

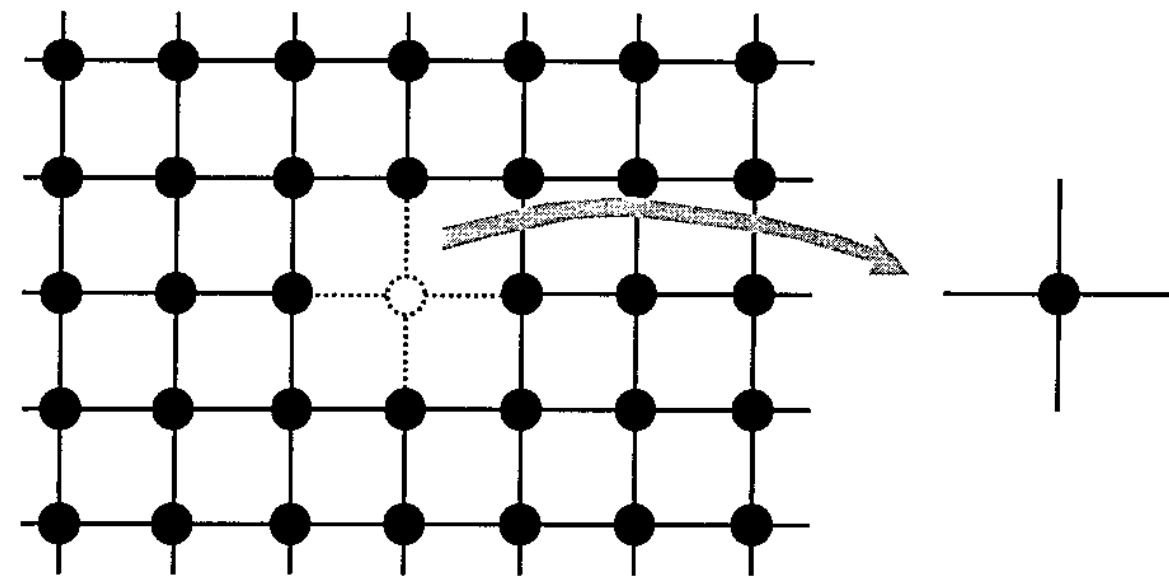
# 流模型： 计算物理视角

王磊 中科院物理研究所  
wanglei@iphy.ac.cn  
<https://wangleiphy.github.io>

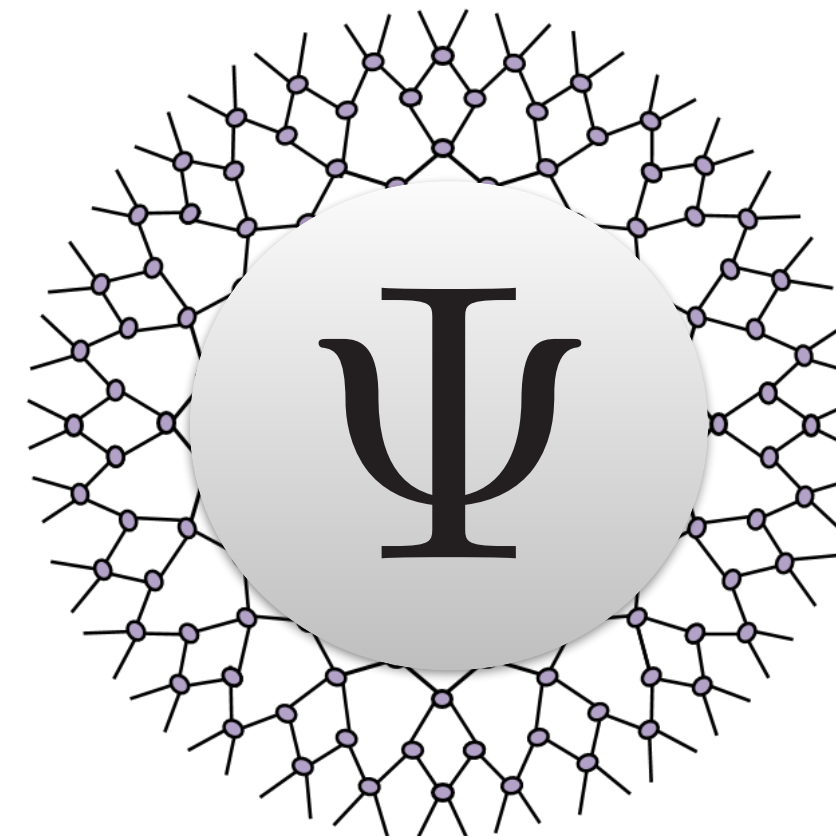


# Physicists' gifts to Machine Learning

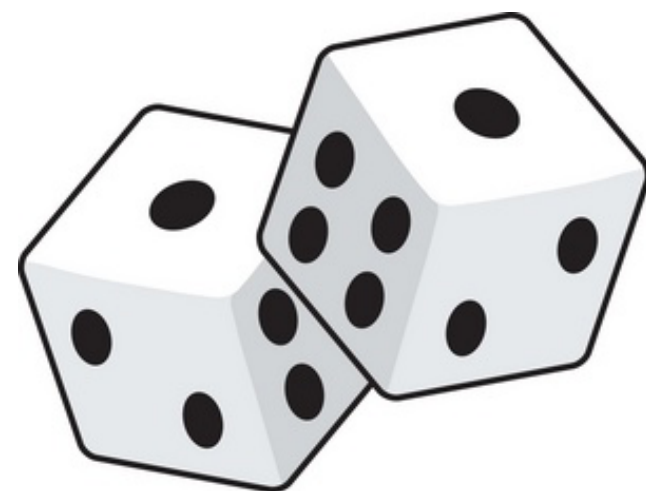
## Mean Field Theory



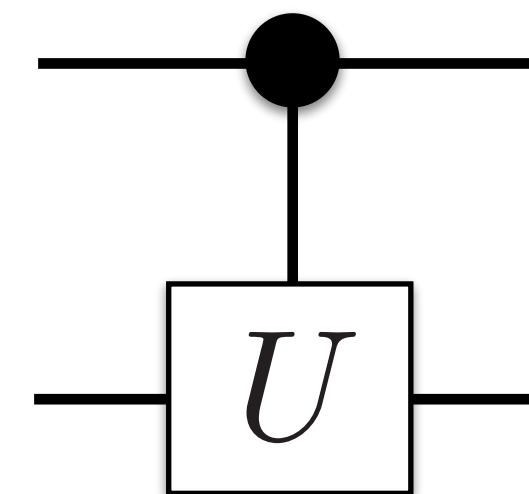
## Tensor Networks



## Monte Carlo Methods



## Quantum Computing





# Deep learning is more than fitting functions



**Discriminative learning**

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

or  $p(y | \mathbf{x})$

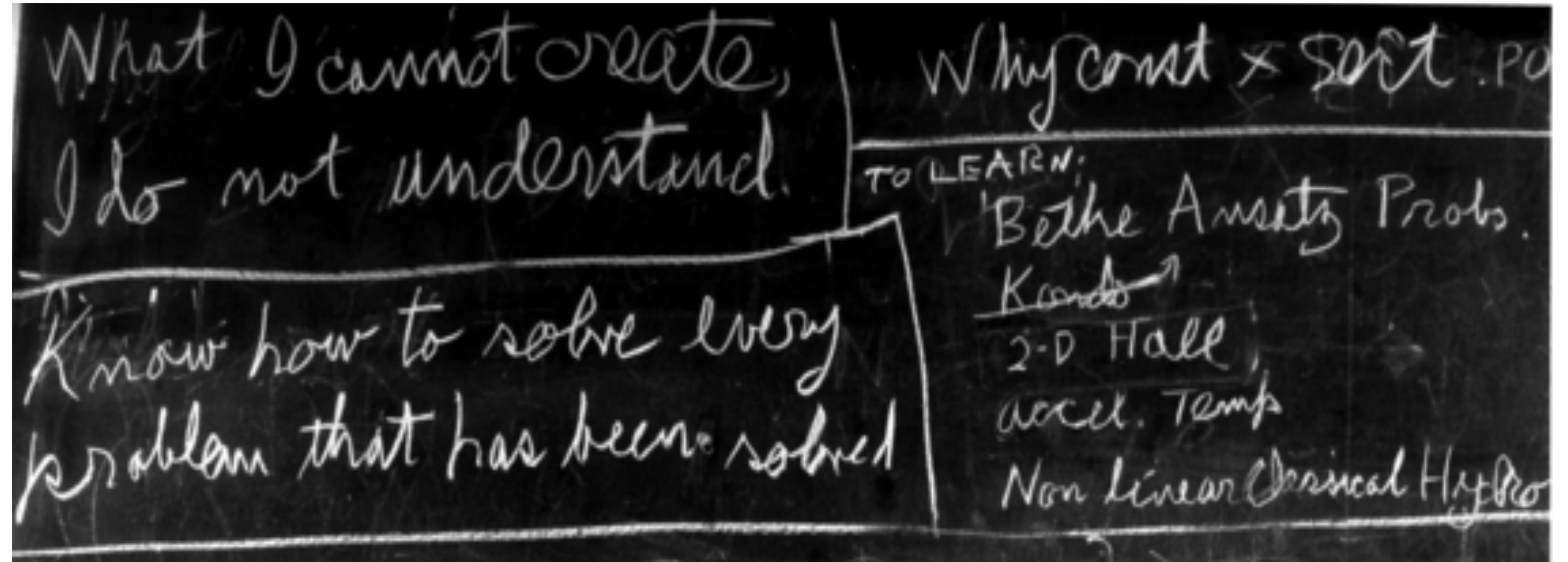
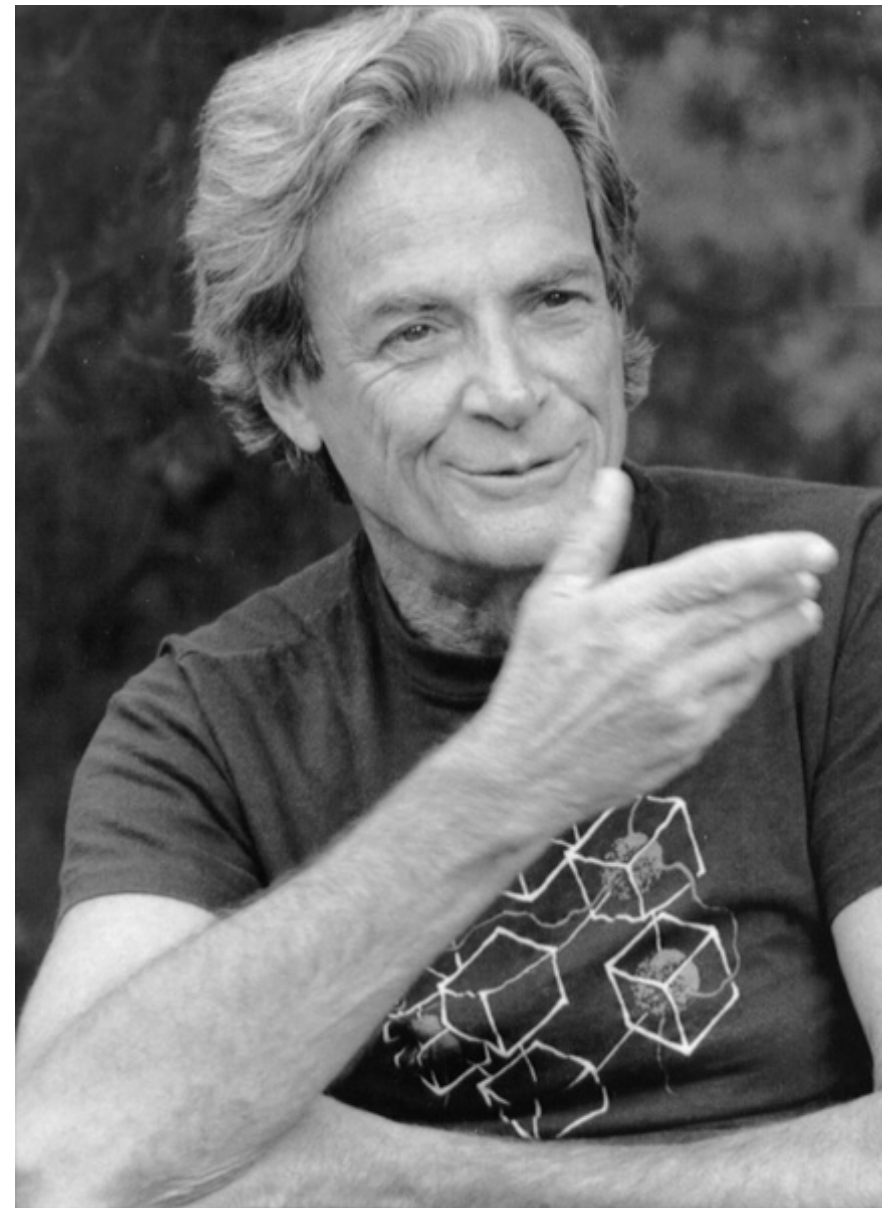


**Generative learning**

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



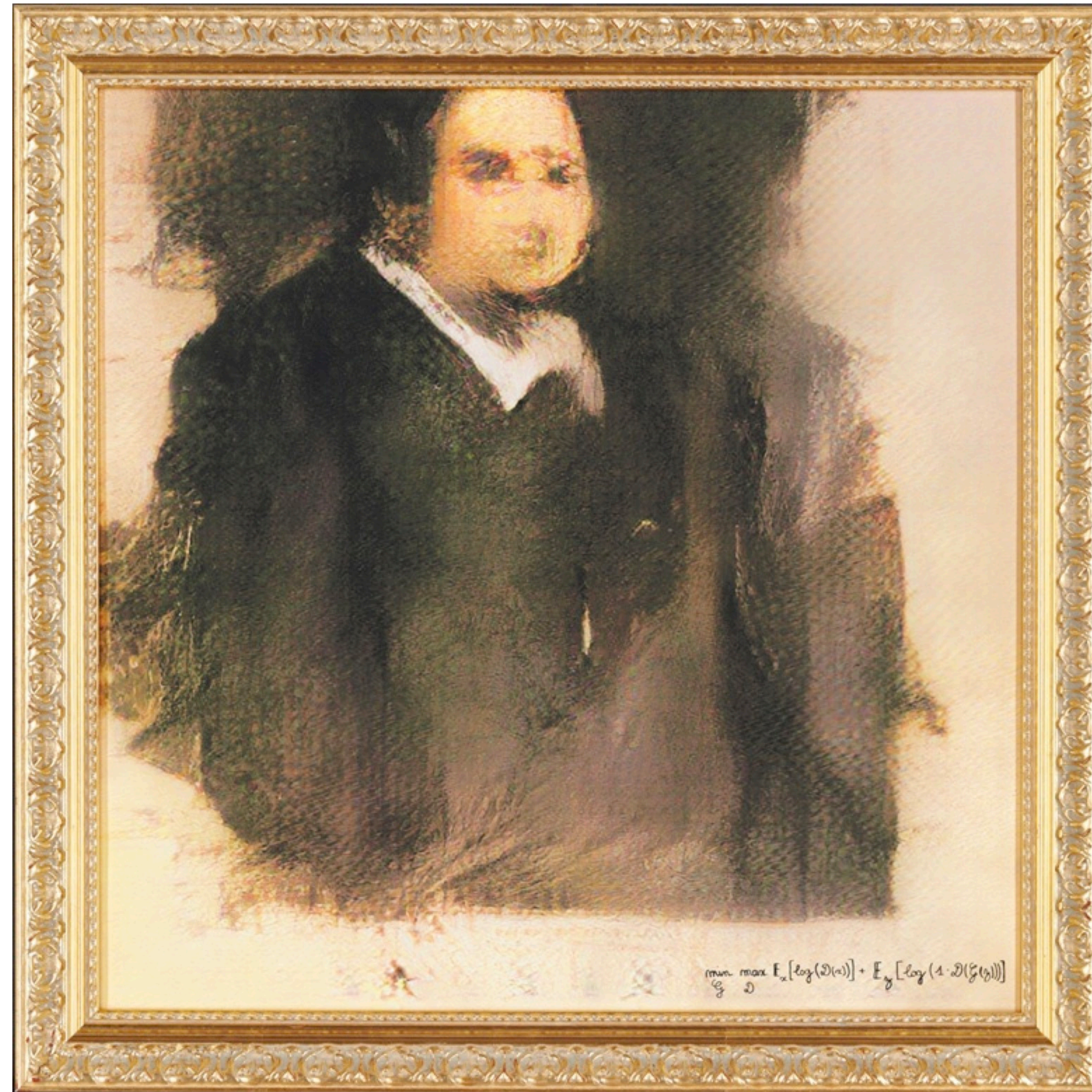
# Deep learning is more than fitting functions



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



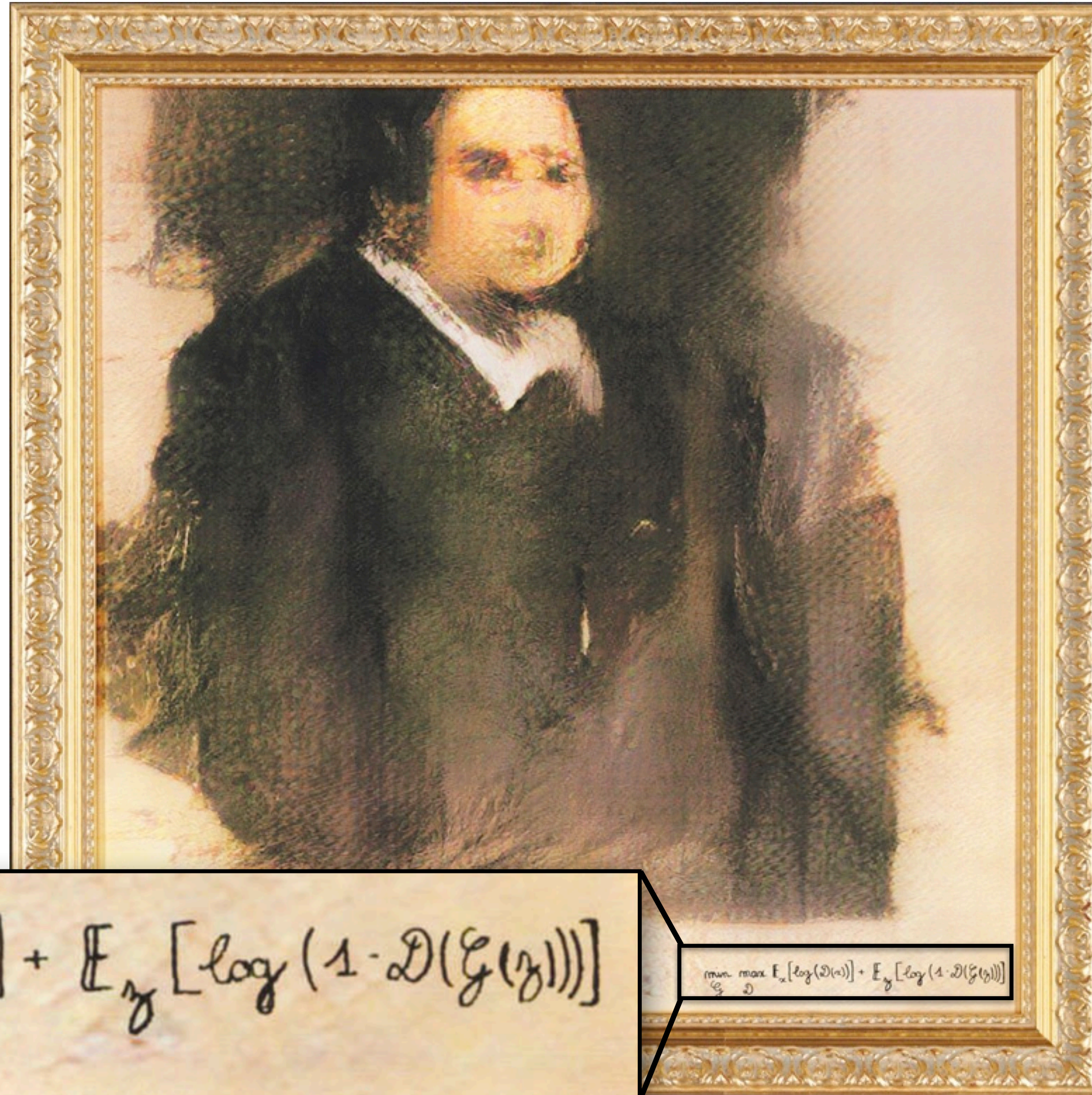
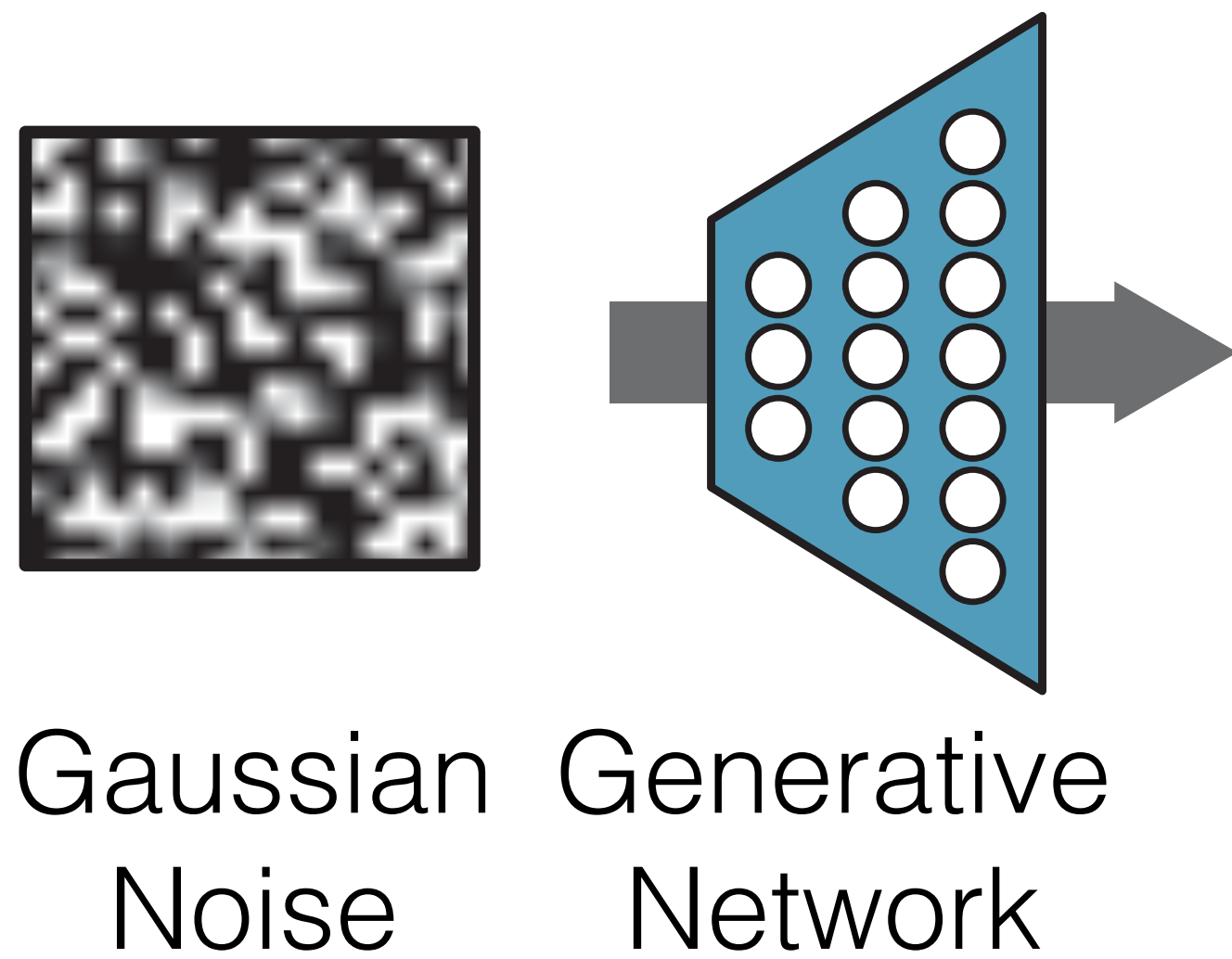
# Generated Arts



**\$432,500**  
**25 October 2018**  
**Christie's New York**



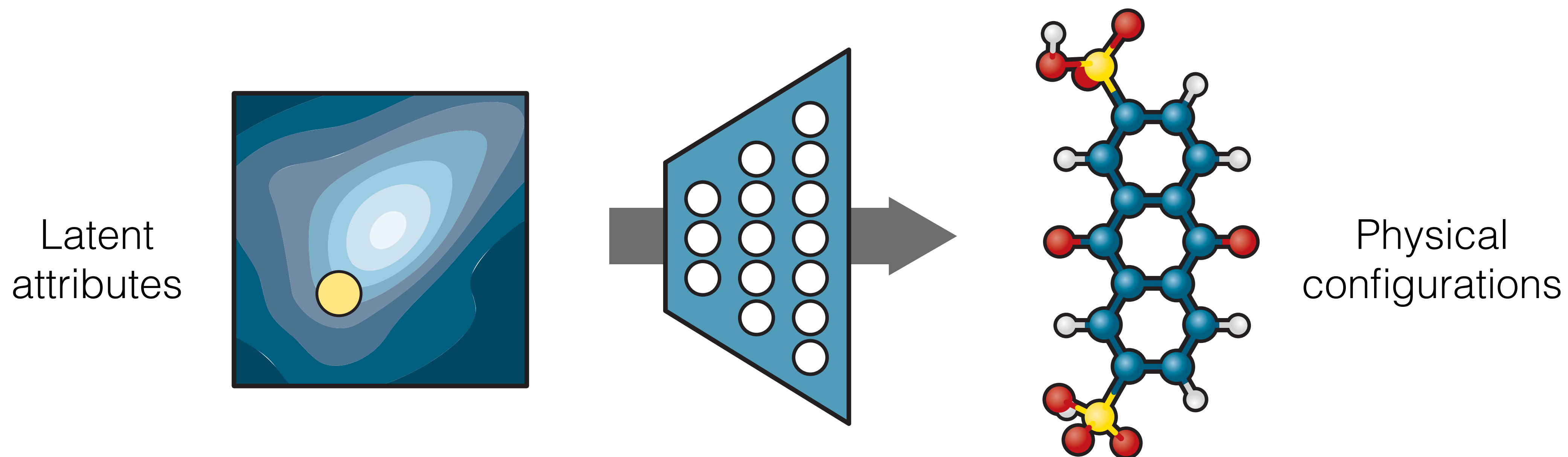
# Generated Arts



**\$432,500**  
**25 October 2018**  
**Christie's New York**



# Generating molecules



Math behind:  
**Probability  
Transformation**

Simple  
Distributions

Generate

Inference

Complex  
Distribution

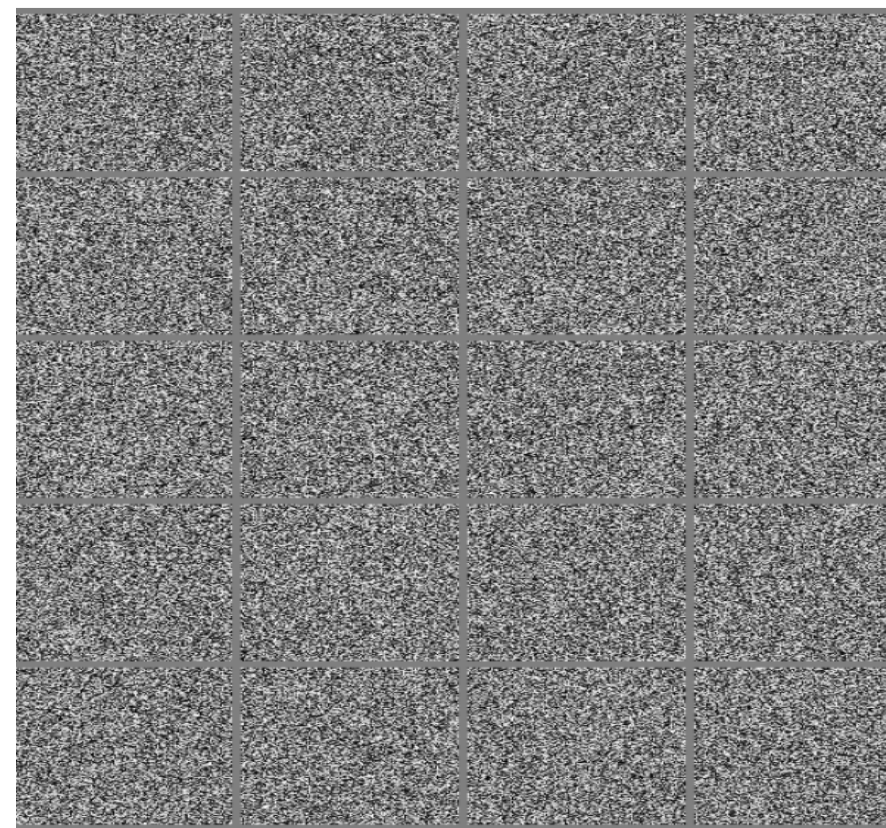
Sanchez-Lengeling & Aspuru-Guzik,  
Inverse molecular design using machine learning:  
Generative models for matter engineering, Science '18



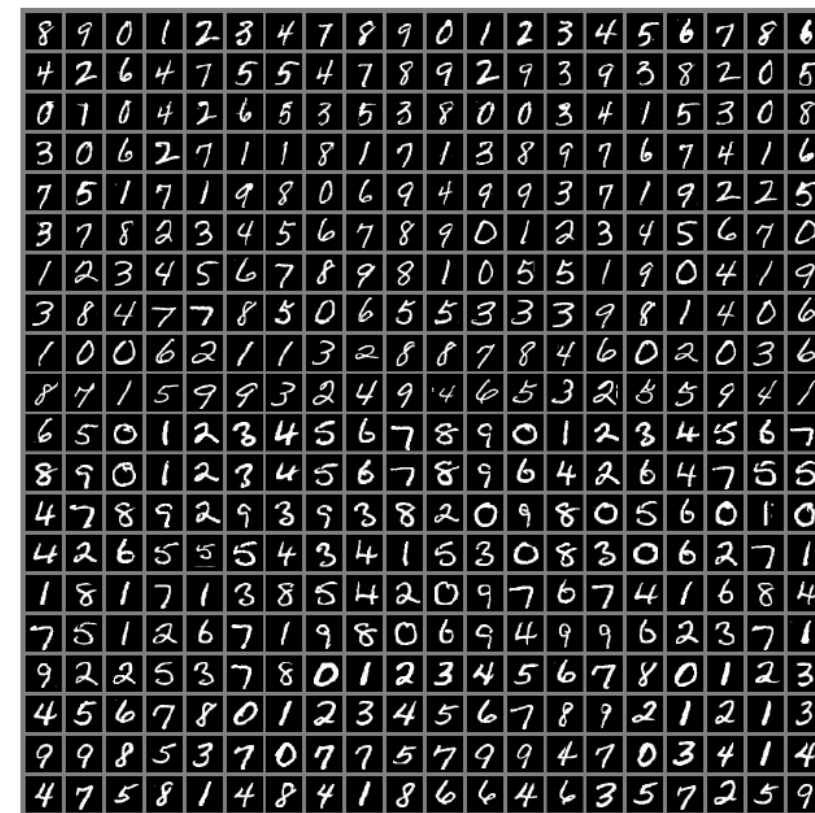
# Probabilistic Generative Modeling

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

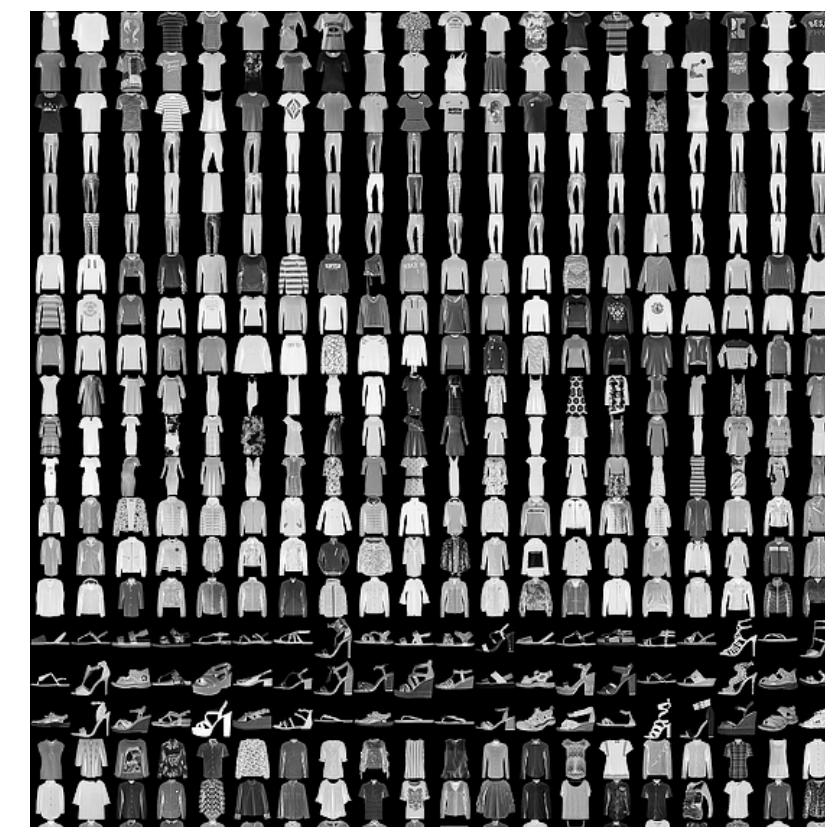
How to **express, learn, and sample** from a high-dimensional probability distribution ?



“random” images



“natural” images





# Probabilistic Modeling

## DEEP LEARNING

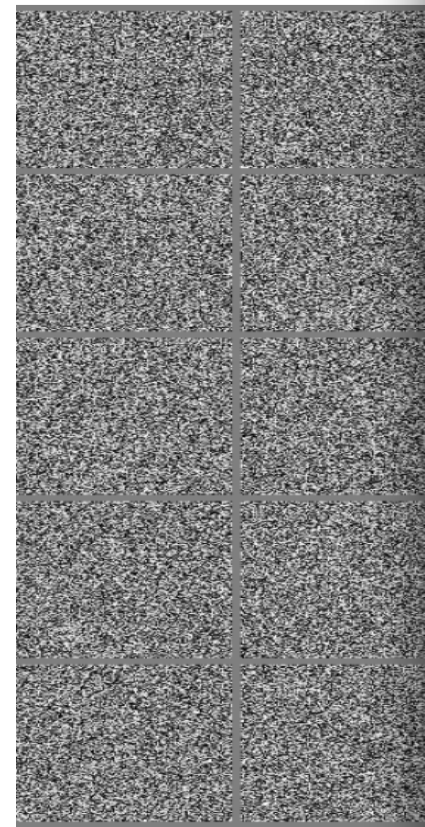
Ian Goodfellow, Yoshua Bengio,  
and Aaron Courville

How to learn from a high-dimensional distribution?

Page 159

*“... the images encountered in AI applications occupy a negligible proportion of the volume of image space.”*

“random

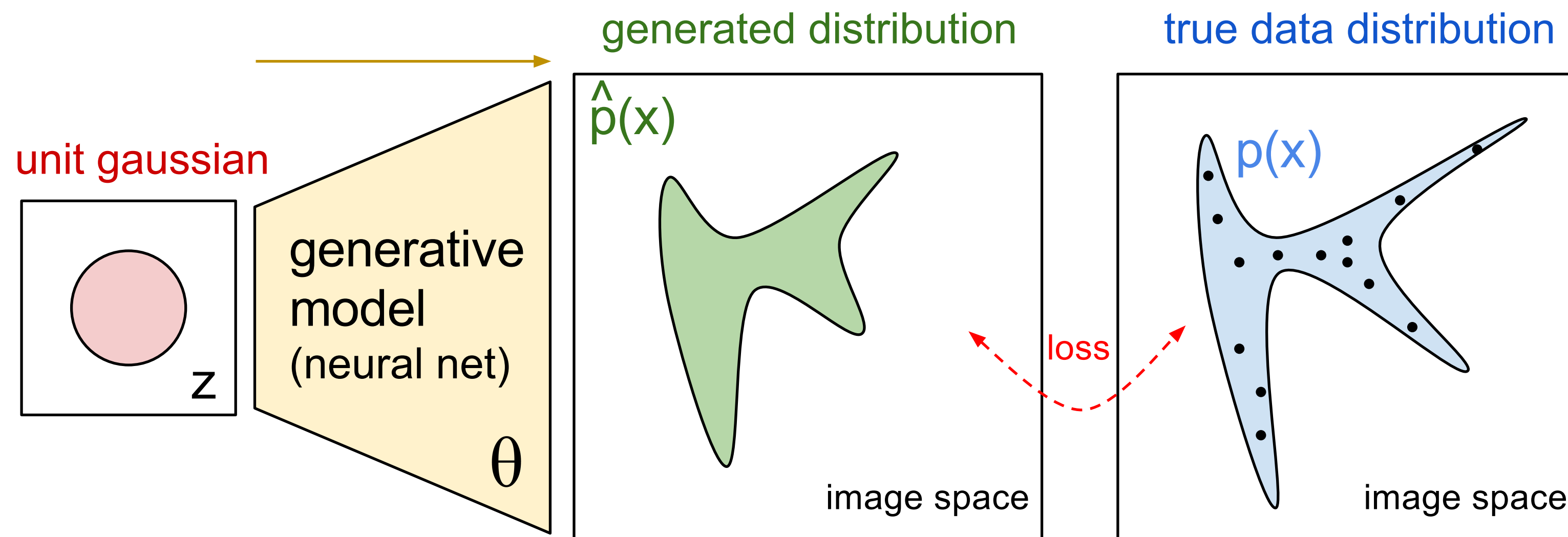




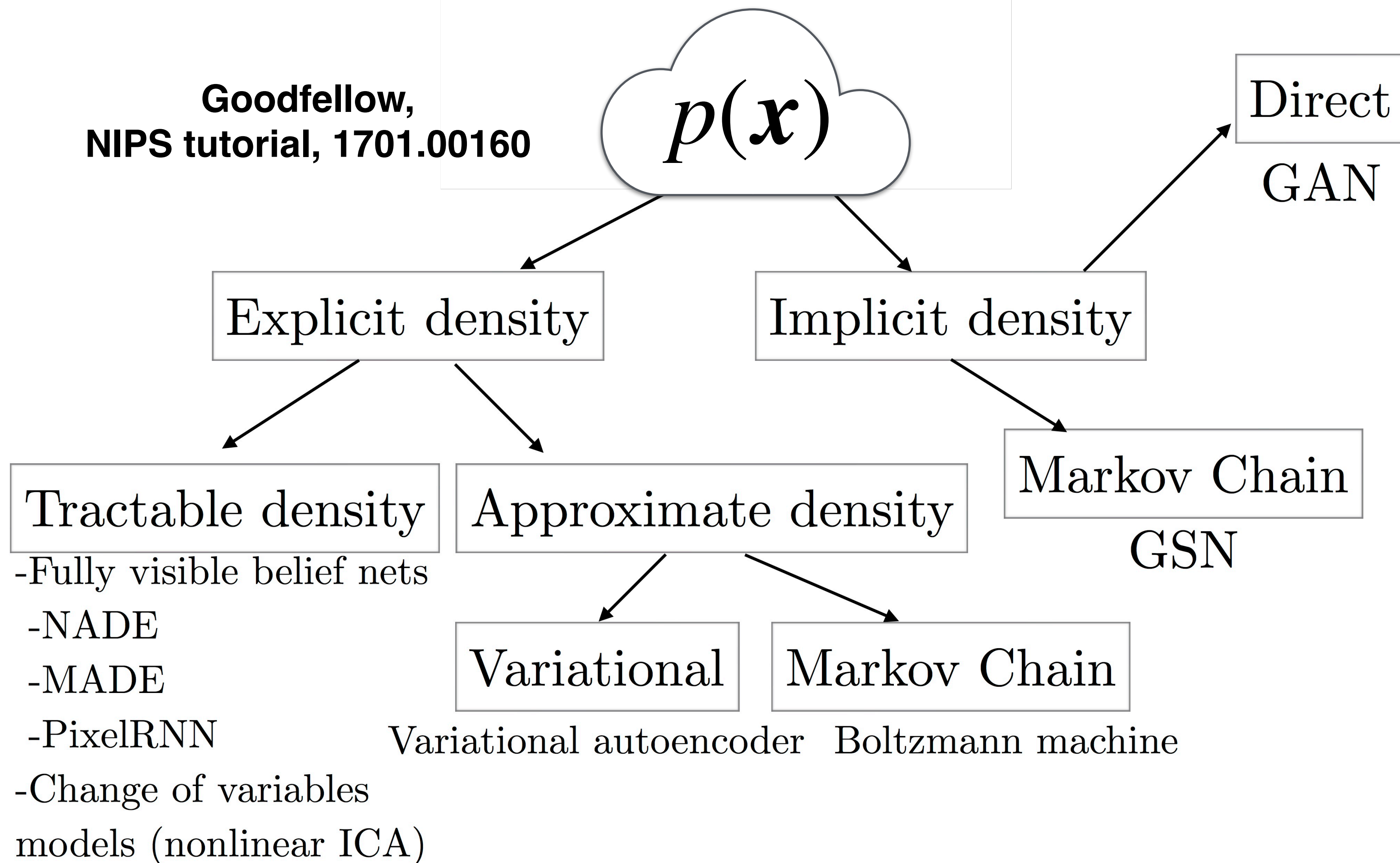
# Probabilistic Generative Modeling

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

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

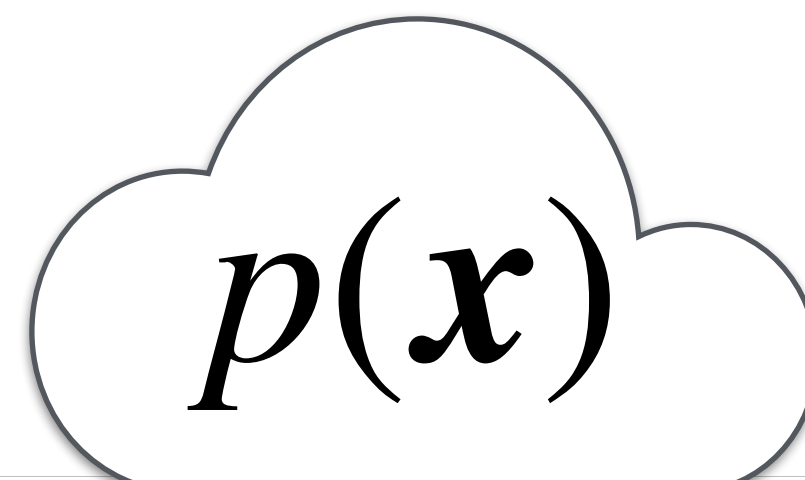


# Physics genes of generative models



# Physics genes of generative models

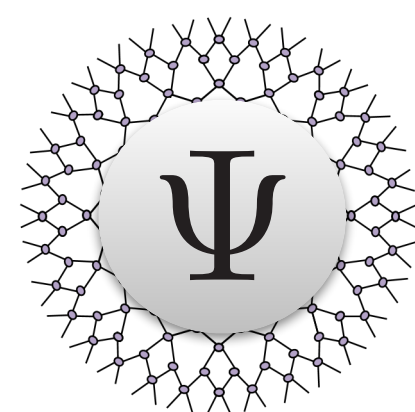
Goodfellow,  
NIPS tutorial, 1701.00160



Explicit density

Implicit density

Direct  
GAN



**Tensor  
Networks**

Tractable density

- Fully visible belief nets
- NADE
- MADE
- PixelRNN
- Change of variables  
models (nonlinear ICA)

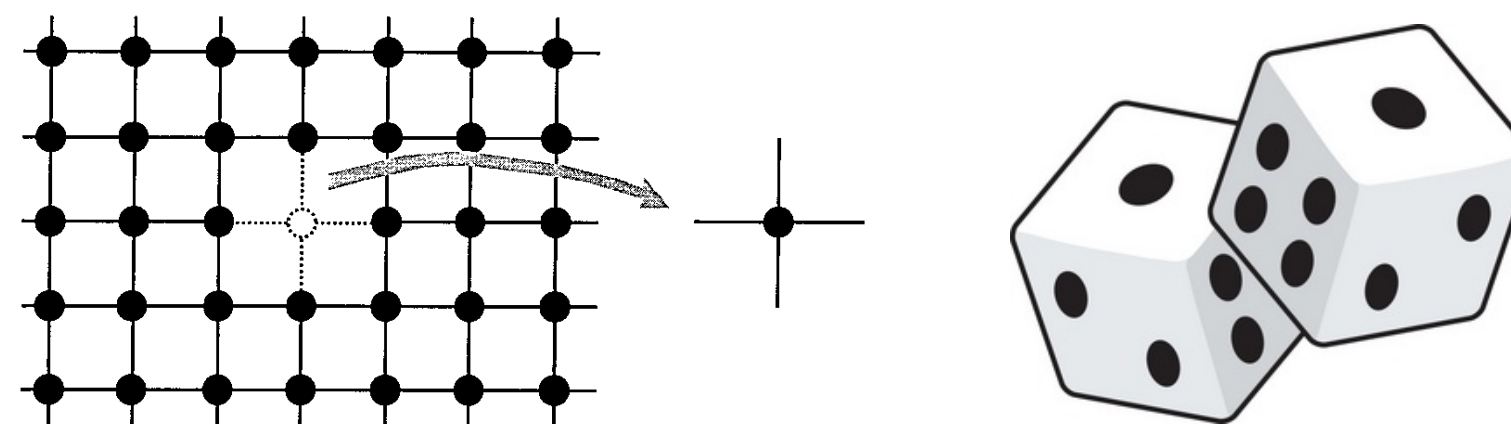
Approximate density

Variational

Variational autoencoder

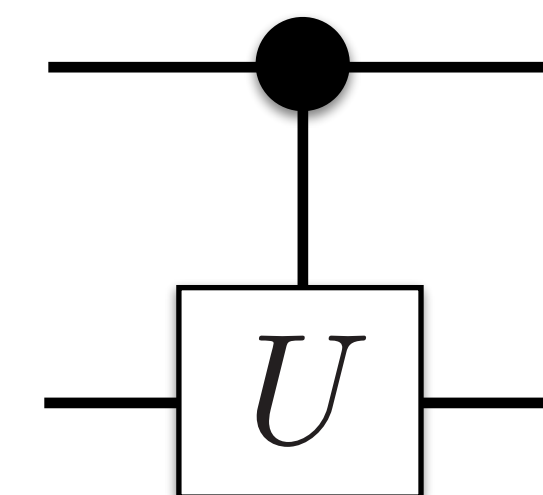
Markov Chain

Boltzmann machine



Markov Chain

GSN



**Quantum  
Circuits**

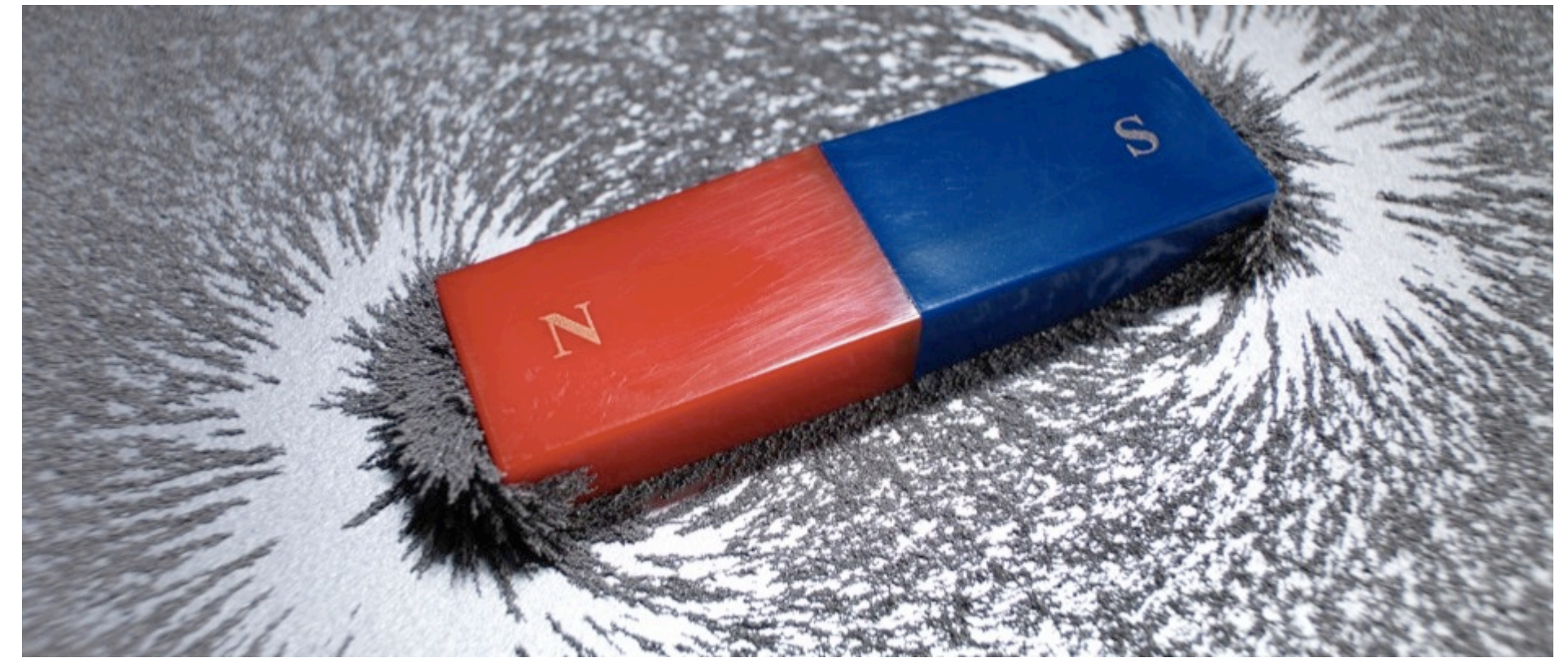


# Generative modeling



Known: samples  
Unknown: generating distribution

# Physics



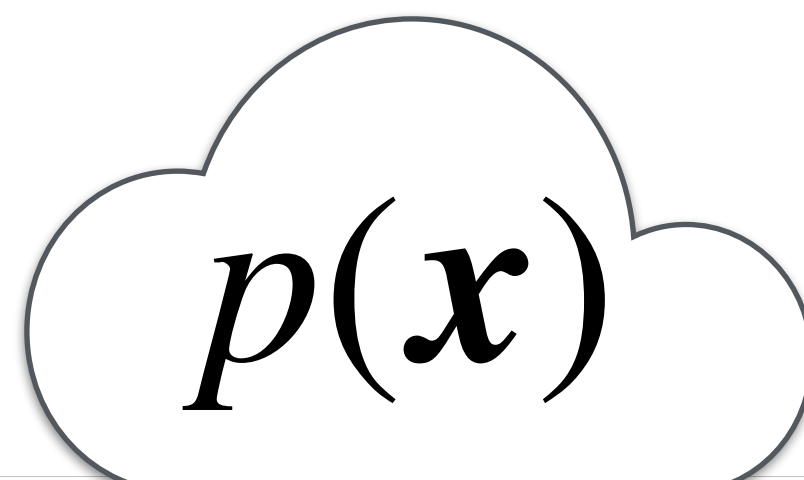
Known: energy function  
Unknown: samples, partition function

**Modern generative models for physics**  
**Physics of and for generative modeling**



# Physics genes of generative models

Goodfellow,  
NIPS tutorial, 1701.00160



Explicit density

Implicit density

Direct  
GAN

Tractable density

- Fully visible belief nets
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- MADE
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Approximate density

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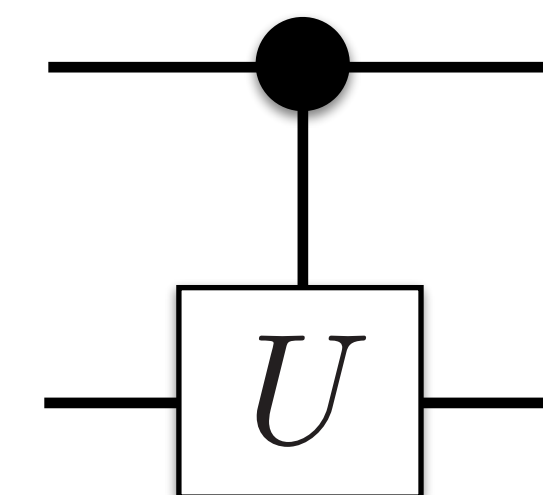
Variational autoencoder

Markov Chain

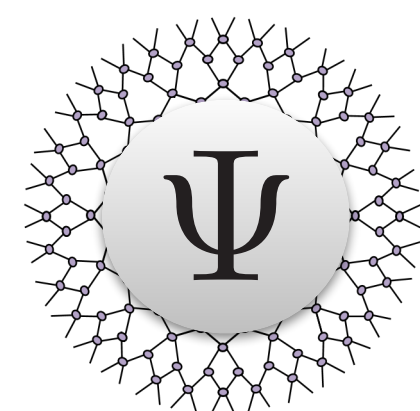
Boltzmann machine

Markov Chain

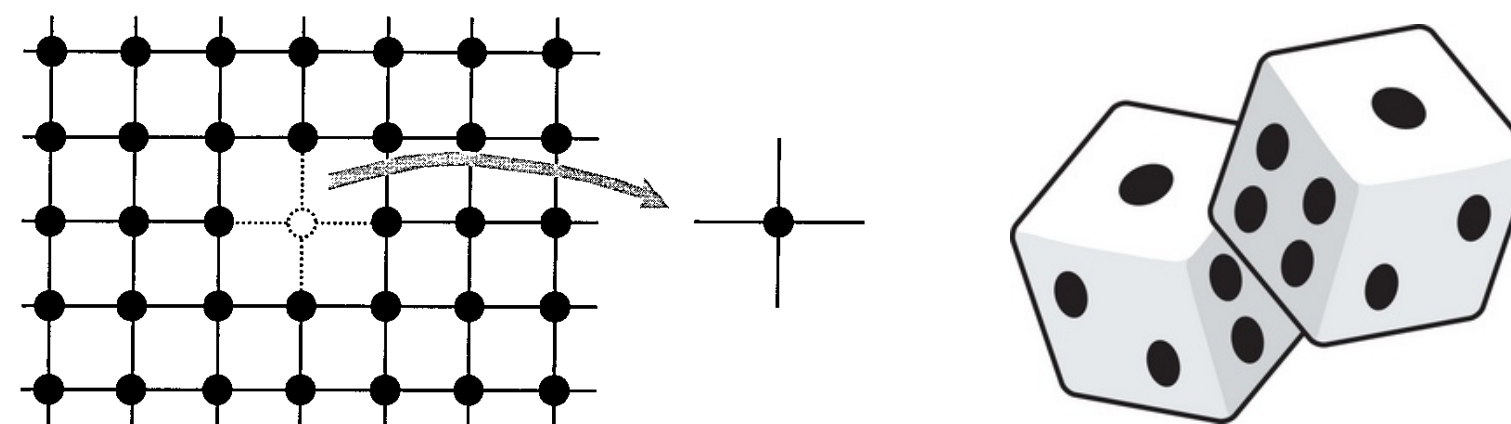
GSN



Quantum  
Circuits

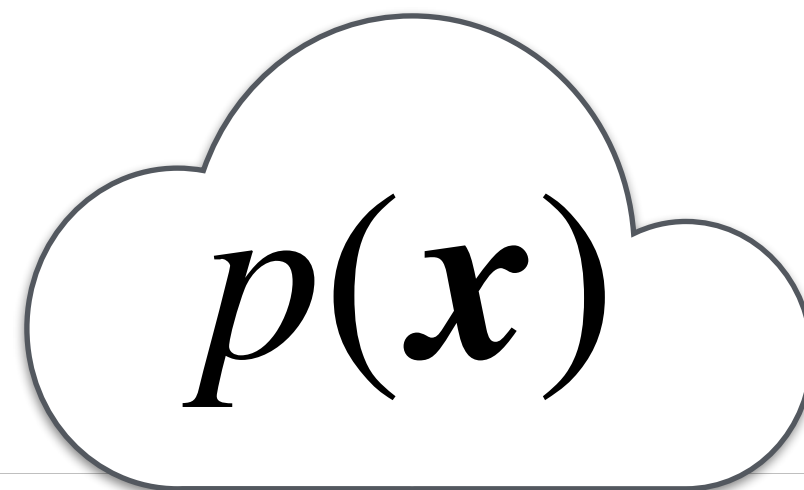


Tensor  
Networks



# Physics genes of generative models

Goodfellow,  
NIPS tutorial, 1701.00160



Explicit density

Implicit density

Direct  
GAN

Tractable density

- Fully visible belief nets
- NADE
- MADE
- PixelRNN

-Change of variables  
models (nonlinear ICA)

Approximate density

Variational

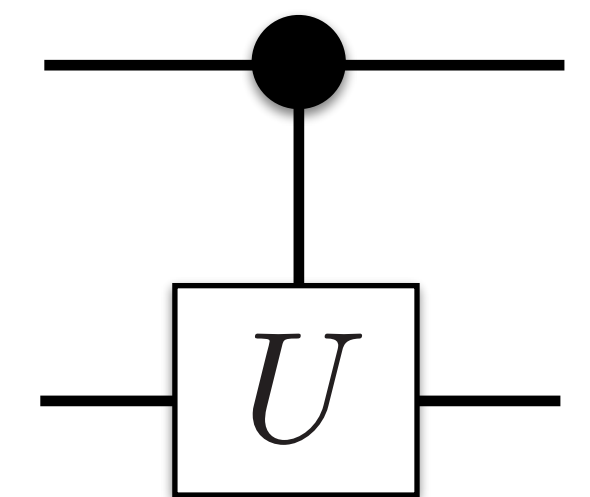
Variational autoencoder

Markov Chain

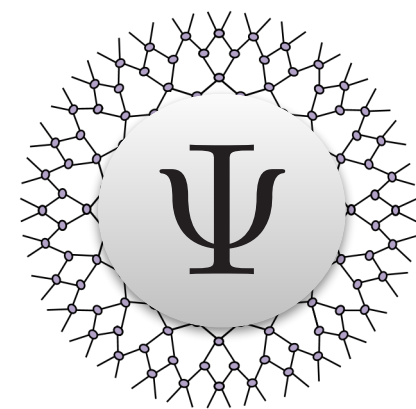
Boltzmann machine

Markov Chain

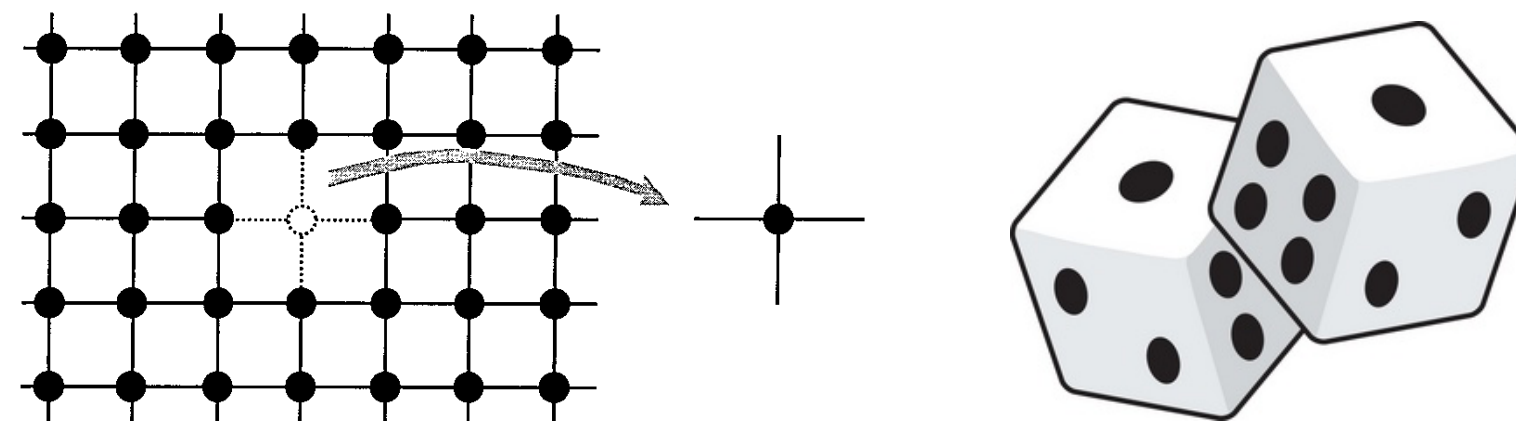
GSN



Quantum  
Circuits



Tensor  
Networks





# Generative Models for Physicists

Lei Wang\*

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

October 28, 2018

## Abstract

Generative models generate unseen samples according to a learned joint probability distribution in the high-dimensional space. They find wide applications in density estimation, variational inference, representation learning and more. Deep generative models and associated techniques (such as differentiable programming and representation learning) are cutting-edge technologies physicists can learn from deep learning.

This note introduces the concept and principles of generative modeling, together with applications of modern generative models (autoregressive models, normalizing flows, variational autoencoders etc) as well as the old ones (Boltzmann machines) to physics problems. As a bonus, this note puts some emphasize on physics-inspired generative models which take insights from statistical, quantum, and fluid mechanics.

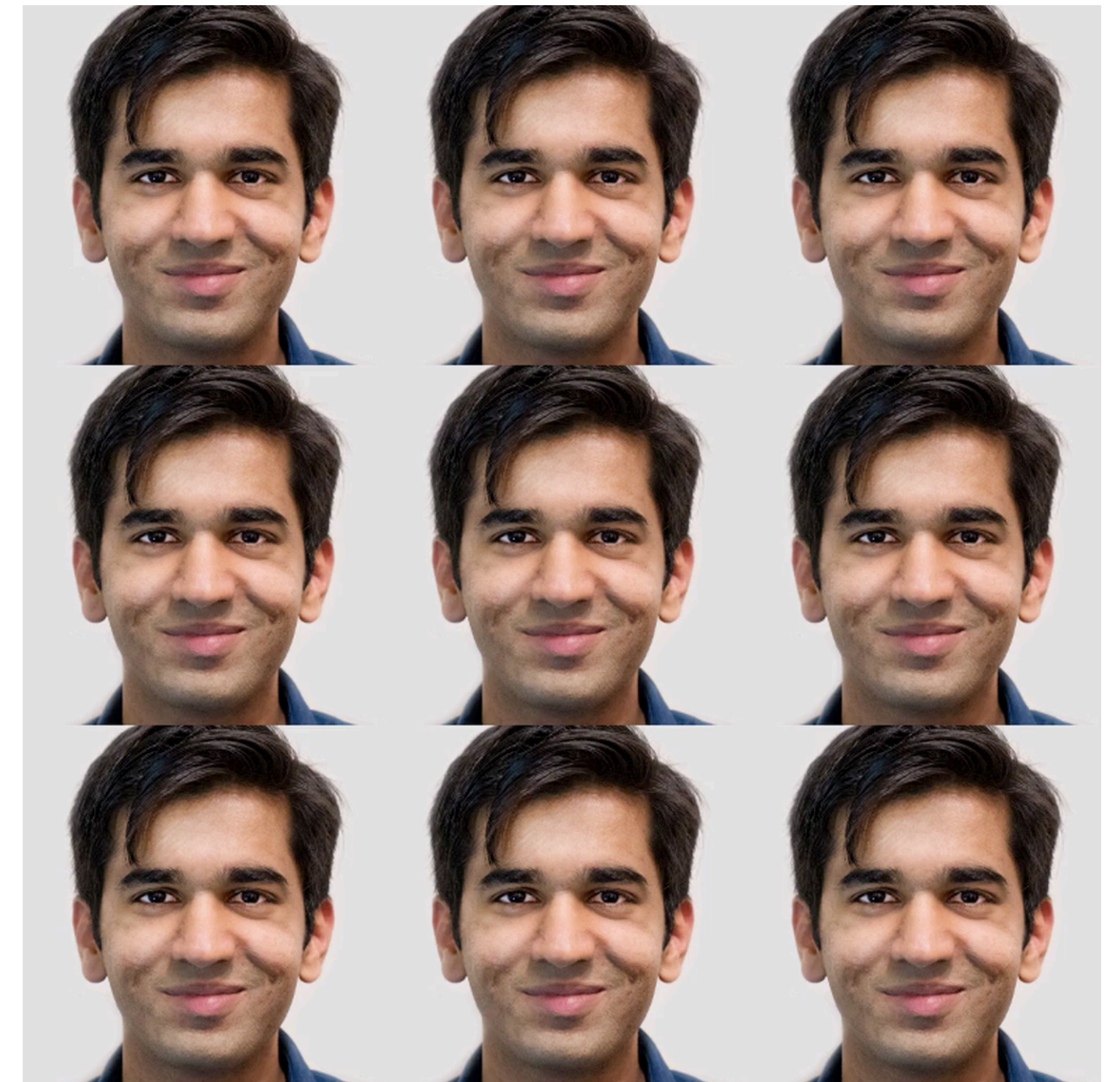
The latest version of the note is at <http://wangleiphy.github.io/>. Please send comments, suggestions and corrections to the email address in below.

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# Generative modeling with normalizing flows



Wavenet 1609.03499 1711.10433

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

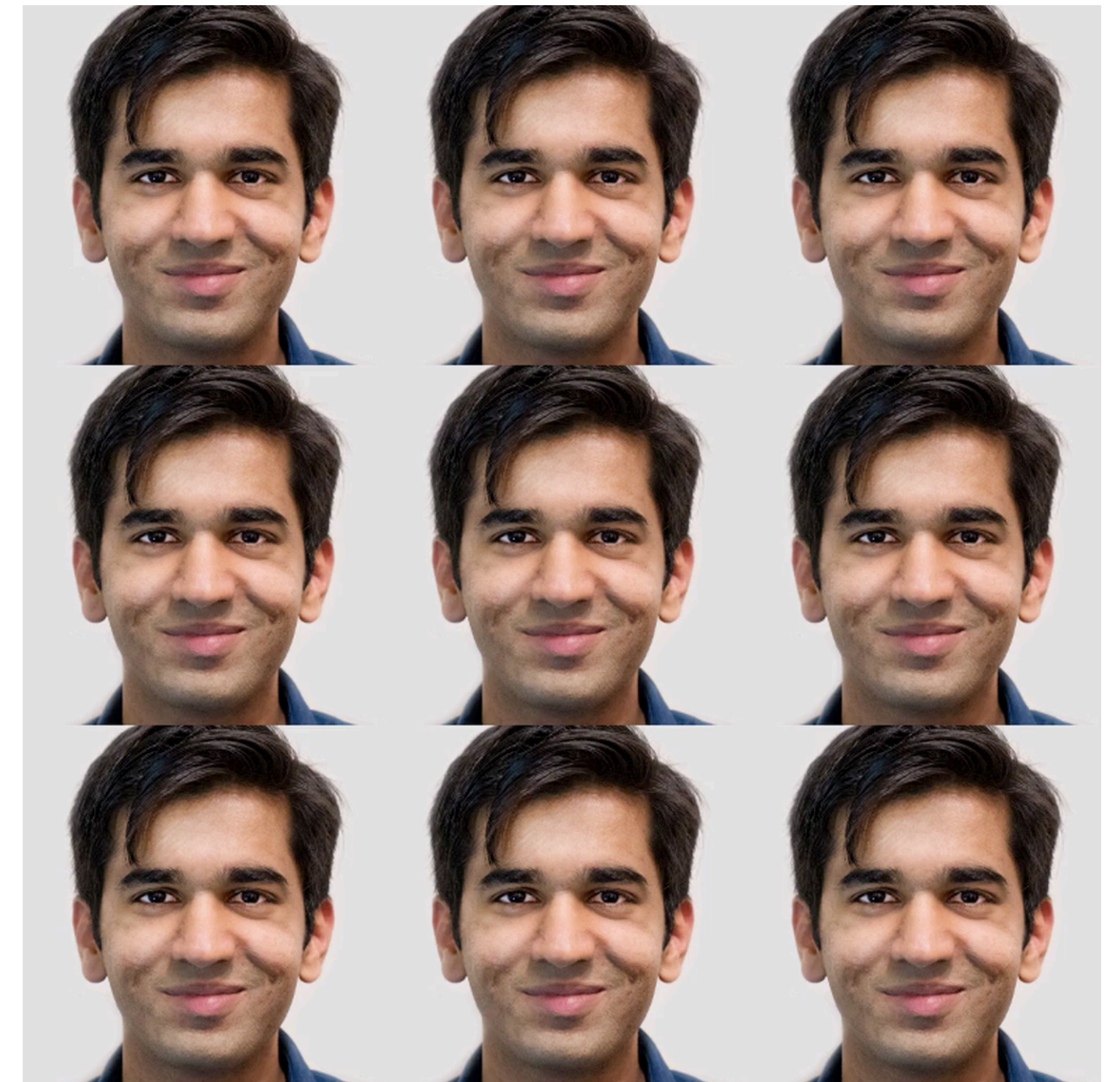


Glow 1807.03039

<https://blog.openai.com/glow/>



# Generative modeling with normalizing flows



Wavenet 1609.03499 1711.10433

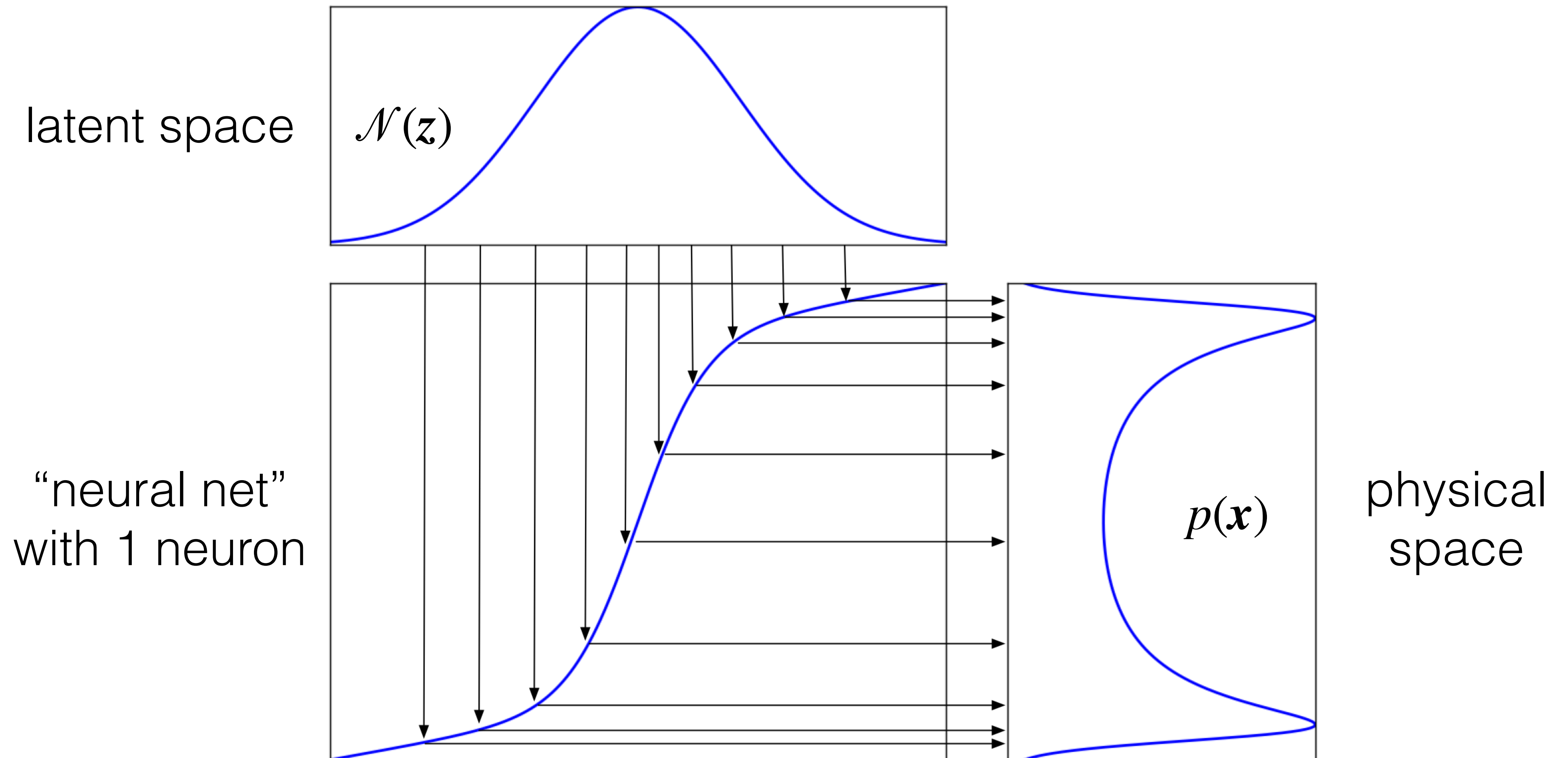
<https://deepmind.com/blog/wavenet-generative-model-raw-audio/>  
<https://deepmind.com/blog/high-fidelity-speech-synthesis-wavenet/>



Glow 1807.03039

<https://blog.openai.com/glow/>

# Normalizing flow in a nutshell



# Normalizing Flows

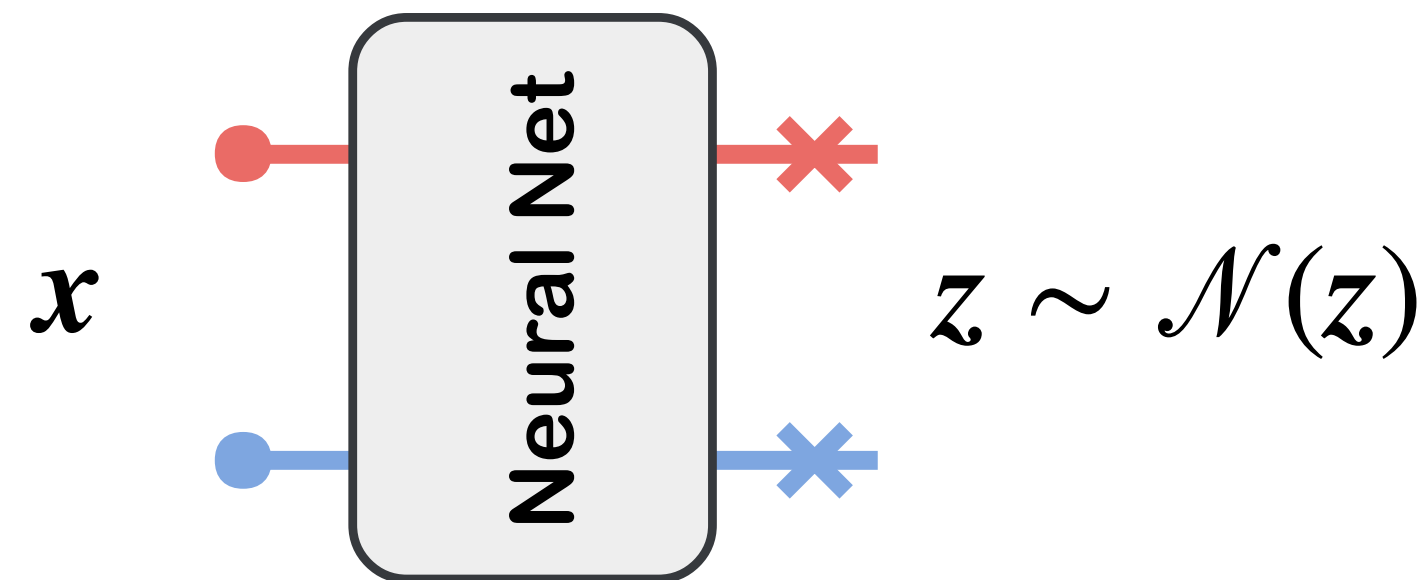
**Change of variables  $x \leftrightarrow z$  with deep neural nets**

$$p(x) = \mathcal{N}(z) \left| \det \left( \frac{\partial z}{\partial x} \right) \right|$$

**Review article** 1912.02762

**Tutorial** [https://iclr.cc/virtual\\_2020/speaker\\_4.html](https://iclr.cc/virtual_2020/speaker_4.html)

composable, differentiable, and invertible mapping between manifolds



**Learn probability transformations with normalizing flows**

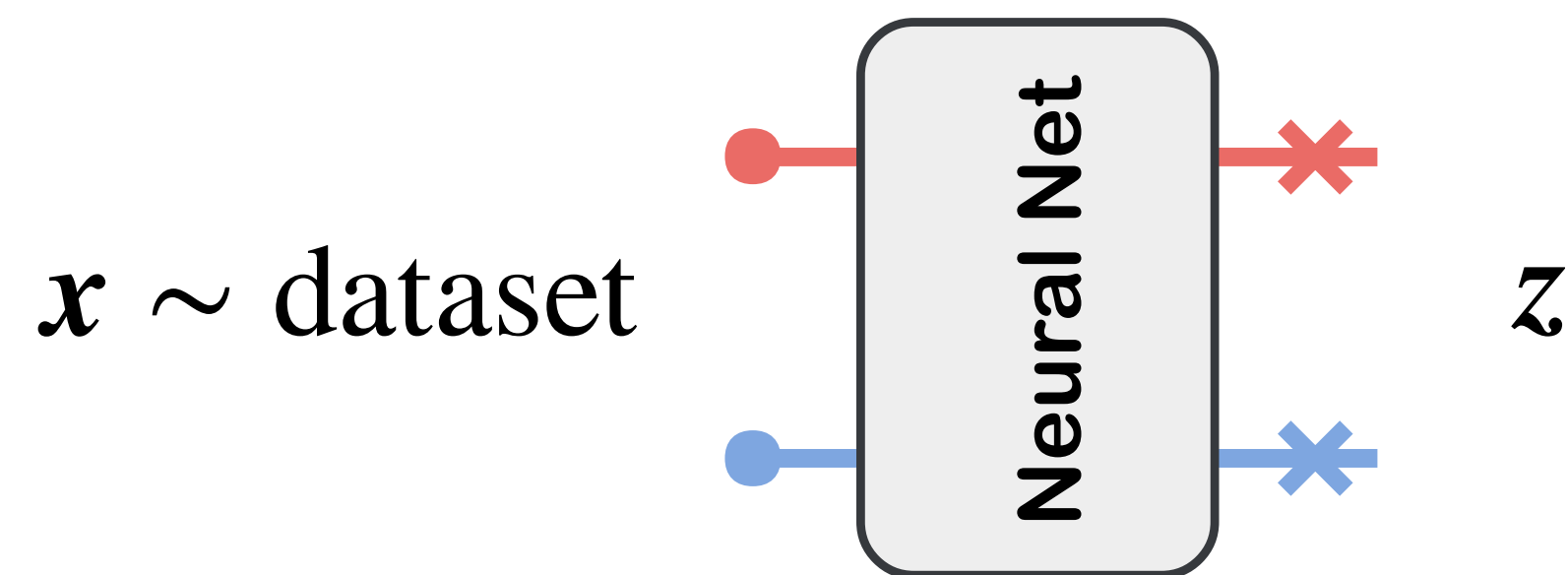


# Training approaches

## Density estimation

“learn from data”

$$\mathcal{L} = - \mathbb{E}_{\mathbf{x} \sim \text{dataset}} [\ln p(\mathbf{x})]$$

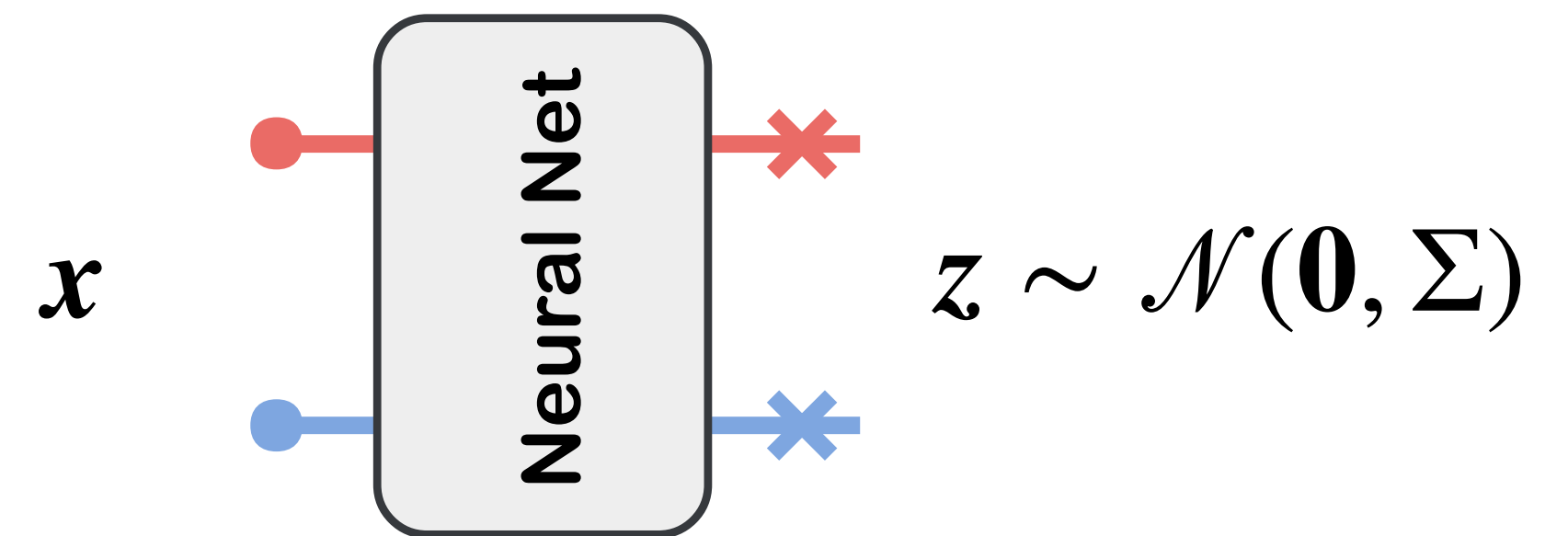


Sample from dataset in the physical space

## Variational calculation

“learn from Hamiltonian”

$$\mathcal{L} = \int d\mathbf{x} p(\mathbf{x}) [\ln p(\mathbf{x}) + \beta H(\mathbf{x})]$$



Sample in the latent space

# Training approaches

## Density estimation

“learn from data”

$$\mathcal{L} = - \mathbb{E}_{\mathbf{x} \sim \text{dataset}} [\ln p(\mathbf{x})]$$

$$\mathbb{KL}(\pi || p) = \sum_{\mathbf{x}} \pi \ln \pi - \underbrace{\sum_{\mathbf{x}} \pi \ln p}_{\mathcal{L}}$$

Sample from dataset in the physical space

## Variational calculation

“learn from Hamiltonian”

$$\mathcal{L} = \int d\mathbf{x} p(\mathbf{x}) [\ln p(\mathbf{x}) + \beta H(\mathbf{x})]$$

$$\mathcal{L} + \ln Z = \mathbb{KL} \left( p || \frac{e^{-\beta H}}{Z} \right) \geq 0$$

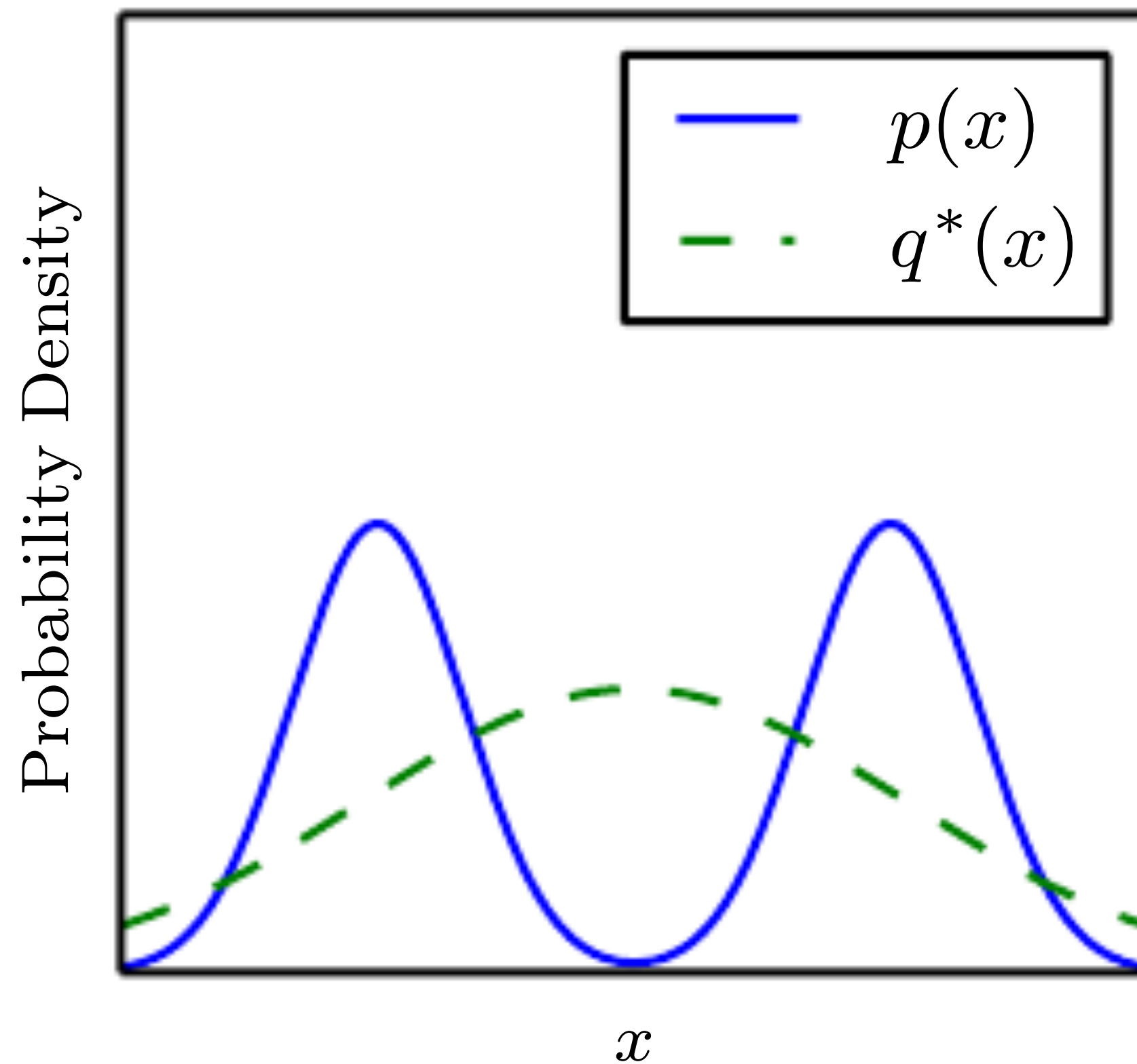
Sample in the latent space



# Forward KL or Reverse KL ?

## Maximum Likelihood Estimation

$$q^* = \operatorname{argmin}_q D_{\text{KL}}(p||q)$$



## Variational Free Energy

$$q^* = \operatorname{argmin}_q D_{\text{KL}}(q||p)$$

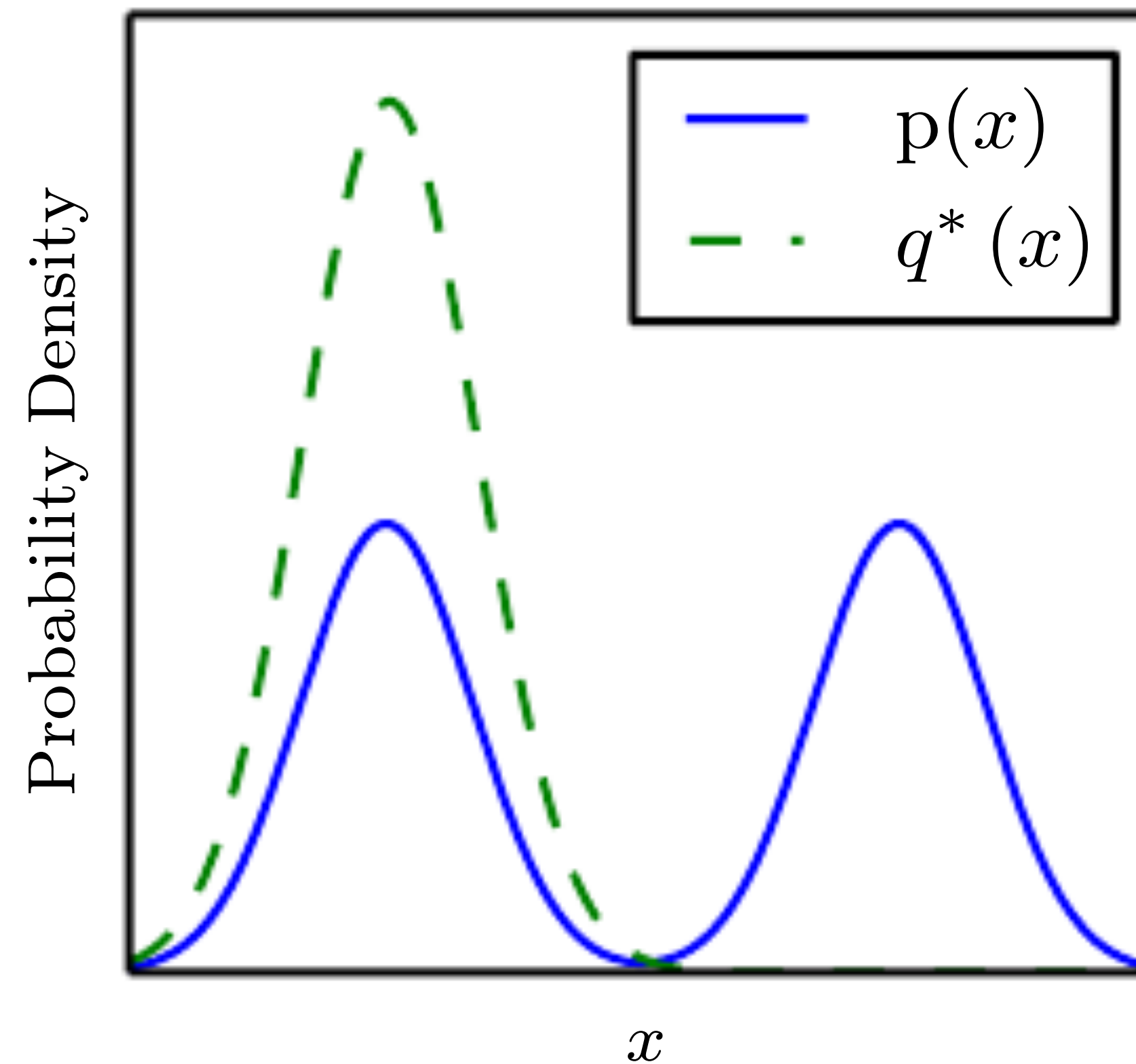


Fig. 3.6, Goodfellow, Bengio, Courville, <http://www.deeplearningbook.org/>

# Monte Carlo Gradient Estimators

**Review: 1906.10652**

$$\nabla_{\theta} \mathbb{E}_{\mathbf{x} \sim p_{\theta}} [f(\mathbf{x})]$$

Reinforcement learning  
Variational inference  
Variational Monte Carlo  
Variational quantum algorithms  
...

Score function estimator (REINFORCE)

$$\nabla_{\theta} \mathbb{E}_{\mathbf{x} \sim p_{\theta}} [f(\mathbf{x})] = \mathbb{E}_{\mathbf{x} \sim p_{\theta}} [f(\mathbf{x}) \nabla_{\theta} \ln p_{\theta}(\mathbf{x})]$$

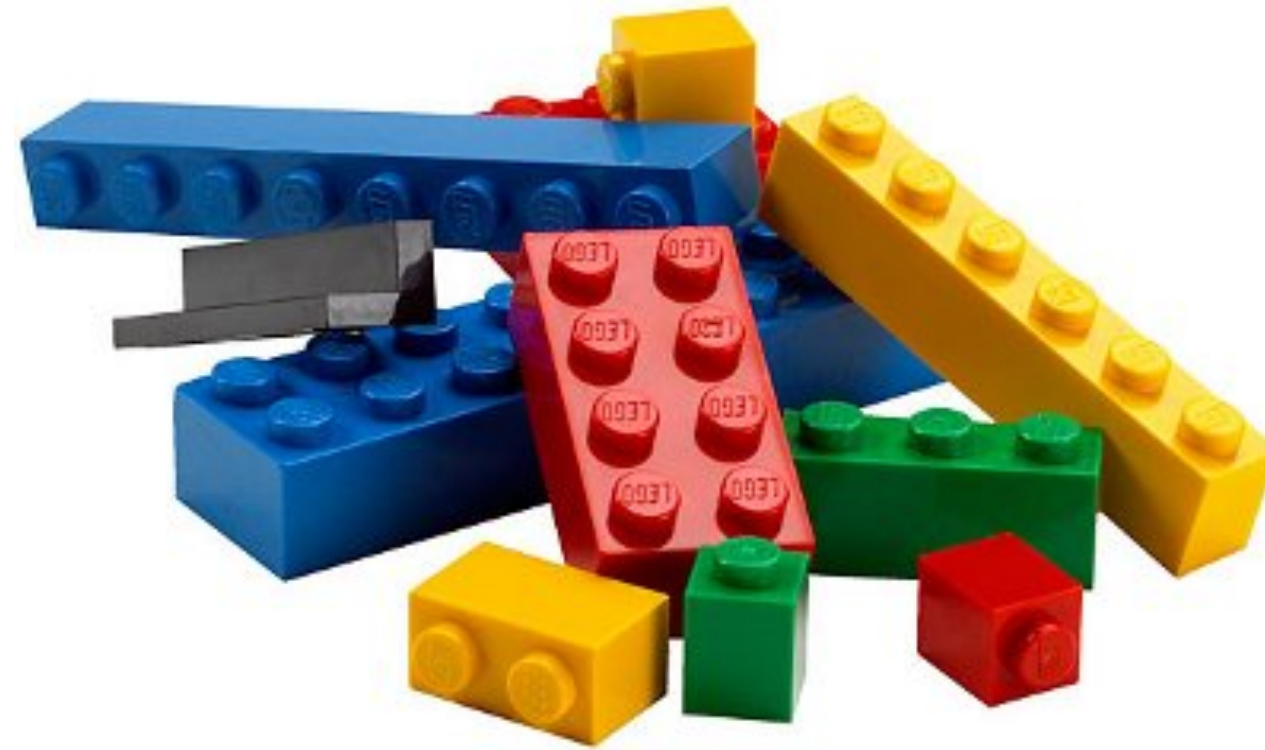
Pathwise estimator (Reparametrization trick)  $\mathbf{x} = g_{\theta}(\mathbf{z})$

$$\nabla_{\theta} \mathbb{E}_{\mathbf{x} \sim p_{\theta}} [f(\mathbf{x})] = \mathbb{E}_{\mathbf{z} \sim \mathcal{N}(\mathbf{z})} [\nabla_{\theta} f(g_{\theta}(\mathbf{z}))]$$

**Choose the one with the lowest variance**

# Design principles

**Composability**

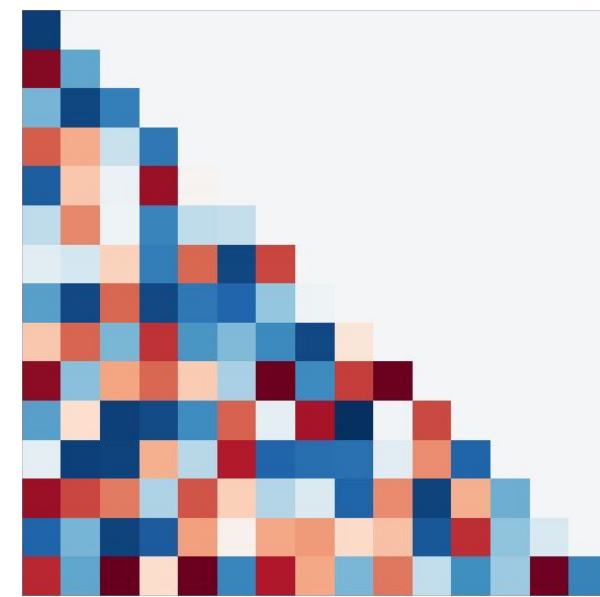


$$\mathbf{z} = \mathcal{T}(\mathbf{x})$$

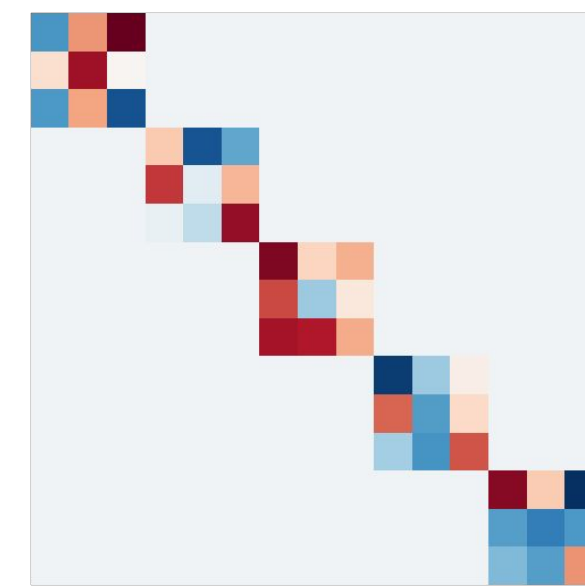
$$\mathcal{T} = \mathcal{T}_1 \circ \mathcal{T}_2 \circ \mathcal{T}_3 \circ \dots$$

**Balanced  
efficiency &  
inductive bias**

$$\left| \det \left( \frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) \right|$$



Autoregressive



Neural RG

$$\frac{\partial \rho(\mathbf{x}, t)}{\partial t} + \nabla \cdot [\rho(\mathbf{x}, t) \mathbf{v}] = 0$$


Continuous flow

# Example of a building block

Forward

$$\begin{cases} \mathbf{x}_{<} = \mathbf{z}_{<} \\ \mathbf{x}_{>} = \mathbf{z}_{>} \odot e^{s(\mathbf{z}_{<})} + t(\mathbf{z}_{<}) \end{cases}$$

arbitrary  
neural nets

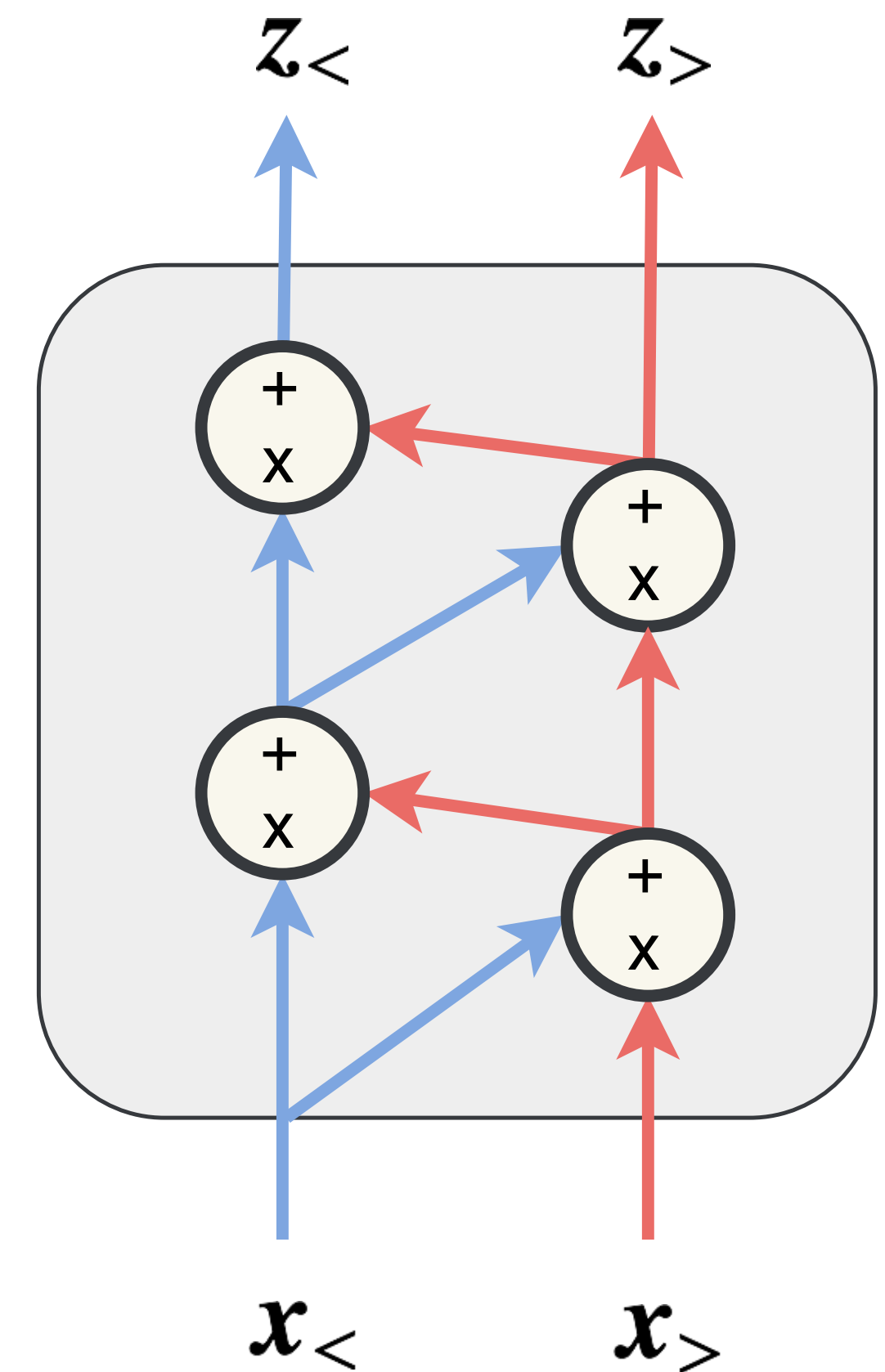


Inverse

$$\begin{cases} \mathbf{z}_{<} = \mathbf{x}_{<} \\ \mathbf{z}_{>} = (\mathbf{x}_{>} - t(\mathbf{x}_{<})) \odot e^{-s(\mathbf{x}_{<})} \end{cases}$$

Log-Abs-Jacobian-Det

$$\ln \left| \det \left( \frac{\partial \mathbf{x}}{\partial \mathbf{z}} \right) \right| = \sum_i [s(\mathbf{z}_{<})]_i$$

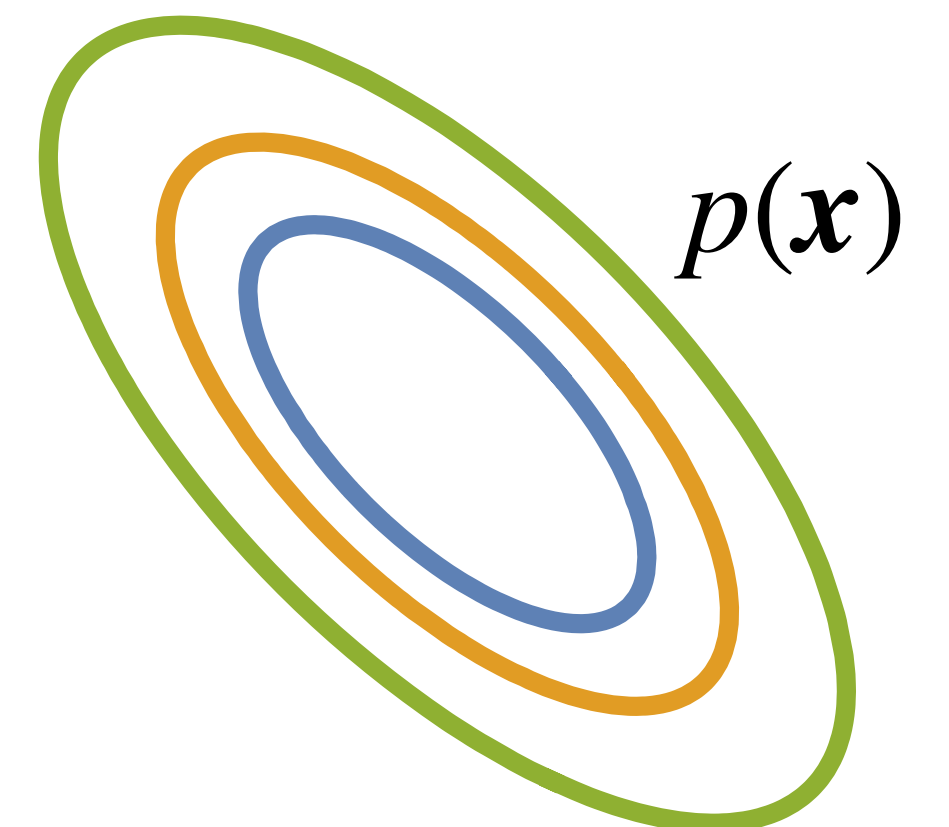
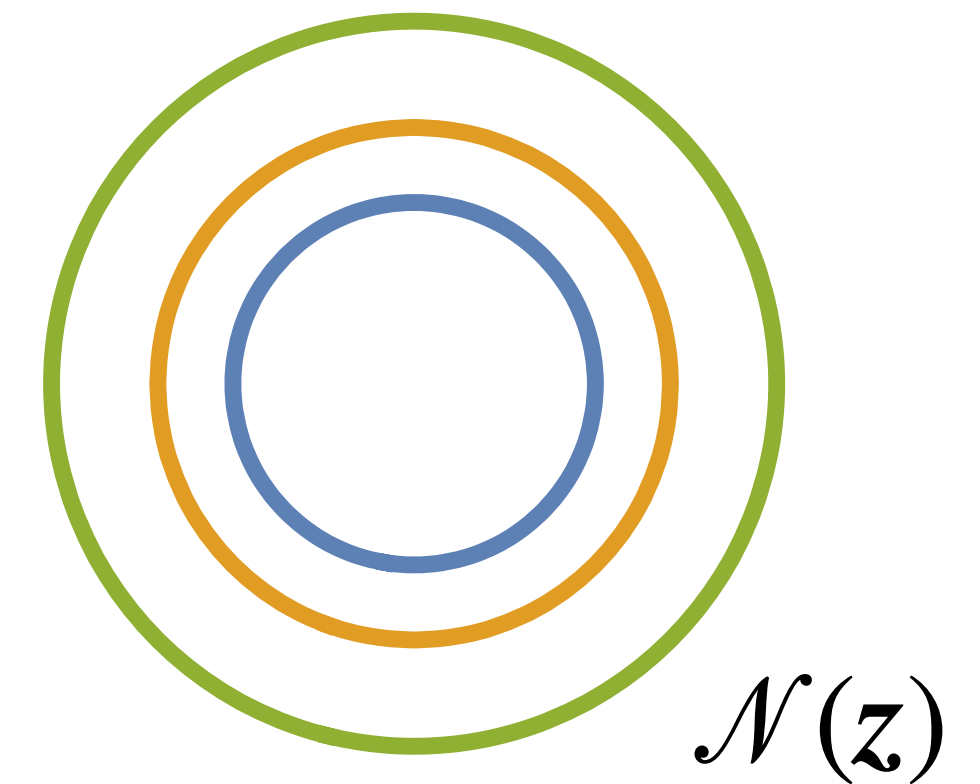
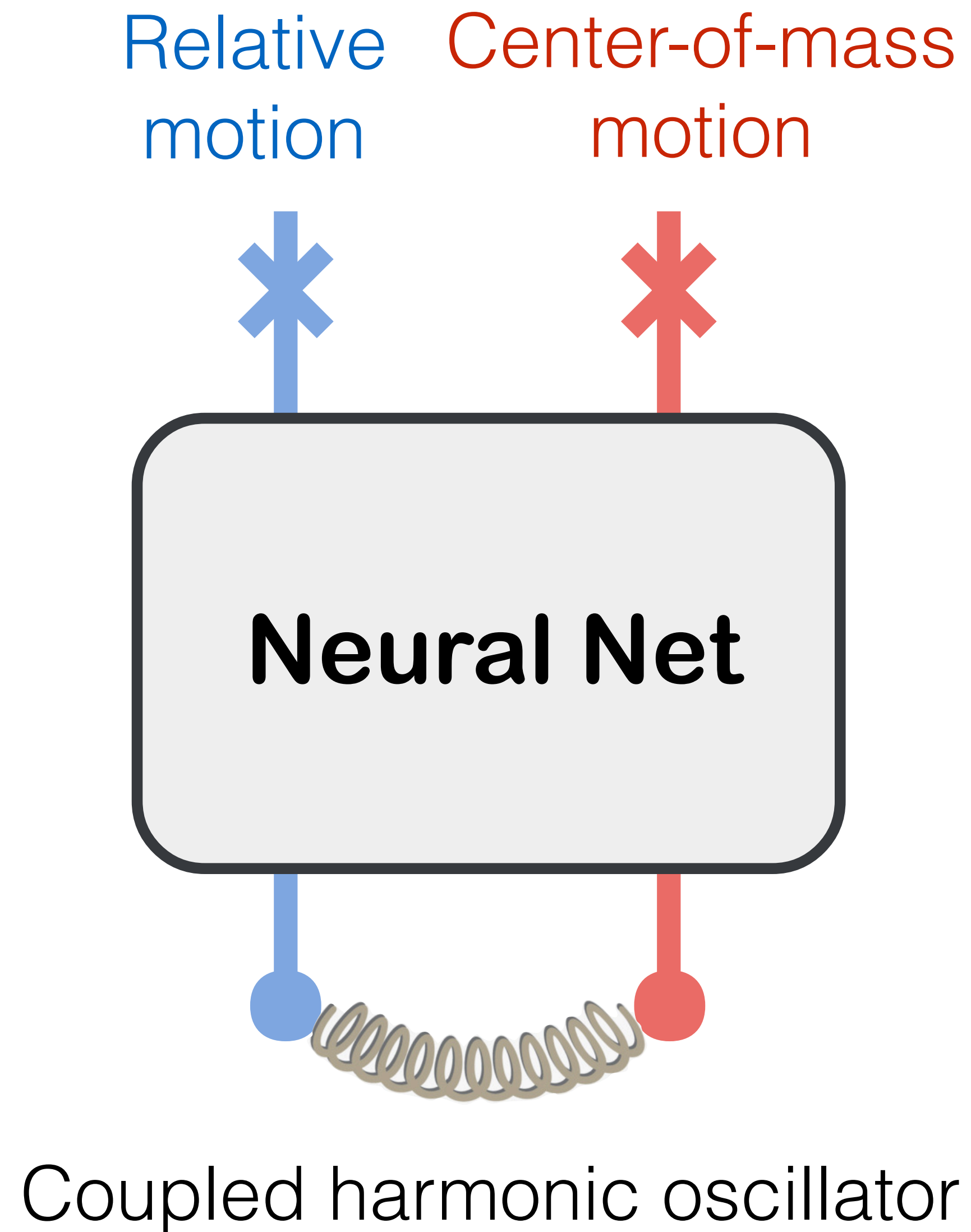


Real NVP, Dinh et al, 1605.08803

Turns out to have surprising connection Störmer–Verlet integration (later)

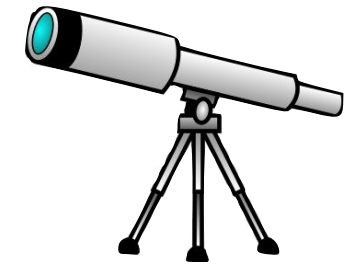


# How it can be useful in physics ?

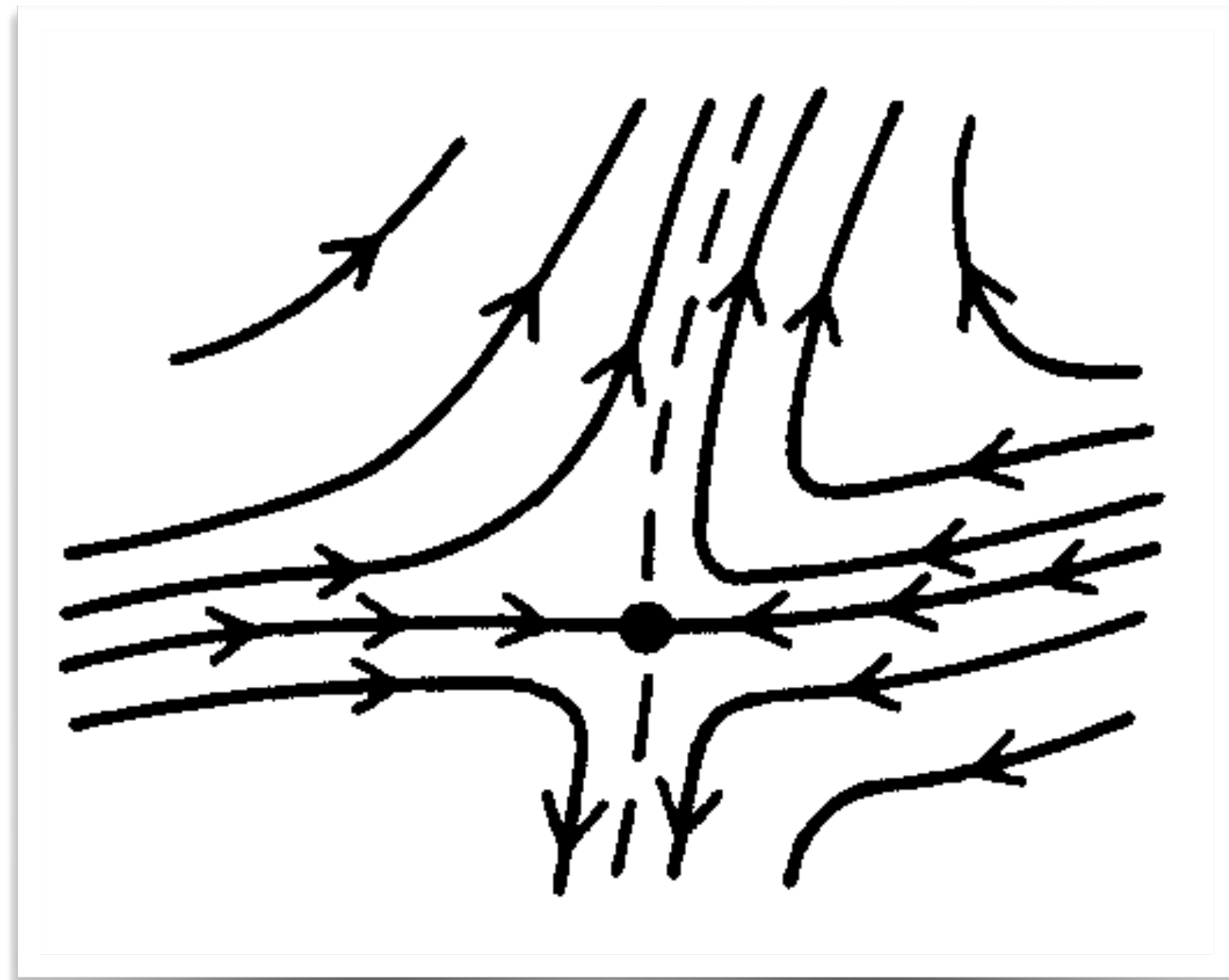




# How it can be useful in physics ?



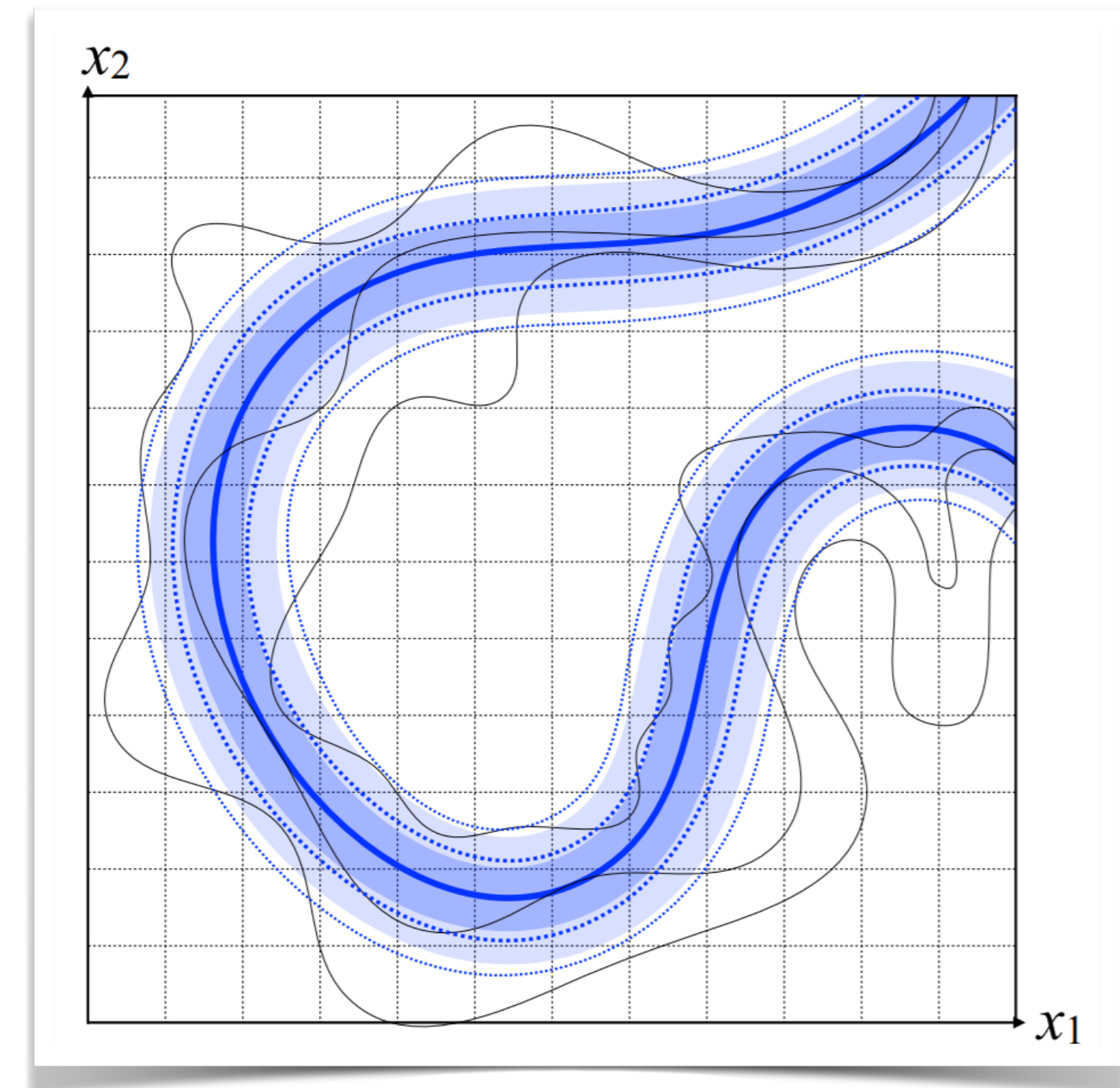
**Renormalization group**



Effective theory emerges upon transformation of the variables



**Monte Carlo update**



Physics happens on a manifold  
Learn neural nets to unfold that manifold

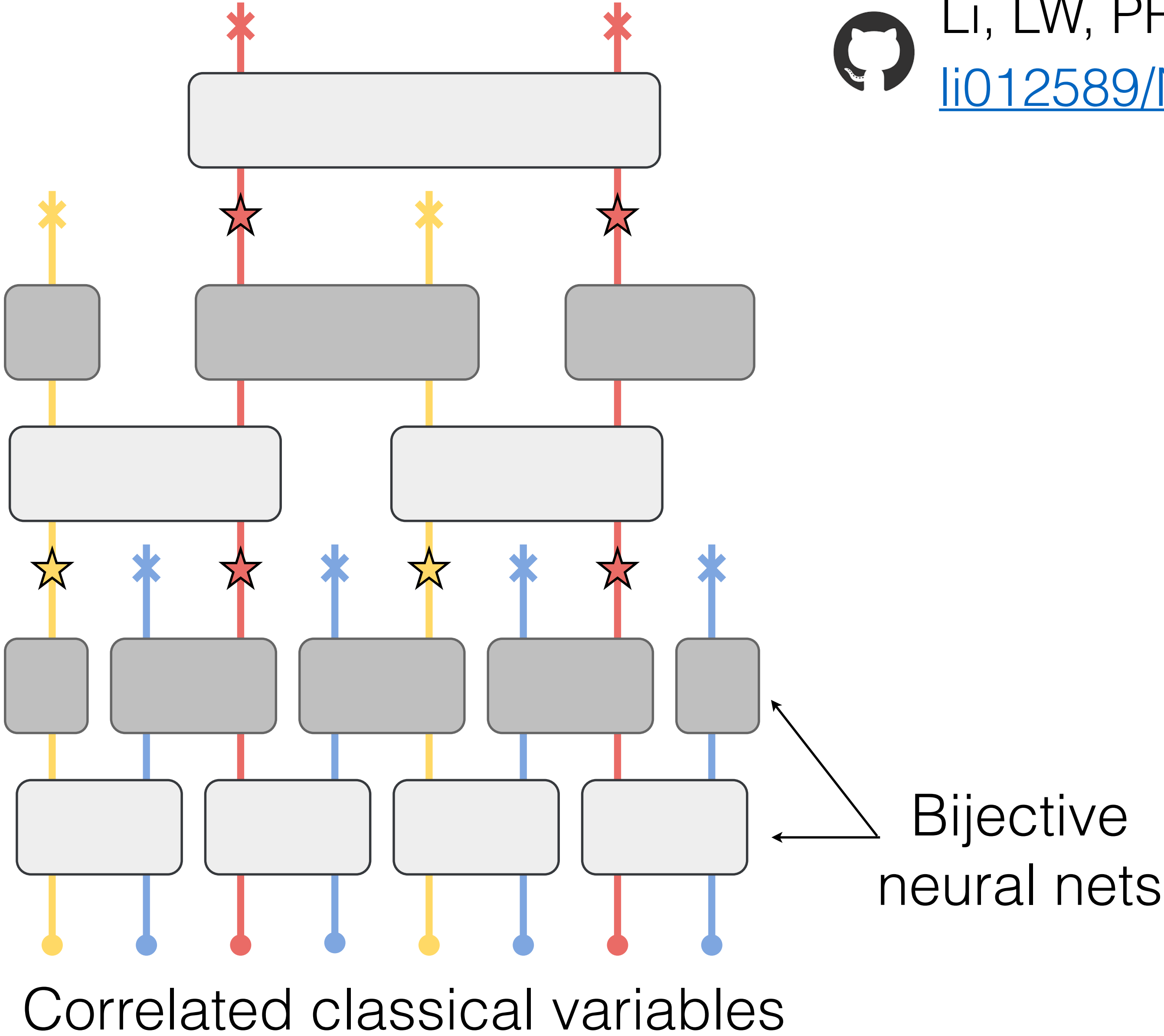


# Neural Network Renormalization Group



Li, LW, PRL '18

[li012589/NeuralRG](https://github.com/li012589/NeuralRG)



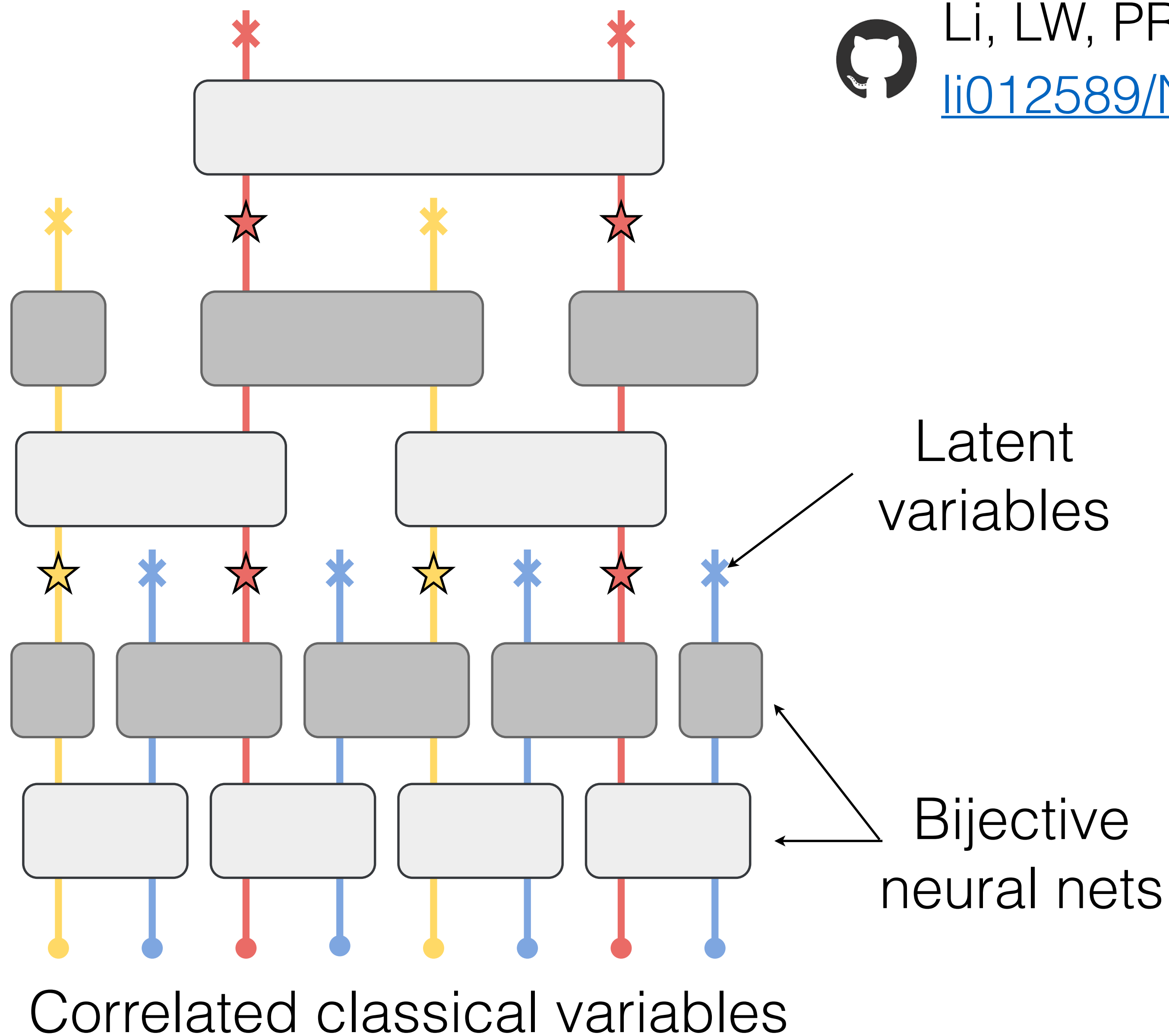


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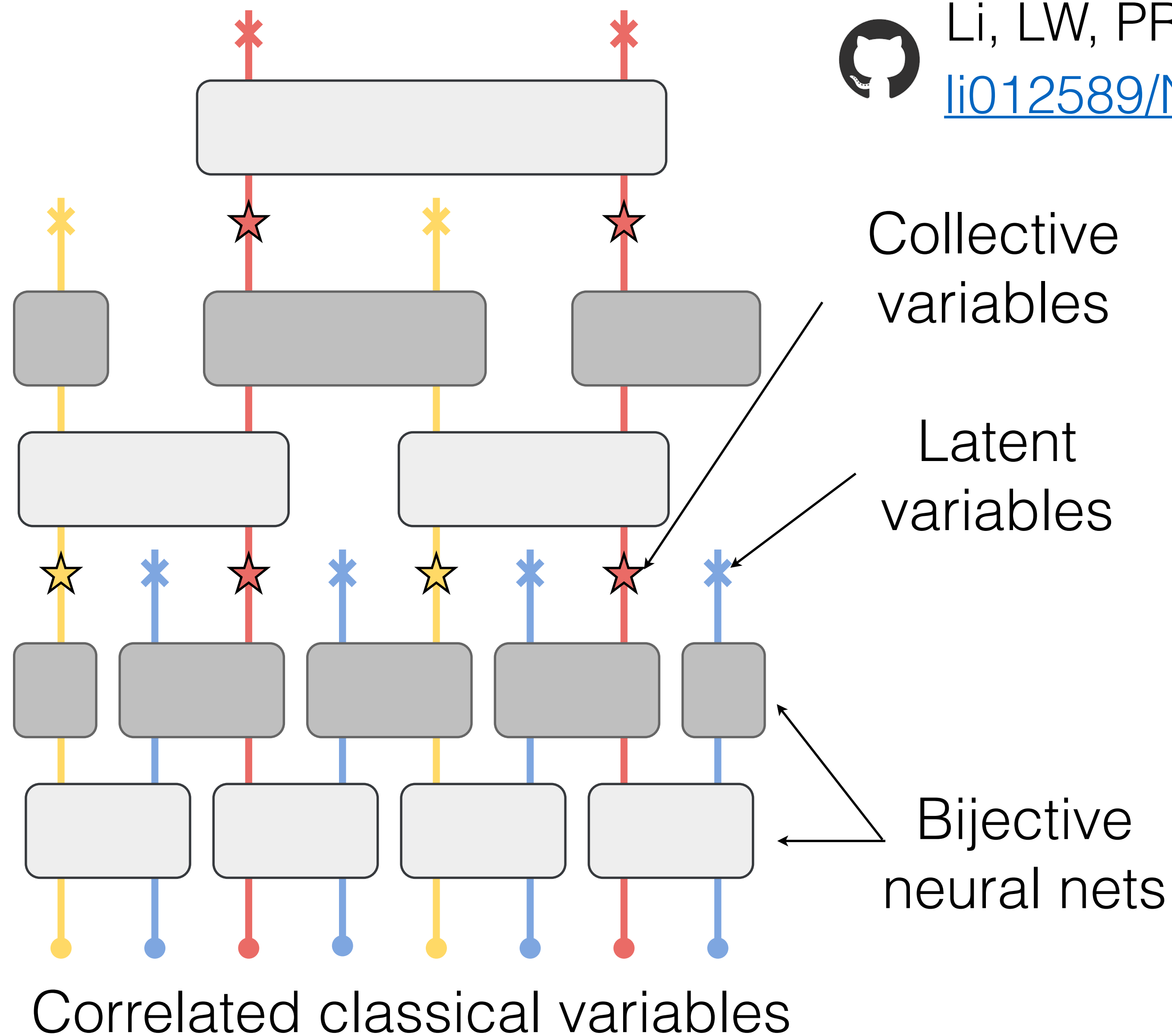


# Neural Network Renormalization Group



Li, LW, PRL '18

[li012589/NeuralRG](https://github.com/li012589/NeuralRG)





# Neural Network Renormalization Group



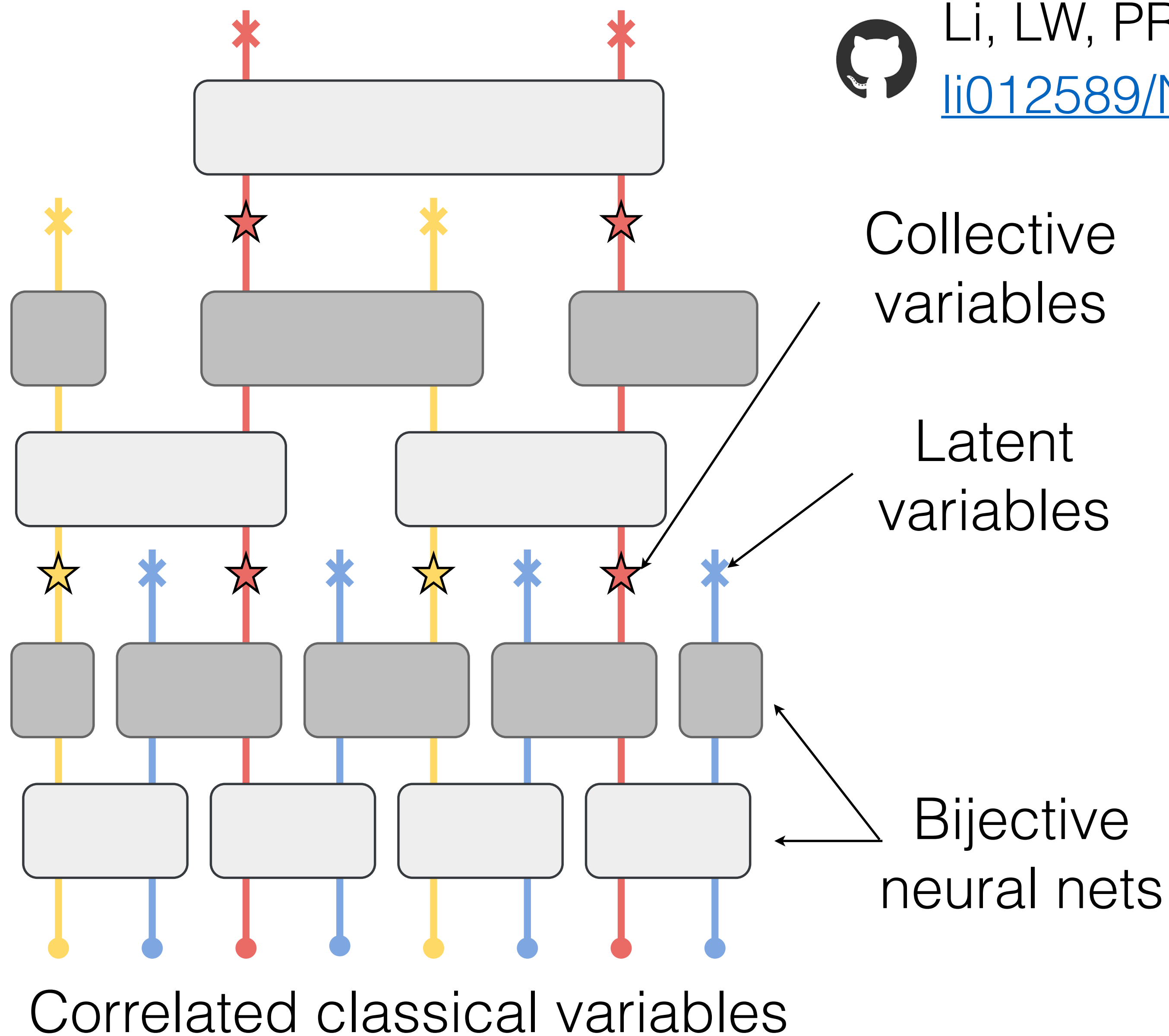
Li, LW, PRL '18

[li012589/NeuralRG](https://github.com/li012589/NeuralRG)

$$\mathbf{z} = g^{-1}(\mathbf{x})$$

Inference  
Generate

$$\mathbf{x} = g(\mathbf{z})$$



# Neural Network Renormalization Group



Li, LW, PRL '18

[li012589/NeuralRG](https://github.com/li012589/NeuralRG)

$$\mathbf{z} = g^{-1}(\mathbf{x})$$

Inference  
Generate

## Probability Transformation

$$\ln p(\mathbf{x}) = \ln \mathcal{N}(\mathbf{z}) - \ln \left| \det \left( \frac{\partial \mathbf{x}}{\partial \mathbf{z}} \right) \right|$$

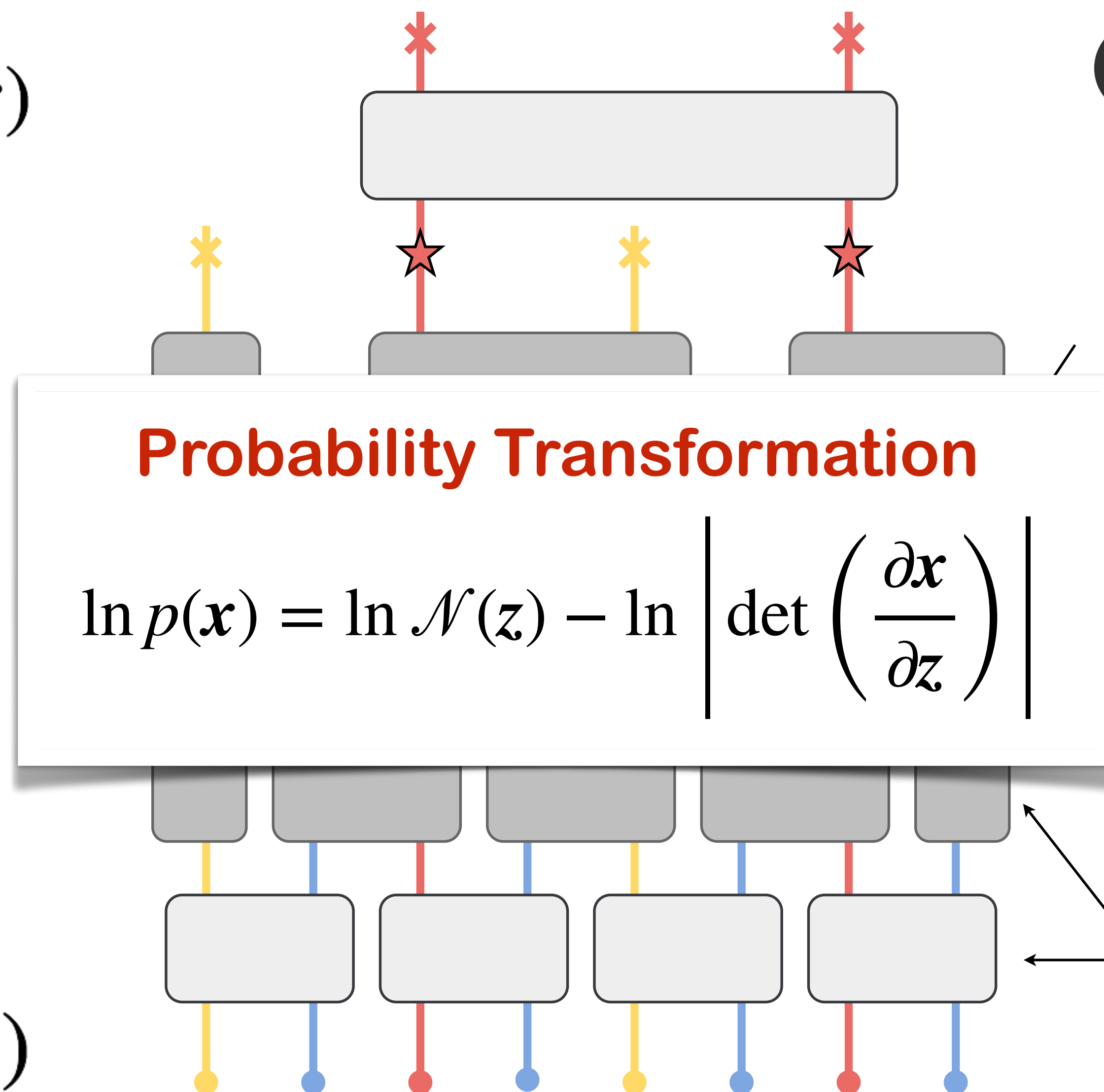
Collective variables

Latent variables

Bijective neural nets

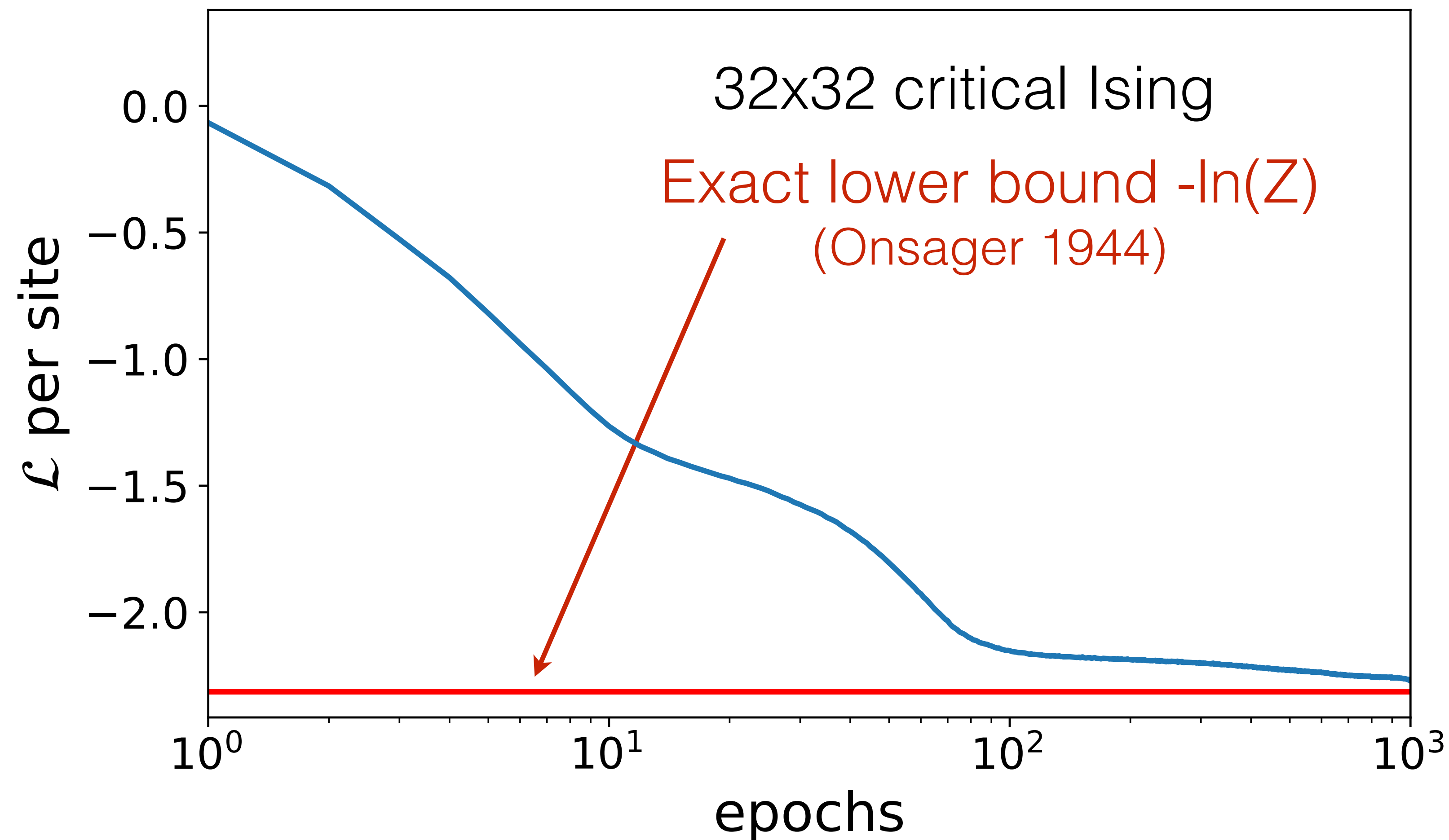
$$\mathbf{x} = g(\mathbf{z})$$

Correlated classical variables





# Variational Loss

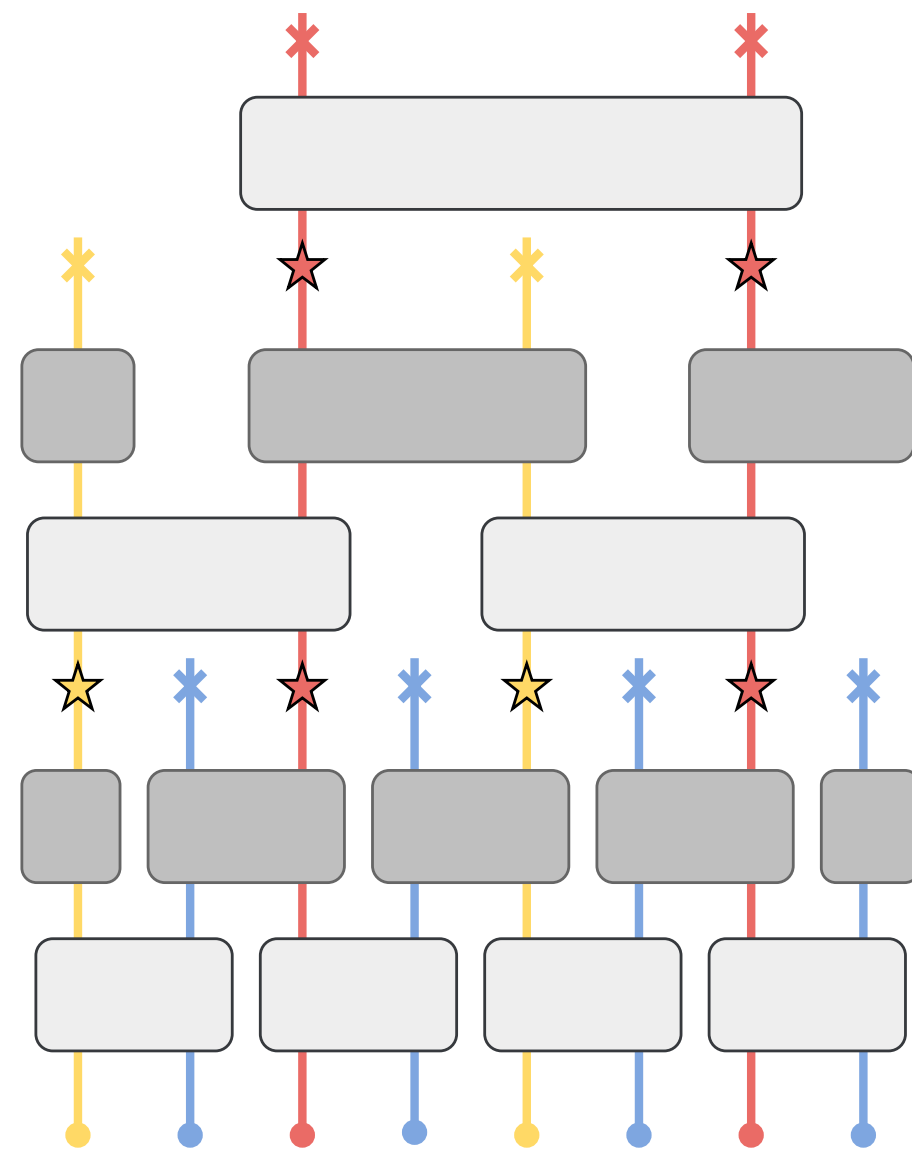


Training = Variational free energy calculation

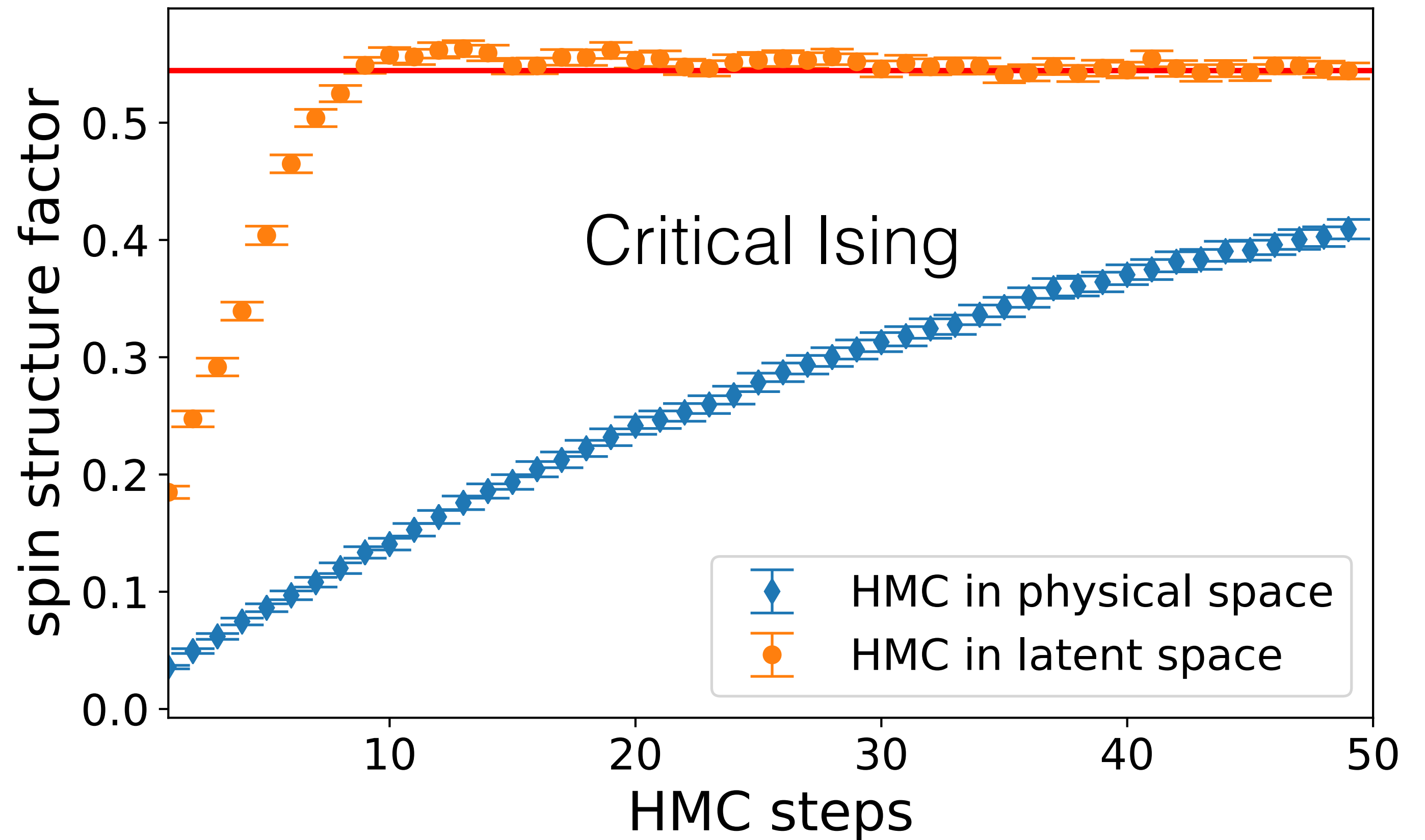
# Sampling in the latent space

Latent space energy function

$$E_{\text{eff}}(\mathbf{z}) = E(g(\mathbf{z})) + \ln p(g(\mathbf{z})) - \ln \mathcal{N}(\mathbf{z})$$



Physical energy function  $E(\mathbf{x})$

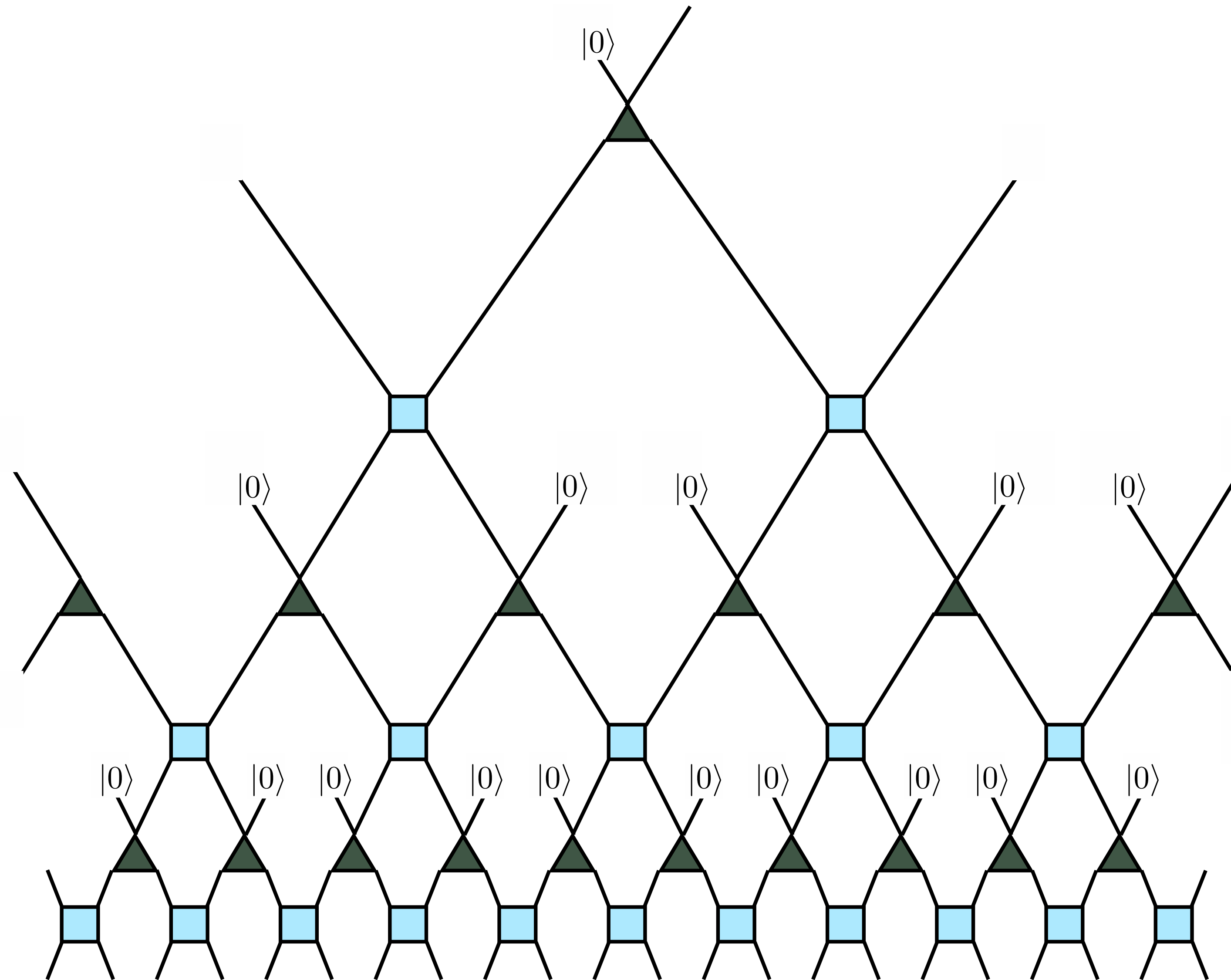


**HMC thermalizes faster in the latent space**

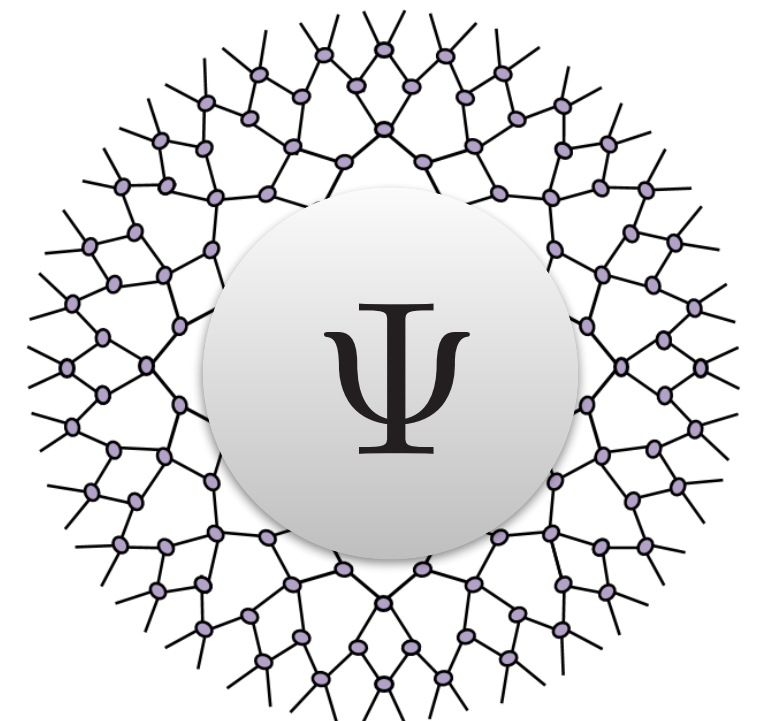
Other ways to de-bias: neural importance sampling, Metropolis rejection of flow proposal ...



# Quantum origin of the architecture

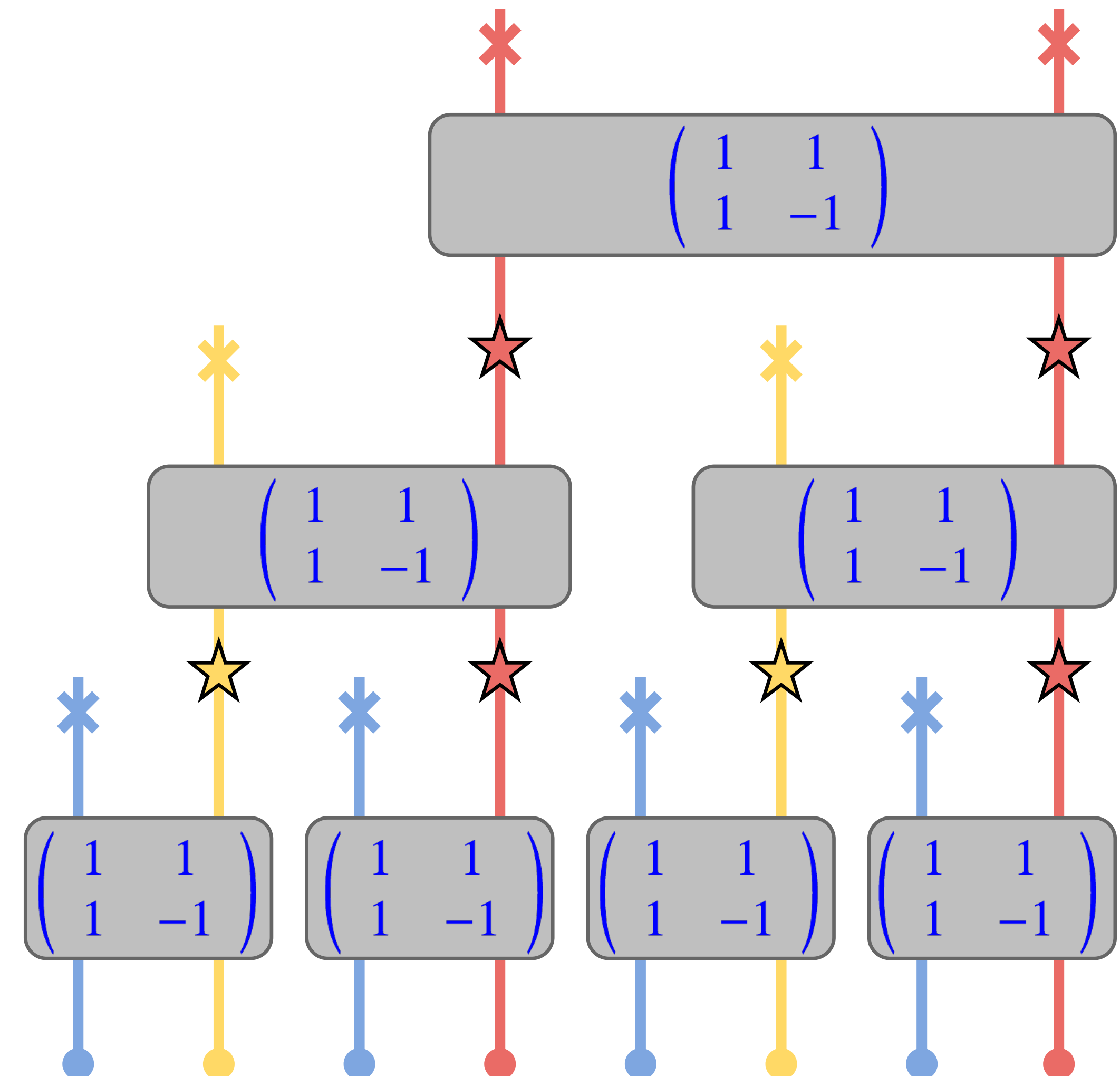
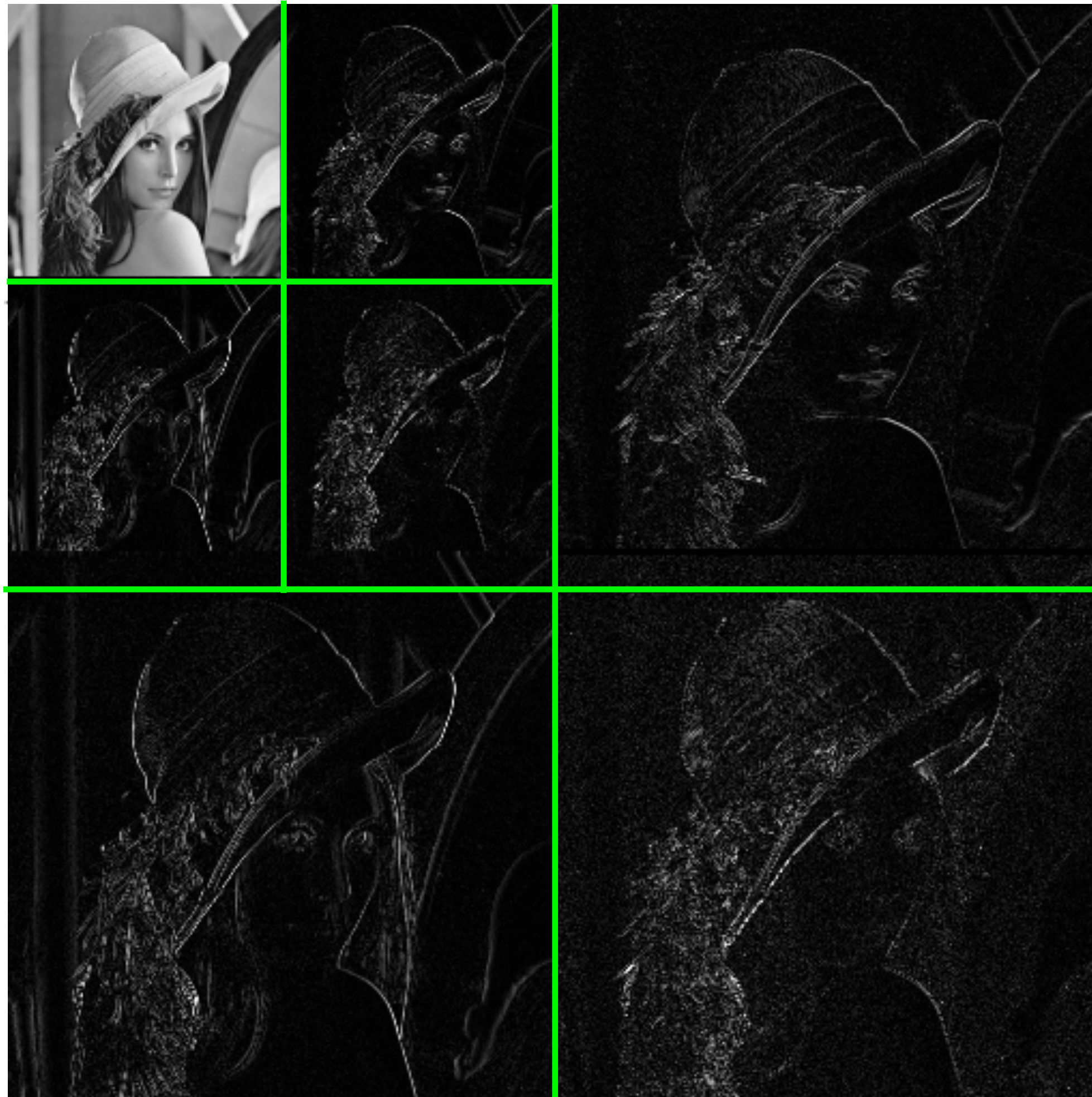


Entangled qubits



**M**ulti-Scale  
**E**ntanglement  
**R**enormalization  
**A**nsatz

# Connection to wavelets



**Nonlinear & adaptive generalizations of wavelets**

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



# Continuous normalizing flows

$$\ln p(\mathbf{x}) = \ln \mathcal{N}(\mathbf{z}) - \ln \left| \det \left( \frac{\partial \mathbf{x}}{\partial \mathbf{z}} \right) \right|$$

Consider infinitesimal change-of-variables Chen et al 1806.07366

$$\mathbf{x} = \mathbf{z} + \varepsilon \mathbf{v} \qquad \ln p(\mathbf{x}) - \ln \mathcal{N}(\mathbf{z}) = - \ln \left| \det \left( 1 + \varepsilon \frac{\partial \mathbf{v}}{\partial \mathbf{z}} \right) \right|$$

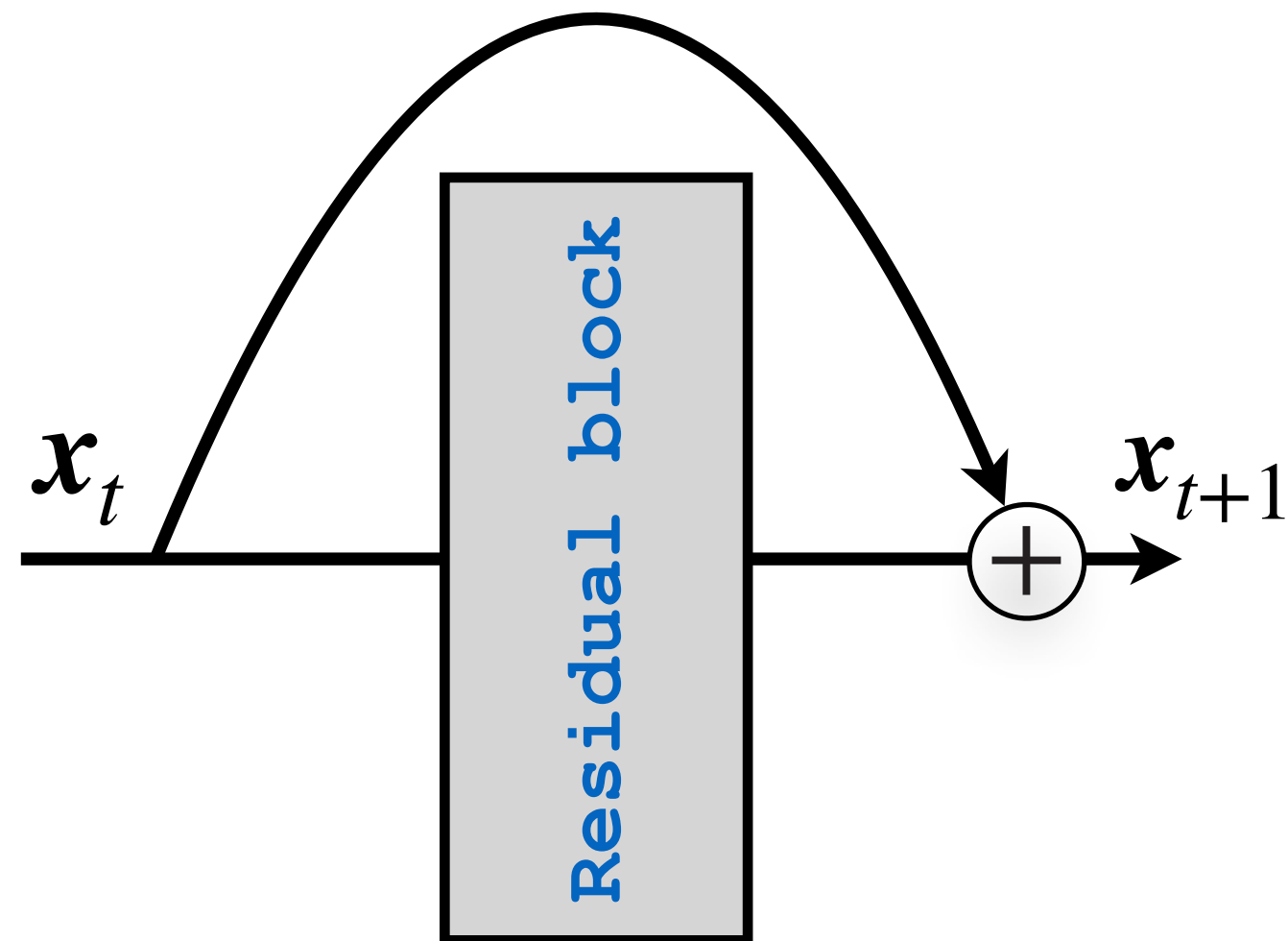
$$\varepsilon \rightarrow 0$$

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}$$

$$\frac{d \ln \rho(\mathbf{x}, t)}{dt} = - \nabla \cdot \mathbf{v}$$

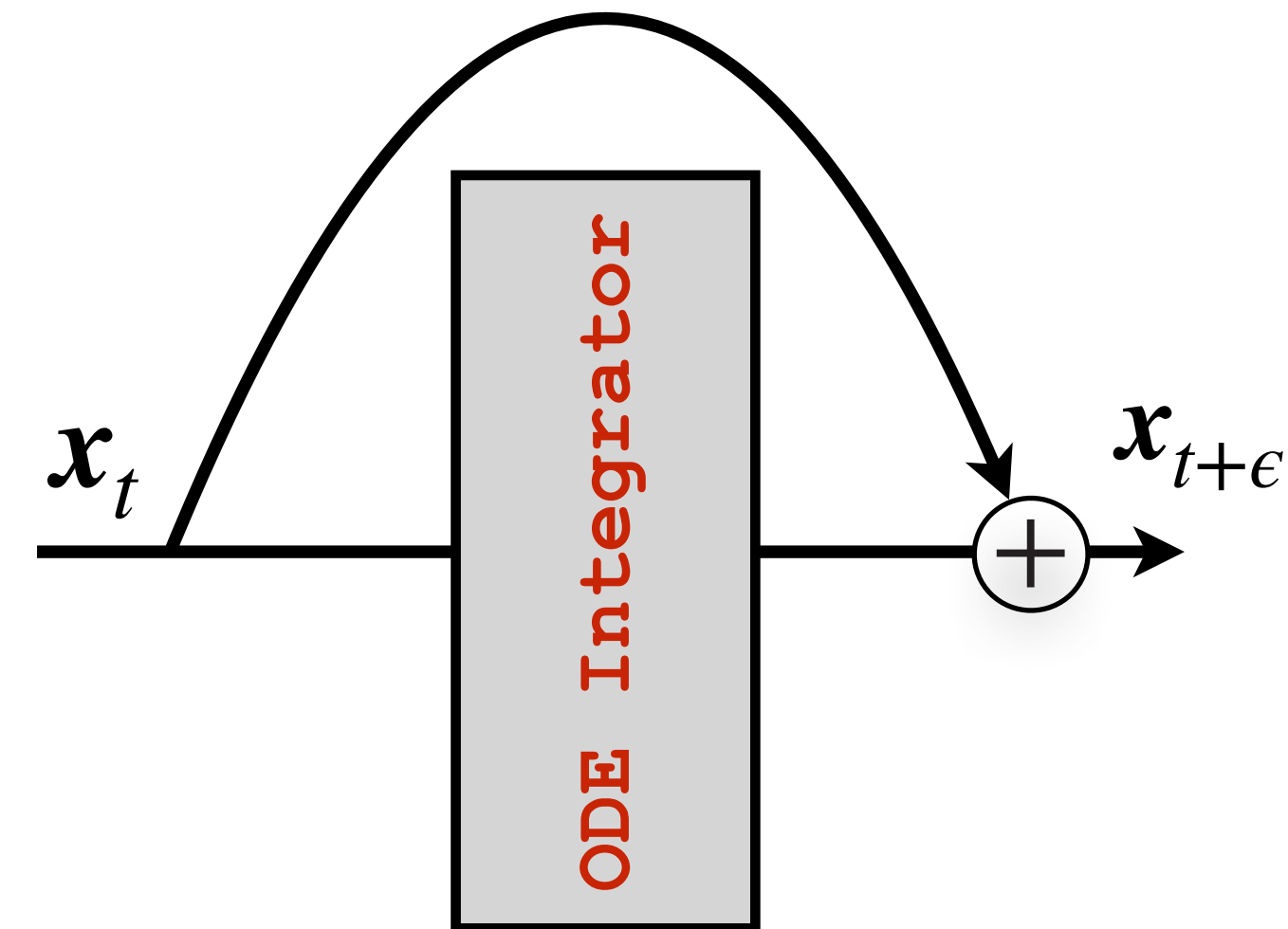
# Neural Ordinary Differential Equations

## Residual network



$$x_{t+1} = x_t + f(x_t)$$

## ODE integration



$$dx/dt = f(x)$$

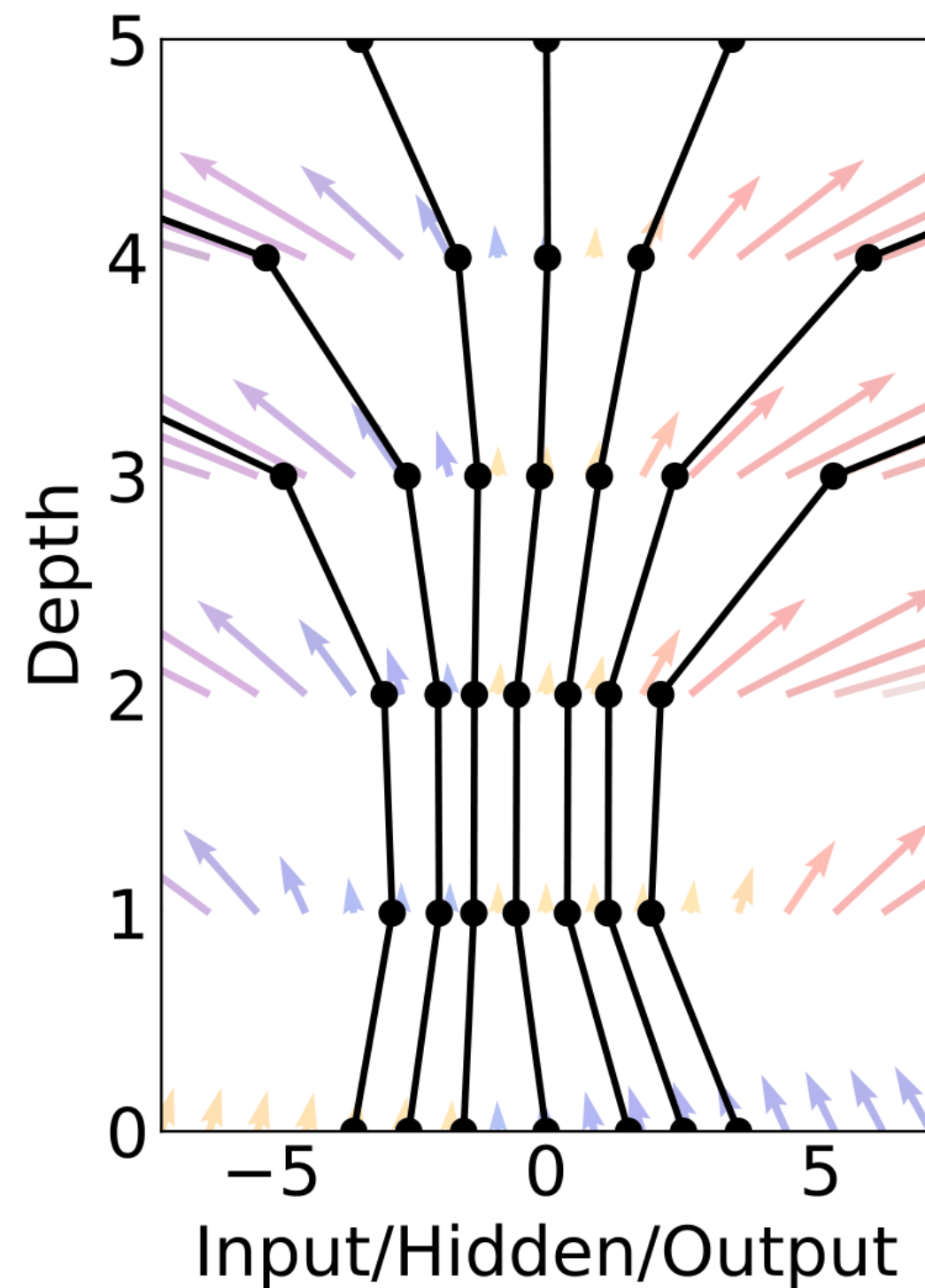
Chen et al, 1806.07366

Harbor et al 1705.03341  
Lu et al 1710.10121,  
E Commun. Math. Stat 17'...



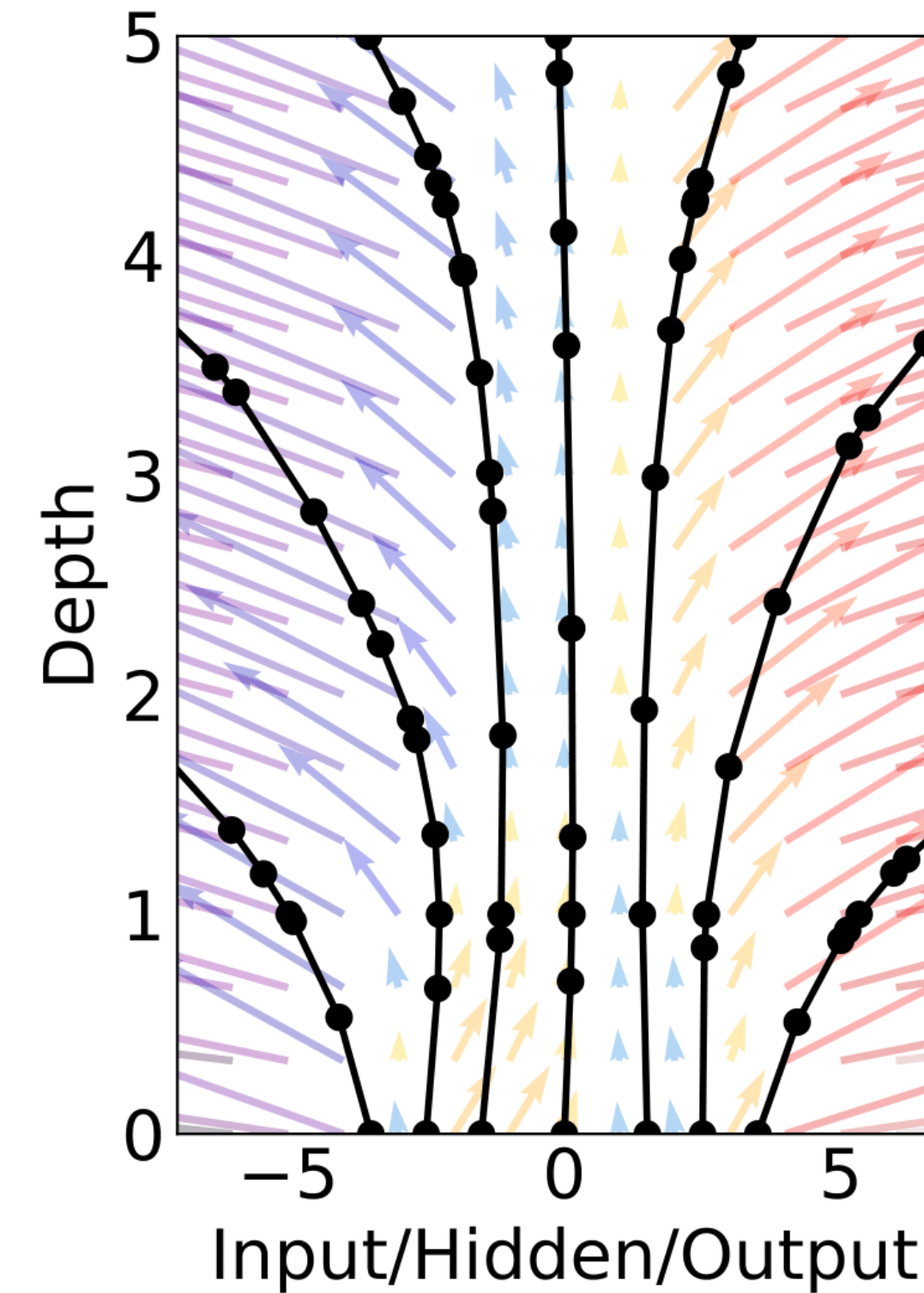
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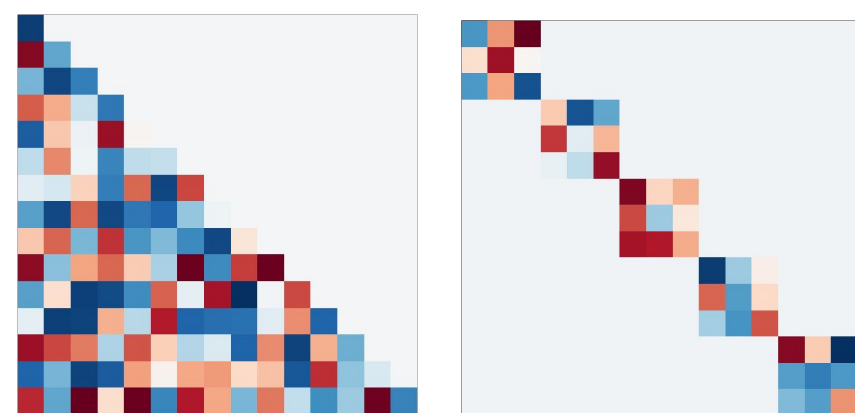
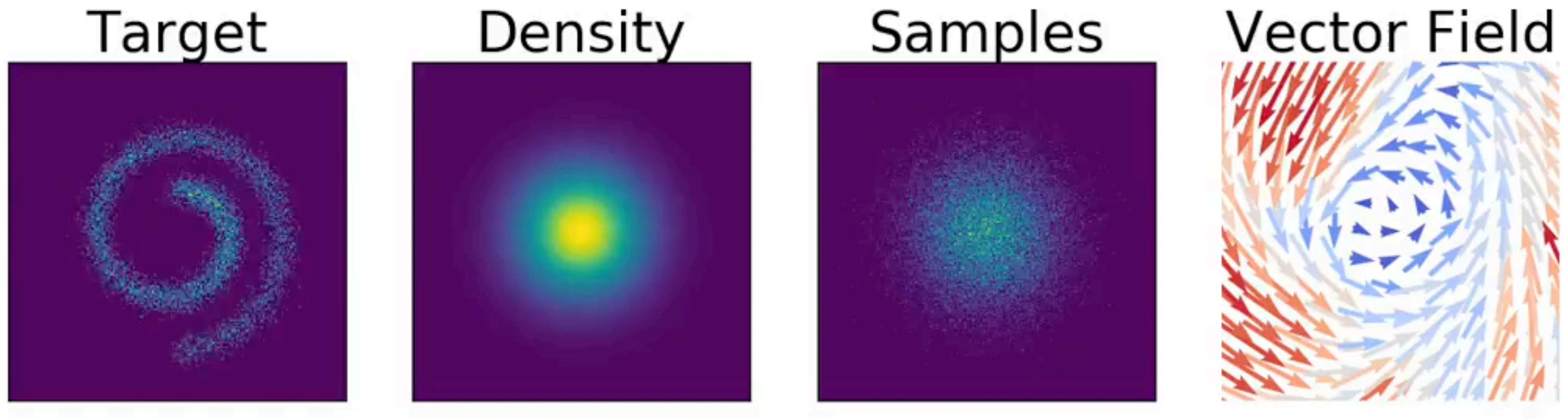
$$d\mathbf{x}/dt = f(\mathbf{x})$$

Chen et al, 1806.07366

Harbor et al 1705.03341  
Lu et al 1710.10121,  
E Commun. Math. Stat 17'...

# Neural Ordinary Differential Equations

Chen et al, 1806.07366, Grathwohl et al 1810.01367

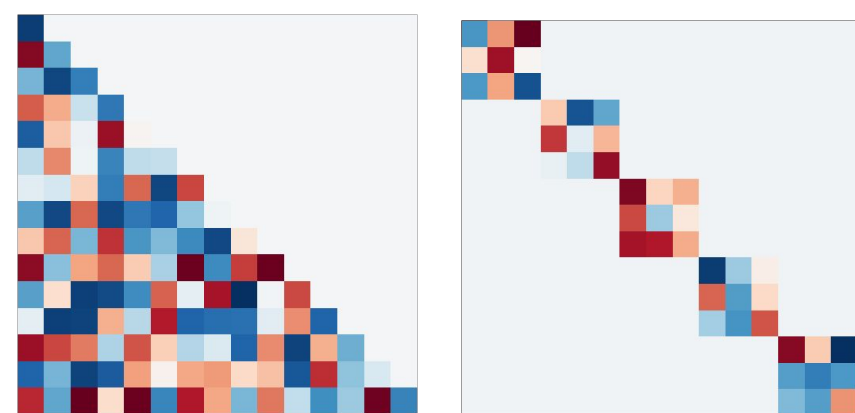
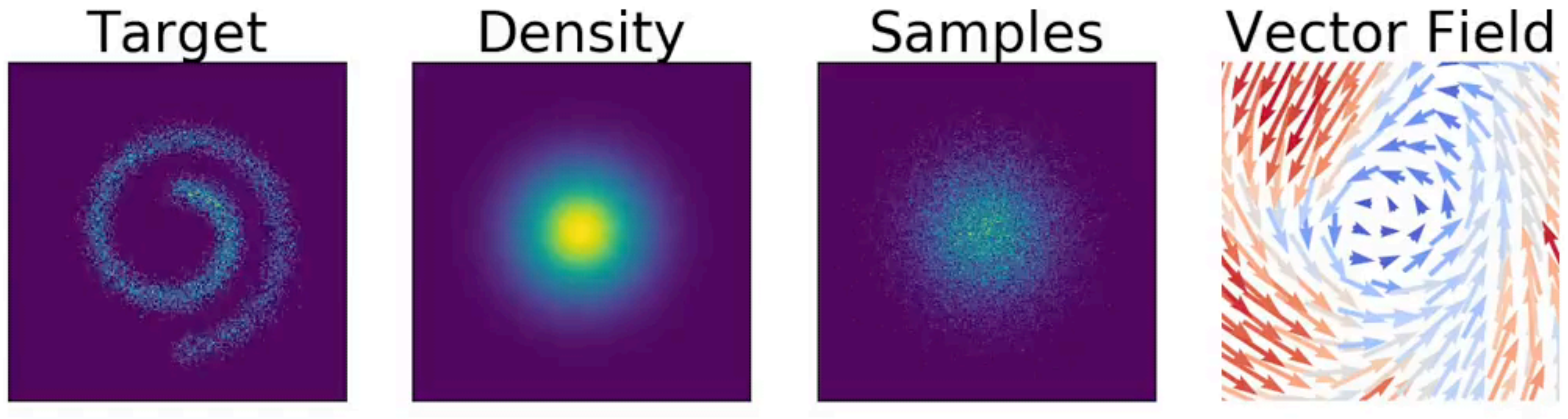


**Continuous normalizing flow have no structural constraints on the transformation Jacobian**



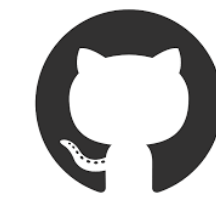
# Neural Ordinary Differential Equations

Chen et al, 1806.07366, Grathwohl et al 1810.01367



**Continuous normalizing flow have no structural constraints on the transformation Jacobian**

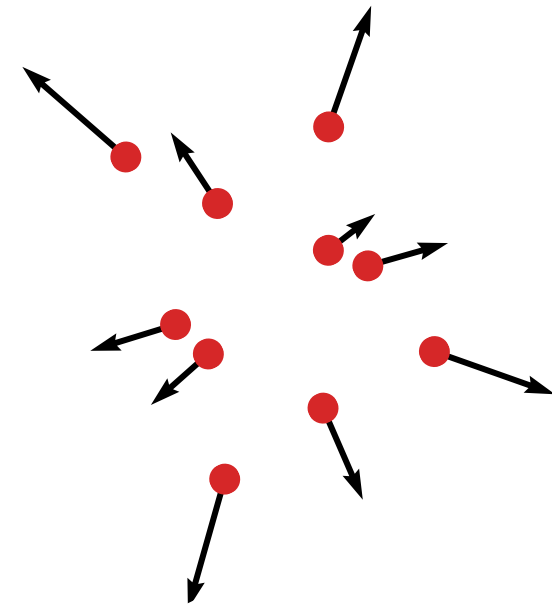
# Fluid physics behind flows



Zhang, E, LW 1809.10188

[wangleiphy/MongeAmpereFlow](https://github.com/wangleiphy/MongeAmpereFlow)

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}$$

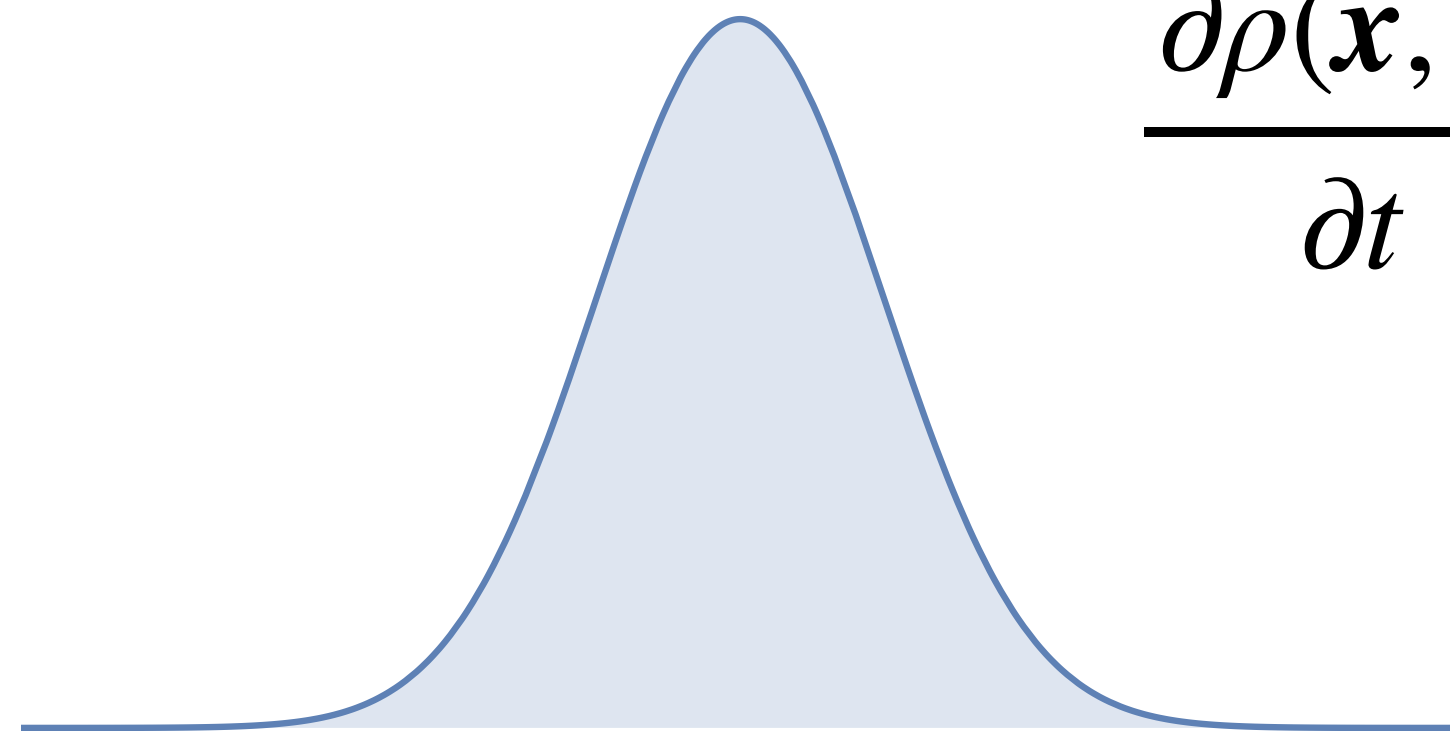


$$\frac{d \ln \rho(\mathbf{x}, t)}{dt} = - \nabla \cdot \mathbf{v}$$

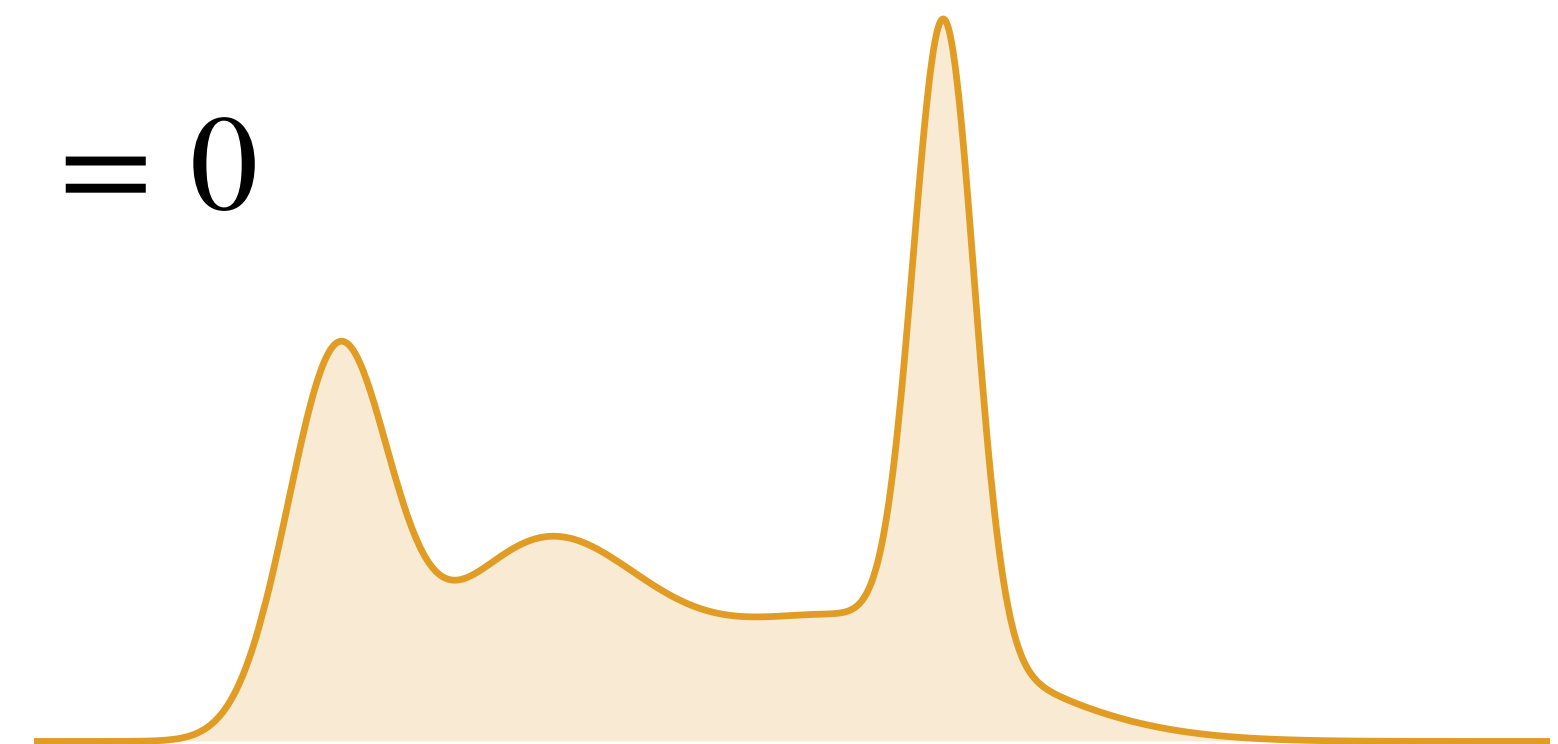
$$\frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla$$

“material  
derivative”

$$\frac{\partial \rho(\mathbf{x}, t)}{\partial t} + \nabla \cdot [\rho(\mathbf{x}, t) \mathbf{v}] = 0$$



Simple density

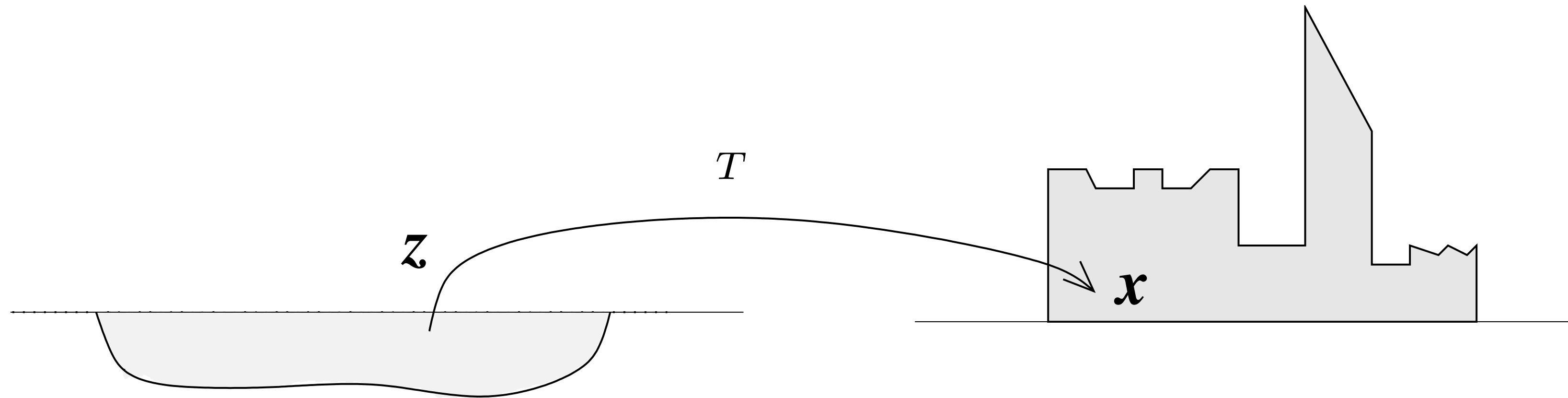


Complex density



# Optimal Transport Theory

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



Monge



Kantorovich



Koopmans



Dantzig



Brenier



Otto



McCann



Villani



Figalli

**Nobel Prize in Economics '75**

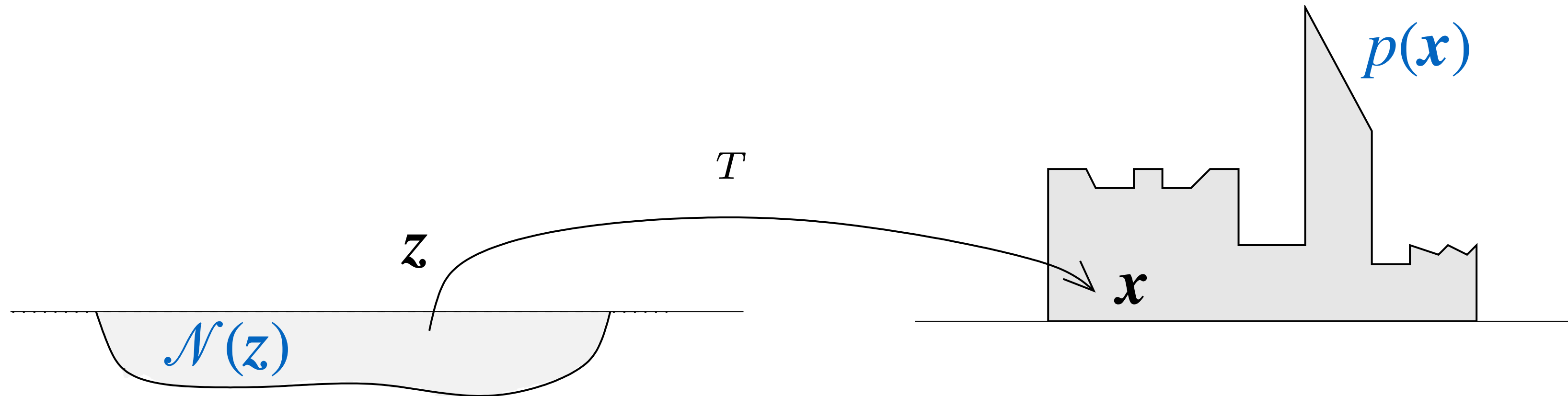
**Fields Metal '10**

**Fields Metal '18**

from Cuturi, Solomon NISP 2017 tutorial

# Optimal Transport Theory

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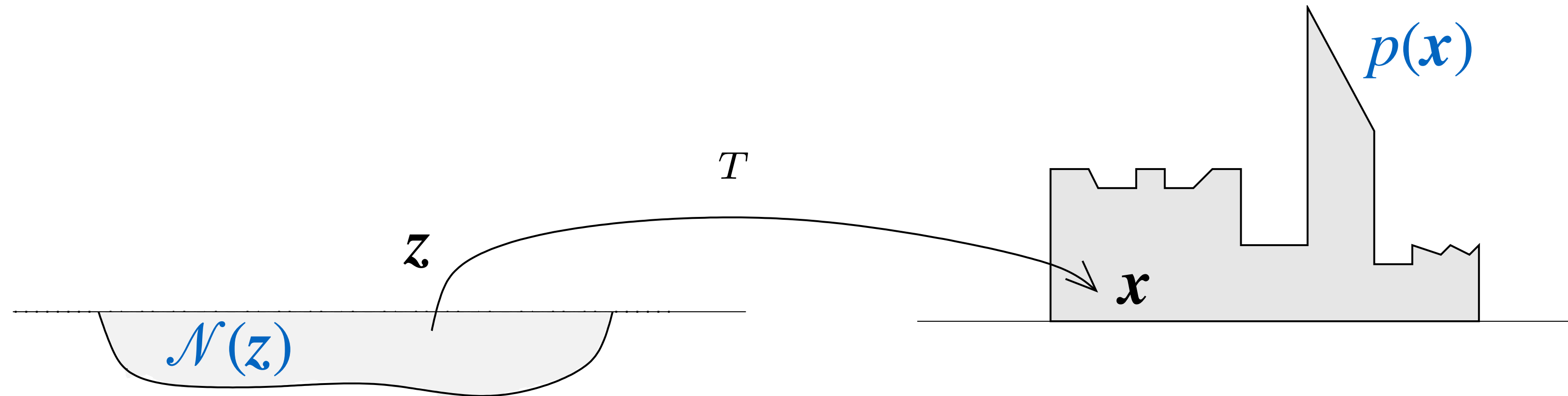
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# Optimal Transport Theory

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



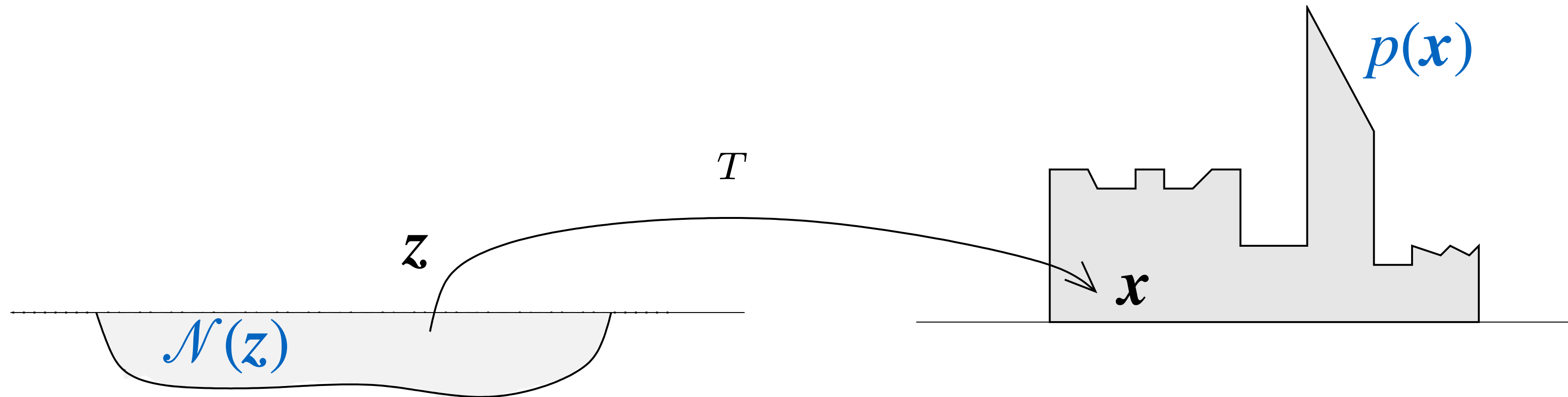
Brenier theorem (1991)

Under certain conditions  
the optimal map is

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

# Optimal Transport Theory

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



Brenier theorem (1991)

Under certain conditions  
the optimal map is

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

Monge-Ampère Equation

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



# Monge-Ampère Flow

Zhang, E, LW 1809.10188



[wangleiphy/MongeAmpereFlow](https://github.com/wangleiphy/MongeAmpereFlow)

$$\frac{\partial \rho(\mathbf{x}, t)}{\partial t} + \nabla \cdot [\rho(\mathbf{x}, t) \nabla \varphi] = 0$$

- ① Drive the flow with an “irrotational” velocity field
- ② Impose symmetry to the scalar valued potential for symmetric generative model

$$\varphi(g \mathbf{x}) = \varphi(\mathbf{x}) \implies \rho(g \mathbf{x}) = \rho(\mathbf{x})$$

# Hamiltonian dynamics: phase space flow

## Hamiltonian equations

$$\begin{cases} \dot{p} = -\frac{\partial H}{\partial q} \\ \dot{q} = +\frac{\partial H}{\partial p} \end{cases}$$



# Hamiltonian dynamics: phase space flow

**Hamiltonian equations**

**Phase space variables**

$$\boldsymbol{x} = (p, q)$$

$$\begin{cases} \dot{p} = -\frac{\partial H}{\partial q} \\ \dot{q} = +\frac{\partial H}{\partial p} \end{cases}$$

**Symplectic metric**

$$J = \begin{pmatrix} & I \\ -I & \end{pmatrix}$$

# Hamiltonian dynamics: phase space flow

**Hamiltonian equations**

$$\begin{cases} \dot{p} = -\frac{\partial H}{\partial q} \\ \dot{q} = +\frac{\partial H}{\partial p} \end{cases}$$

**Phase space variables**

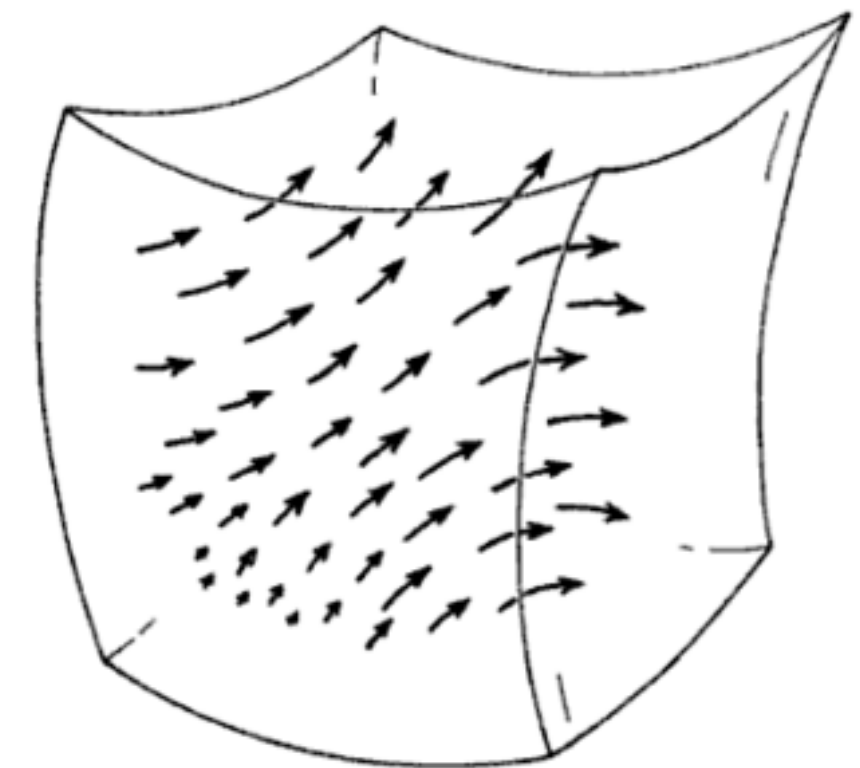
$$\boldsymbol{x} = (p, q)$$

**Symplectic metric**

$$J = \begin{pmatrix} & I \\ -I & \end{pmatrix}$$

**Symplectic gradient flow**

$$\dot{\boldsymbol{x}} = \nabla_{\boldsymbol{x}} H(\boldsymbol{x}) J$$

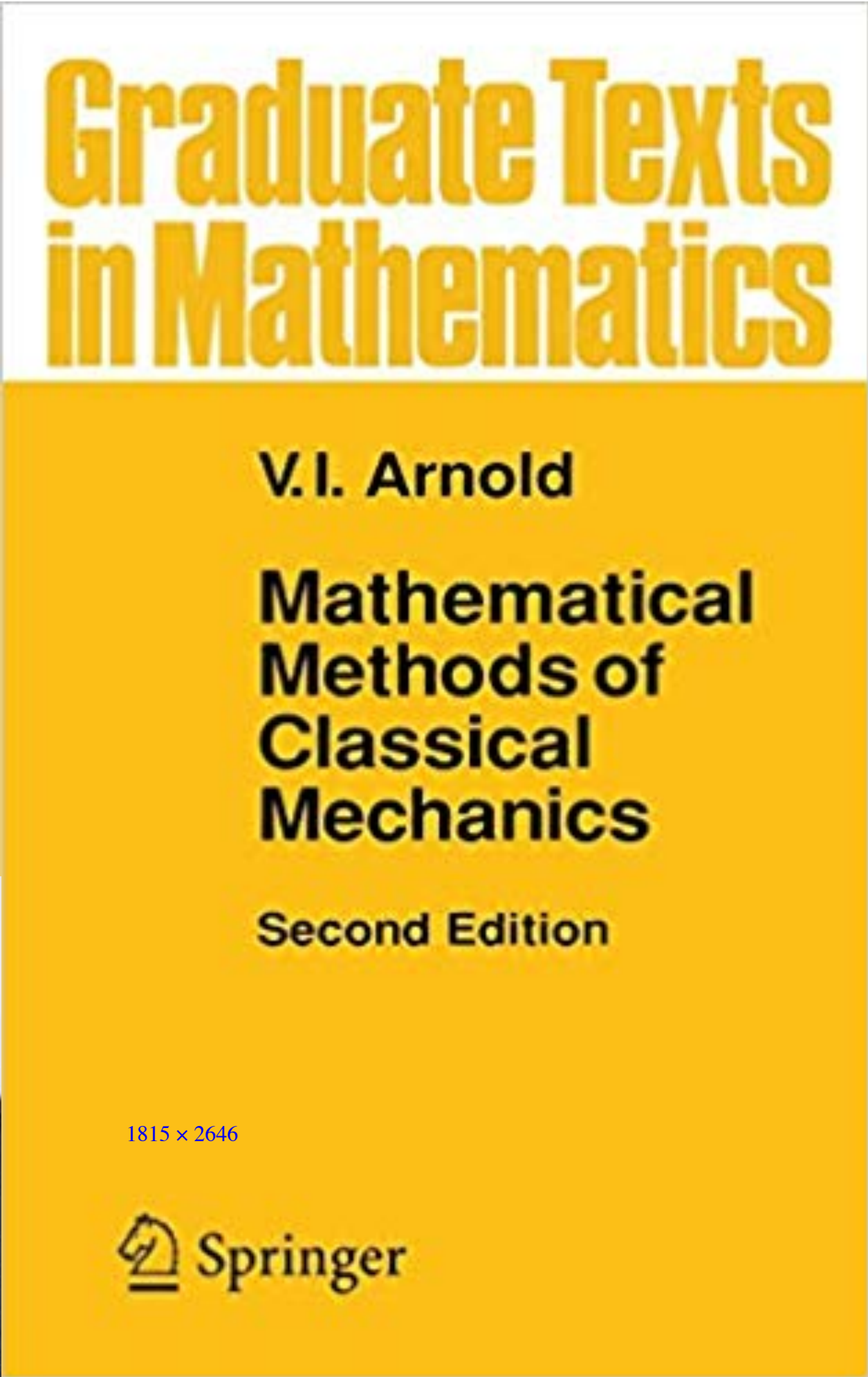




# Hamiltonian dynamics: phase space flow

Hamiltonian eq

$$\begin{cases} \dot{p} = -\frac{\partial H}{\partial q} \\ \dot{q} = +\frac{\partial H}{\partial p} \end{cases}$$



phase va

$$= (p, q)$$

lectic m

$$\begin{pmatrix} & I \\ -I & \end{pmatrix}$$



ic gradient flow

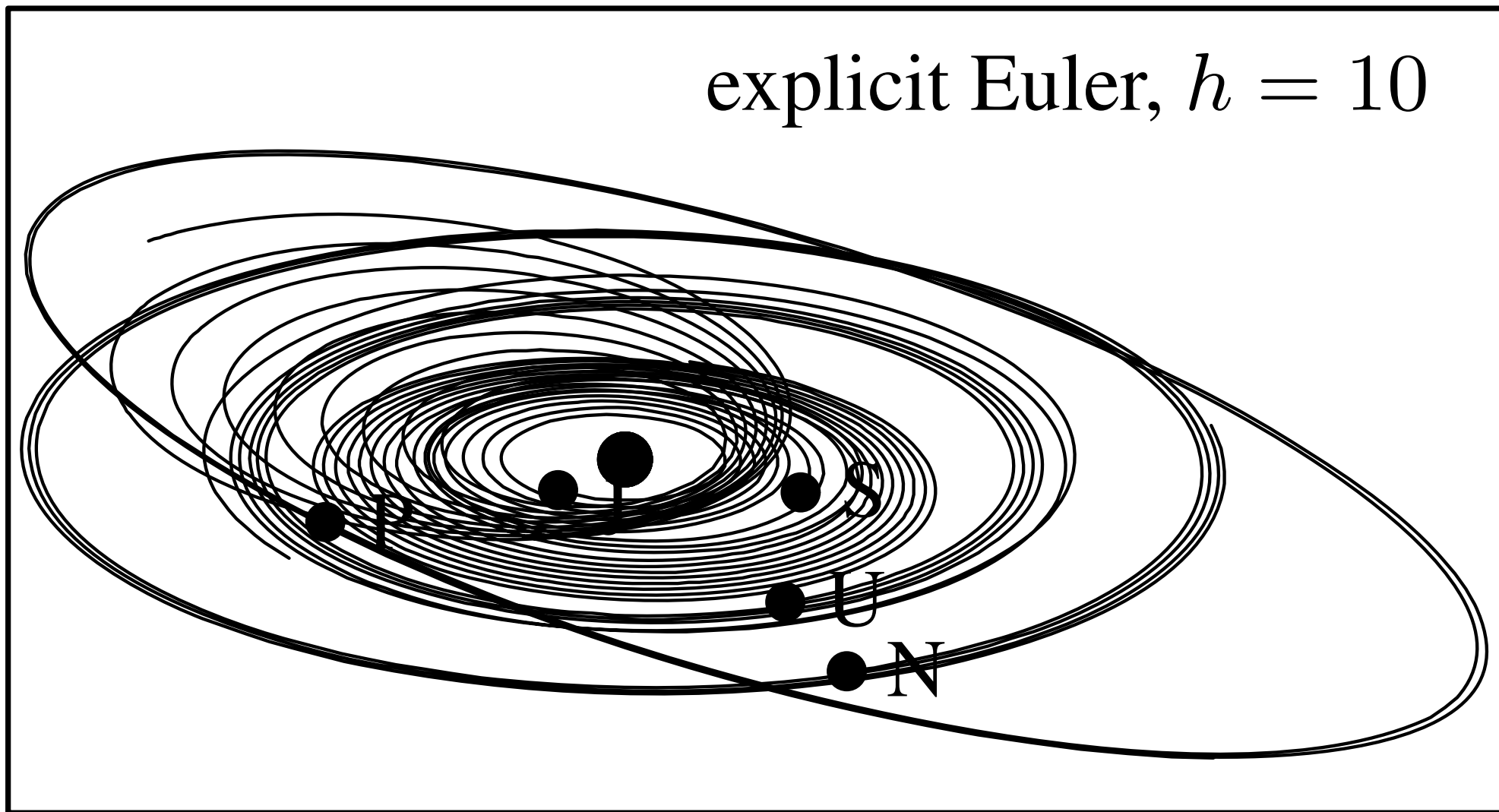
$$\nabla_x H(x)J$$



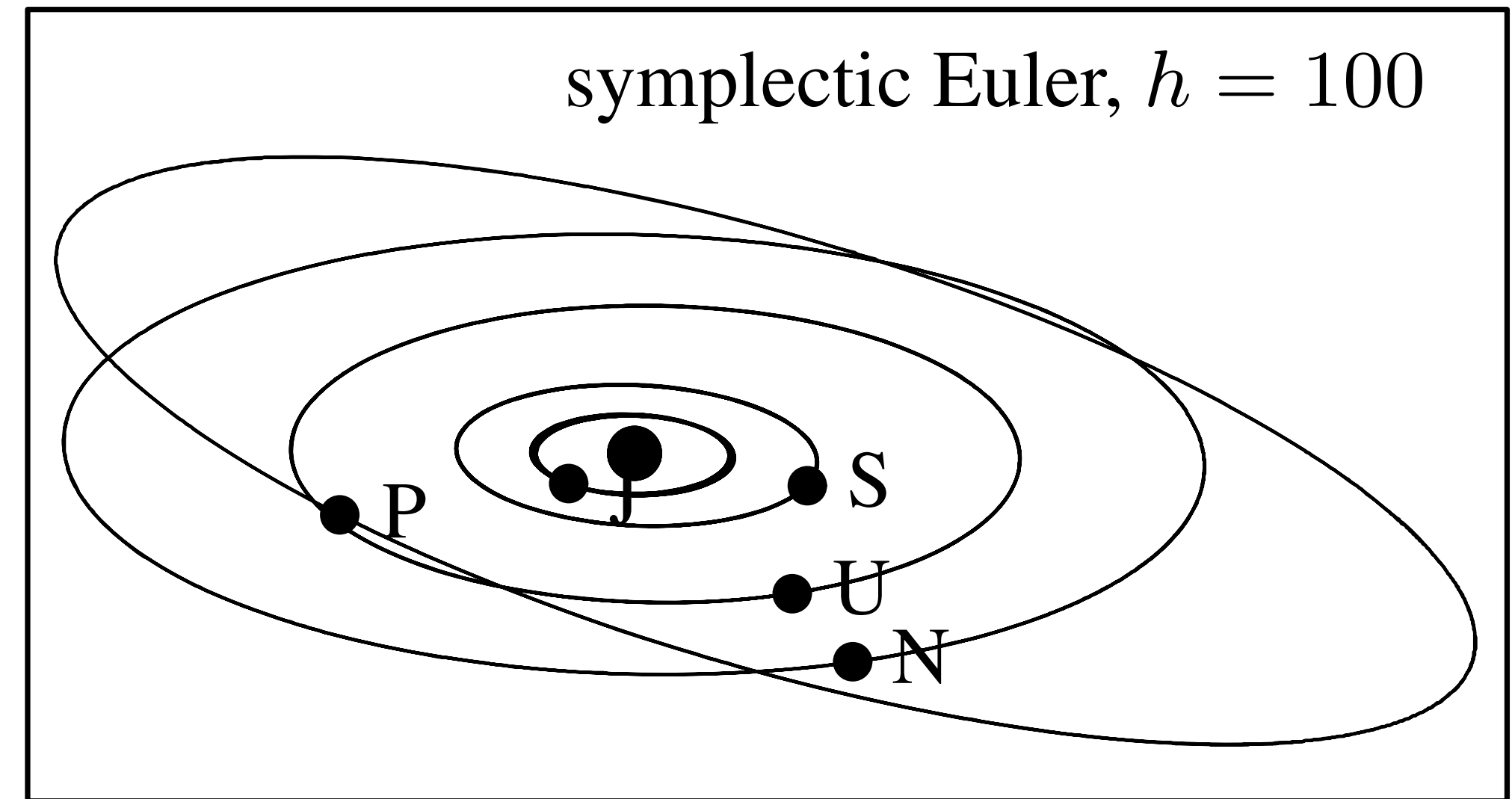


# Symplectic Integrators

explicit Euler,  $h = 10$



symplectic Euler,  $h = 100$





# Canonical Transformations

$$\mathbf{x} = (p, q) \xleftrightarrow{\text{Change of variables}} \mathbf{z} = (P, Q)$$

which satisfies  $\left( \nabla_{\mathbf{x}} \mathbf{z} \right) J \left( \nabla_{\mathbf{x}} \mathbf{z} \right)^T = J$  symplectic condition

# Canonical Transformations

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one has  $\dot{\mathbf{z}} = \nabla_{\mathbf{z}} K(\mathbf{z}) J$  where  $K(\mathbf{z}) = H \circ \mathbf{x}(\mathbf{z})$

**Preserves Hamiltonian dynamics in the “latent phase space”**



# Canonical transformation for Moon-Earth-Sun 3-body problem

Gutzwiller, RMP, '98

634 THÉORIE DU MOUVEMENT DE LA LUNE.

$$\left. \begin{aligned} (E_{11}) \quad & + \left( \frac{3}{8} e^2 - \frac{3}{4} \gamma^2 e^2 - \frac{3}{2} e^2 - \frac{411}{16} e^2 e^2 \right) \frac{n^2}{n_1^2} \\ & + \left( \frac{219}{64} e^2 - \frac{99}{4} \gamma^2 e^2 - \frac{619}{32} e^2 - \frac{9843}{128} e^2 e^2 \right) \frac{n^2}{n_1^2} \\ & + \left[ \frac{189}{128} e^2 \frac{n^2}{n_1^2} - \frac{65337}{1024} e^2 \frac{n^2}{n_1^2} - \frac{5}{64} e^2 \frac{n^2}{n_1^2} \cdot \frac{n_1^2}{a^2} \right] \cos \phi_*(t+c) \\ & - \frac{99}{128} e^2 \frac{n^2}{n_1^2} \cos 2\phi_*(t+c), \\ (F_{11}) \quad & - \left[ \left( \frac{3}{4} - \frac{3}{2} \gamma^2 + \frac{3}{8} e^2 - \frac{15}{8} e^2 + \frac{3}{4} \gamma^2 + \frac{15}{4} \gamma^2 e^2 - \frac{171}{64} e^2 - \frac{15}{16} e^2 e^2 \right) \frac{n^2}{n_1^2} \right. \\ & + \left( \frac{3}{8} - \frac{3}{4} \gamma^2 + \frac{21}{16} e^2 - \frac{411}{16} e^2 \right) \frac{n^2}{n_1^2} \\ & + \left( \frac{219}{64} - \frac{99}{4} \gamma^2 + \frac{1399}{128} e^2 - \frac{9843}{128} e^2 \right) \frac{n^2}{n_1^2} \\ & + \left. \frac{189}{128} \frac{n^2}{n_1^2} - \frac{65229}{1024} \frac{n^2}{n_1^2} - \frac{5}{64} e^2 \frac{n^2}{n_1^2} \cdot \frac{n_1^2}{a^2} \right] \sin \phi_*(t+c) \\ & + \left[ \left( \frac{9}{64} - \frac{9}{16} \gamma^2 - \frac{45}{128} e^2 - \frac{45}{64} e^2 \right) \frac{n^2}{n_1^2} + \frac{9}{64} \frac{n^2}{n_1^2} + \frac{675}{512} \frac{n^2}{n_1^2} \right] \sin 2\phi_*(t+c) \\ & - \frac{9}{256} \frac{n^2}{n_1^2} \sin 3\phi_*(t+c), \\ (G_{11}) \quad & a = a_0 \left\{ 1 + \left[ \left( \frac{3}{2} e^2 - 3 \gamma^2 e^2 - \frac{15}{4} e^2 - \frac{15}{4} e^2 e^2 + \frac{3}{2} \gamma^2 e^2 + \frac{15}{2} \gamma^2 e^2 \right. \right. \right. \\ & + \left. \frac{15}{2} \gamma^2 e^2 e^2 + \frac{101}{32} e^2 + \frac{75}{8} e^2 e^2 \right) \frac{n^2}{n_1^2} \right. \\ & + \left( \frac{3}{4} e^2 - \frac{3}{2} \gamma^2 e^2 - \frac{15}{8} e^2 - \frac{411}{8} e^2 e^2 \right) \frac{n^2}{n_1^2} \\ & + \left. \left( \frac{219}{32} e^2 - \frac{99}{2} \gamma^2 e^2 - \frac{1819}{64} e^2 - \frac{9843}{64} e^2 e^2 \right) \frac{n^2}{n_1^2} \right. \\ & + \left. \frac{189}{64} e^2 \frac{n^2}{n_1^2} - \frac{77349}{512} e^2 \frac{n^2}{n_1^2} - \frac{5}{32} e^2 \frac{n^2}{n_1^2} \cdot \frac{n_1^2}{a^2} \right] \cos \phi_*(t+c) \\ & - \frac{9}{16} e^2 \frac{n^2}{n_1^2} \cos 2\phi_*(t+c) \left. \right\}, \\ (H_{11}) \quad & \gamma^2 = \gamma_1^2 - \left[ \left( \frac{3}{8} \gamma^2 e^2 - \frac{3}{4} \gamma^2 e^2 - \frac{3}{4} \gamma^2 e^2 - \frac{15}{16} \gamma^2 e^2 e^2 \right) \frac{n^2}{n_1^2} \right. \\ & + \left. \frac{3}{16} \gamma^2 e^2 \frac{n^2}{n_1^2} + \frac{219}{128} \gamma^2 e^2 \frac{n^2}{n_1^2} \right] \cos \phi_*(t+c). \end{aligned} \right\}$$

640 THÉORIE DU MOUVEMENT DE LA LUNE.

$$\begin{aligned} & + \left( \frac{13}{64} + \frac{187}{32} \gamma^2 - \frac{237}{128} e^2 + \frac{195}{128} e^2 - \frac{1389}{32} \gamma^2 - \frac{599}{64} \gamma^2 e^2 + \frac{2805}{64} \gamma^2 e^2 \right. \\ & \quad \left. - \frac{103173}{1024} e^2 - \frac{3105}{256} e^2 e^2 \right) \frac{n^2}{n_1^2} \\ & + \left( \frac{79}{16} + \frac{55}{48} \gamma^2 - \frac{1063}{48} e^2 + \frac{2133}{32} e^2 \right) \frac{n^2}{n_1^2} + \left( \frac{153}{8} + \frac{3245}{96} \gamma^2 - \frac{73159}{768} e^2 + \frac{240085}{512} e^2 \right) \frac{n^2}{n_1^2} \\ & + \frac{22441}{288} \frac{n^2}{n_1^2} + \frac{99916415}{442368} \frac{n^2}{n_1^2} + \frac{4431}{2048} \frac{n^2}{n_1^2} \cdot \frac{n_1^2}{a^2} \left. \right\} \end{aligned}$$

De ces valeurs de L, G, H, on déduit

$$\begin{aligned} \frac{da}{dt} &= \frac{1}{an} \left\{ 2 + \left( \frac{1969}{32} - \frac{1629}{8} \gamma^2 + \frac{34985}{128} e^2 + \frac{28635}{64} e^2 \right) \frac{n^2}{n_1^2} \right. \\ & \quad \left. + \left( \frac{415}{2} - \frac{2745}{4} \gamma^2 + \frac{31449}{16} e^2 + \frac{43299}{16} e^2 \right) \frac{n^2}{n_1^2} + \frac{61185}{64} \frac{n^2}{n_1^2} + \frac{1532167}{576} \frac{n^2}{n_1^2} \right\}, \\ \frac{dG}{dt} &= -\frac{1}{an} \left\{ \left( \frac{527}{8} - \frac{3633}{16} \gamma^2 - \frac{9991}{128} e^2 + 480 e^2 \right) \frac{n^2}{n_1^2} \right. \\ & \quad \left. + \left( \frac{2757}{8} - \frac{2493}{2} \gamma^2 - \frac{7161}{16} e^2 + \frac{36459}{8} e^2 \right) \frac{n^2}{n_1^2} + \frac{104117}{64} \frac{n^2}{n_1^2} + \frac{277537}{48} \frac{n^2}{n_1^2} \right\}, \\ \frac{dH}{dt} &= -\frac{1}{an} \left\{ \left( \frac{15}{16} + \frac{15}{16} \gamma^2 - \frac{1809}{32} e^2 + \frac{225}{32} e^2 \right) \frac{n^2}{n_1^2} \right. \\ & \quad \left. + \left( \frac{167}{8} - 66 \gamma^2 - \frac{2625}{8} e^2 + \frac{4509}{16} e^2 \right) \frac{n^2}{n_1^2} + \frac{895}{16} \frac{n^2}{n_1^2} + \frac{176531}{576} \frac{n^2}{n_1^2} \right\}, \\ \frac{de}{dt} &= \frac{1}{a^2 ne} \left\{ 1 - e^2 + \left( \frac{1901}{64} - \frac{1113}{16} \gamma^2 - \frac{40571}{128} e^2 + \frac{28065}{128} e^2 \right) \frac{n^2}{n_1^2} + \frac{3323}{24} \frac{n^2}{n_1^2} + \frac{62483}{96} \frac{n^2}{n_1^2} \right\}, \\ \frac{d\gamma}{dt} &= -\frac{1}{a^2 ne} \left\{ 1 - \frac{1}{2} e^2 - \frac{1}{8} e^2 - \frac{1}{16} e^2 \right. \\ & \quad \left. + \left( \frac{1901}{64} - \frac{1113}{16} \gamma^2 - \frac{3831}{8} e^2 + \frac{28065}{128} e^2 \right) \frac{n^2}{n_1^2} + \frac{3323}{24} \frac{n^2}{n_1^2} + \frac{62483}{96} \frac{n^2}{n_1^2} \right\}, \\ \frac{dL}{dt} &= \frac{1}{a^2 ne} \cdot \frac{141}{8} e^2 \frac{n^2}{n_1^2}, \\ \frac{d\gamma}{dt} &= \frac{1}{a^2 ne} \cdot \frac{183}{32} \gamma^2 \frac{n^2}{n_1^2}, \end{aligned}$$

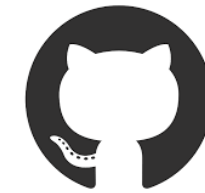


Charles Delaunay

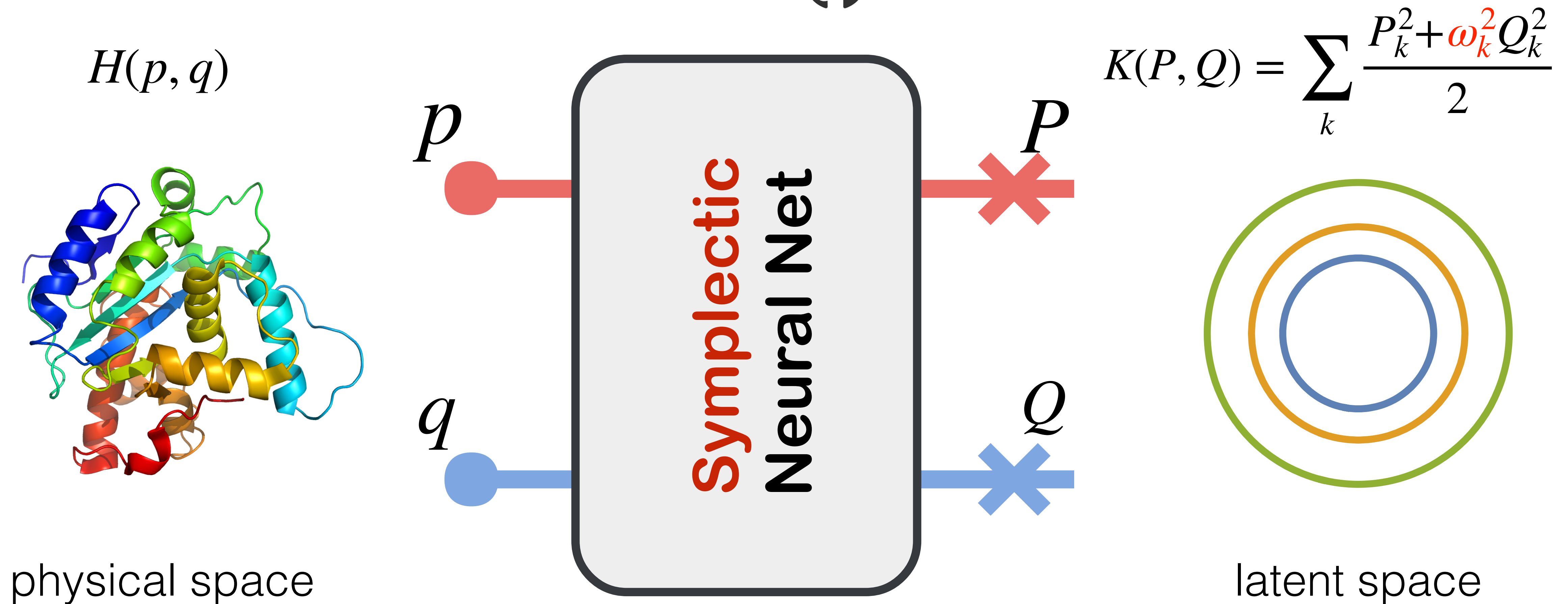
More than 1800 pages of this, ~20 years of efforts (1846-1867)

# Neural Canonical Transformations

Li, Dong, Zhang, LW, PRX '20



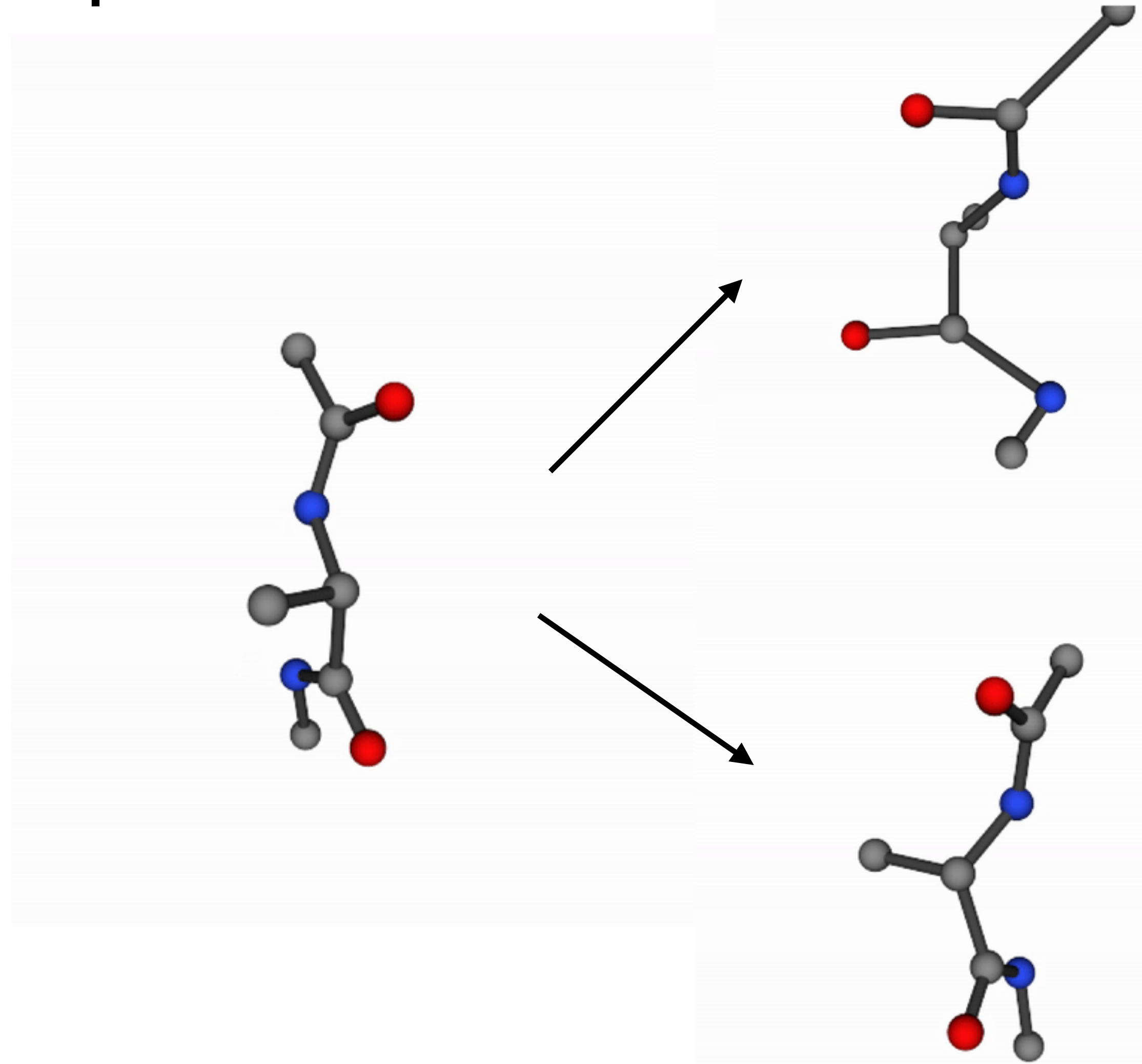
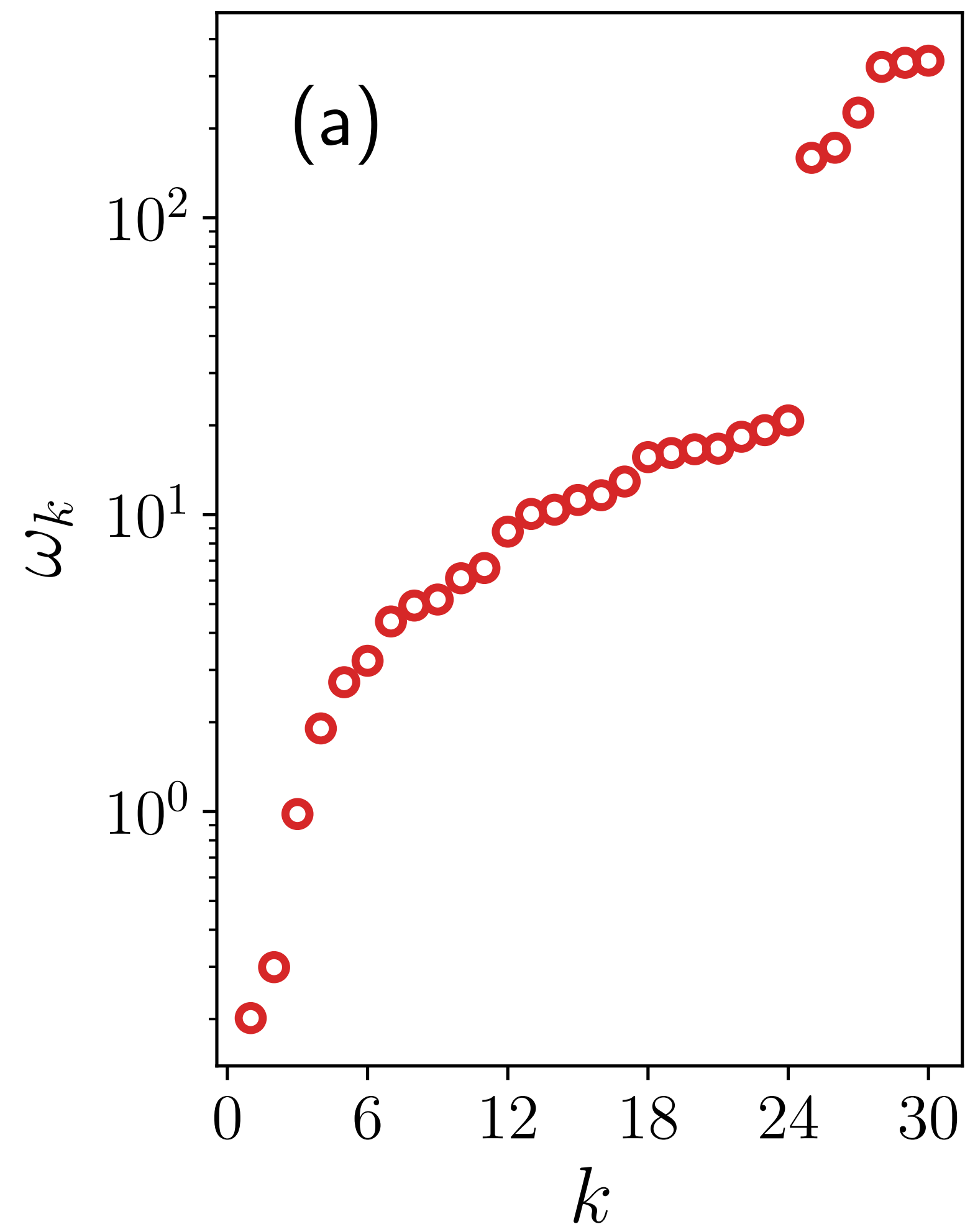
[li012589/neuralCT](https://github.com/li012589/neuralCT)



**Learn the network parameter and the latent harmonic frequency**

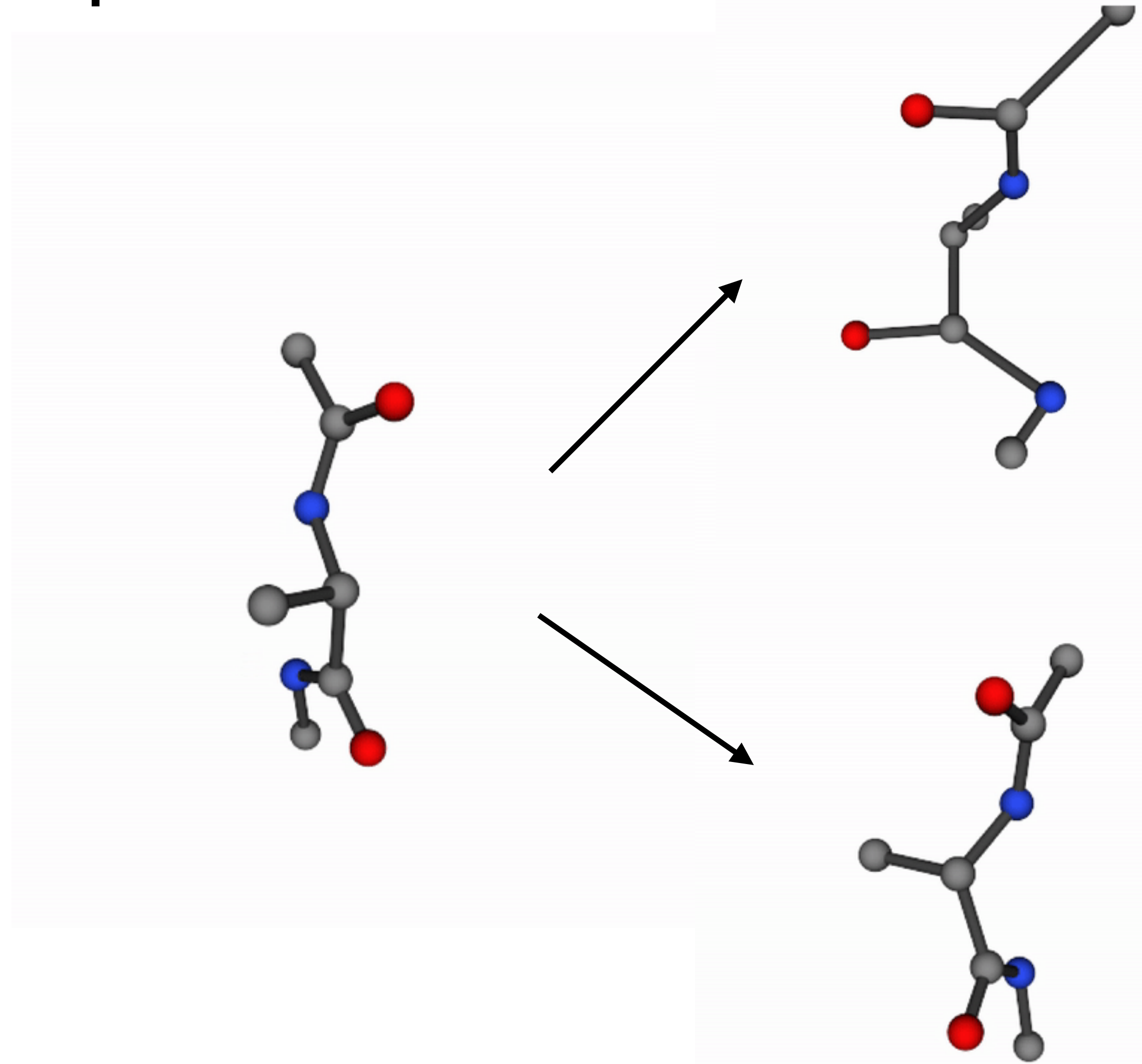
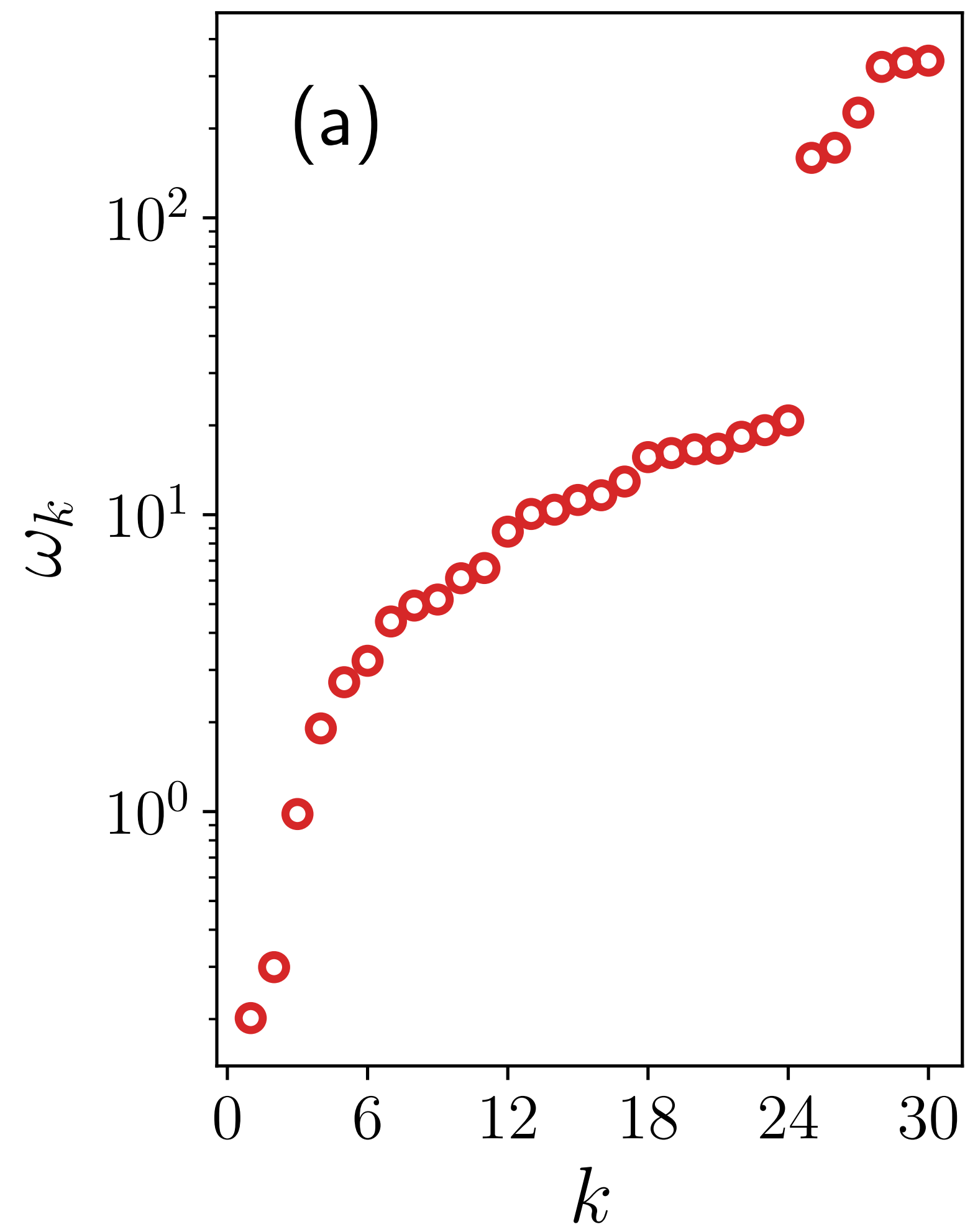


# Alanine dipeptide slow modes



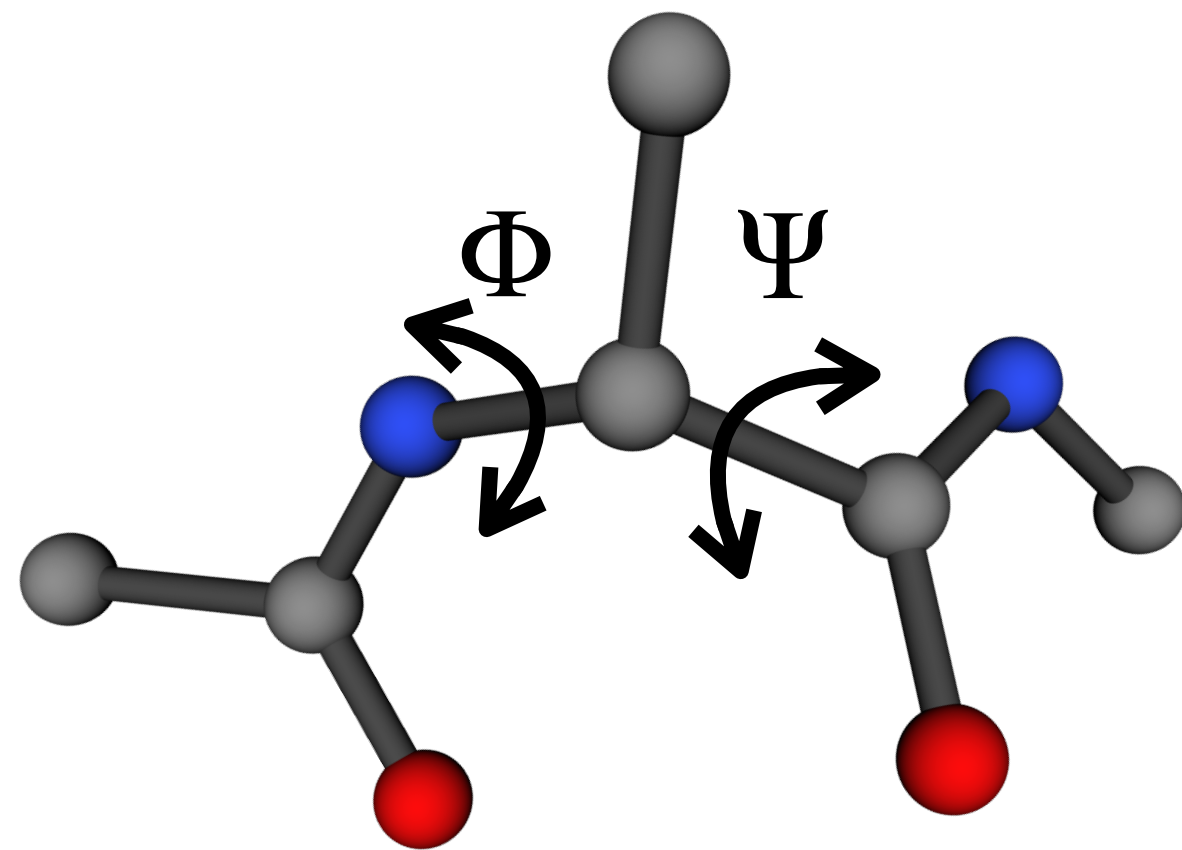
**Neural canonical transformation identifies nonlinear slow modes!**

# Alanine dipeptide slow modes

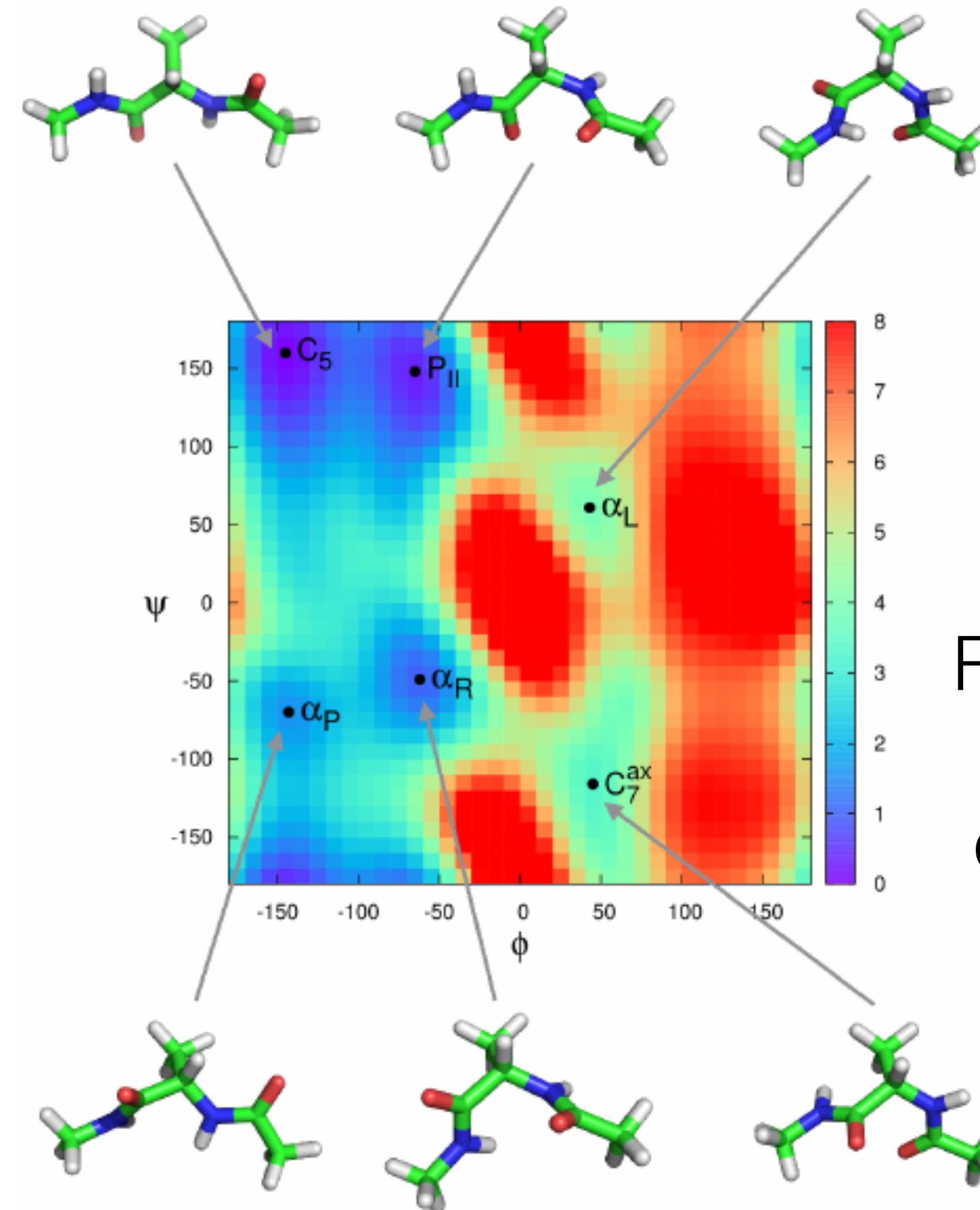
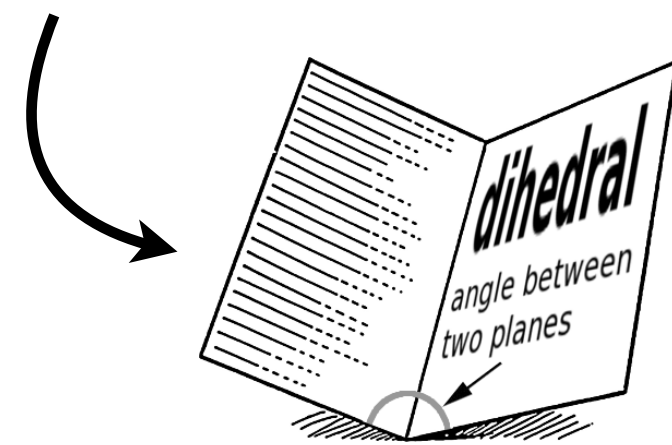


**Neural canonical transformation identifies nonlinear slow modes!**





slow motion of the  
two torsion angles



Ramachandran  
plot of stable  
conformations

**Dimensional reduction to slow collective variables  
useful for control, prediction, enhanced sampling...**

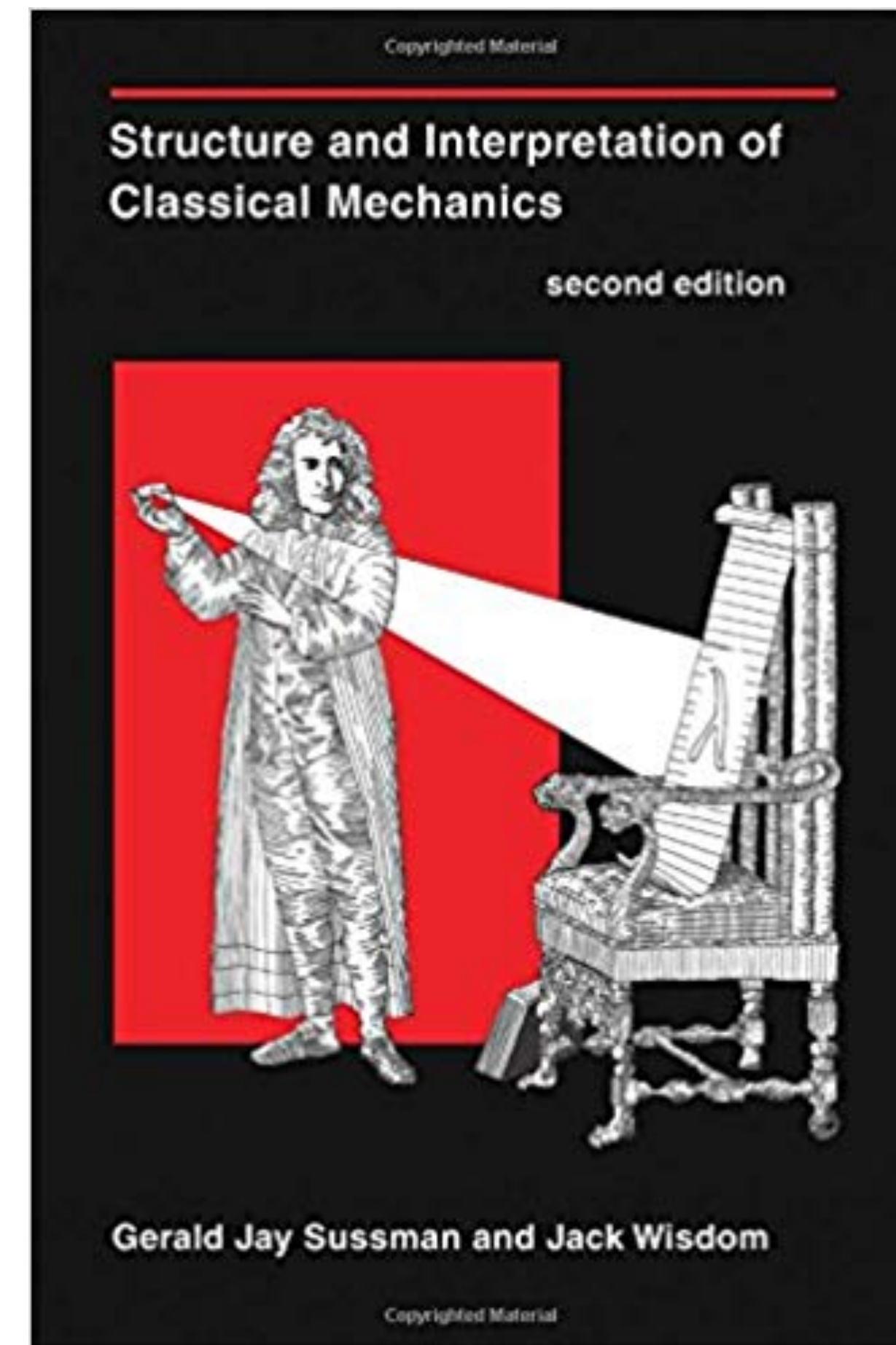
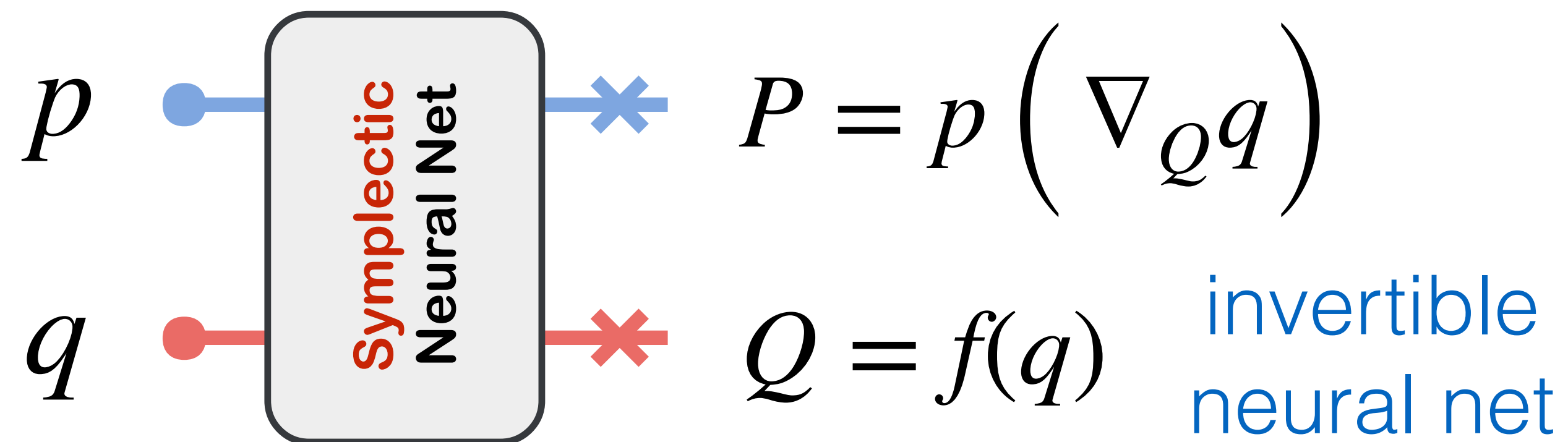
check the paper 1910.00024, PRX '20 for more examples & applications

# Symplectic primitives

- Linear transformation: Symplectic Lie algebra
- Continuous-time flow: Symplectic generating functions

Symplectic integrator of neural ODE, Chen et al 1806.07366

- **Neural point transformation**








# “A Hamiltonian Extravaganza”

—Danilo J. Rezende@DeepMind


Sep 25 **ICLR 2020 paper submission deadline**

Sep 26 *Symplectic ODE-Net*, 1909.12077  **SIEMENS**

Sep 27 *Hamiltonian Graph Networks with ODE Integrators*, 1909.12790  

Sep 29 *Symplectic RNN*, 1909.13334   

Sep 30 *Equivariant Hamiltonian Flows*, 1909.13739 

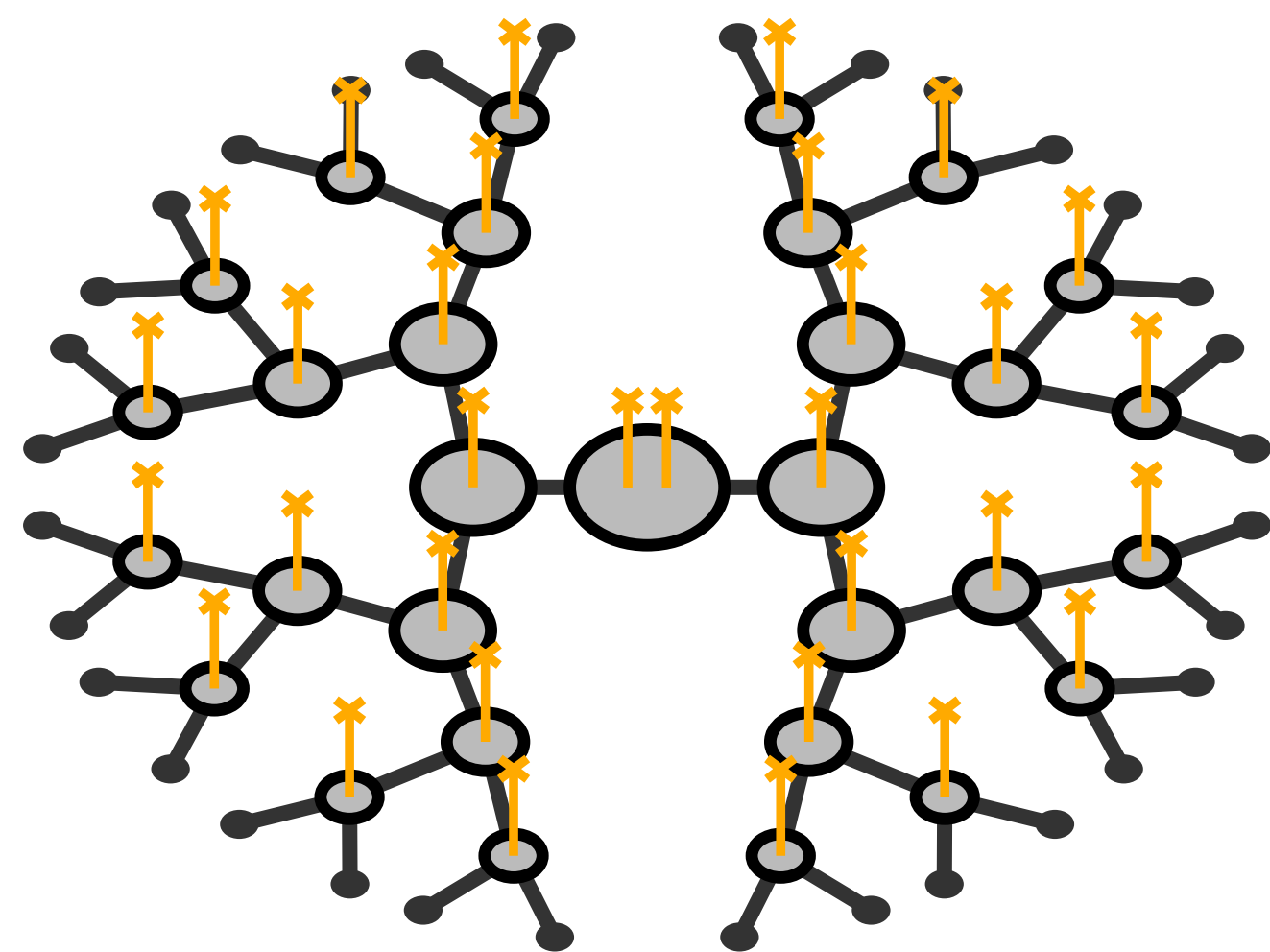
*Hamiltonian Generative Network*, 1909.13789  <http://tiny.cc/hgn>

*Neural Canonical Transformation with Symplectic Flows*, 1910.00024  

See also Bondesan & Lamacraft, *Learning Symmetries of Classical Integrable Systems*, 1906.04645

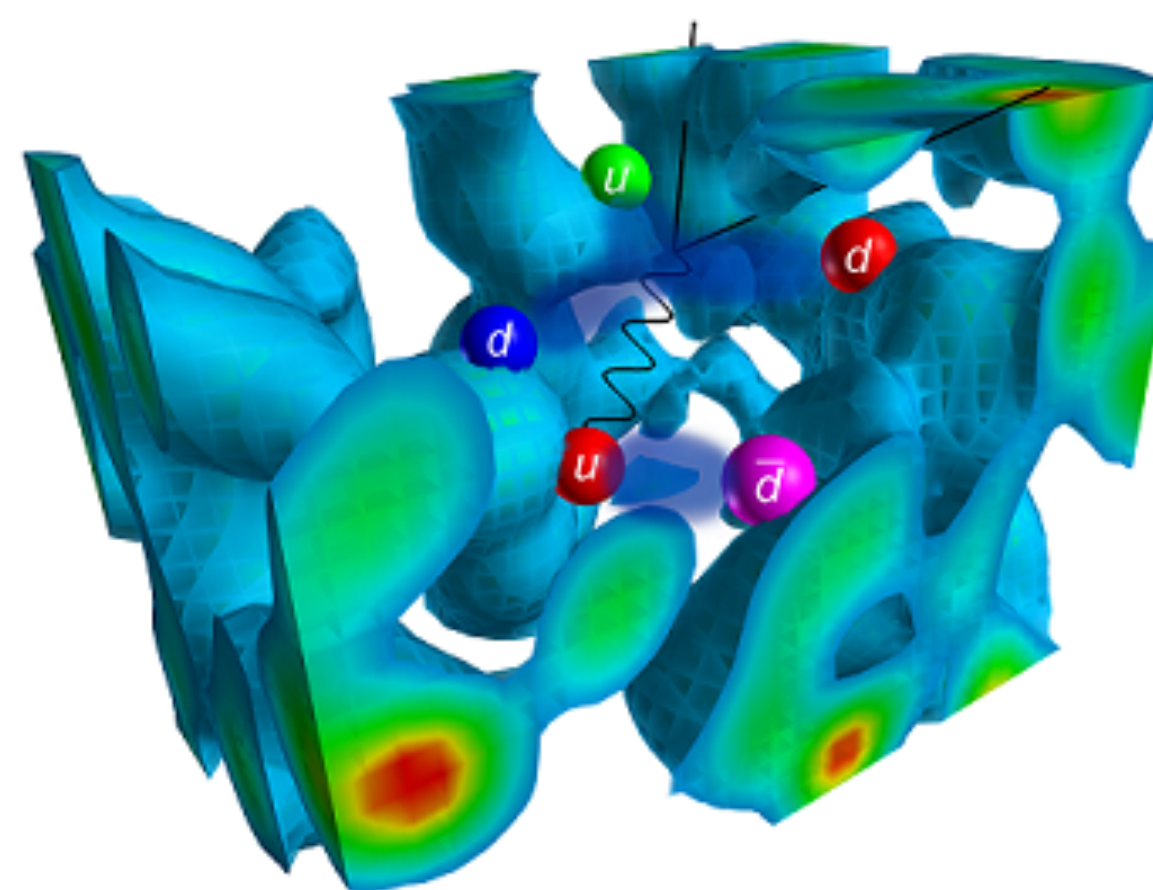
# Killer application in science ?

## Renormalization group



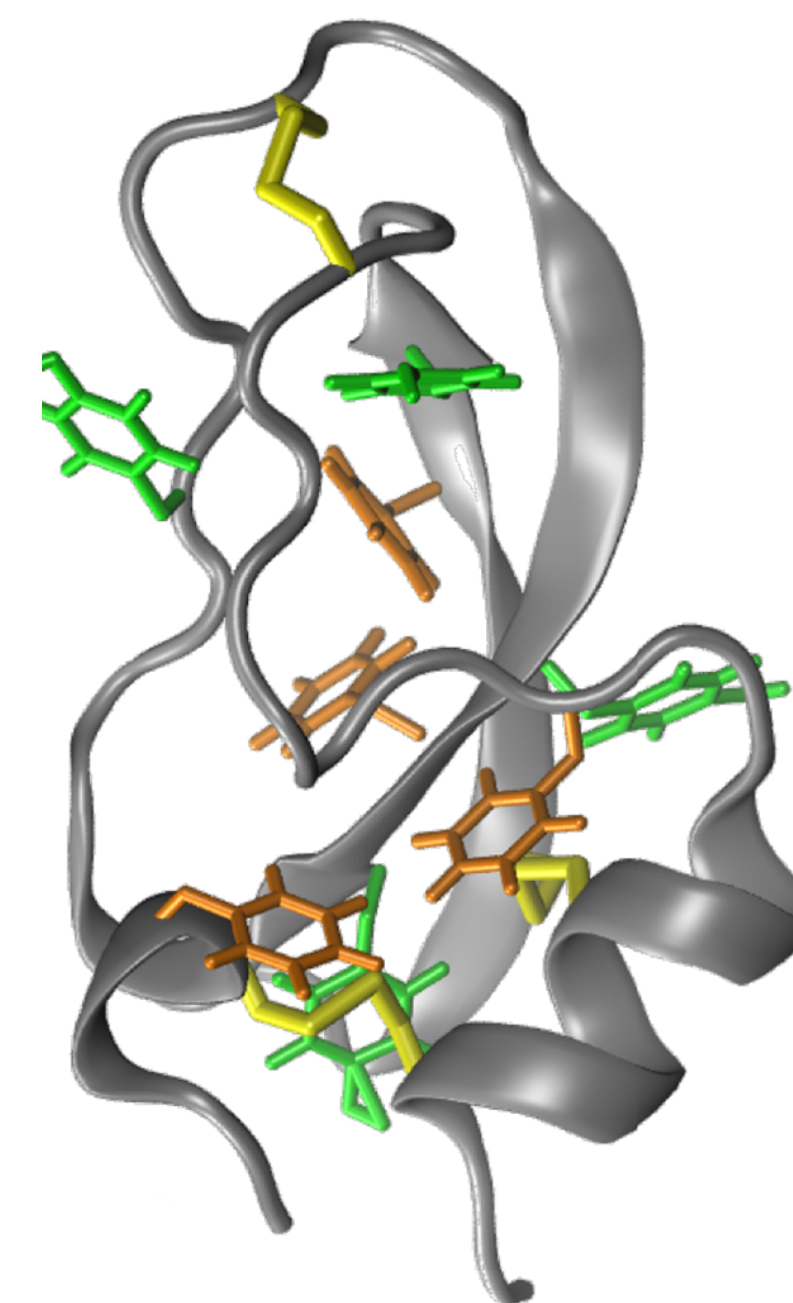
Li and LW, PRL '18  
Hu et al, PRRResearch '20

## Lattice field theory



Albergo et al, PRD '19  
Kanwar et al, PRL '20

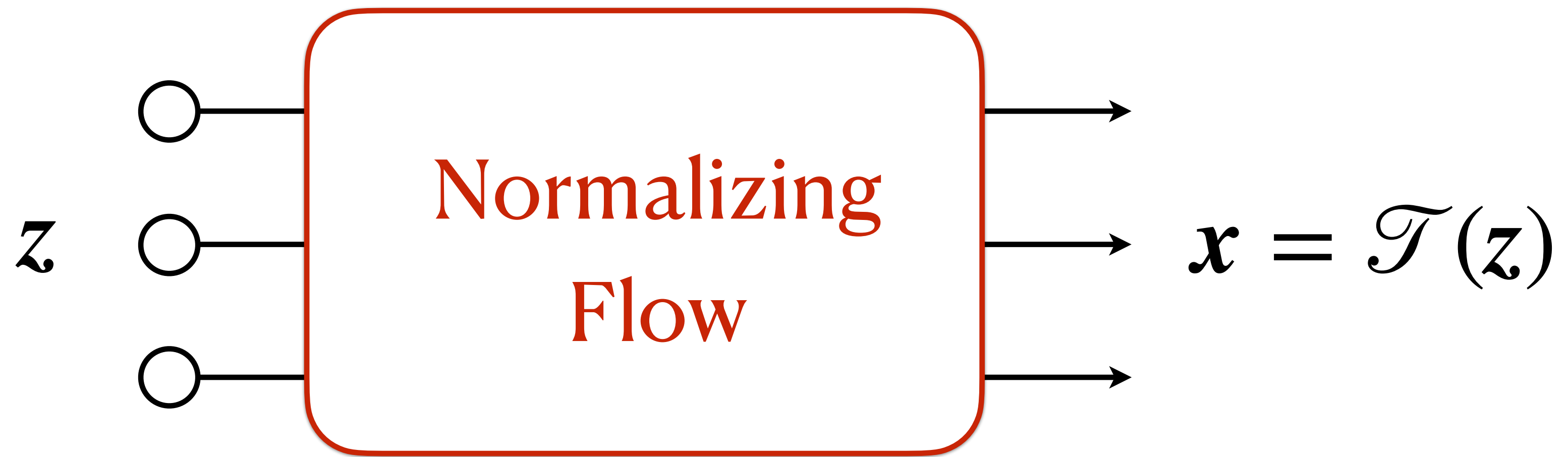
## Molecular simulation



Noe et al, Science '19  
Wirnsberger et al, JCP '20



# Symmetries



Invariance

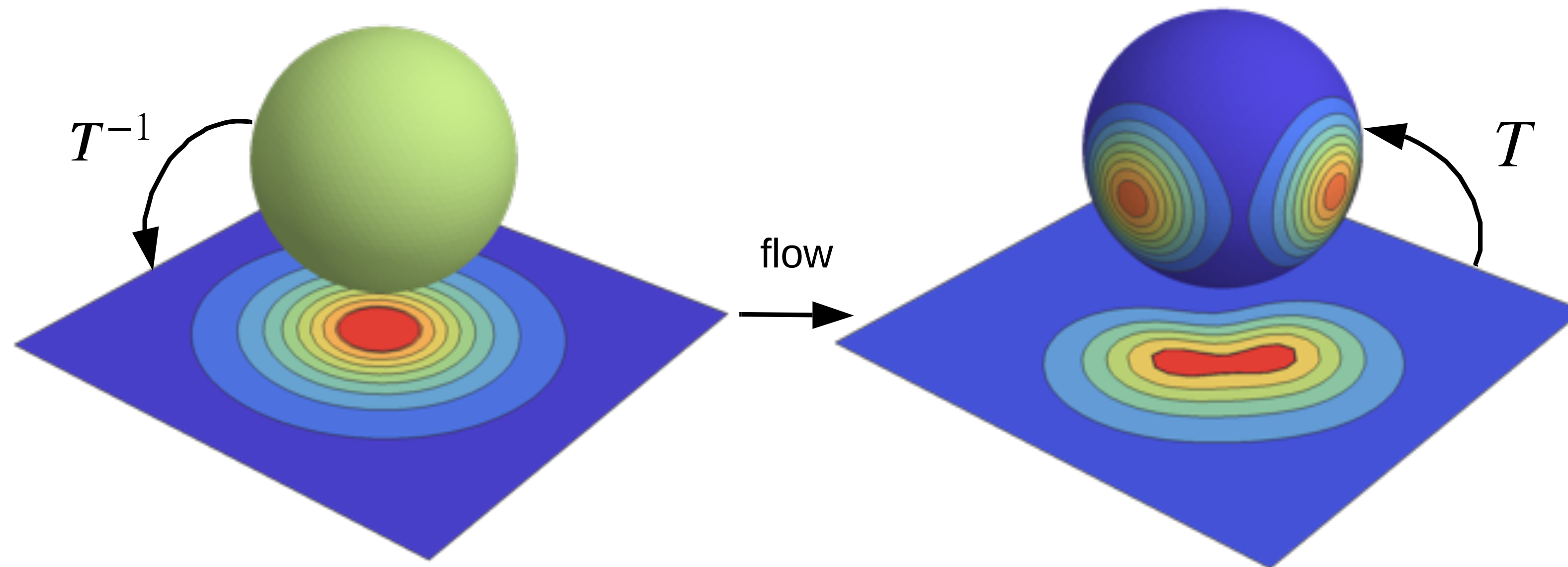
$$\rho(g \mathbf{x}) = \rho(\mathbf{x})$$

Equivariance

$$\mathcal{T}(g \mathbf{z}) = g \mathcal{T}(\mathbf{z})$$

Spatial symmetries, permutation symmetries, gauge symmetries...

# Flow on manifolds



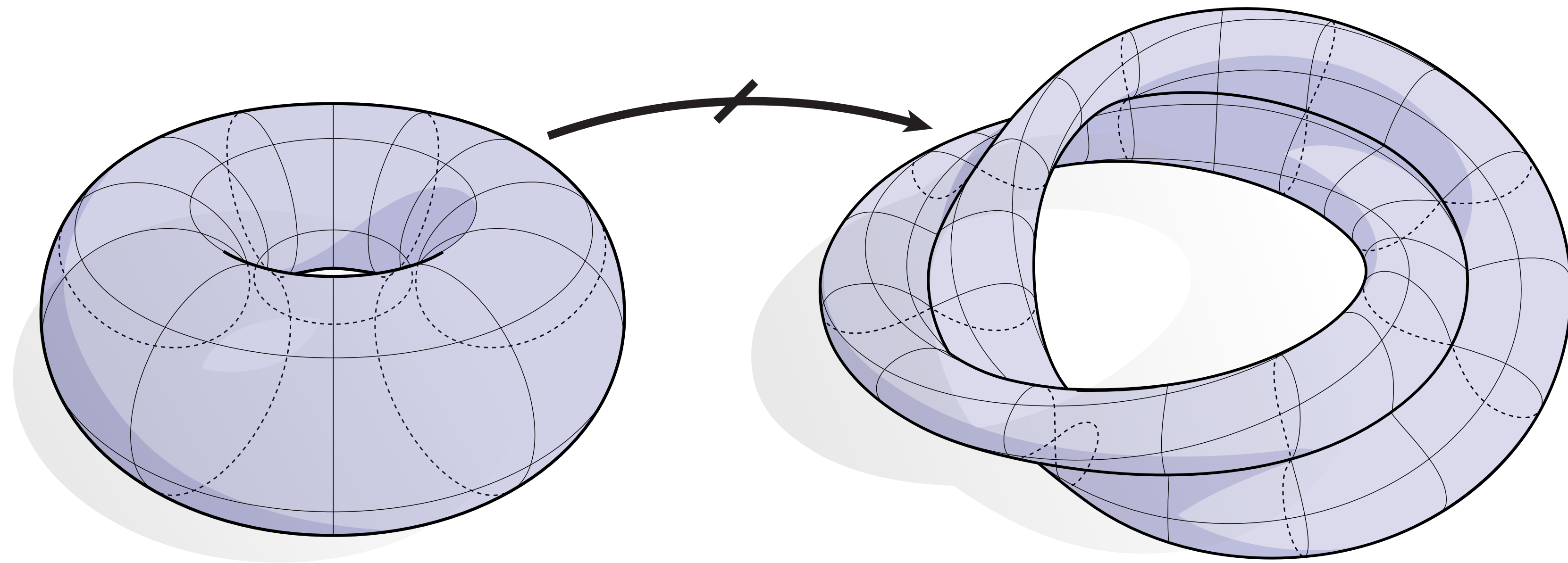
Periodic variables, gauge fields, ...

Gemici et al 1611.02304, Rezende et al, 2002.02428, Boyda et al, 2008.05456

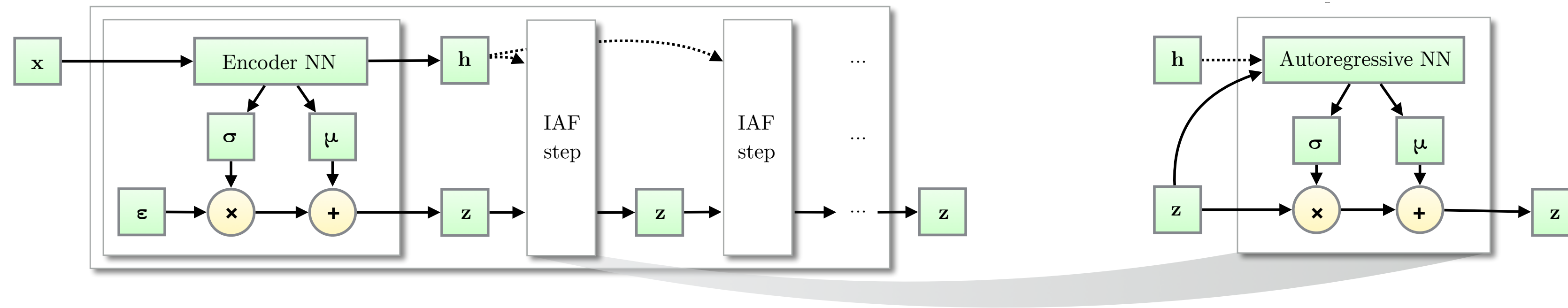
Neural ODE on manifolds, Falorsi et al, 2006.06663, Lou et al, 2006.10254, Mathieu et al, 2006.10605



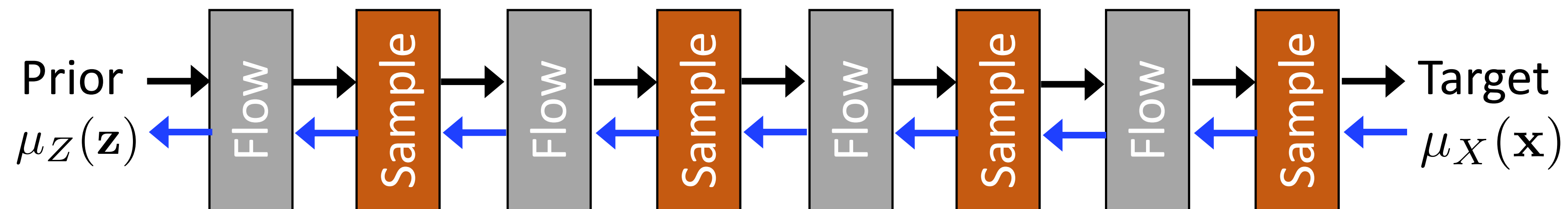
# Obstructions



# Mix with other approaches



Kingma et al, 1606.04934,...

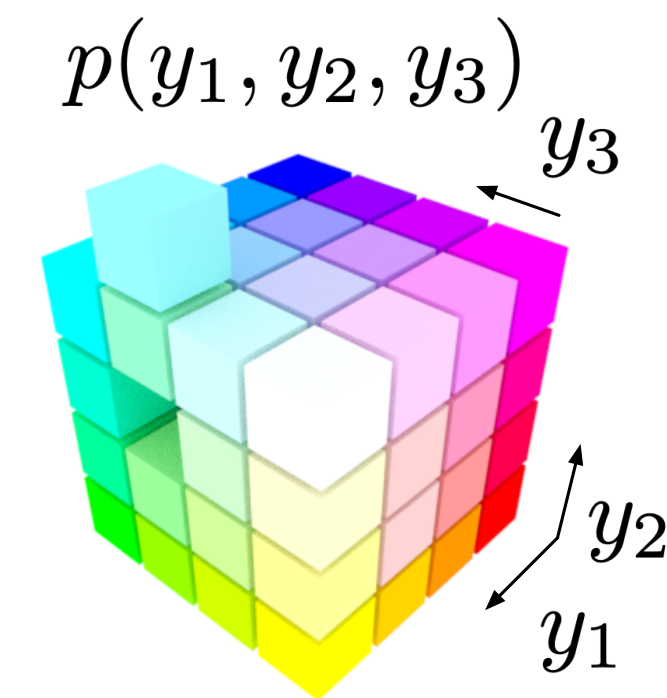
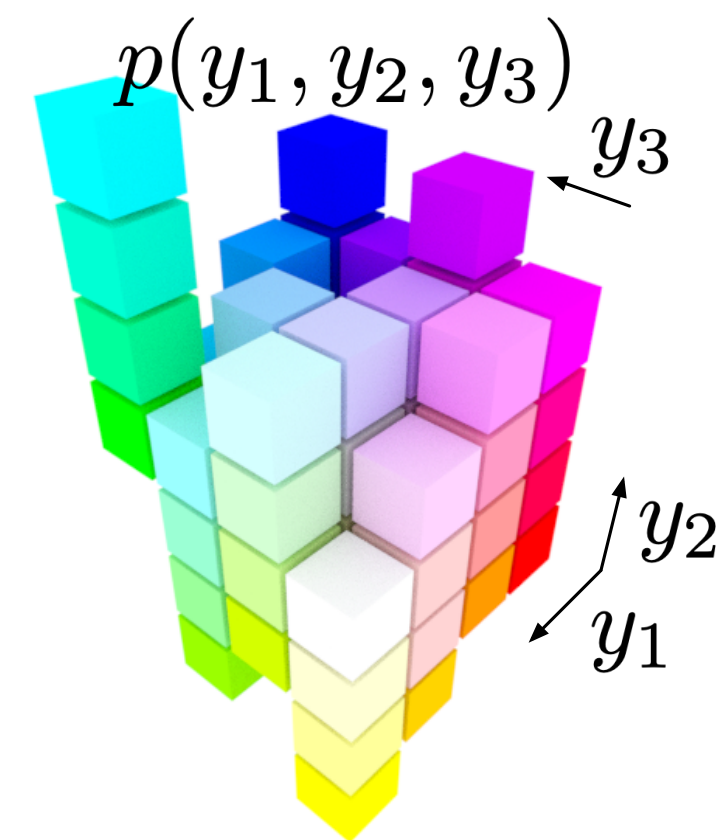
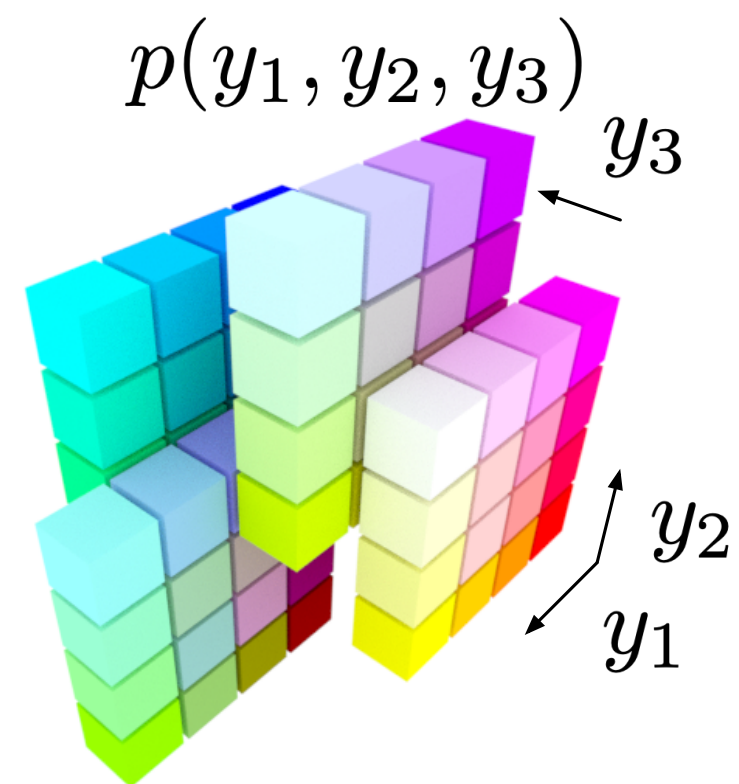
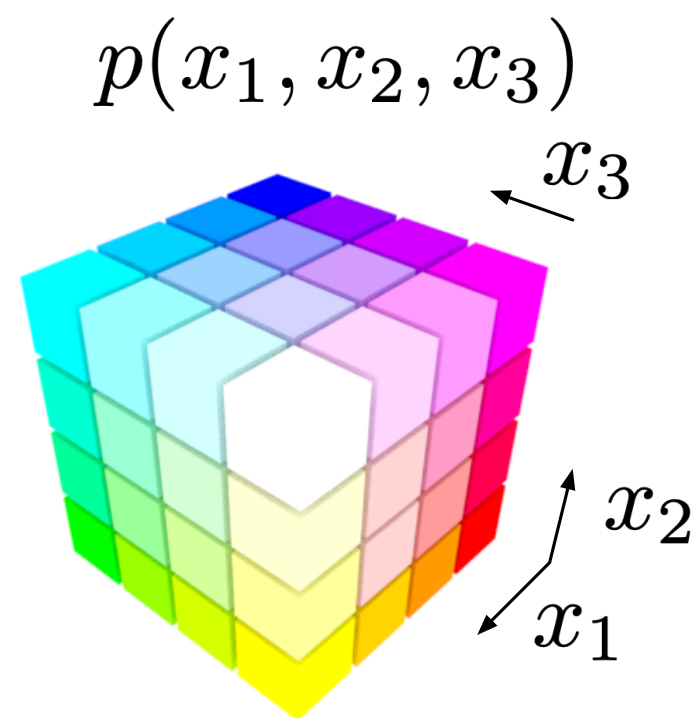


Levy et al, 1711.09268, Wu et al 2002.06707, ...



# Discrete flows

$$p(\mathbf{x}) = p(\mathbf{y} = \mathcal{T}(\mathbf{x}))$$



# Representation learning: what and how ?

What is a good representation ?

1812.02230

## Towards a Definition of Disentangled Representations

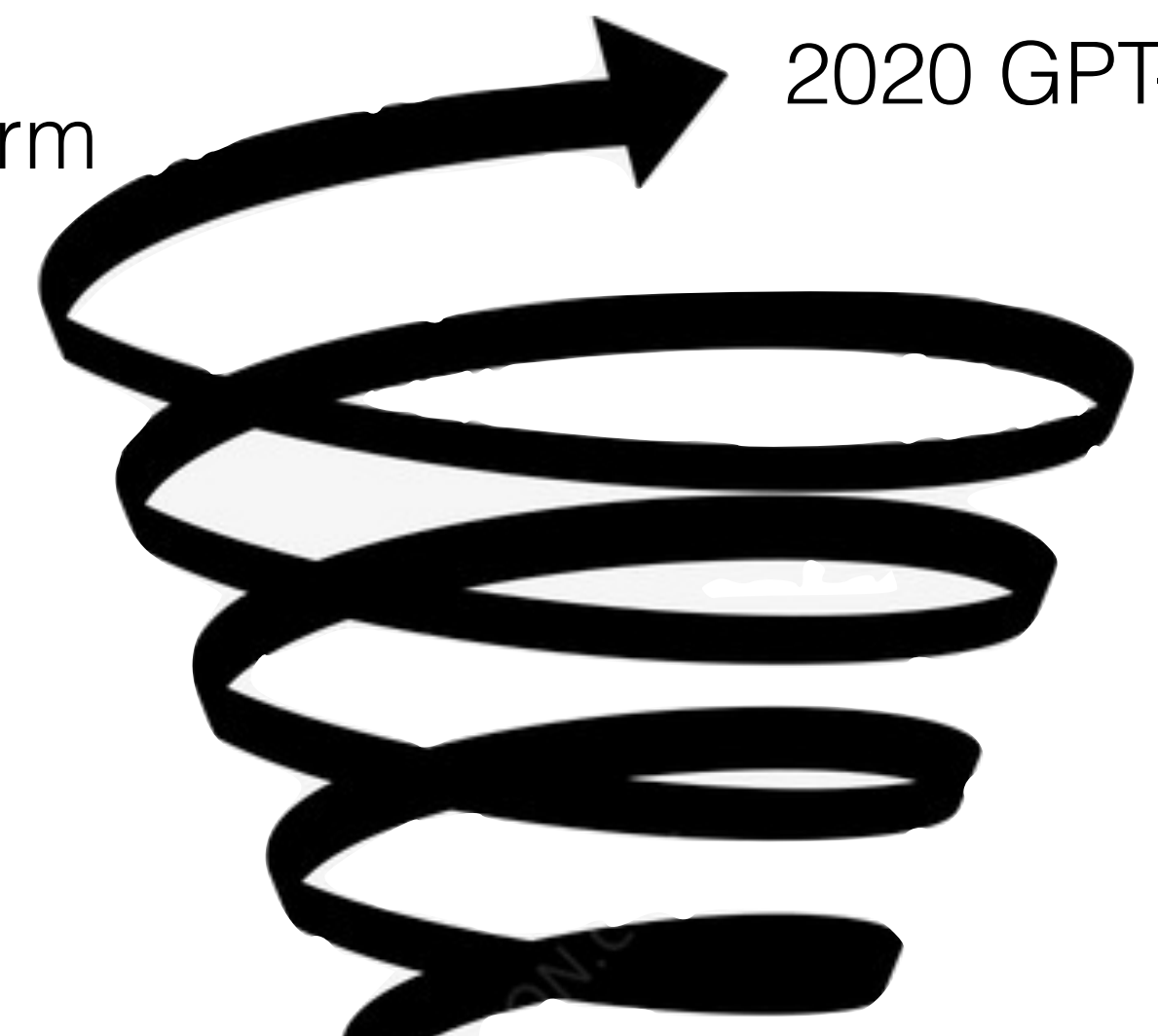
Irina Higgins\*, David Amos\*, David Pfau, Sebastien Racaniere,  
Loic Matthey, Danilo Rezende, Alexander Lerchner  
DeepMind

**G**enerative **P**re-**T**raining appears to be a successful way in learning good representations

2010  
relu, batchnorm  
resnet ...

2020 GPT-3

2006  
deep  
belief net





# Thank You!

## Explore more in the interface of machine learning & physics

### 量子纠缠:从量子物质态到深度学习

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(2 中国科学院大学 北京 100049)

《物理》2017年7月

### 微分万物:深度学习的启示\*

王 磊<sup>1,2,†</sup> 刘金国<sup>3</sup>

(1 中国科学院物理研究所 北京 100190)

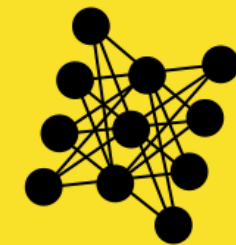
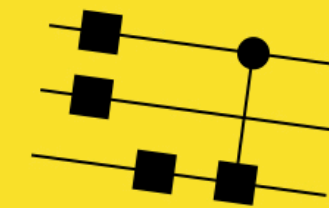
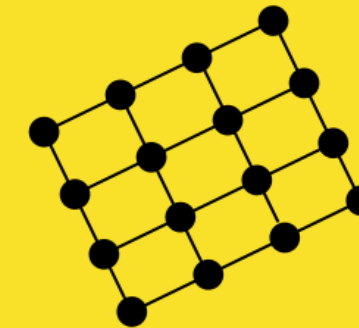
(2 松山湖材料实验室 东莞 523808)

(3 哈佛大学物理系 剑桥 02138)

《物理》2021年2月

# Spring School

## 深度学习&量子编程



王磊

深度学习: 从理论到实践

以微分编程和表示学习为重点  
介绍深度学习技术, 并讲解它们在  
统计物理和量子多体计算中的应用实例

张潘

从机器学习角度理解张量网络

从表述, 优化, 学习与泛化这  
四个角度介绍张量网络及其在  
应用数学和机器学习中的应用

罗秀哲

面向物理学家的Julia编程实践

以量子物理的工程实践为重点介绍  
Julia语言, 量子计算的基础概念, Julia  
语言中的CUDA编程和量子物理工具链

刘金国

量子编程实践

介绍量子机器学习, 量子优化算法和  
量子化学中的研究前沿, 基于Julia量子  
计算库Yao.jl实现这些算法, 介绍自动  
微分与GPU编程在量子编程中的应用

报名方式:



<https://bit.ly/2CE5J8H>

教学资料:

<https://github.com/QuantumBFS/SSSS>

授课形式:

中文授课+程序演示+Hackathon (有奖品)

时间: 2019年5月6-10日

地点: 广东东莞

松山湖材料实验室

粤港澳交叉科学中心

Quantum Hackathon:

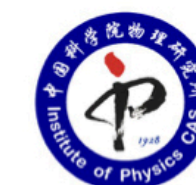
学员将通过组队的形式, 完成  
一个量子物理相关的编程挑战。  
我们将评出表现突出的团队,  
给予奖励。

Contact: [wanglei@iphy.ac.cn](mailto:wanglei@iphy.ac.cn)



QuantumBFS  
Yao Framework

julia



SONGSHAN LAKE  
MATERIALS LABORATORY  
松山湖材料实验室