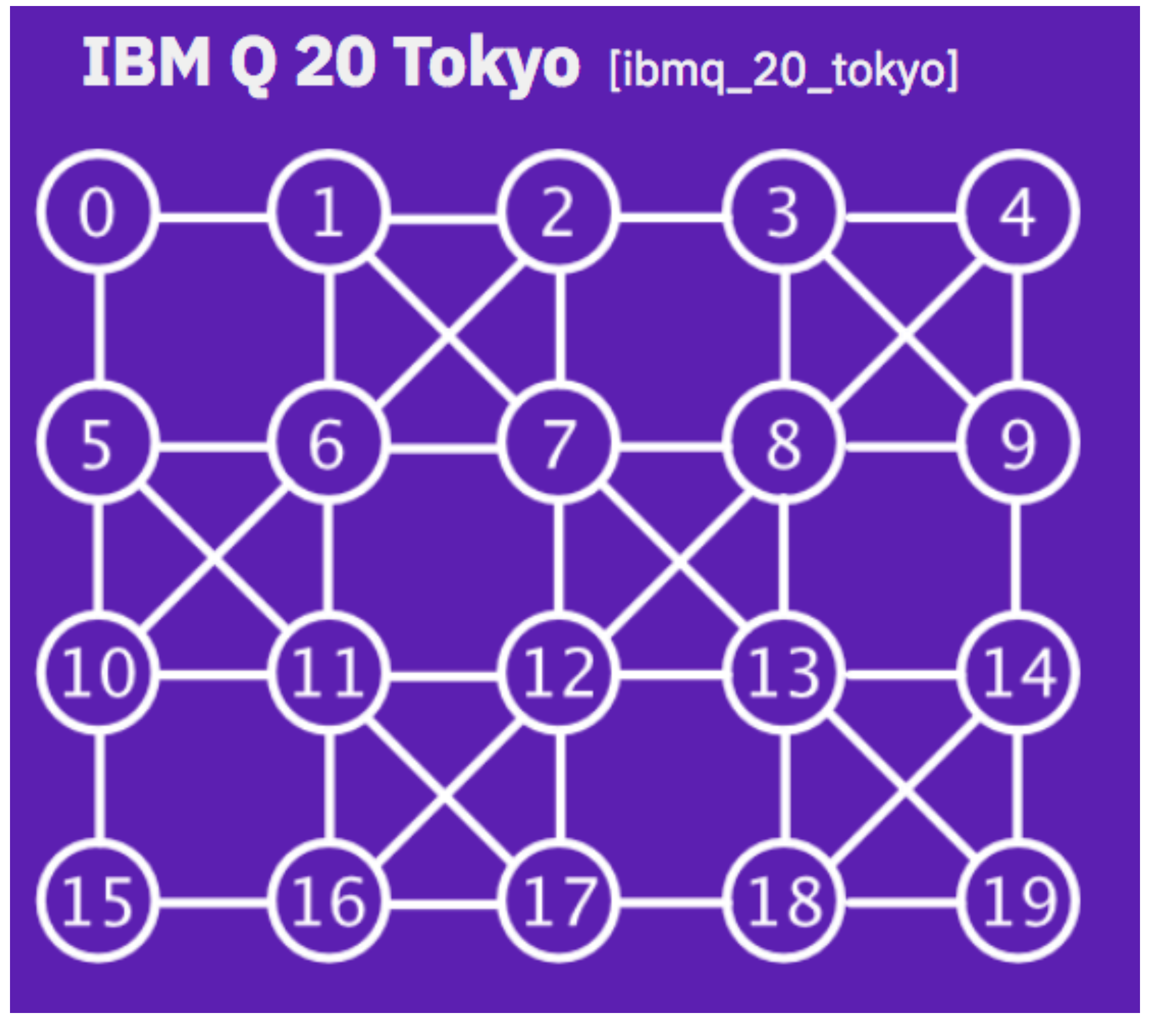
JQI+IonQ+UCL+Cambridge Q+…
1801.07686, 1812.08862





“Bars-and-Stripes”
Han et al, 1709.01662, PRX ’18
cf Mackay’s book “Information Theory, Inference, and Learning”

Oak Ridge, 1811.09905



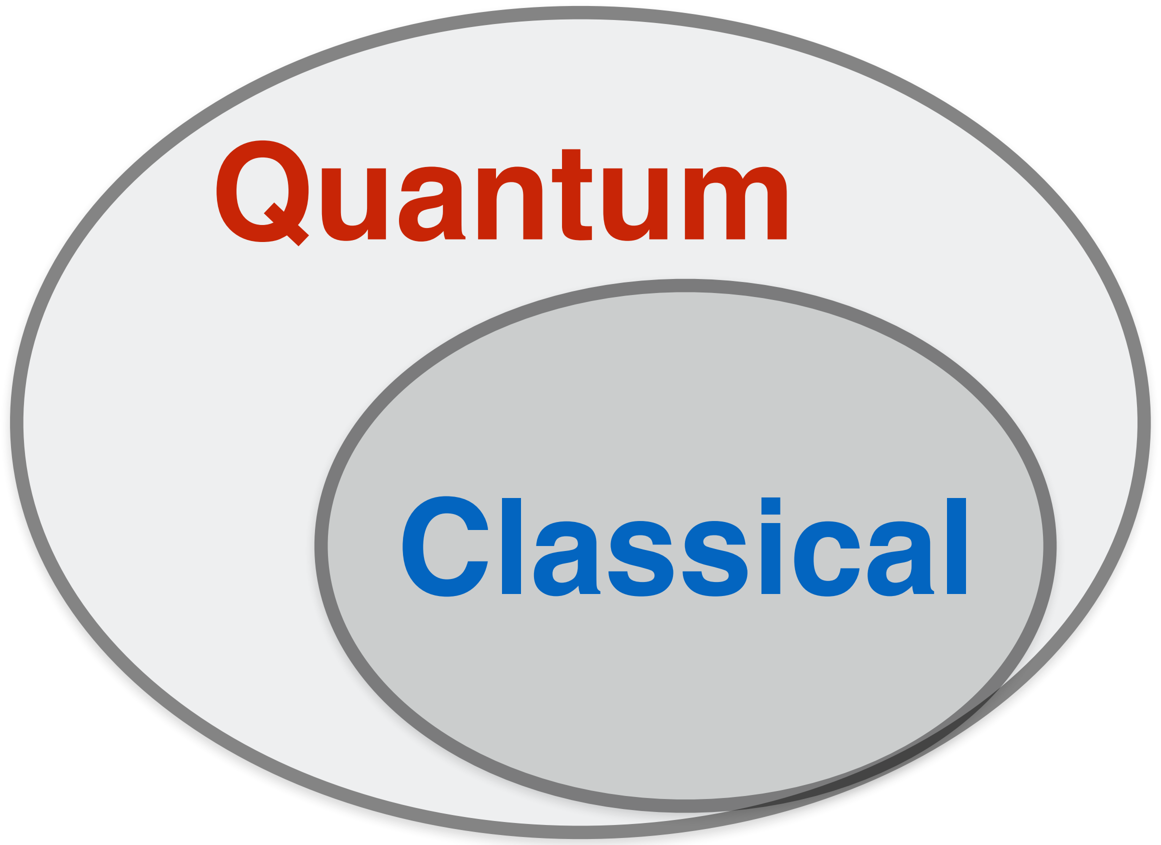
Generative modeling now becomes a calibration score for quantum circuits

Key questions to the future of QCBM

❶ **Is it really useful?**

A killer problem distribution where quantum **really helps**

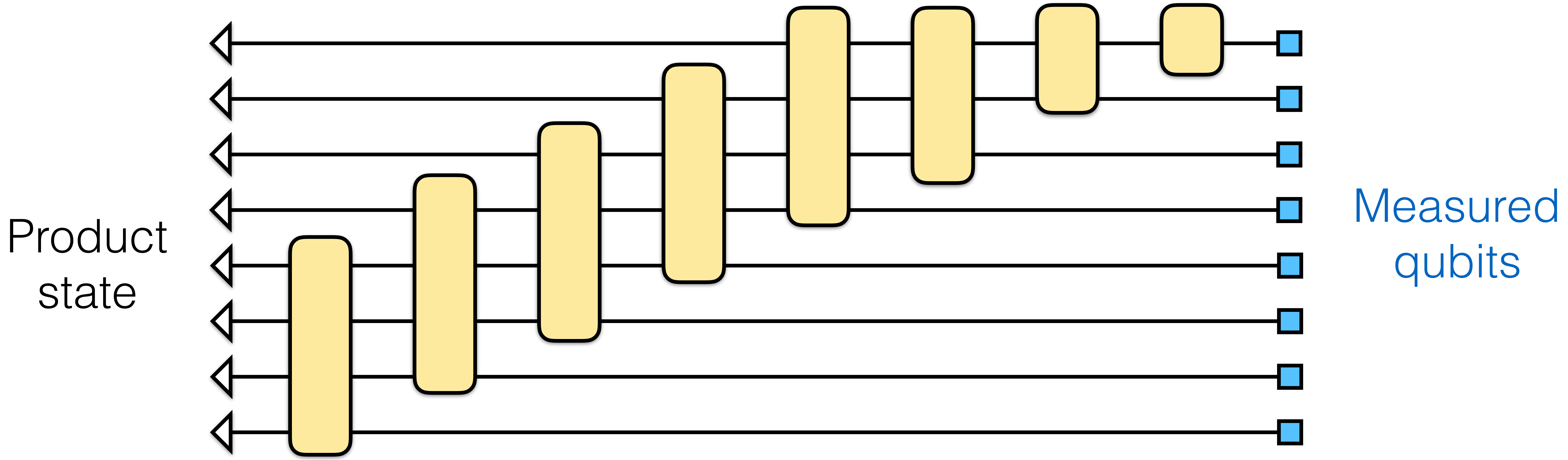
Probability space



❷ **Scale it up**

- Algorithmically saving qubit number
- Quantum circuit architecture design & learning
- Differentiable learning of quantum circuits

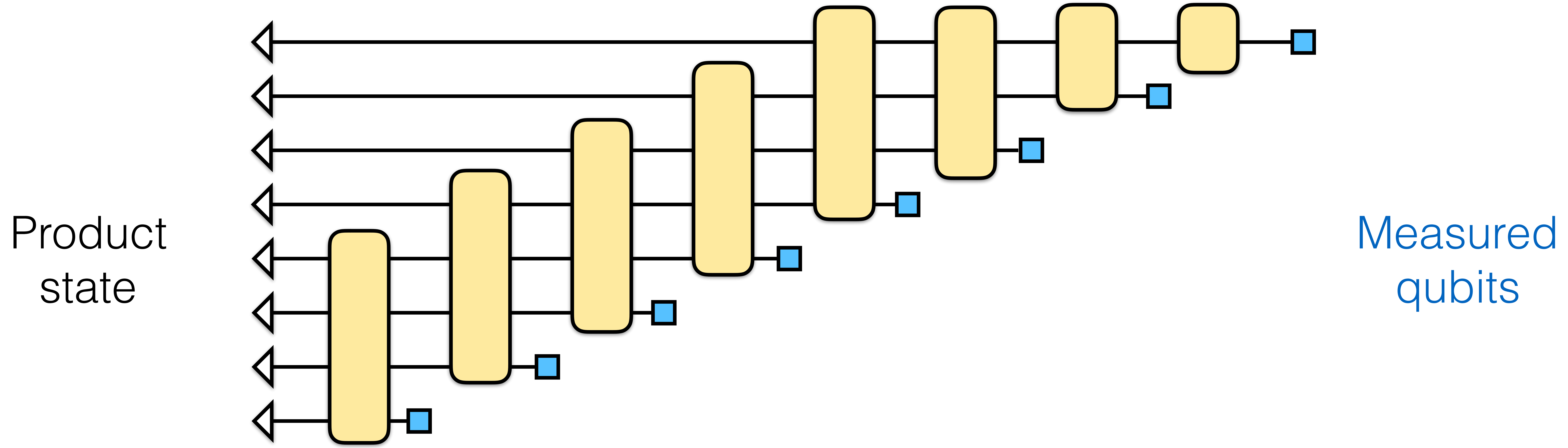
Architecture: Qubit efficient scheme



Huggins, Patel, Whaley, Stoudenmire, 1803.11537
see also Cramer et al, Nat. Comm. 2010

Tensor network inspired quantum circuit architecture

Architecture: Qubit efficient scheme



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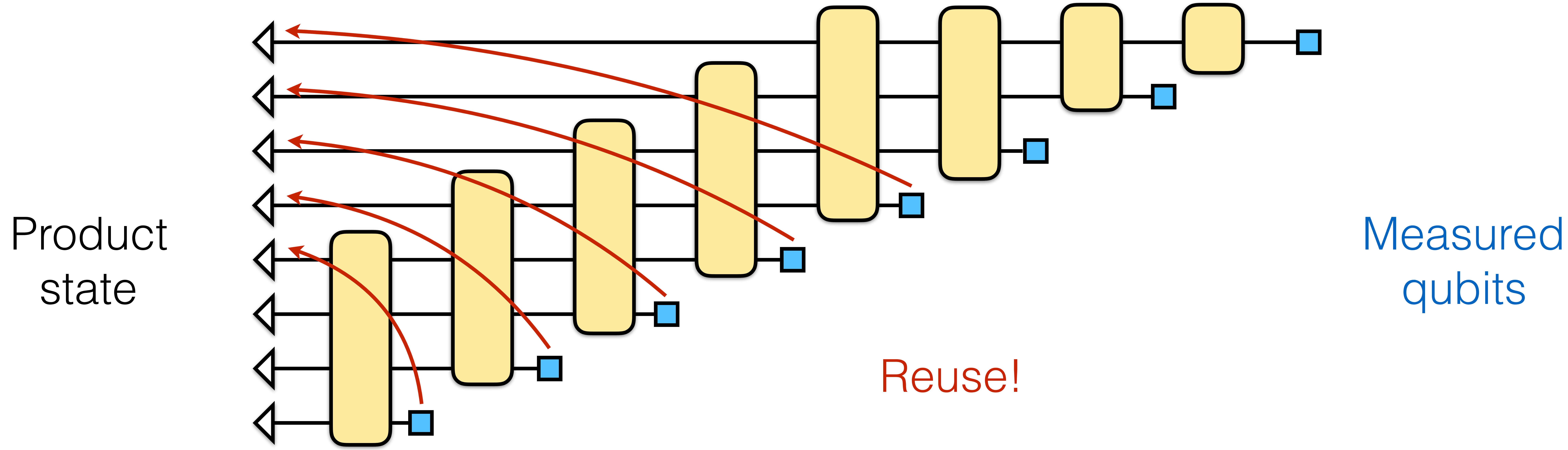

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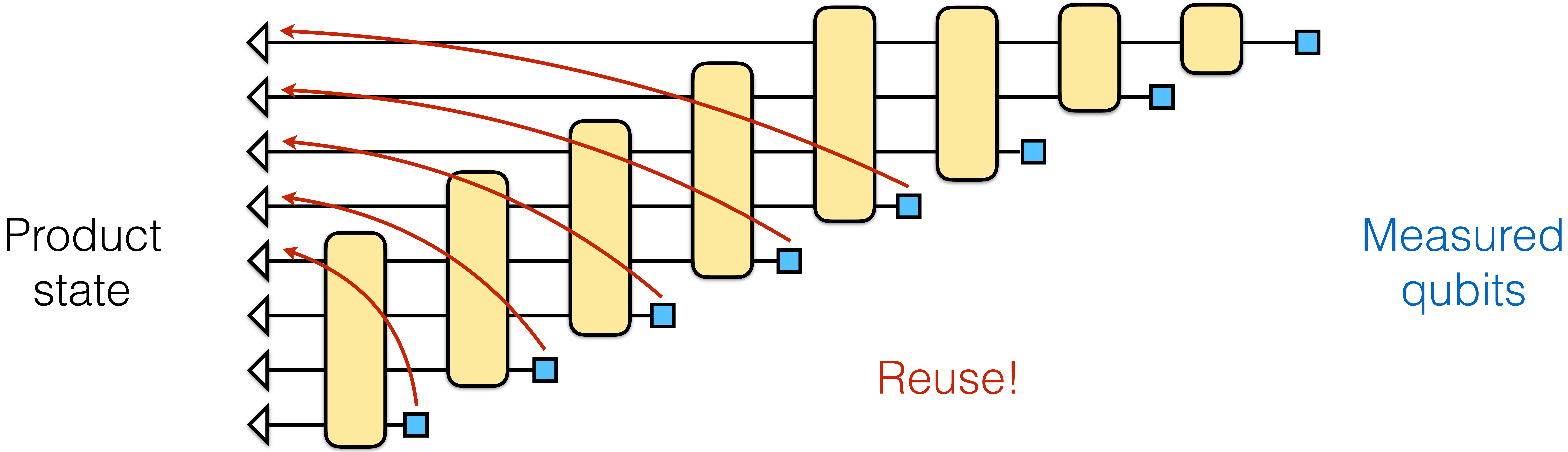

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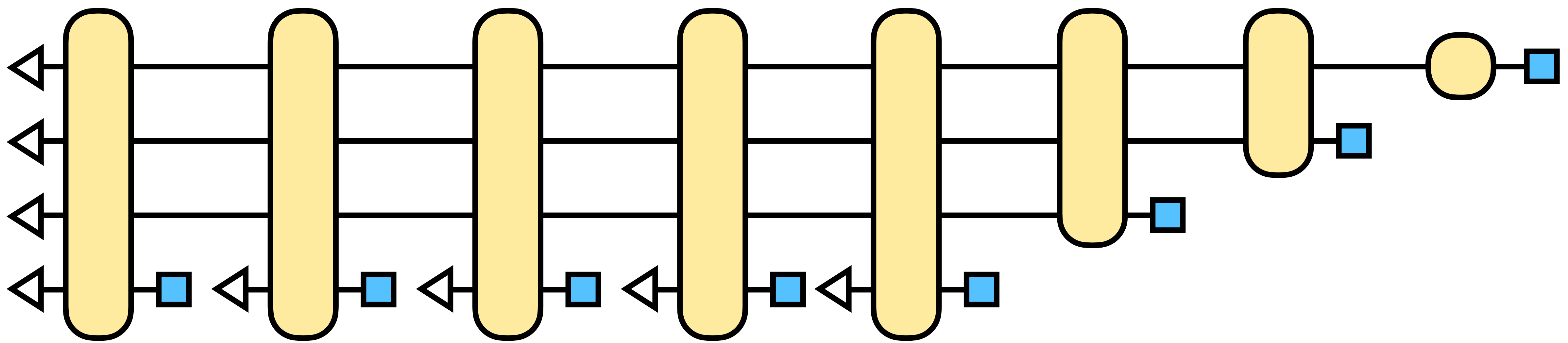

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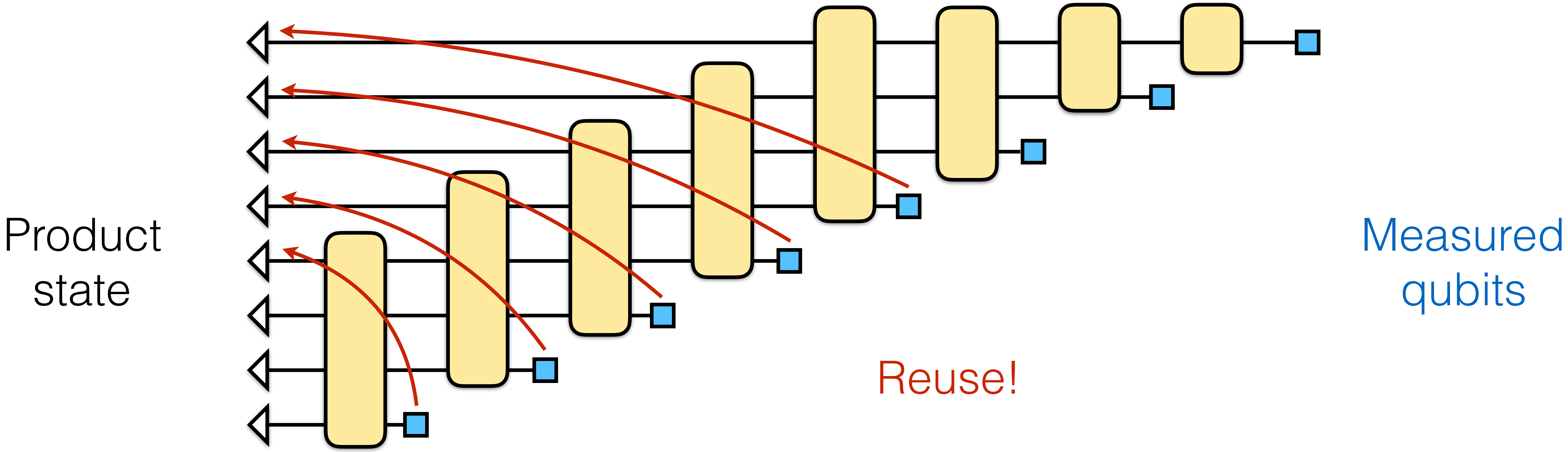

Huggins, Patel, Whaley, Stoudenmire, 1803.11537
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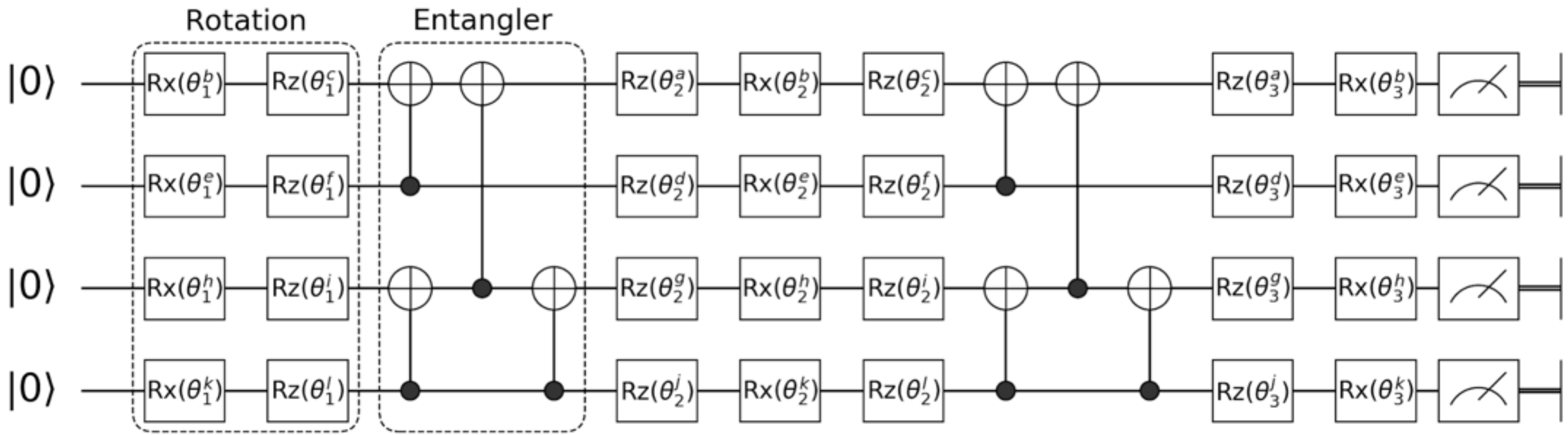
MPS with exponentially large bond dimensions

Training: differentiable learning

Gradient based optimization is the engine of deep learning

Differentiable quantum circuits



Parametrized gate of the form

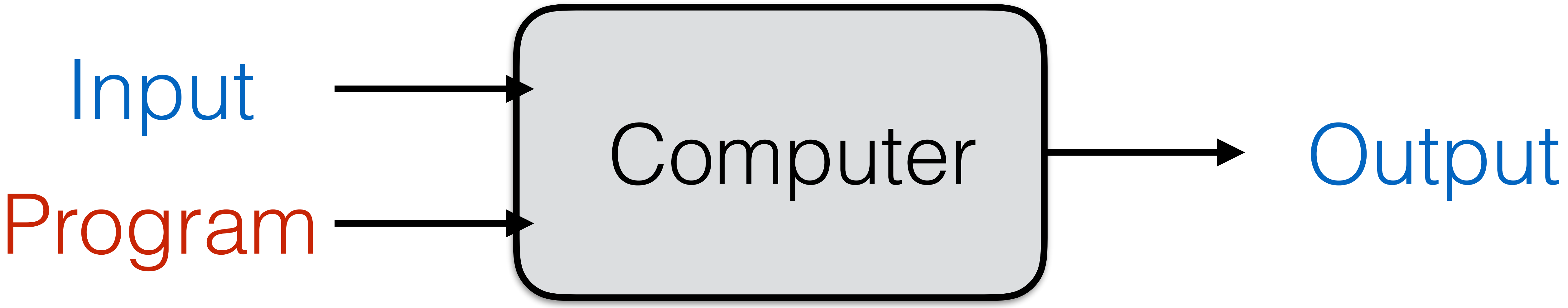
$$e^{-\frac{i\theta}{2}\Sigma} \quad \text{with} \quad \Sigma^2 = 1$$

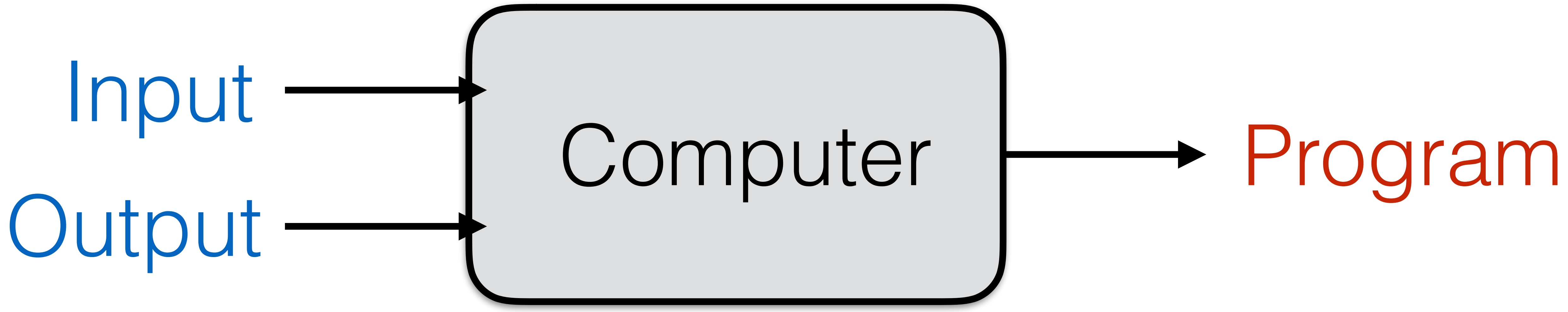
eg, X, Y, Z, CNOT, SWAP…

With Liu 1804.04168, c.f. Li et al 1608.00677
Mitarai et al 1803.00745 Xanadu 1811.04968

$$\boxed{\nabla \langle O \rangle_\theta = \left(\langle O \rangle_{\theta+\pi/2} - \langle O \rangle_{\theta-\pi/2} \right) / 2}$$

Differentiable Programming

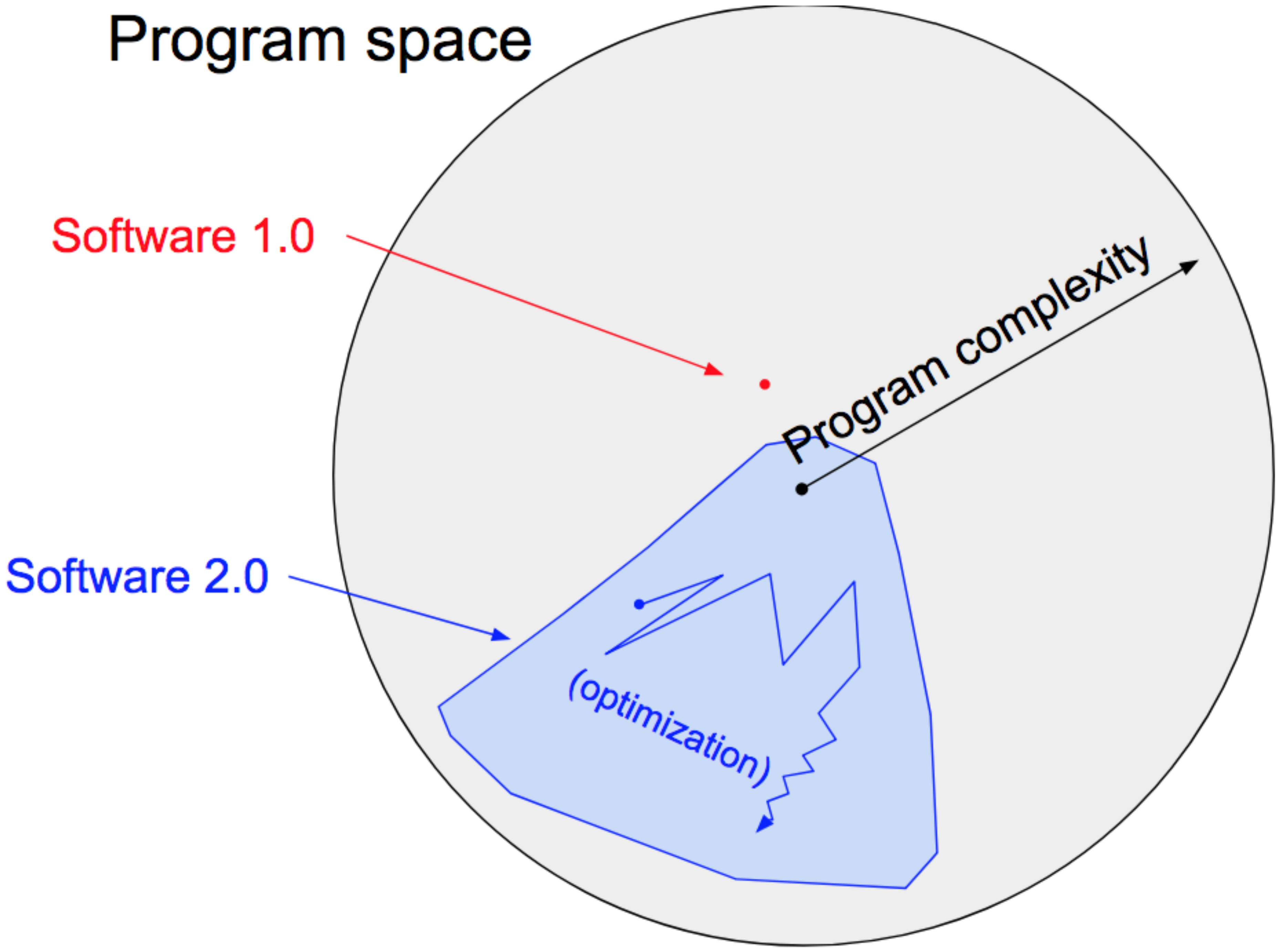




Andrej Karpathy

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



Writing software 2.0 by gradient search in the program space

Differentiable Programming

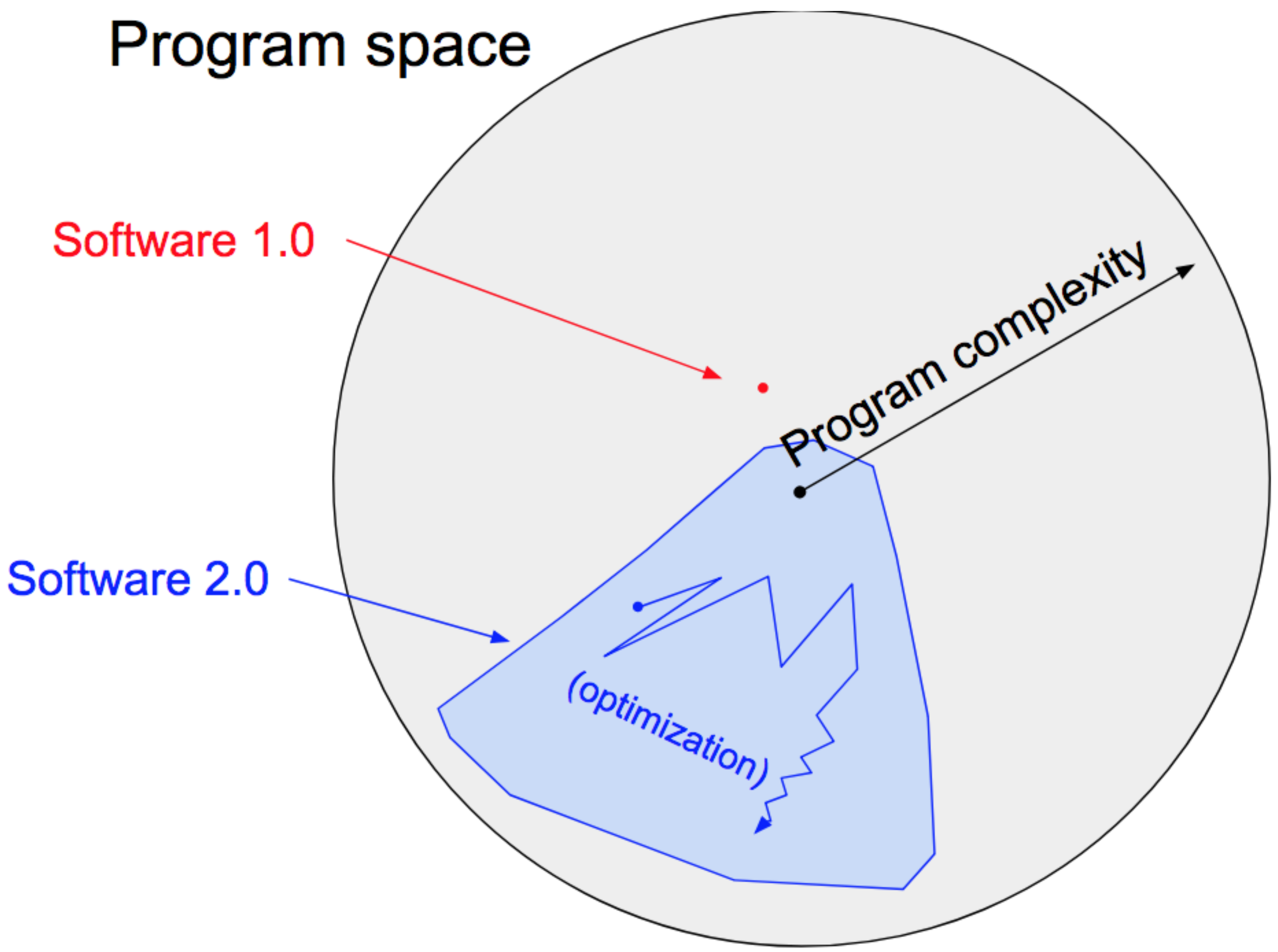
Benefits of Software 2.0

- 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

Andrej Karpathy

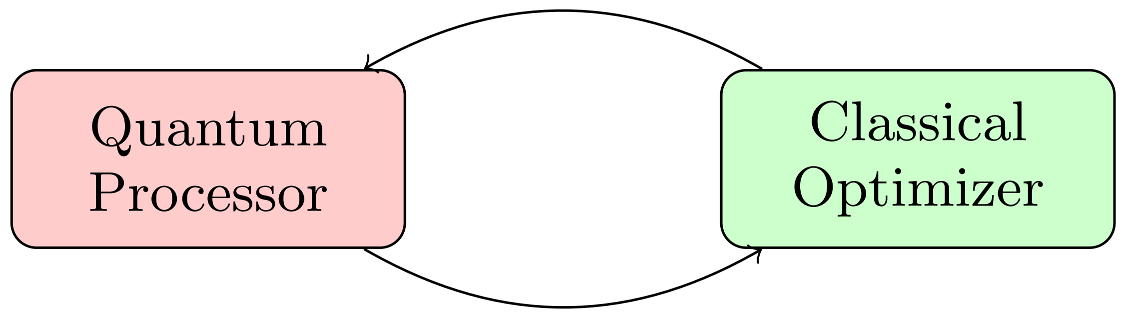
Director of AI at Tesla. Previously Research Scientist at OpenAI and PhD student at Stanford. I like to train deep neural nets on large datasets.

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



Writing software 2.0 by gradient search in the program space

Differentiable Quantum Programming

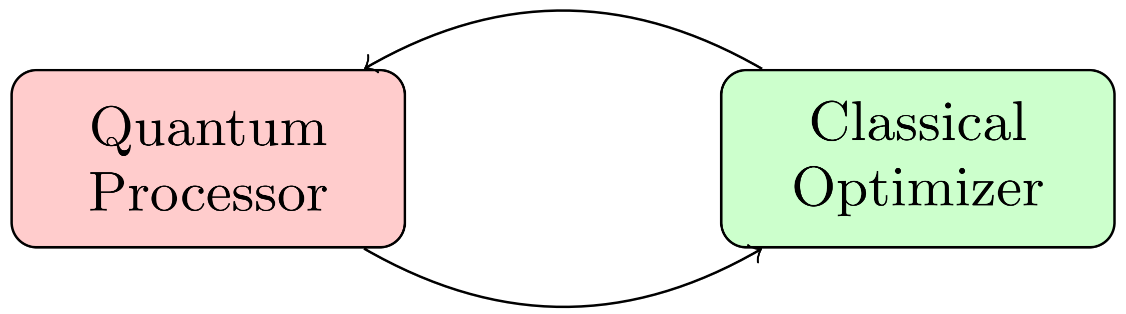


- Variational quantum eigensovler (VQE)
- Quantum approximate optimization algorithm (QAOA)
- Quantum pattern recognition
- Quantum circuit Born machine (QCBM)

…

Quantum circuit classifier	Farhi, Neven, 1802.06002 Havlicek et al, 1804.11326
Born machine experiment	Benedetti, Garcia-Pintos, Nam, Perdomo-Ortiz, 1801.07686
TNS inspired circuit architecture	Huggins, Patel, Whaley, Stoudenmire, 1803.11537
Quantum generative model	Gao, Zhang, Duan, 1711.02038
Quantum adversarial training	Dallaire-Demers, Lloyd, Benedetti 1804.08641,1804.09139, 1806.00463

Differentiable Quantum Programming



It is a paradigm beyond quantum-classical hybrid

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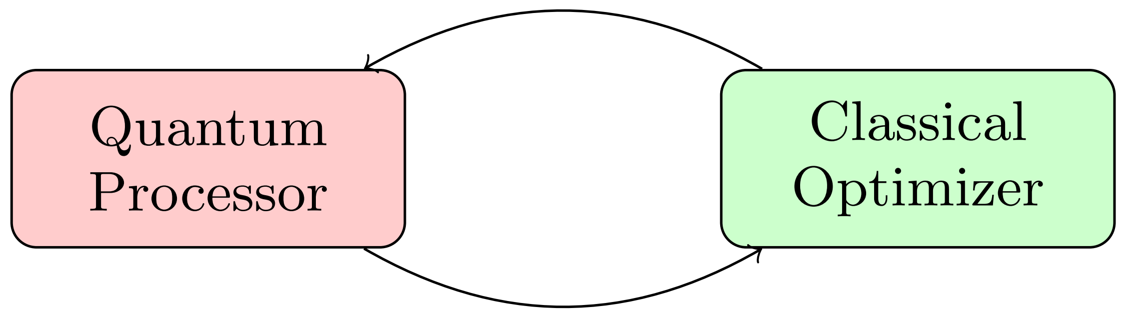
Differentiable Quantum Programming



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Short term：
What can we do with circuits of limited depth ?

Long term:
Are we really good at programing quantum computers ?

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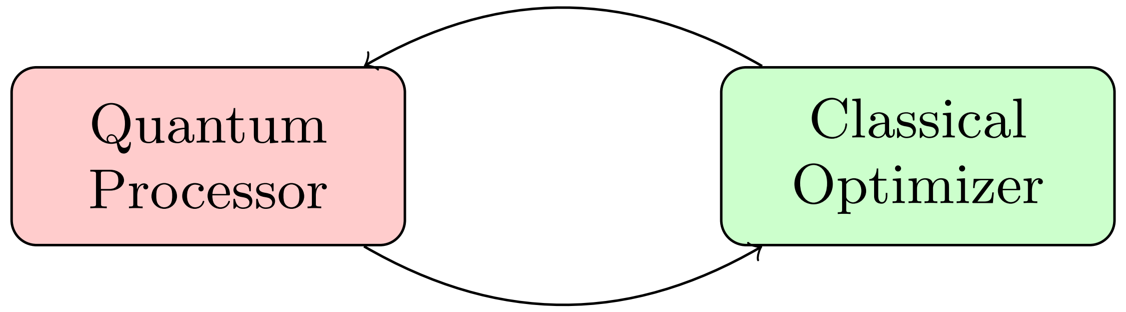
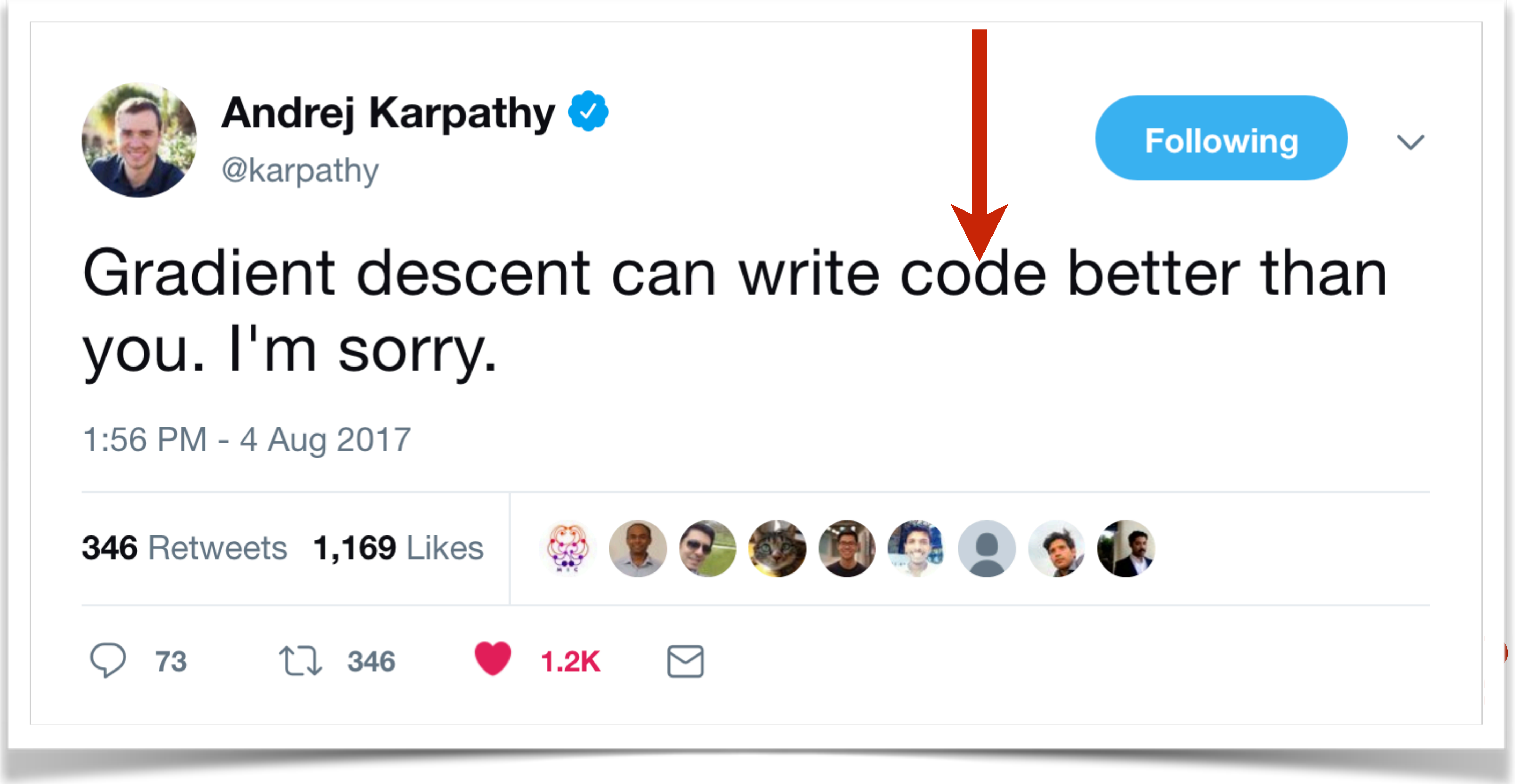


It is a paradigm beyond quantum-classical hybrid

Quantum code



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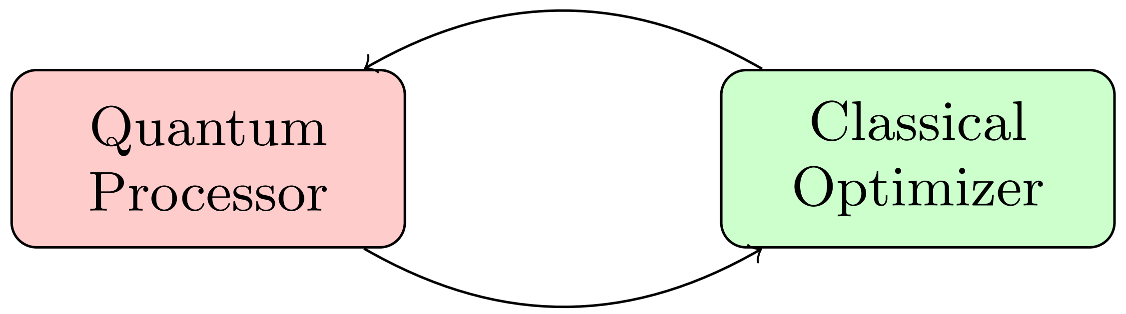

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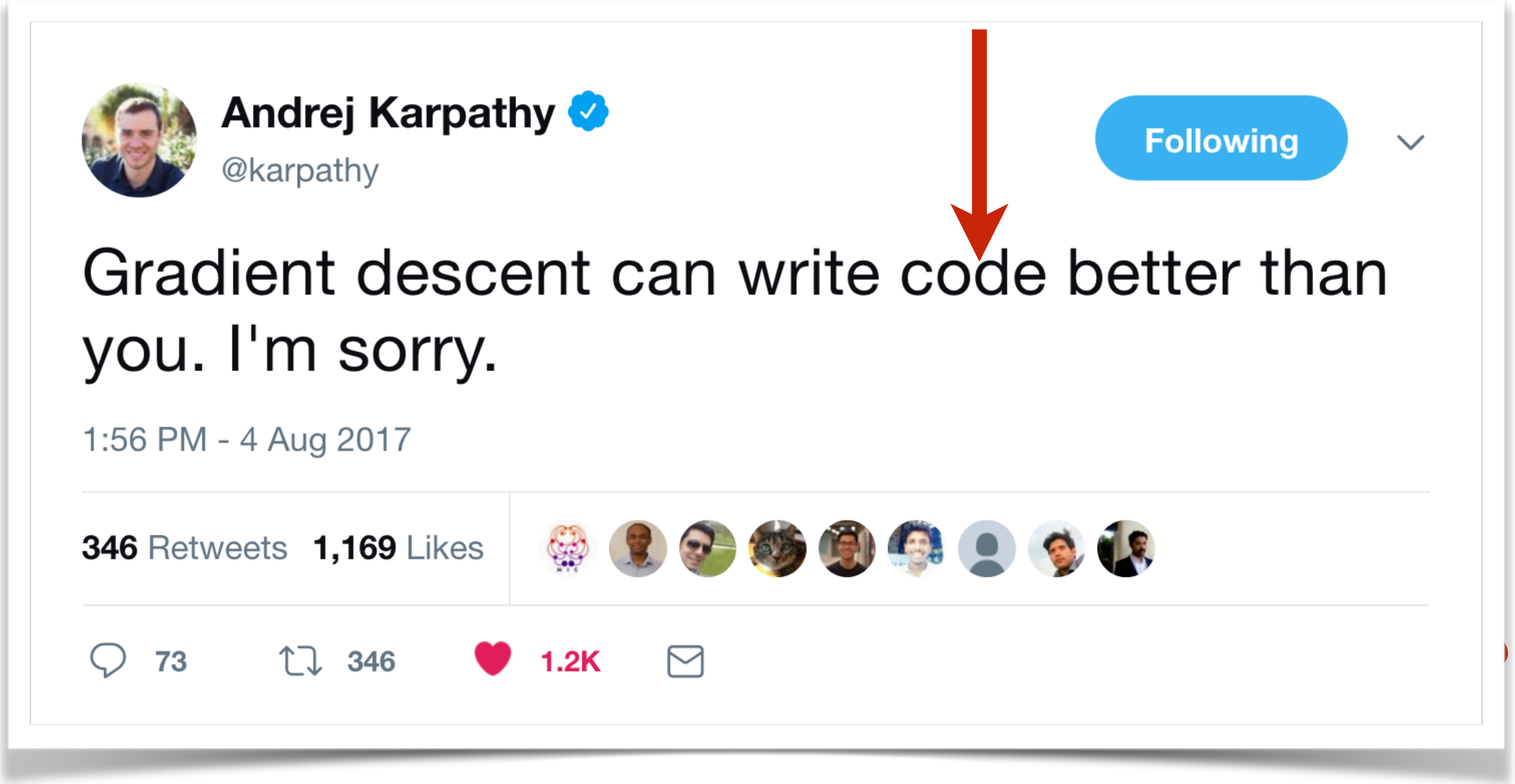

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…

Quantum ci
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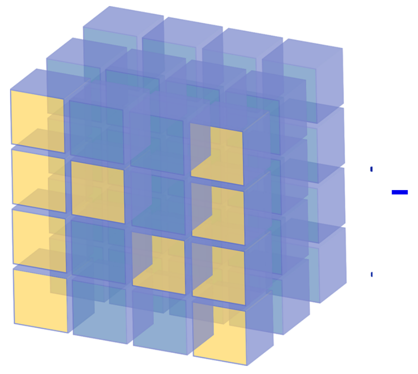
Quantum ad 1806.00463

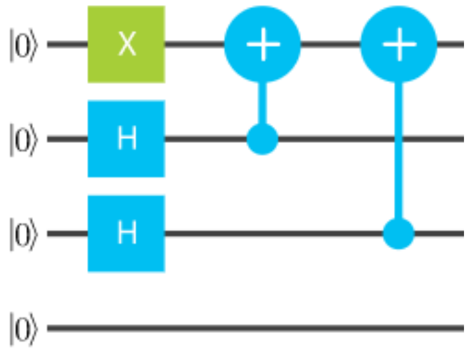
"Quantum Software 2.0"

Try it yourself!

http://lib.itp.ac.cn/html/panzhang/mps/tutorial/

https://github.com/wangleiphy/DL4CSRC

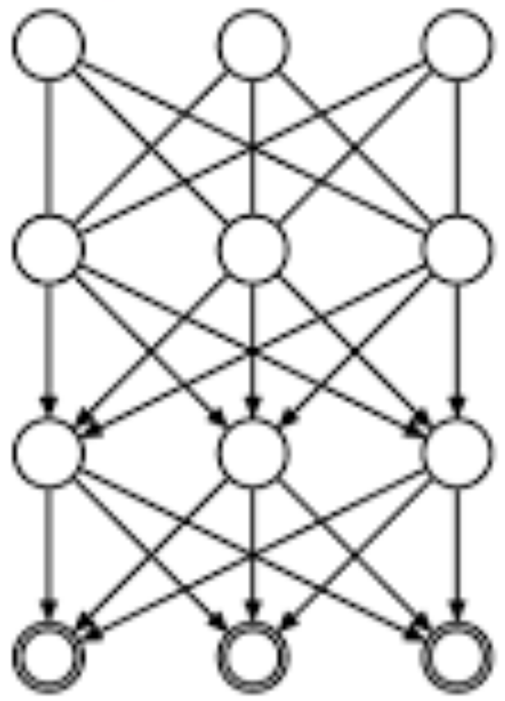




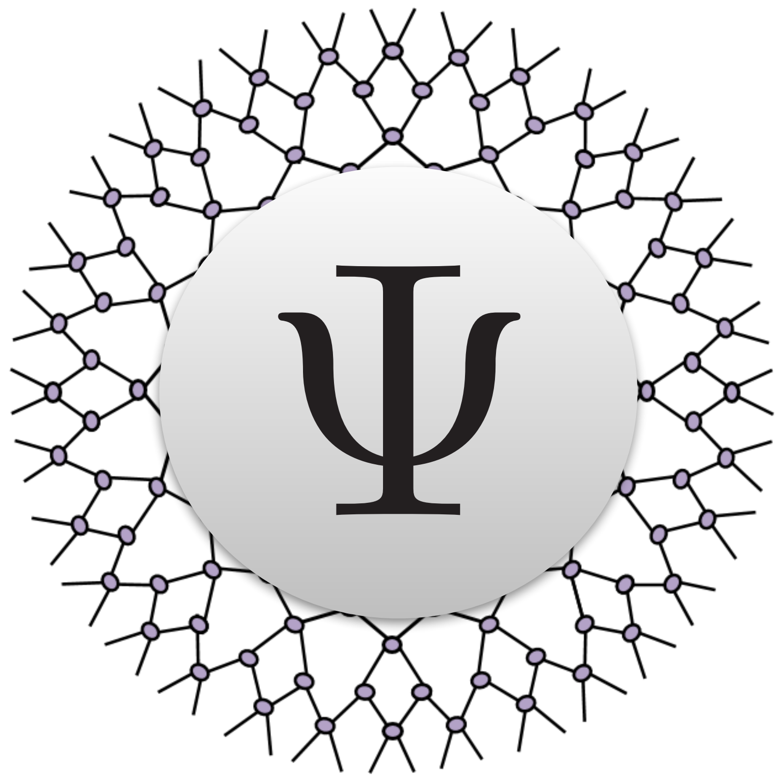
https://github.com/GiggleLiu/QuantumCircuitBornMachine

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

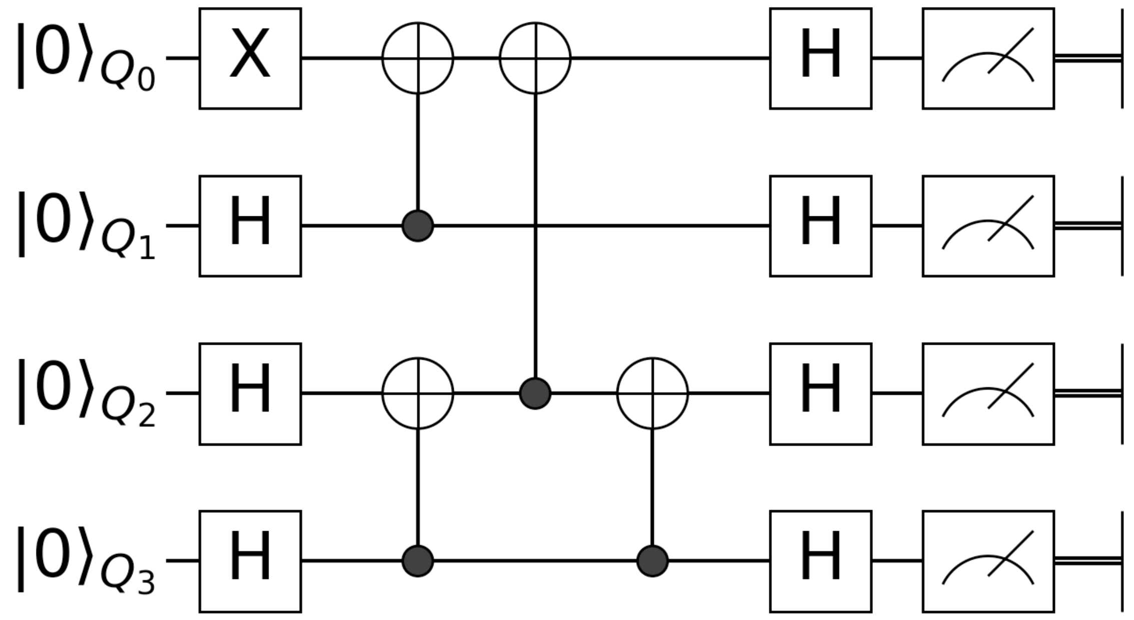
Neural Networks



Tensor Networks



Quantum Circuits



“三重境界”

1. Function Approximation
2. Probabilistic Transformation
3. Information Processing Device

Thank You!

Pan Zhang **Jun Wang** **Jinfeng Zeng** **Song Cheng**

Jin-Guo Liu **Zhao-Yu Han** **Xiu-Zhe Luo** **Tao Xiang**

量子纠缠:从量子物质态到深度学习

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(1 中国科学院物理研究所 北京 100190)

(2 中国科学院大学 北京 100049)

2017－06－05收到

† email: wanglei@iphy.ac.cn

DOI: 10.7693/wl20170702

Quantum entanglement: from quantum states of matter to deep learning

CHENG Song[1,2] CHEN Jing[1,2] WANG Lei[1,†]

(1 Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China)

(2 University of Chinese Academy of Sciences, Beijing 100049, China)

摘 要 量子纠缠在量子物质态的研究中扮演着日趋重要的角色，它可以标记传统范式难以区分的新奇量子态和量子相变，并指导设计高效的数值算法来精确地研究量子多体问题。最近，随着一些深度学习技术在量子物理问题中的应用，人们惊奇地发现：从量子纠缠的视角审视深度学习，或许有助于反过来理解和解决一些深度学习中的问题。量子纠缠定量化地刻画了现实数据集的复杂度，并指导相应的人工神经网络结构设计。沿着这个思路，物理学家们对于量子多体问题所形成的种种洞察和理论可以以一种意想不到的方式应用在现实世界中。

关键词 量子纠缠，张量网络，人工神经网络，深度学习

《物理》杂志
2017年7月刊

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

Google Colab
free GPU access

Lecture Note on Deep Learning and Quantum Many-Body Computation

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

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

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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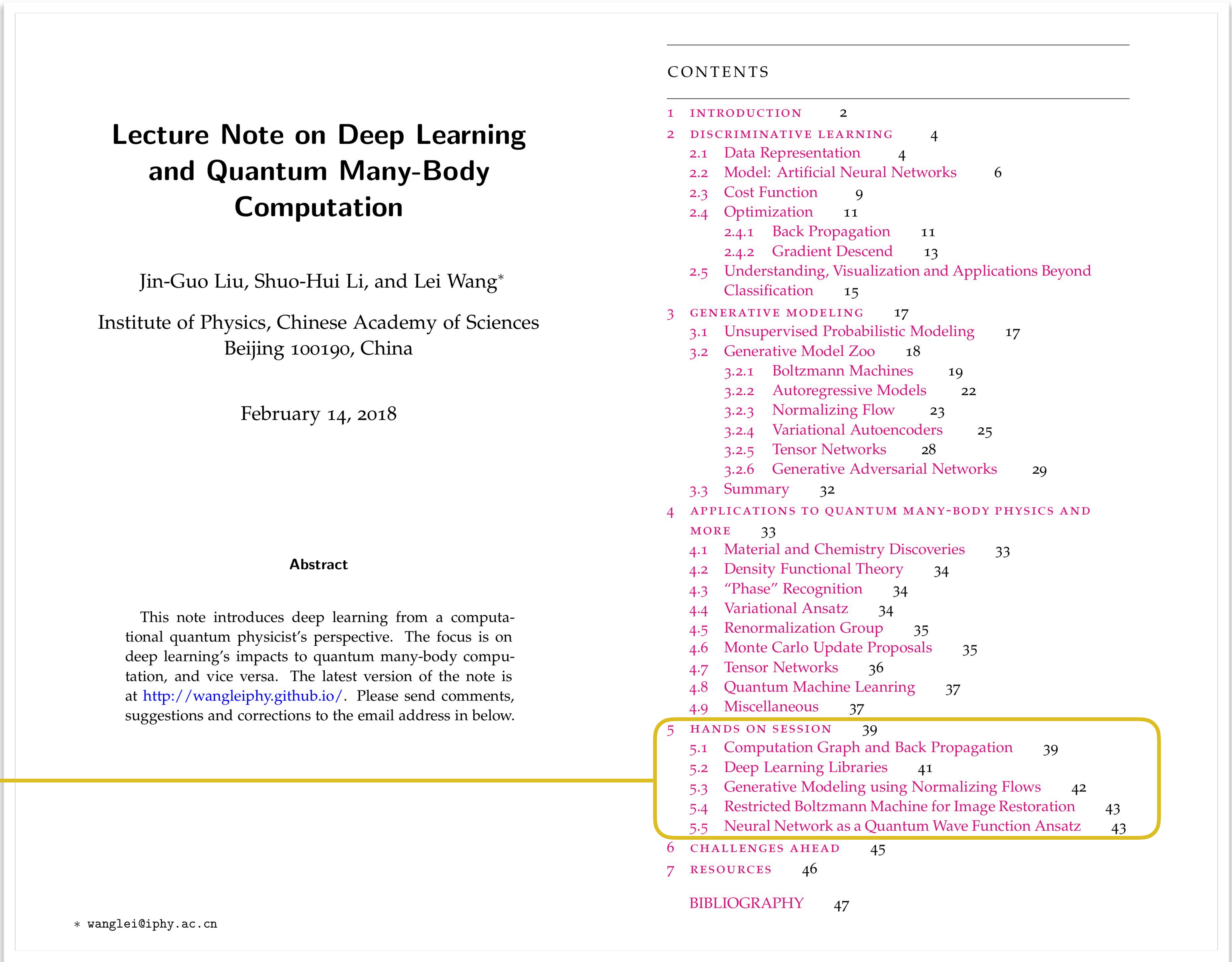

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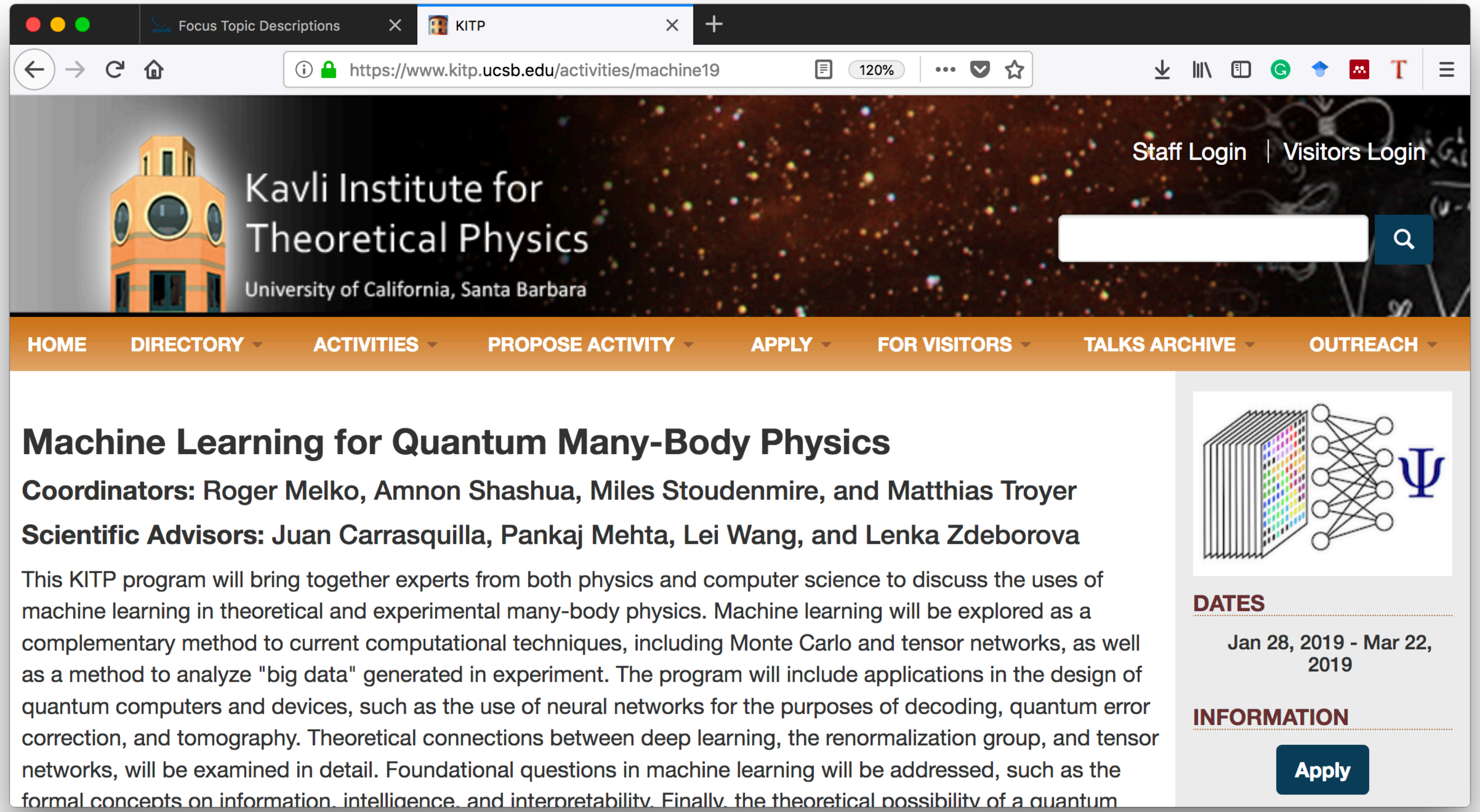

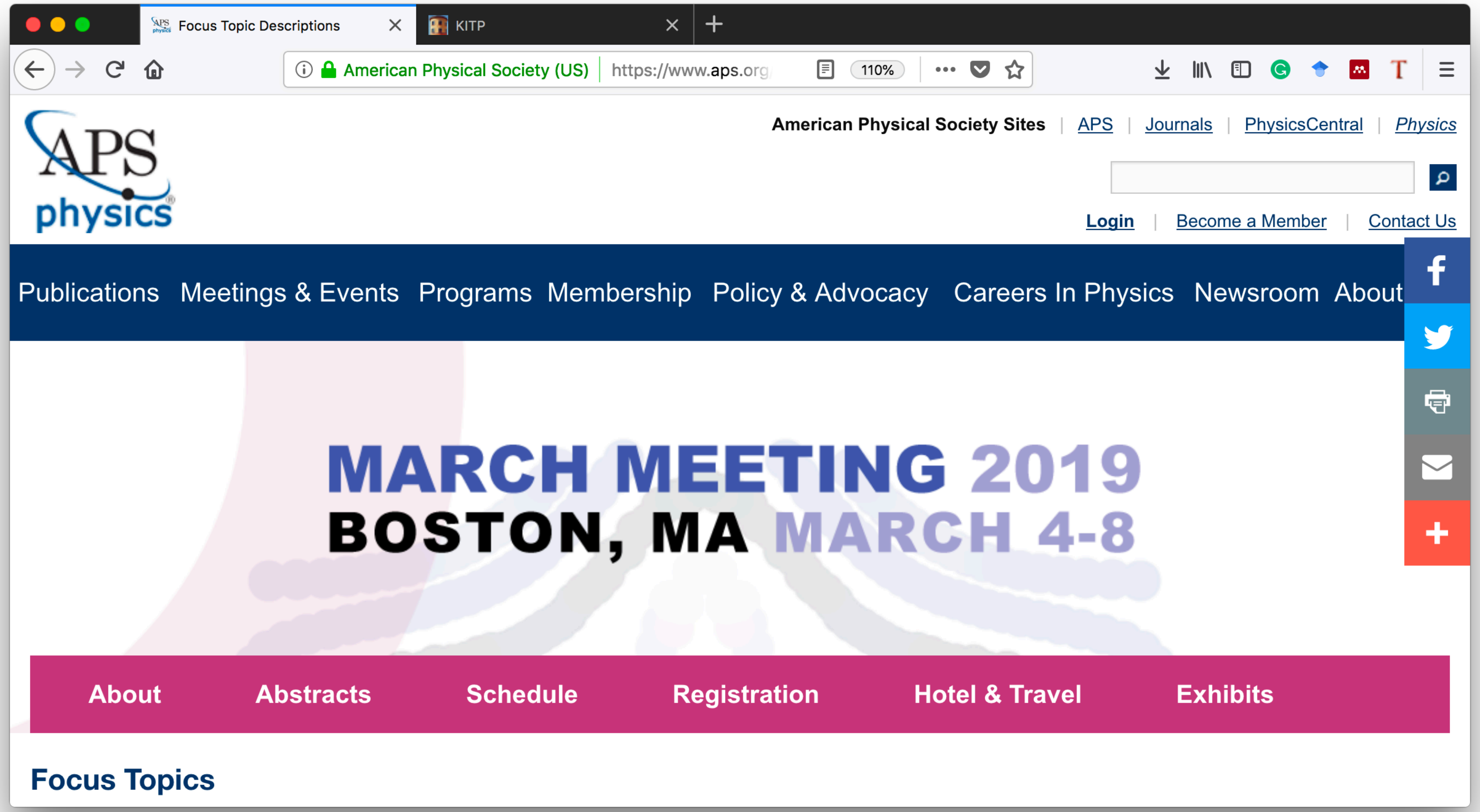

KITP, Santa Barbara Program
ML for Quantum Many-Body Physics
Jan 28-Mar 22, 2019

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