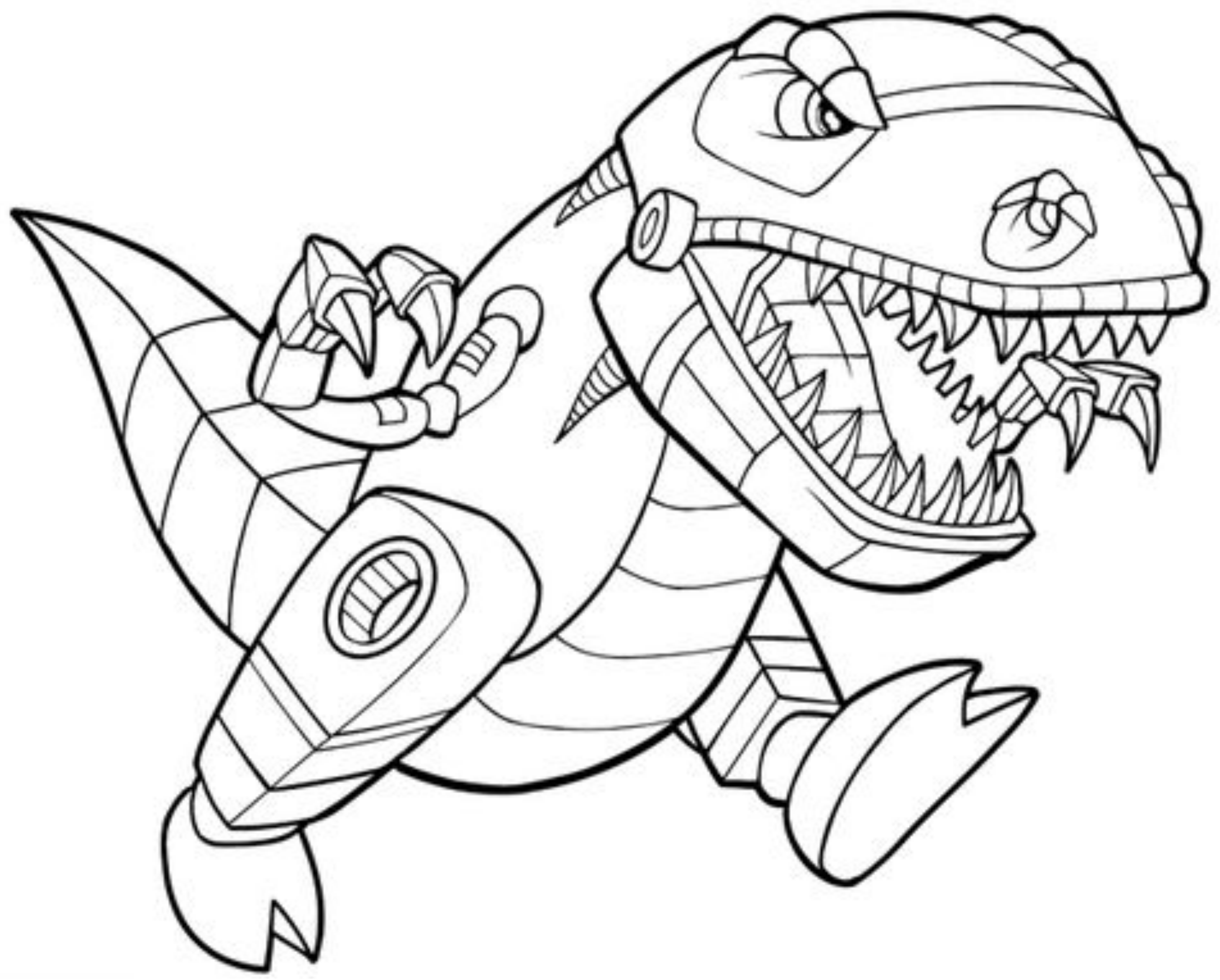

Neural Canonical Transformations

Lei Wang (王磊)

https://wangleiphy.github.io

Institute of Physics, CAS

Hamiltonian dynamics

Hamiltonian equations

$$\begin{cases} \dot{p} = -\dfrac{\partial H}{\partial q} \\[2ex] \dot{q} = +\dfrac{\partial H}{\partial p} \end{cases}$$

Hamiltonian dynamics

Hamiltonian equations

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

Phase space variables

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

Symplectic metric

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

Hamiltonian dynamics

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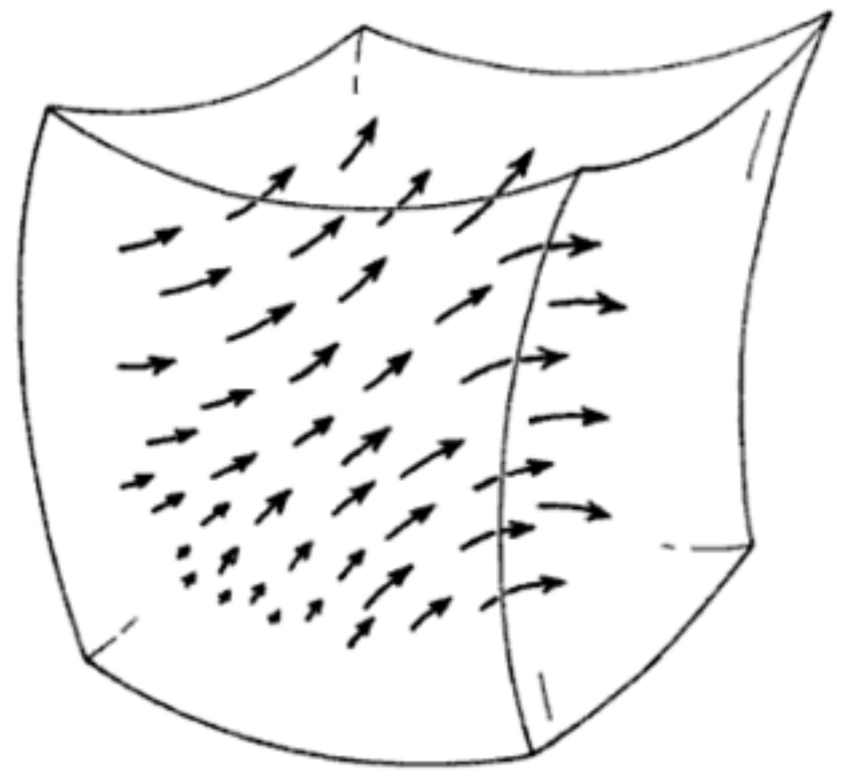
Symplectic metric

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

Symplectic gradient flow

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



Hamiltonian dynamics

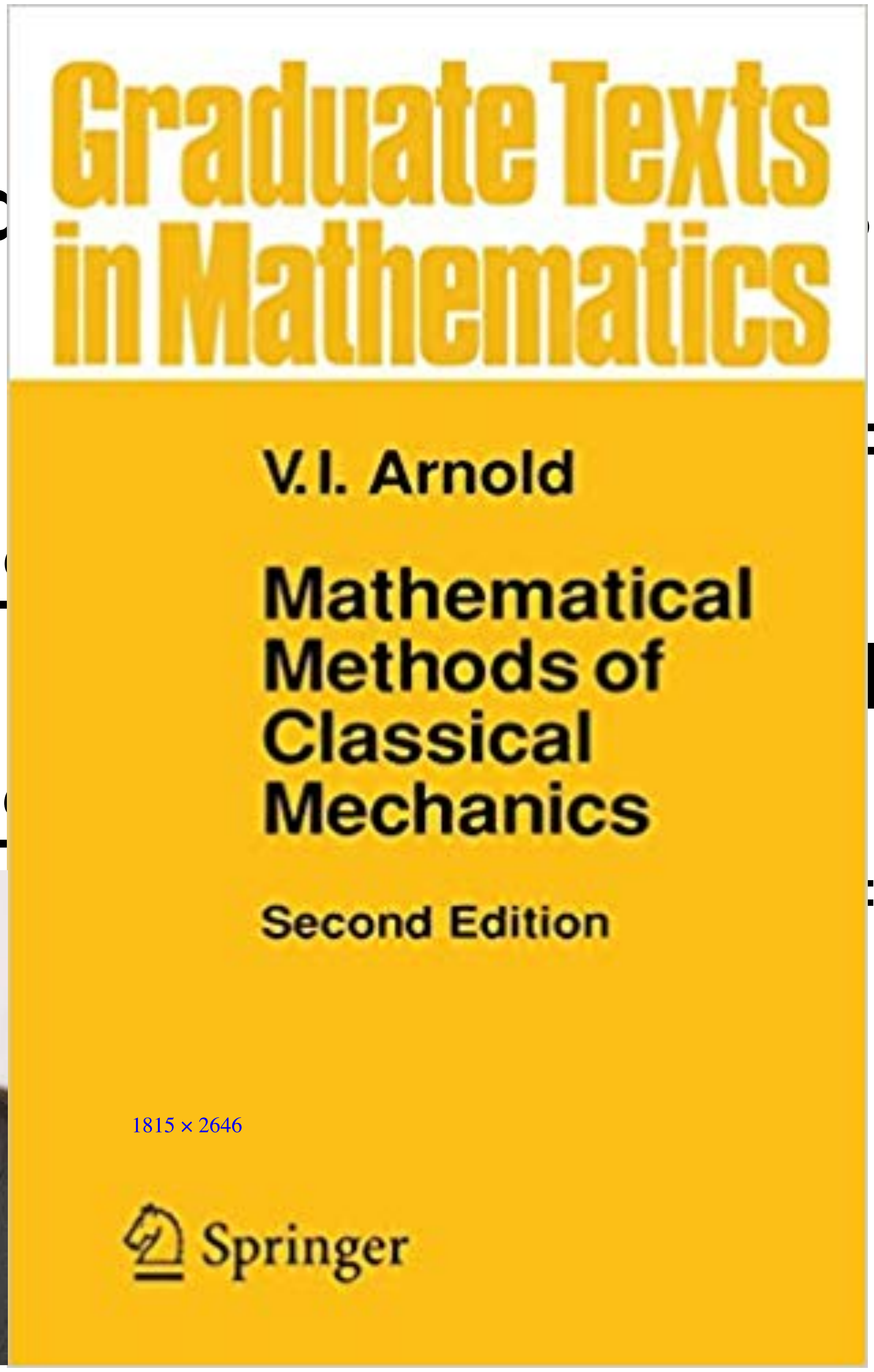
Hamiltonian ec **pace va** **ic gradient flow**

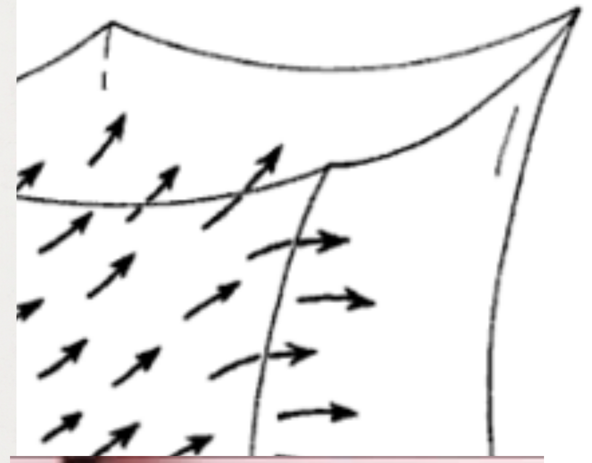
$= (p, q$ $\nabla_x H(\boldsymbol{x}) J$

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

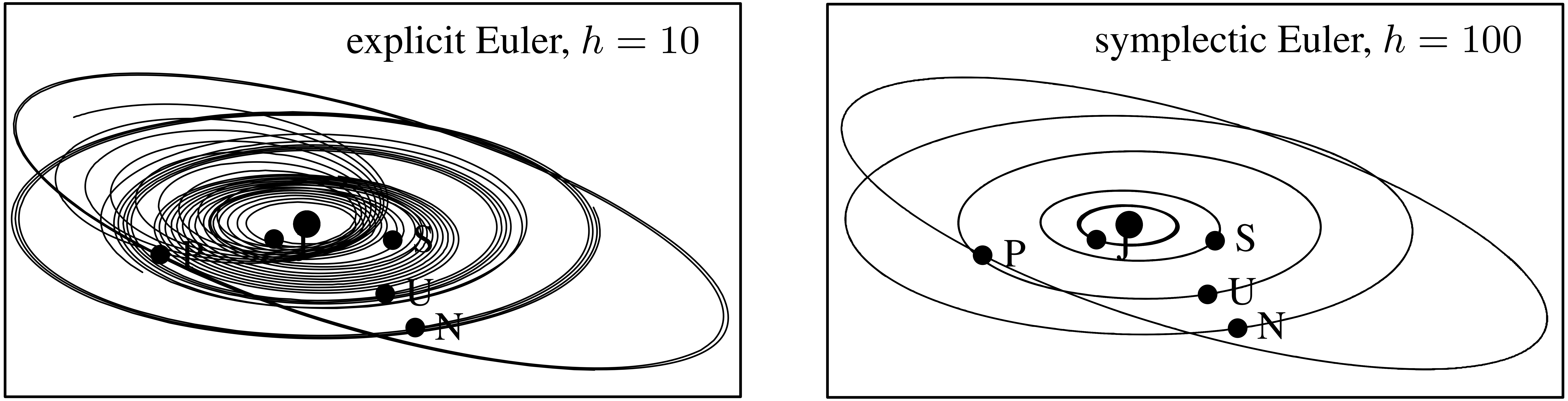
lectic m

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





Symplectic Integrators



from Hairer et al, Geometric Numerical Integration

Canonical Transformations

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

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

Canonical Transformations

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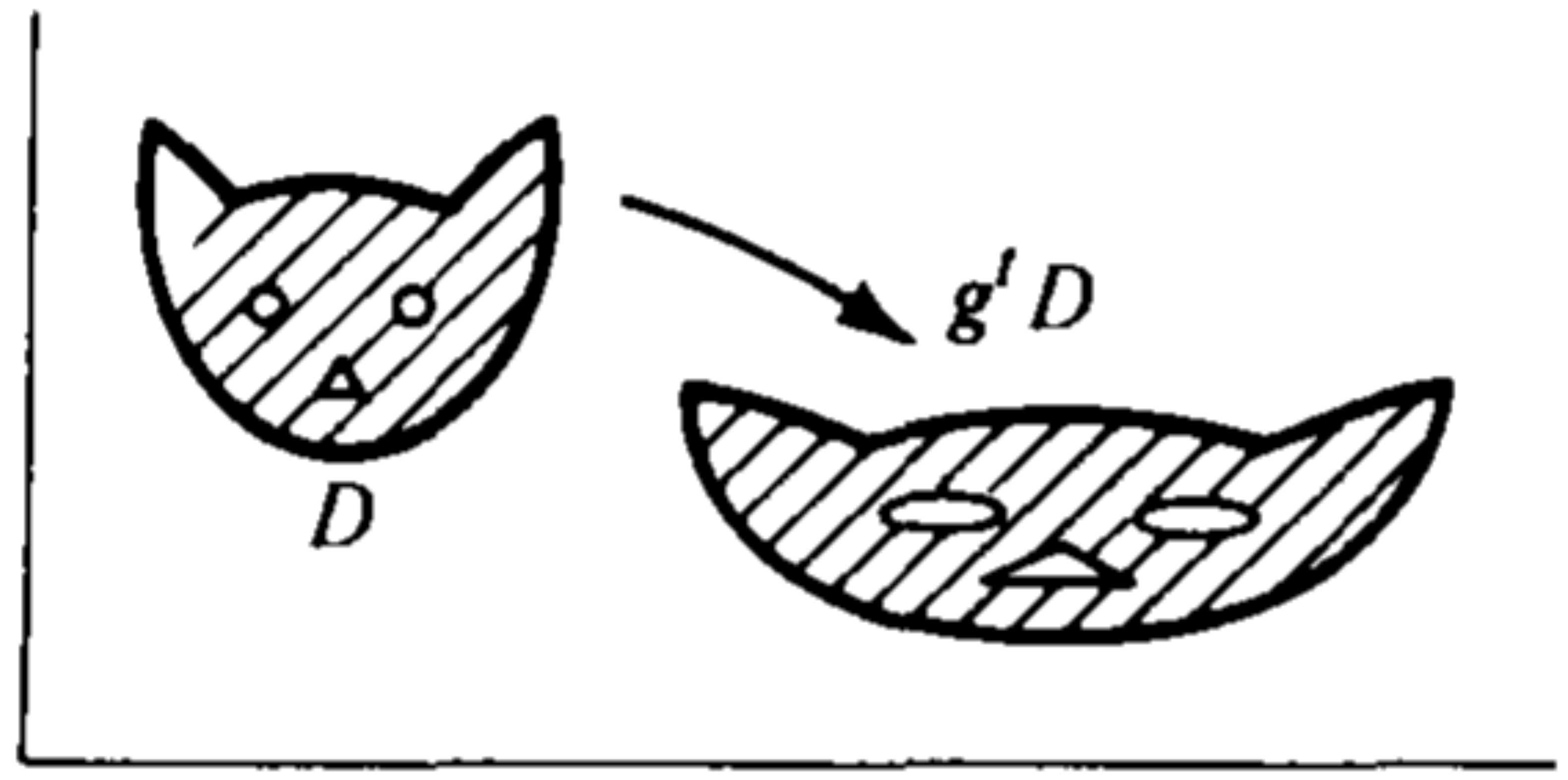
one has $\dot{\boldsymbol{z}} = \nabla_{\boldsymbol{z}} K(\boldsymbol{z}) J$ where $K(\boldsymbol{z}) = H \circ \boldsymbol{x}(\boldsymbol{z})$

Preserves Hamiltonian dynamics in the "latent phase space"

Statistical mechanics perspective

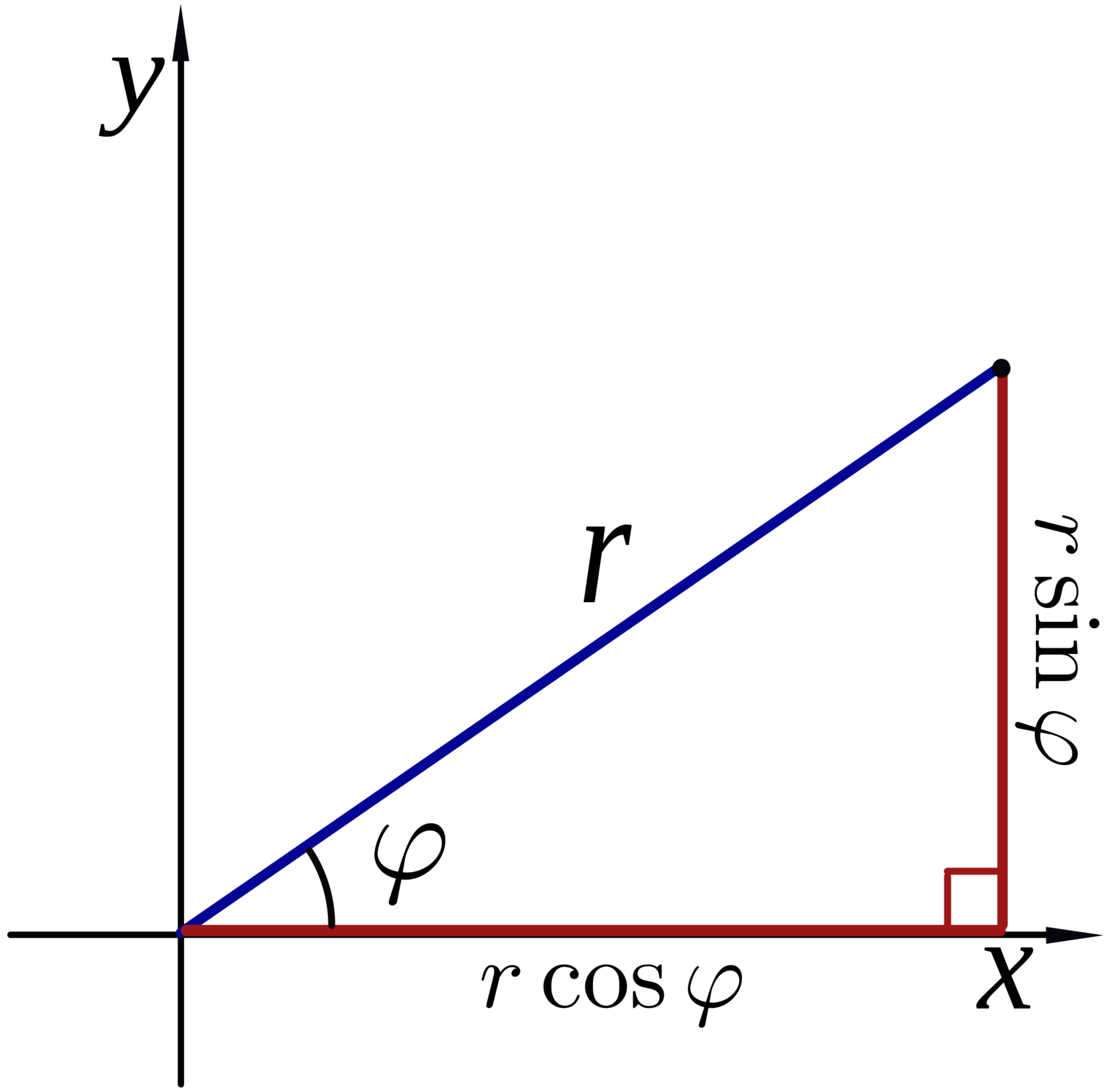
- Canonical transformation deforms phase space density $\rho(\boldsymbol{x}) = e^{-\beta H(\boldsymbol{x})}$
- Symplectic condition => Jacobian determinant = 1
- **Liouville theorem:** incompressible flow in phase space



Example: Cartesian <—> Polar

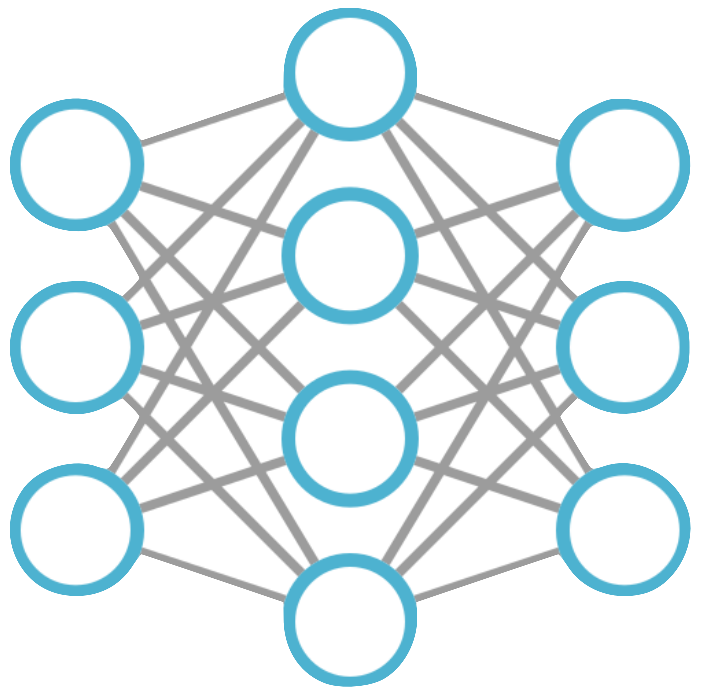
$$(p_x, p_y, x, y) \longleftrightarrow (p_r, p_\varphi, r, \varphi)$$

$$H = \frac{1}{2}\left(p_x^2 + p_y^2\right) + V(x, y)$$



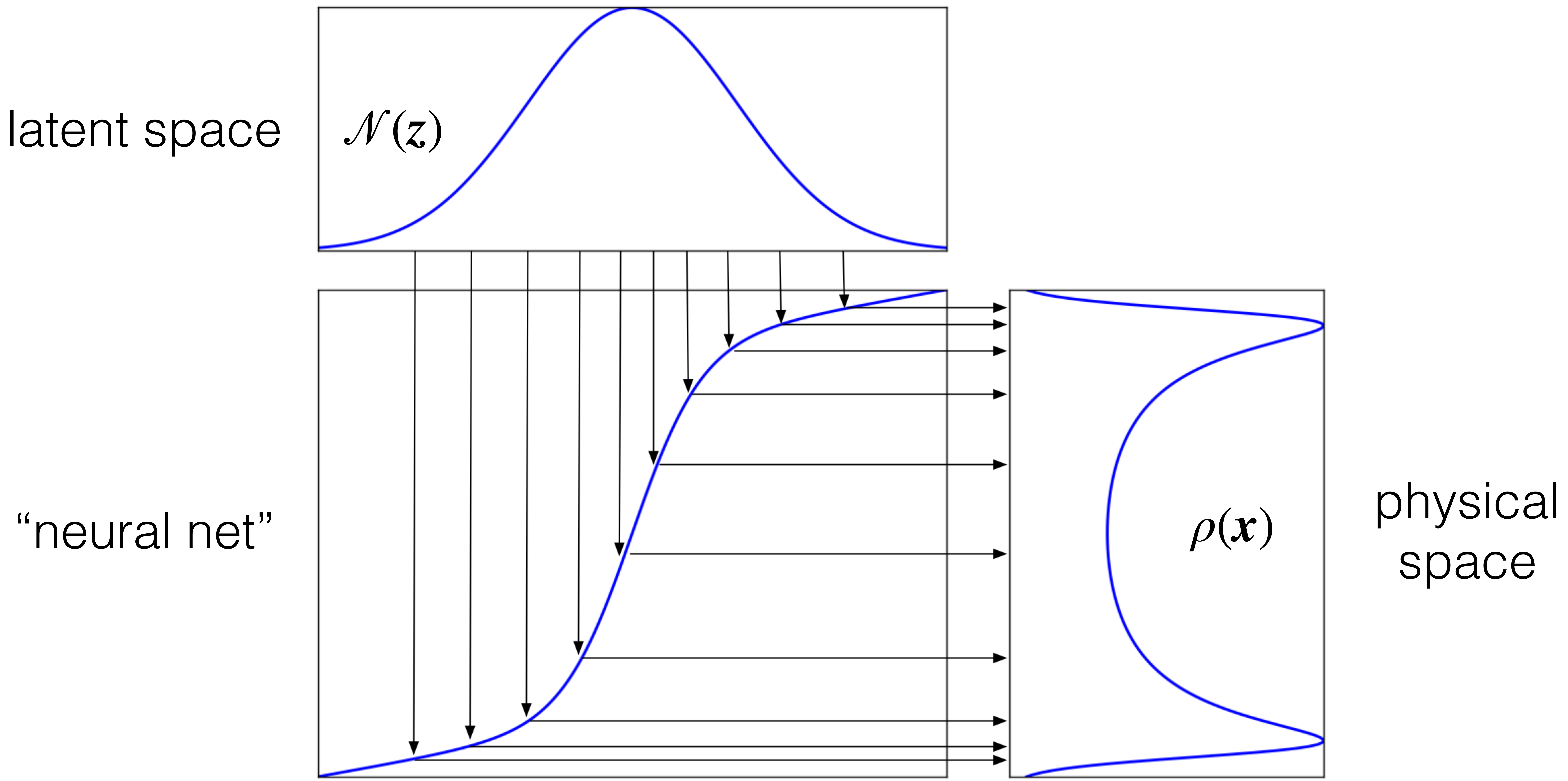
$$K = \frac{1}{2}\left(p_r^2 + \frac{1}{r^2} p_\varphi^2\right) + V(r, \varphi)$$

How to design "useful" canonical transformations ?

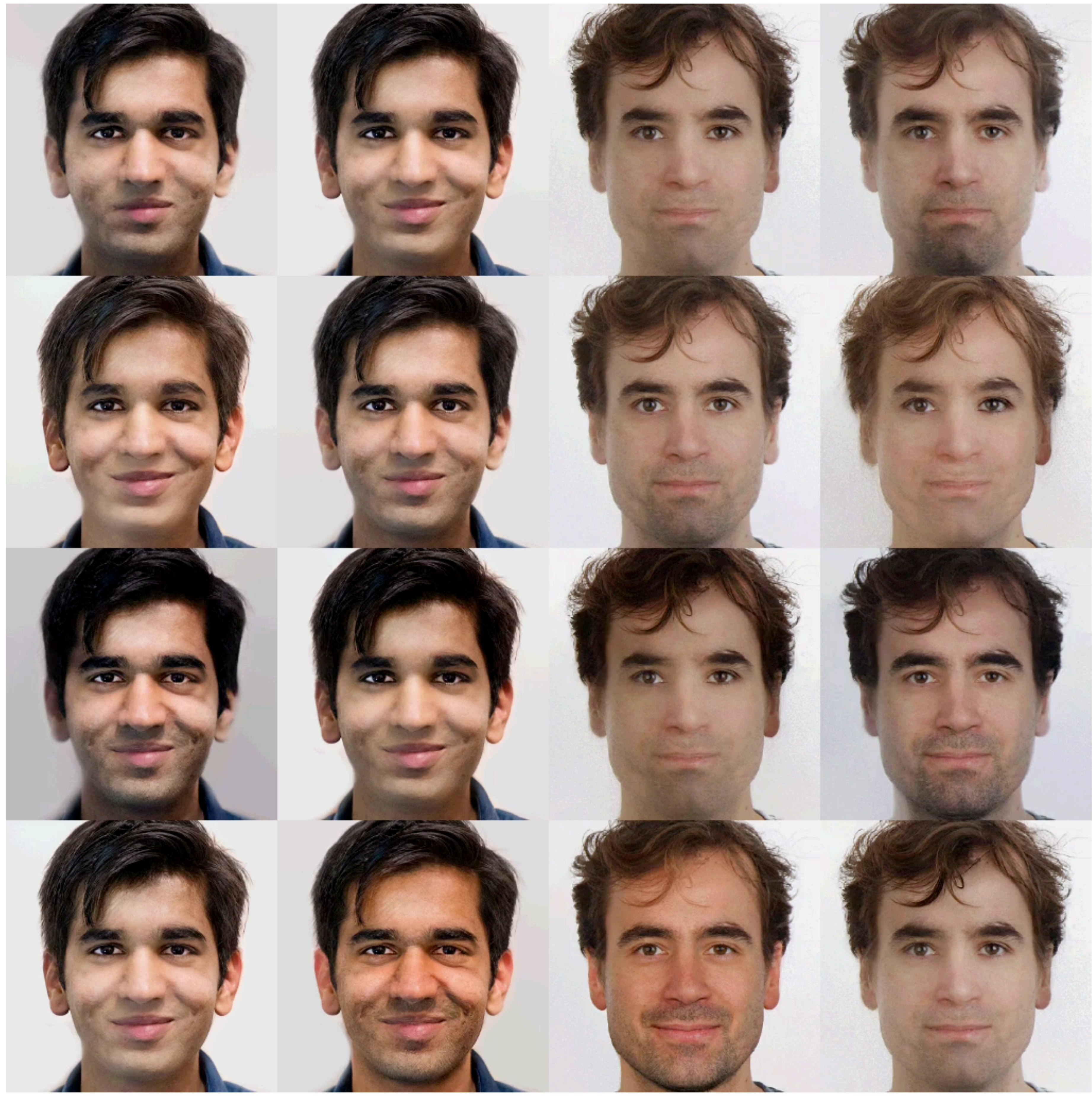


Neural Canonical Transformations

Neural transformation in 1d



Neural transformations in higher dims



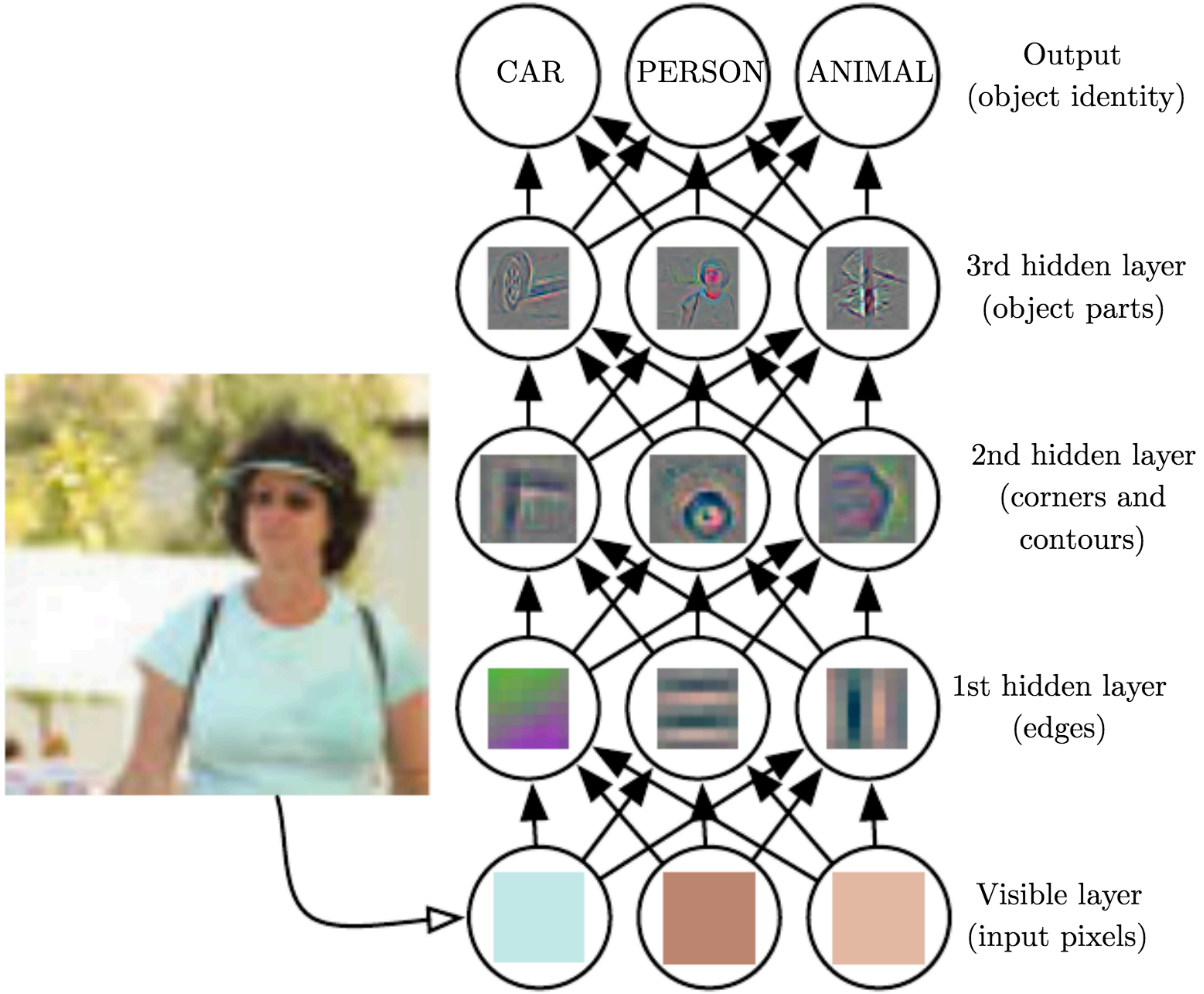
WaveNet 1609.03499 1711.10433

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

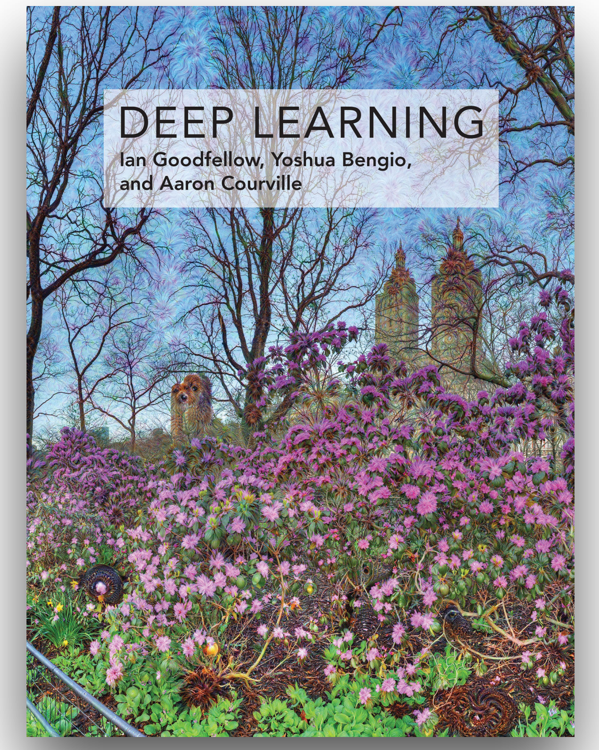
Glow 1807.03039

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

Representation Learning

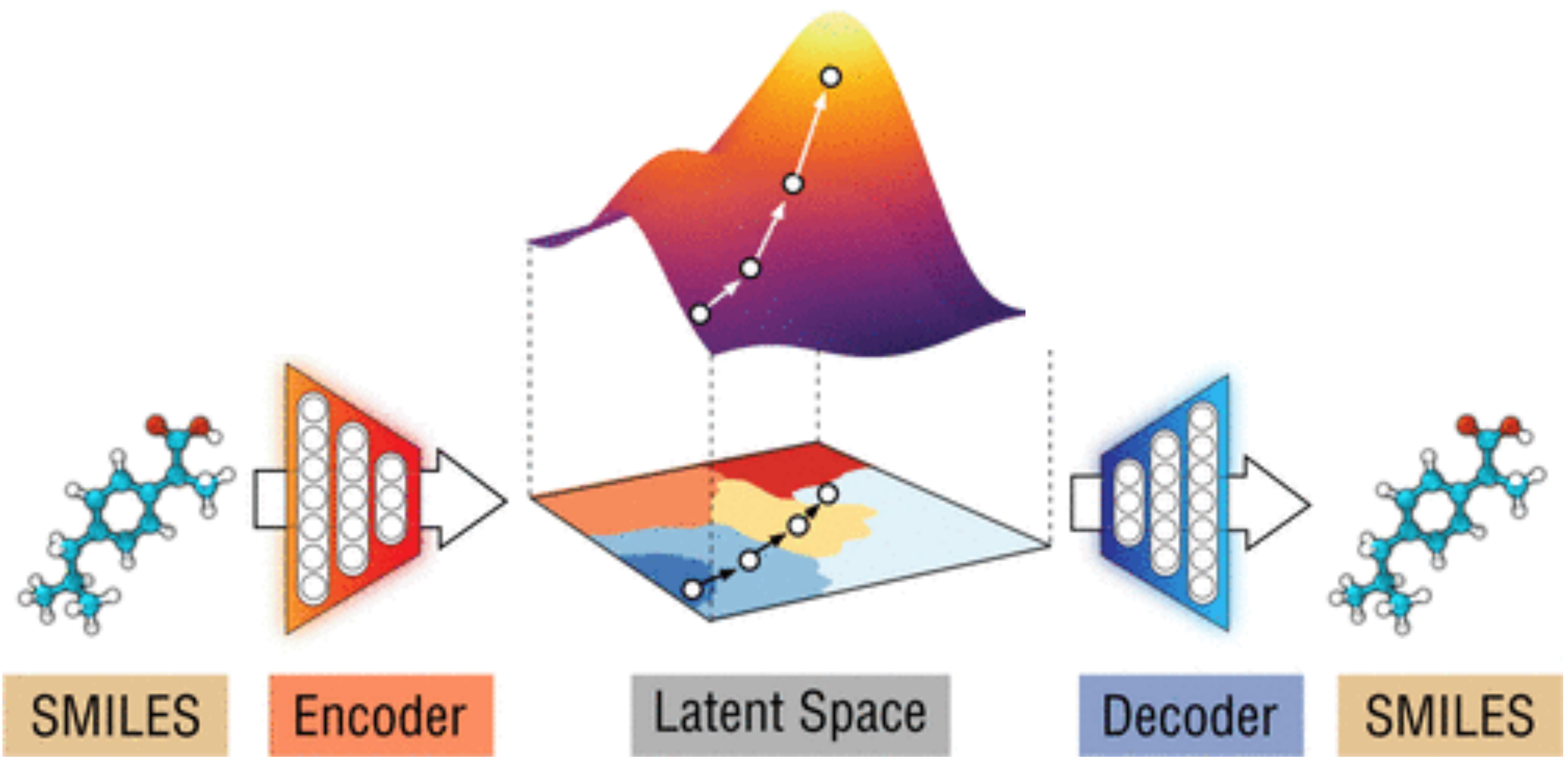


Page 6
Figure 1.2

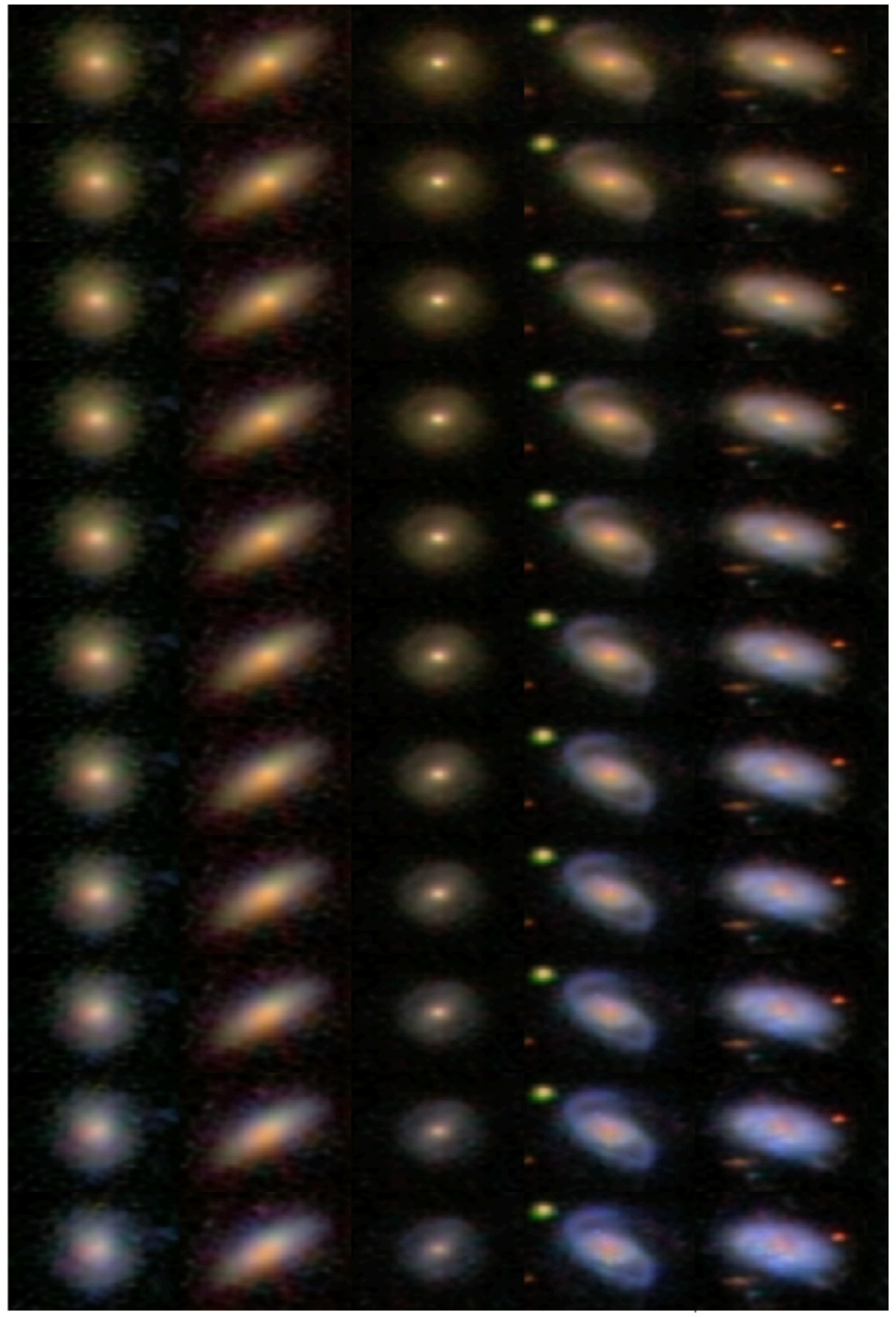


Goodfellow, Bengio, Courville, http://www.deeplearningbook.org/

Learning representation for science

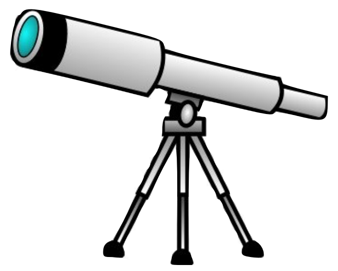


Automatic chemical design
Gomez-Bombarelli et al,1610.02415

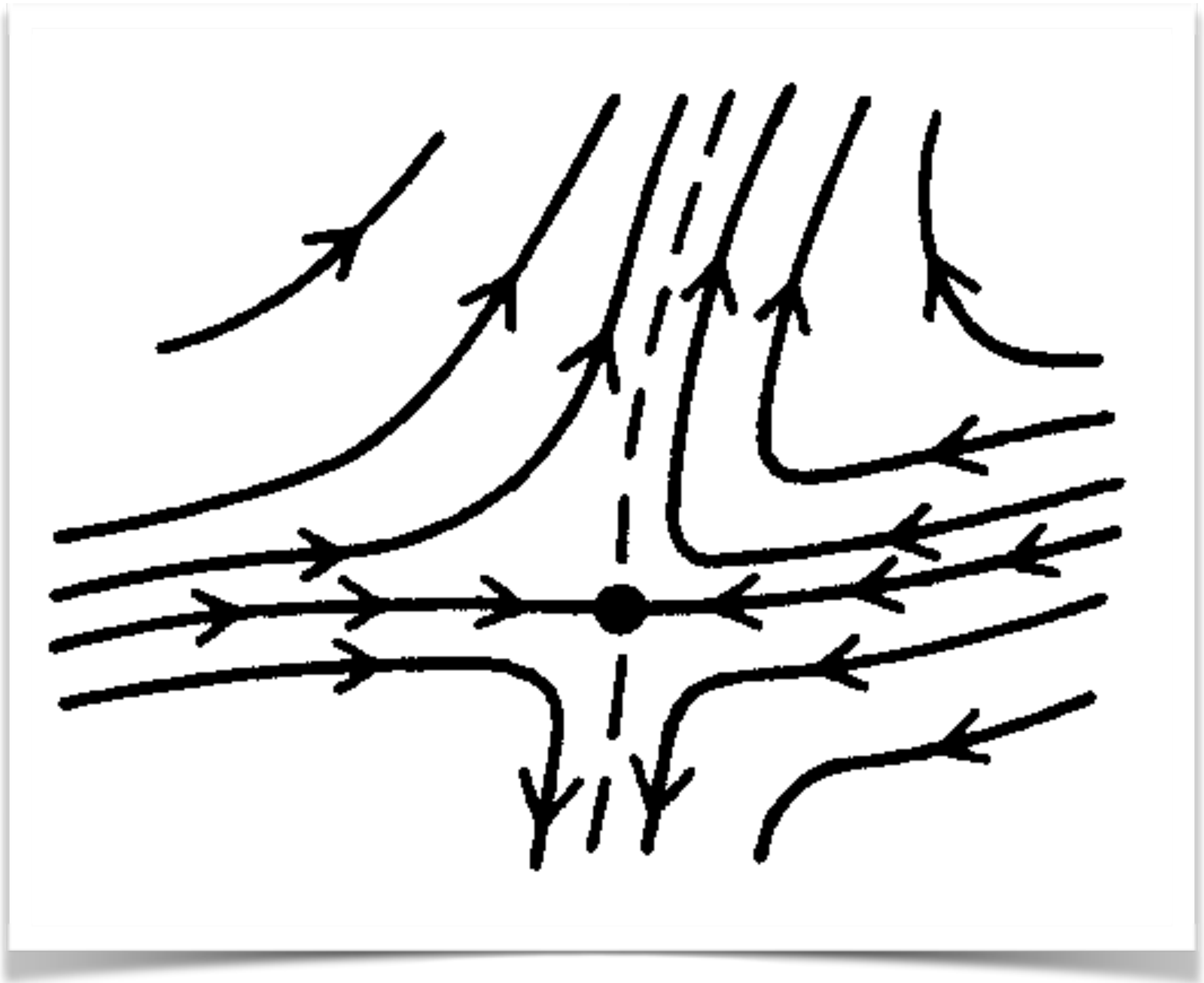


Galaxy evolution
Schawinski et al, 1812.01114

Representation learning in statistical physics

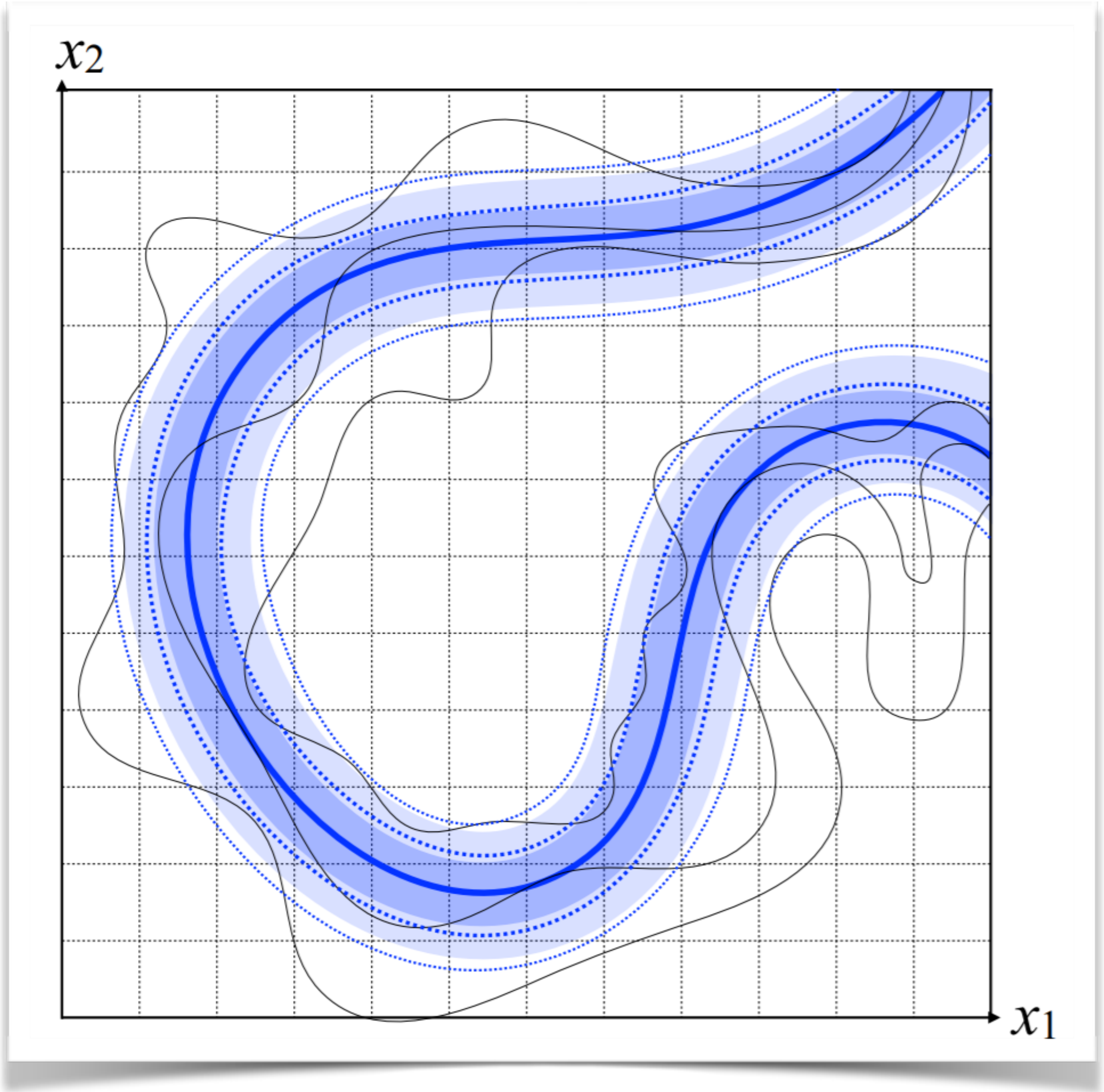


Renormalization group



Effective theory emerges upon transformation of the variables

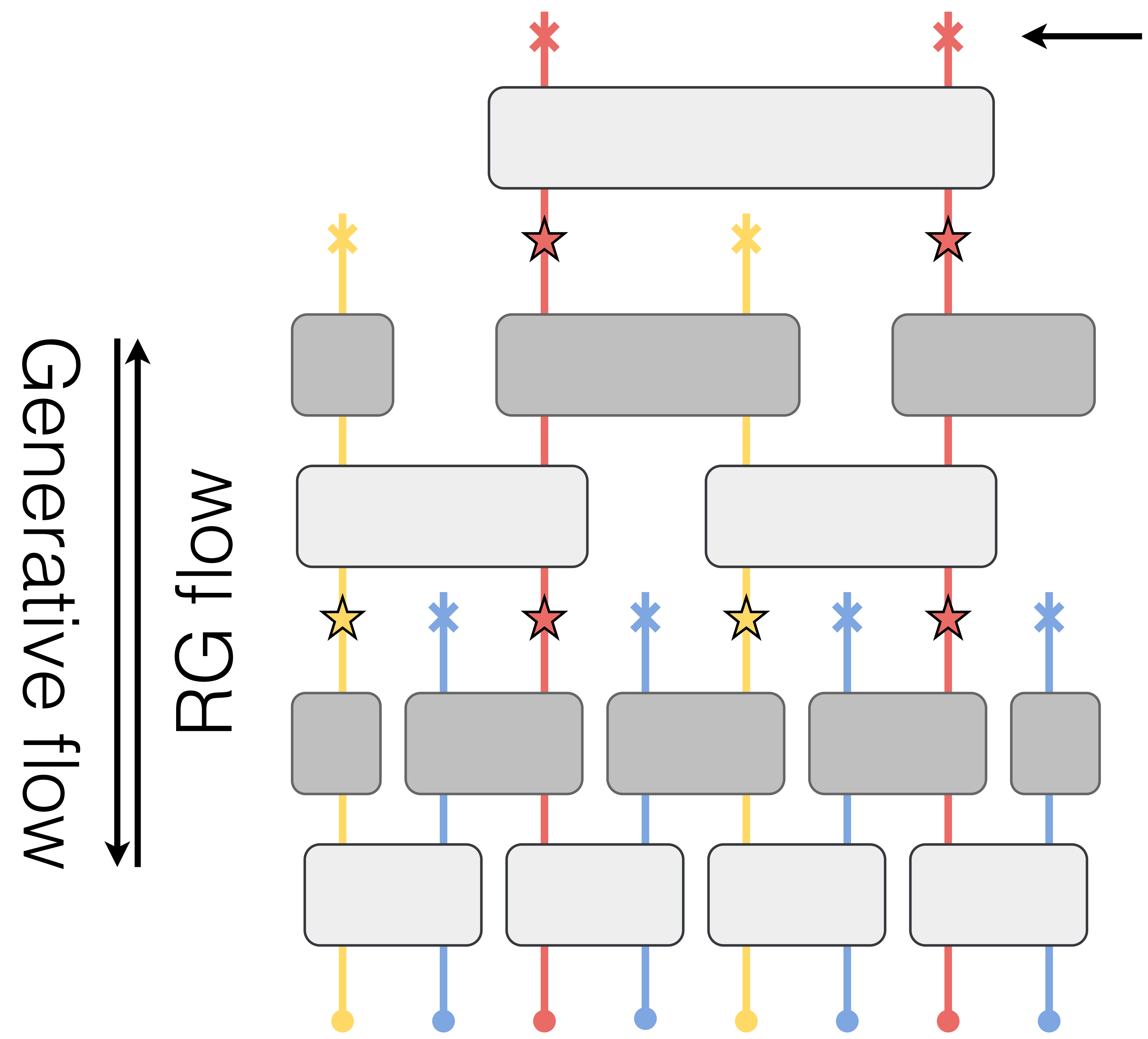
Monte Carlo update

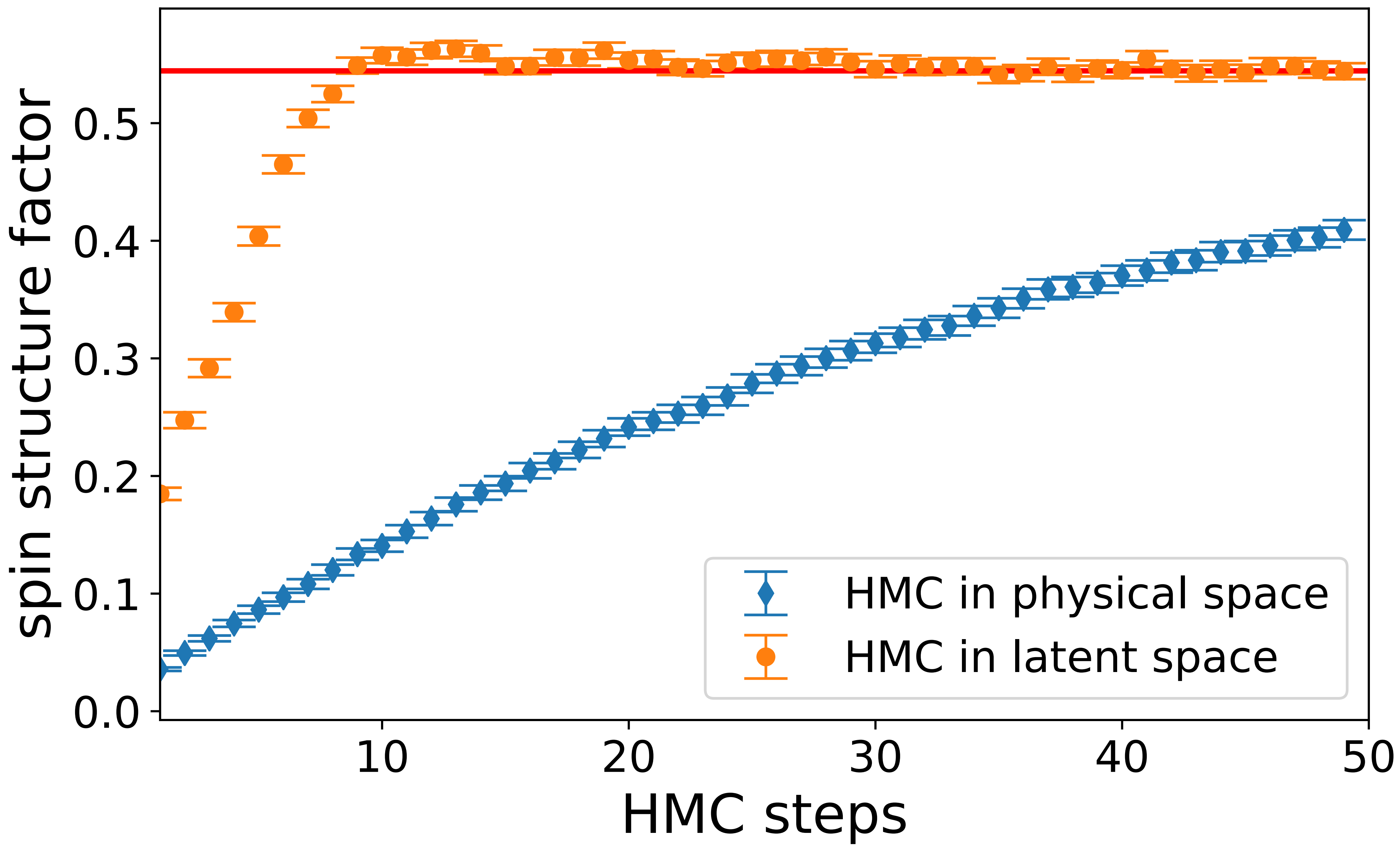


Physics happens on a manifold
Learn neural nets to unfold that manifold

Neural Renormalization Group

Normalizing flow with multi-scale neural network Li and LW, PRL '18



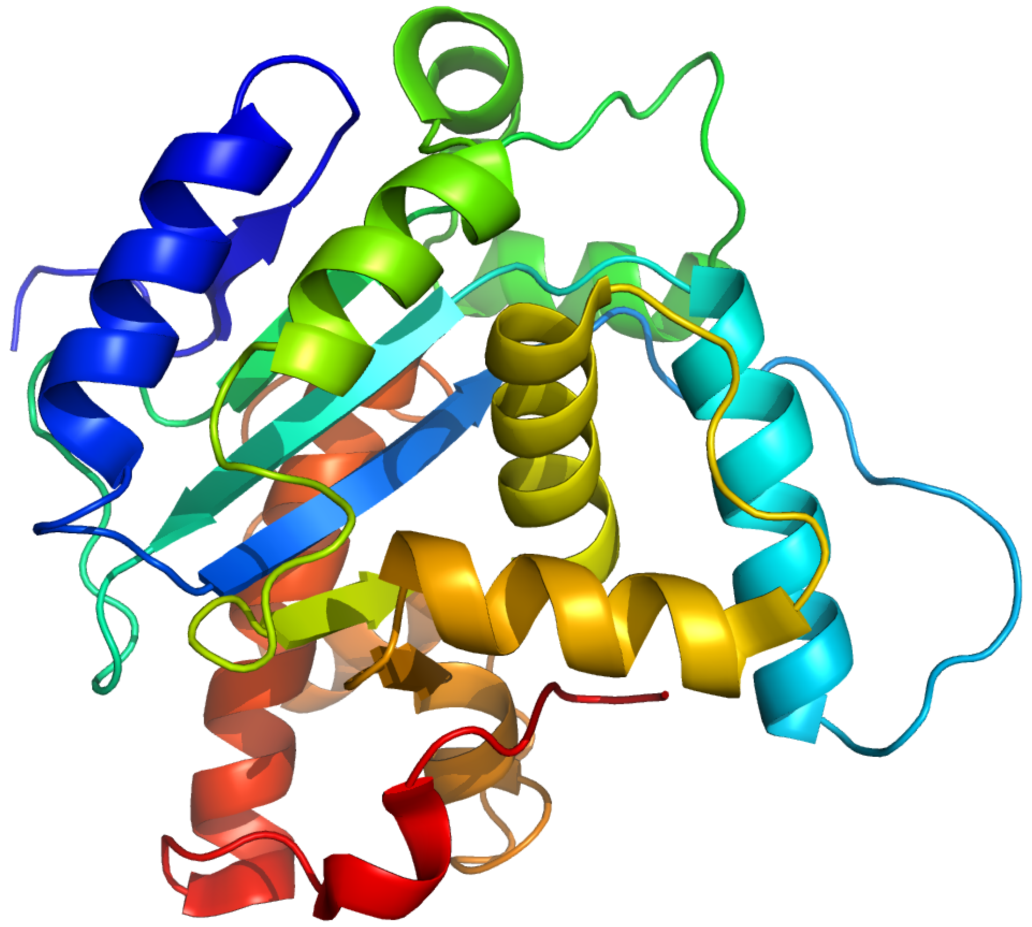


https://github.com/li012589/NeuralRG

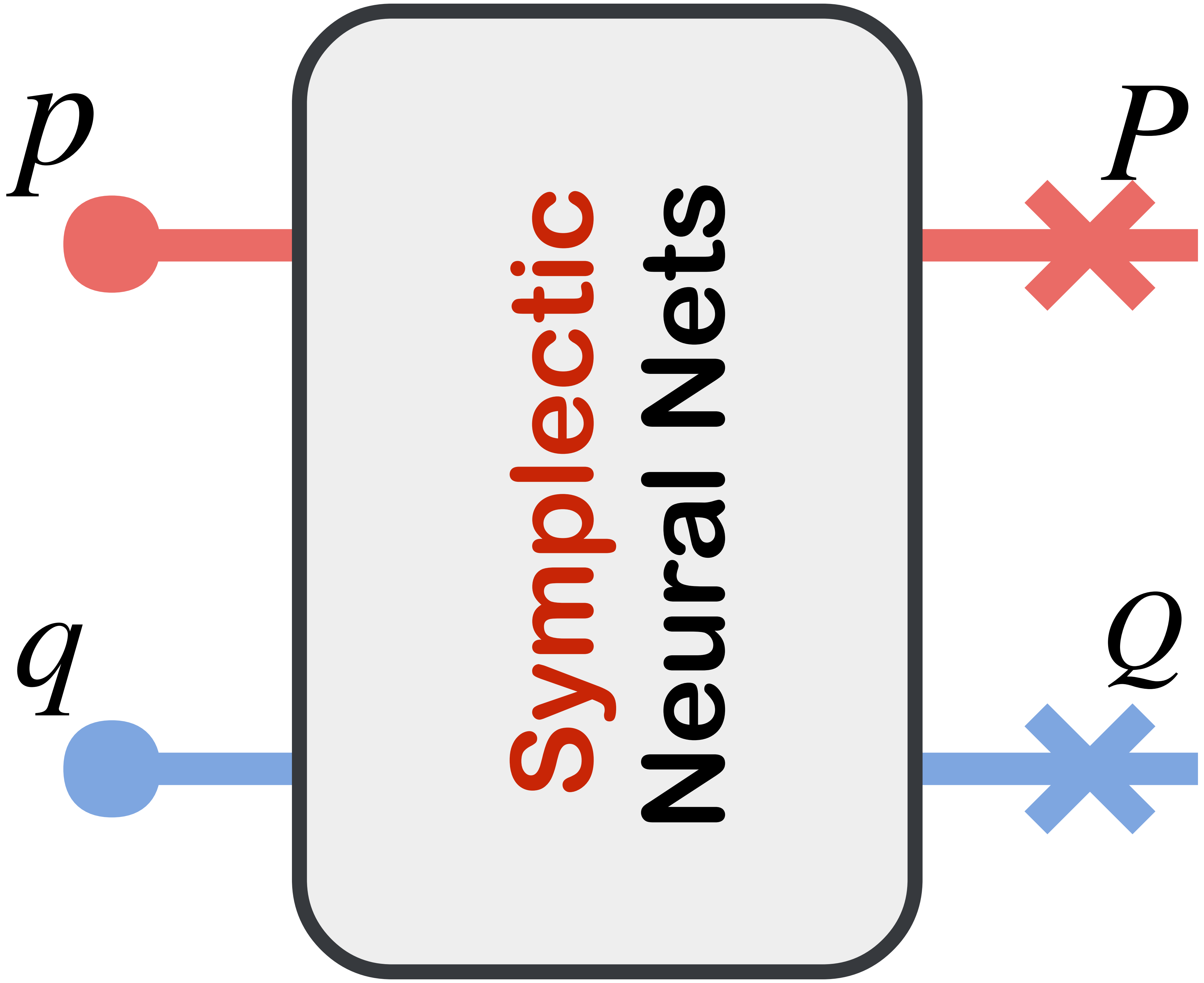
Identify collective variables; and fast sampling w/ learned representation

Neural Canonical Transformations

$H(p, q)$



physical



$$K(P, Q) = \sum_k \frac{P_k^2 + \omega_k^2 Q_k^2}{2}$$

latent

Learn the network and the latent harmonic frequency together

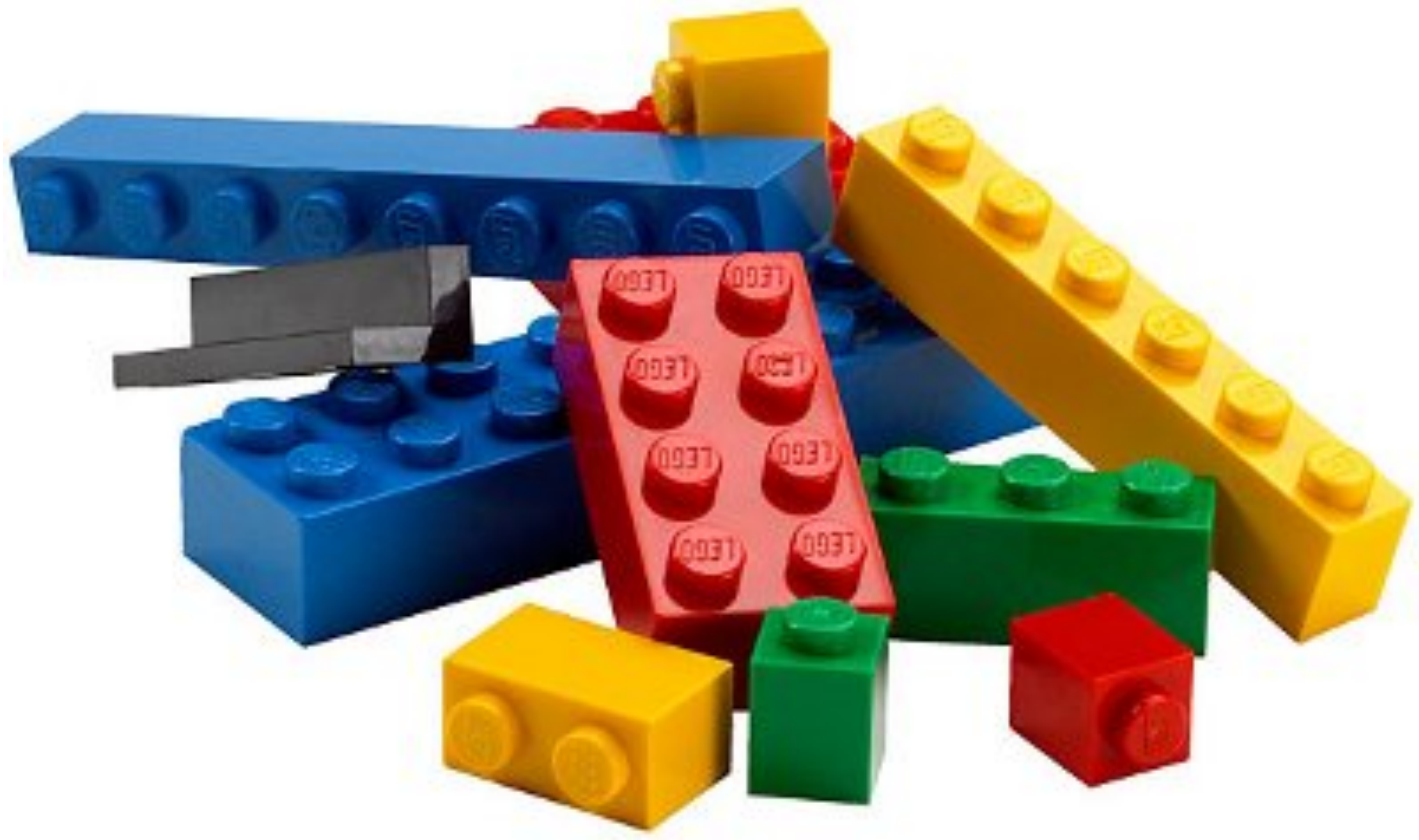
Modular design of the symplectic network

$$z = \mathscr{T}(\boldsymbol{x})$$

$$\mathscr{T} = \mathscr{T}_1 \circ \mathscr{T}_2 \circ \mathscr{T}_3 \circ \cdots$$

$$\boxed{\left(\nabla_x z\right) J \left(\nabla_x z\right)^T = J}$$

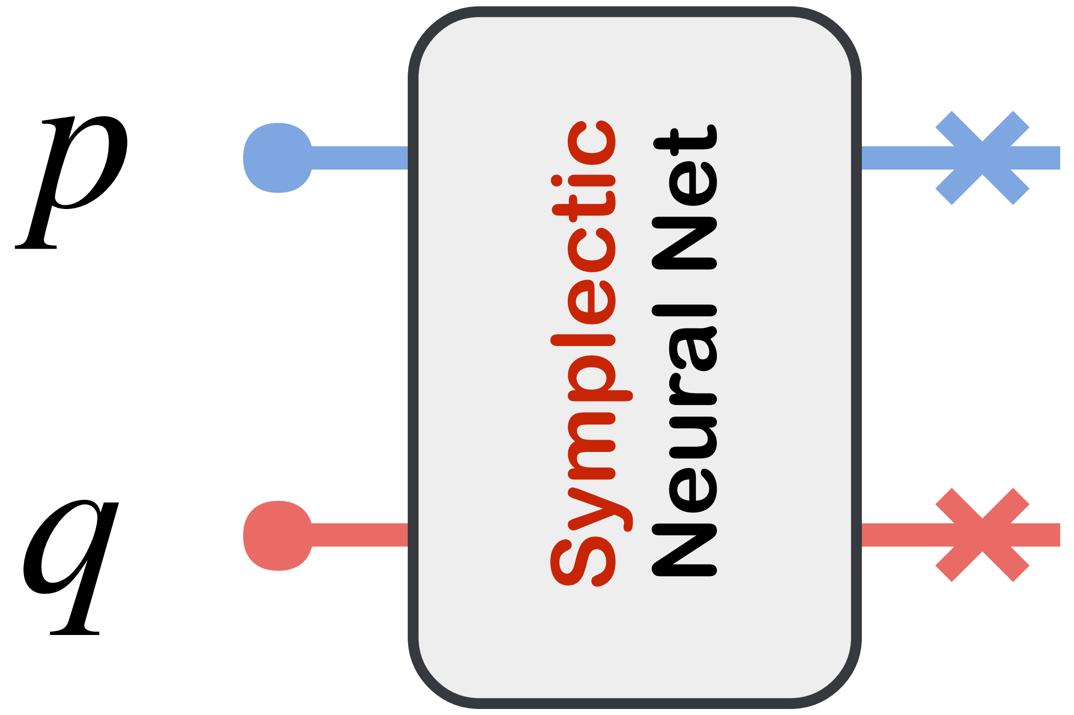
symplectic group



Compose symplectic primitives to a deep neural network

Neural symplectic primitives

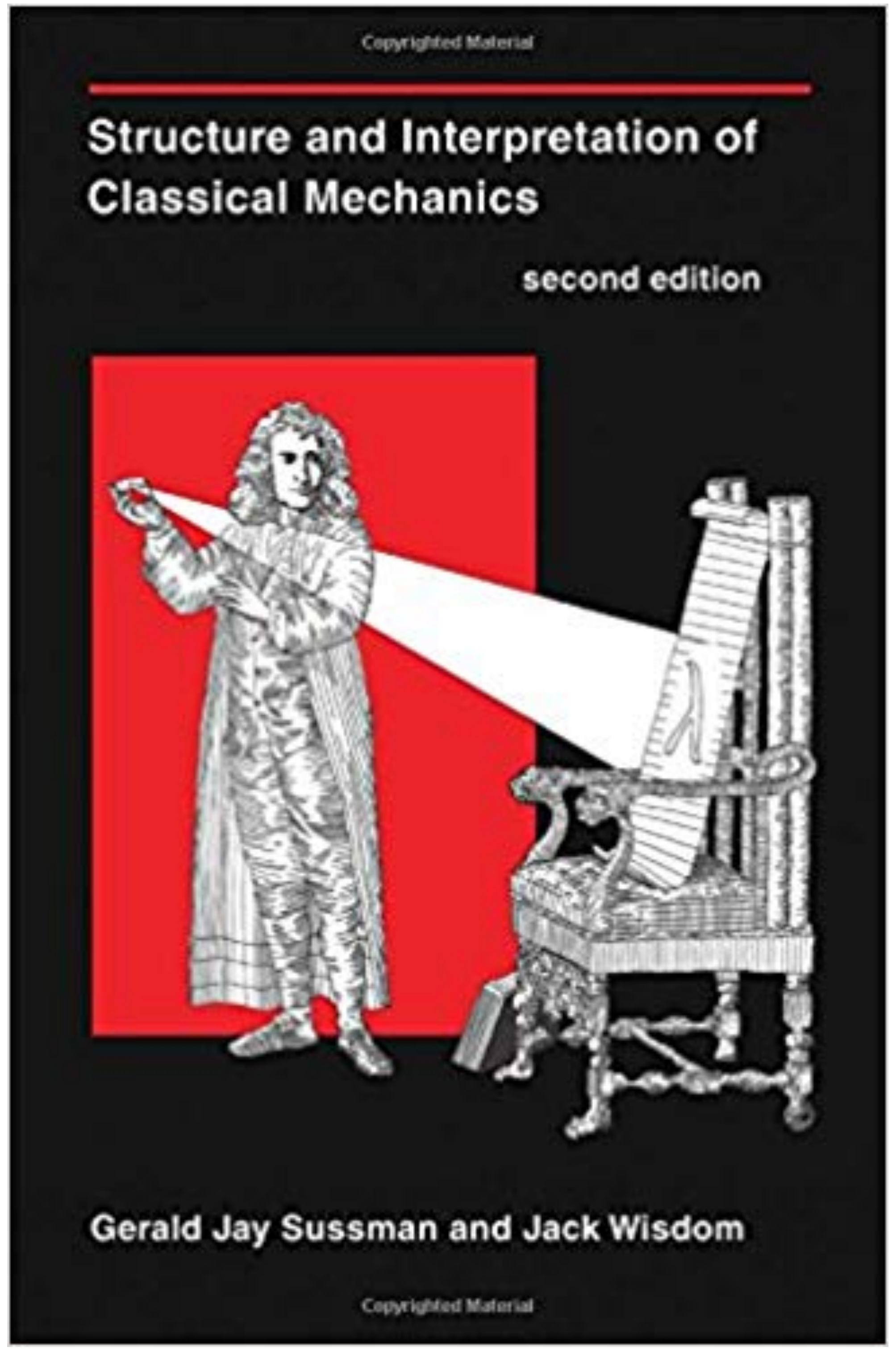
- **Neural coordinate transformation**



$$P = p\left(\nabla_Q q\right)$$

$$Q = f(q)$$

invertible neural net



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

See also Bondesan, Lamacraft, 1906.04645

Neural ODE, Chen et al, 1806.07366, Monge-Ampere flow, Zhang et al 1809.10188

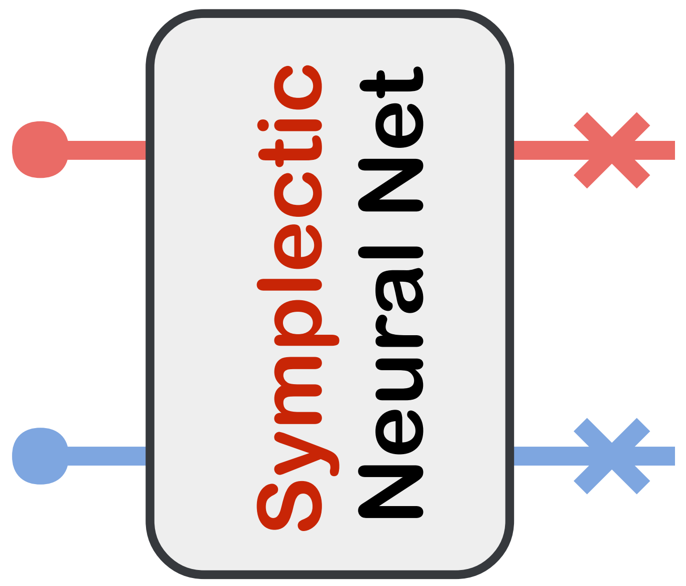
Training approaches

Variational calculation

"learn from Hamiltonian"

$$\mathscr{L} = \int d\boldsymbol{x}\,\rho(\boldsymbol{x})\left[\ln\rho(\boldsymbol{x}) + \beta H(\boldsymbol{x})\right]$$

$\boldsymbol{x}$



$\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{0}, \Sigma)$

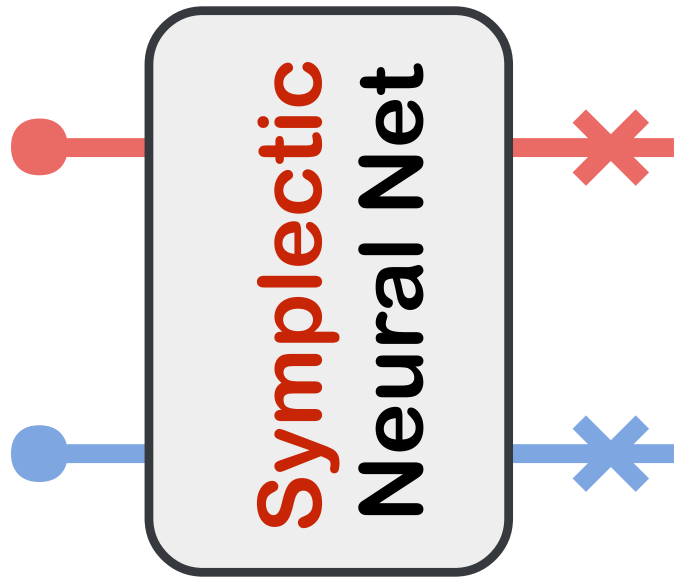
Sample in the latent space

Density estimation

"learn from data"

$$\mathscr{L} = -\,\mathbb{E}_{\boldsymbol{x}\sim\text{dataset}}\left[\ln\rho(\boldsymbol{x})\right]$$

$\boldsymbol{x} \sim \text{dataset}$

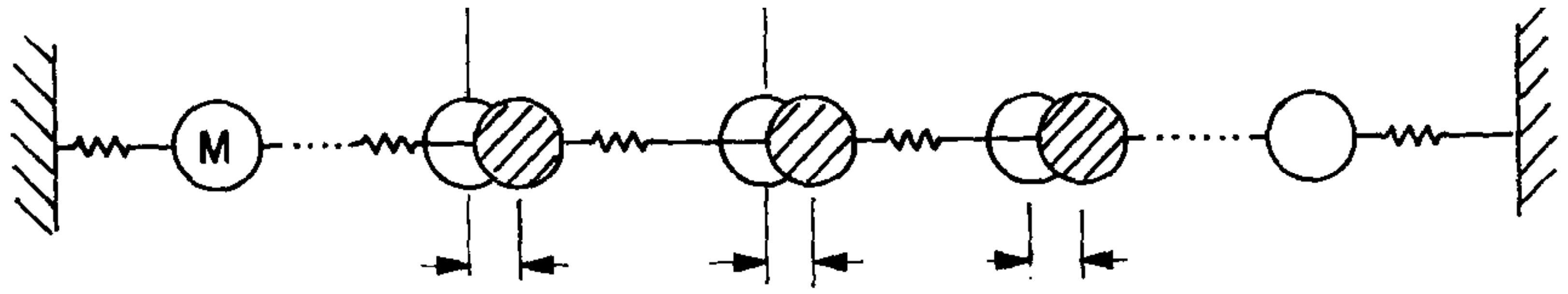


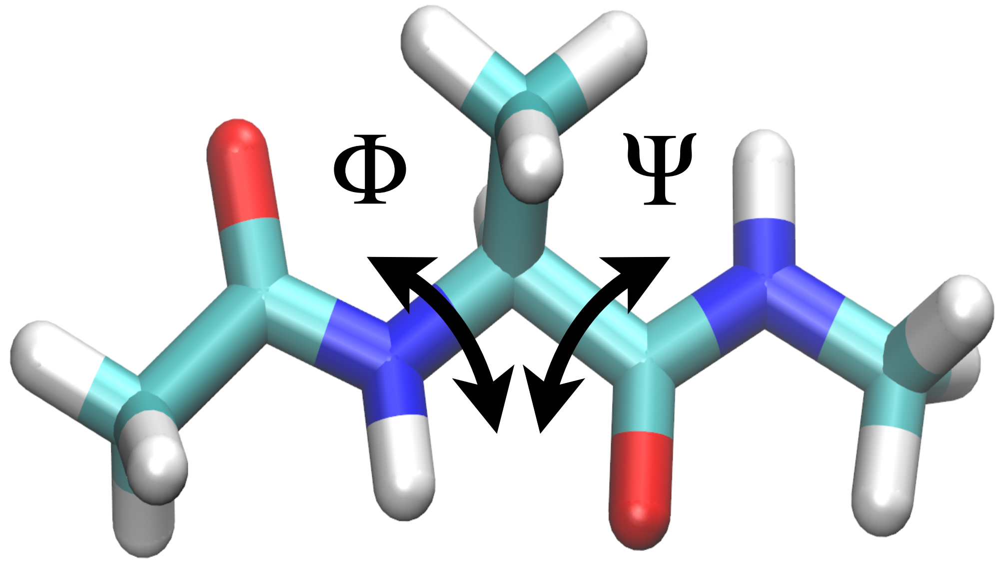
$\boldsymbol{z}$

Sample from dataset in the physical space

How is this going to be useful ?

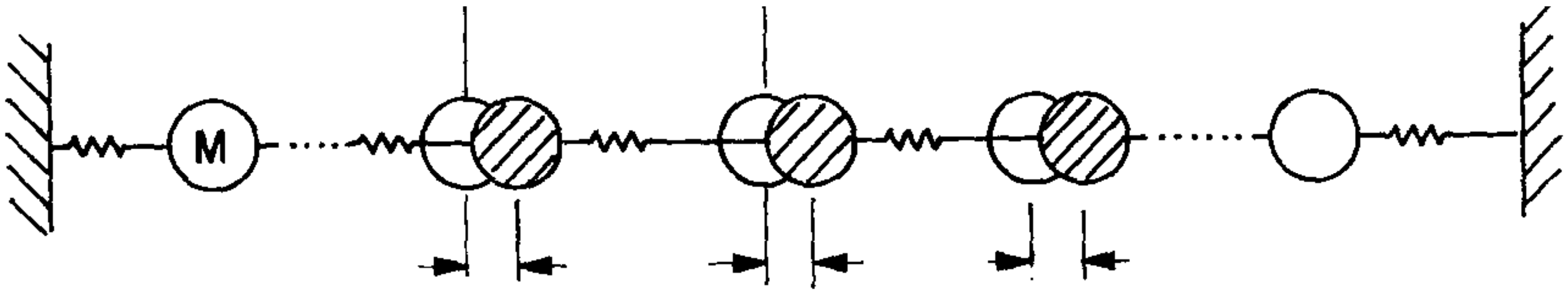
Let's play with examples!





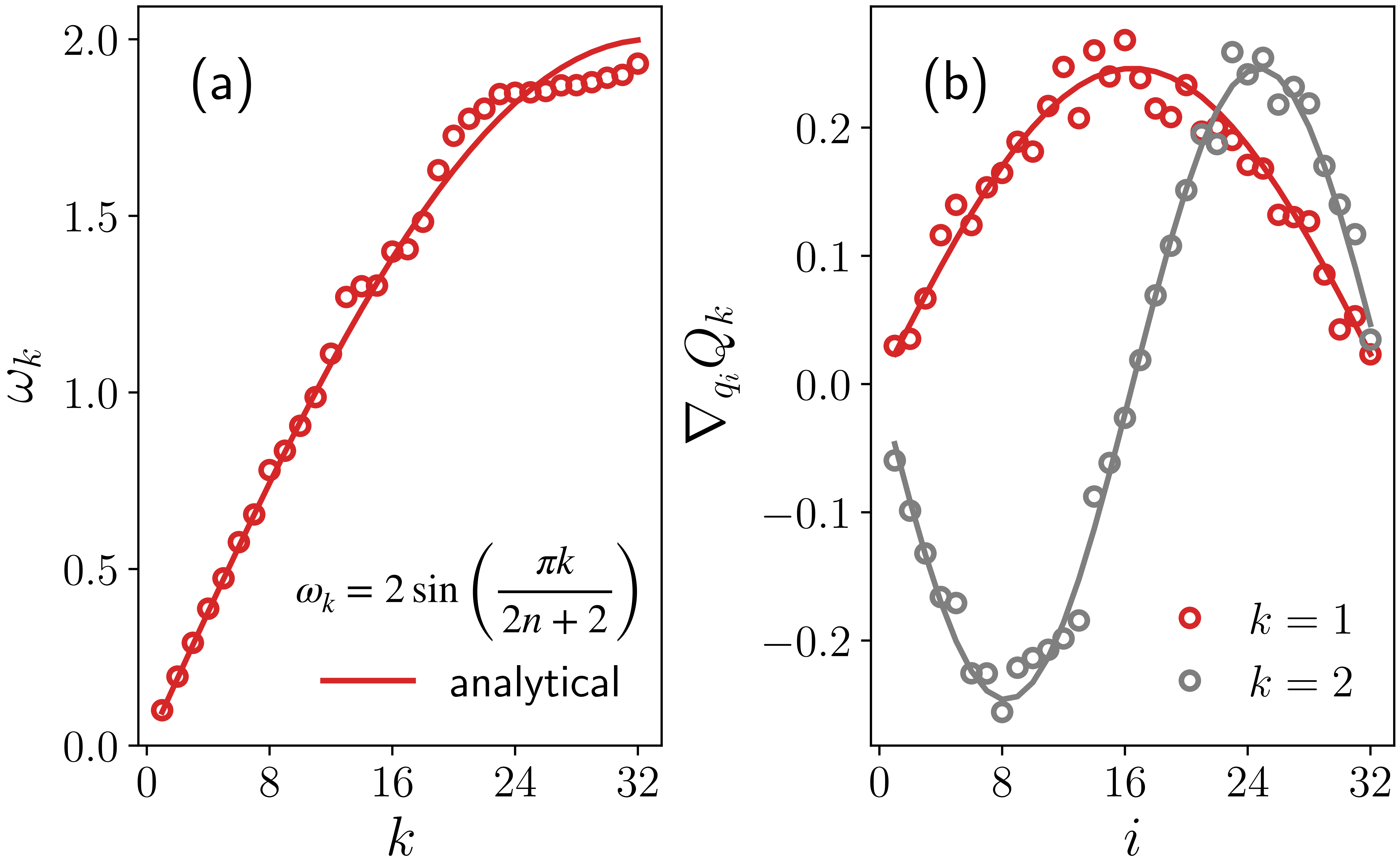
Example 1: Harmonic Chain

$$H = \frac{1}{2} \sum_{i=1}^{n} \left[p_i^2 + (q_i - q_{i-1})^2 \right]$$



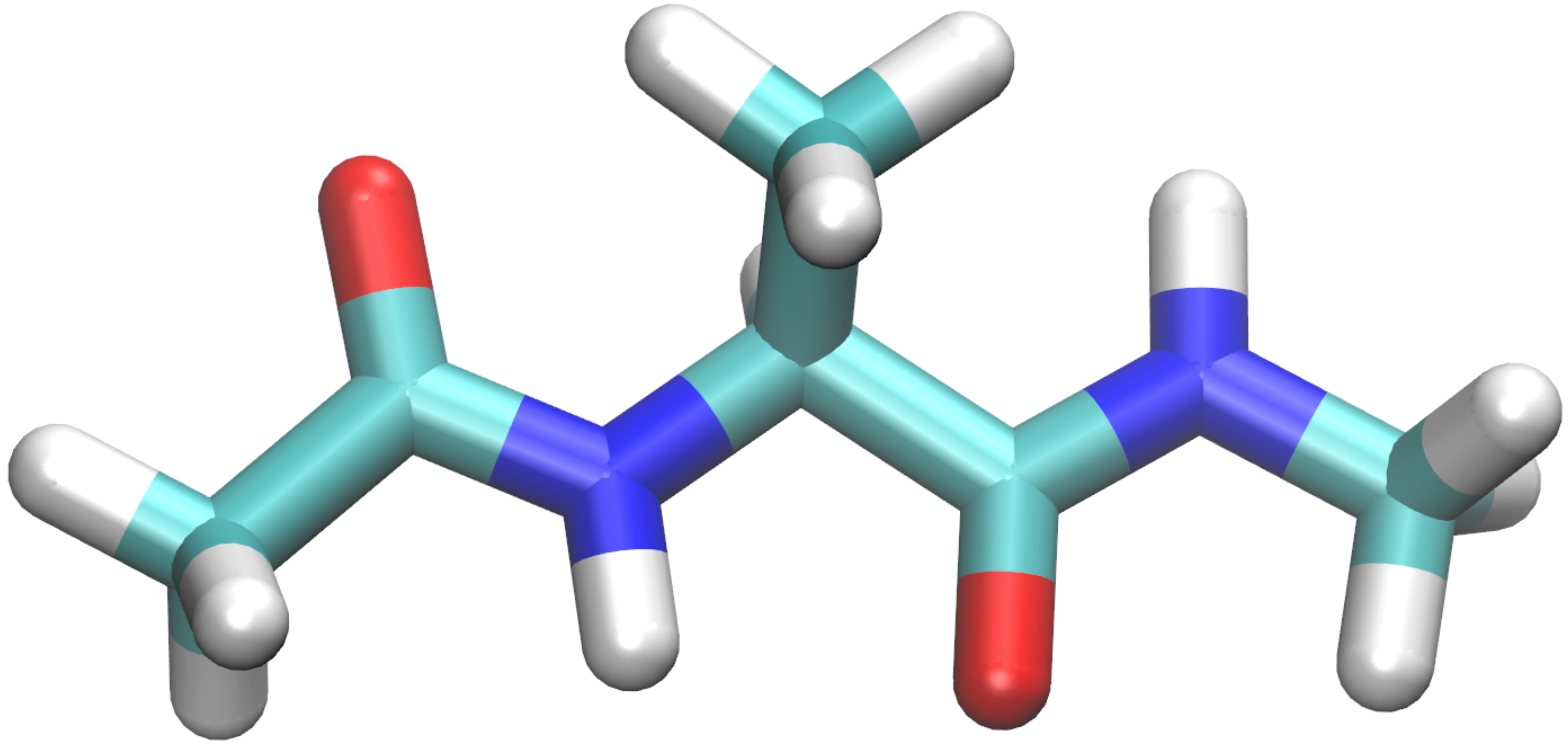
Fermi–Pasta–Ulam–Tsingou problem w/o nonlinearity

Learning the normal modes



Consistency check: neural nets can learn linear coordinate transformations

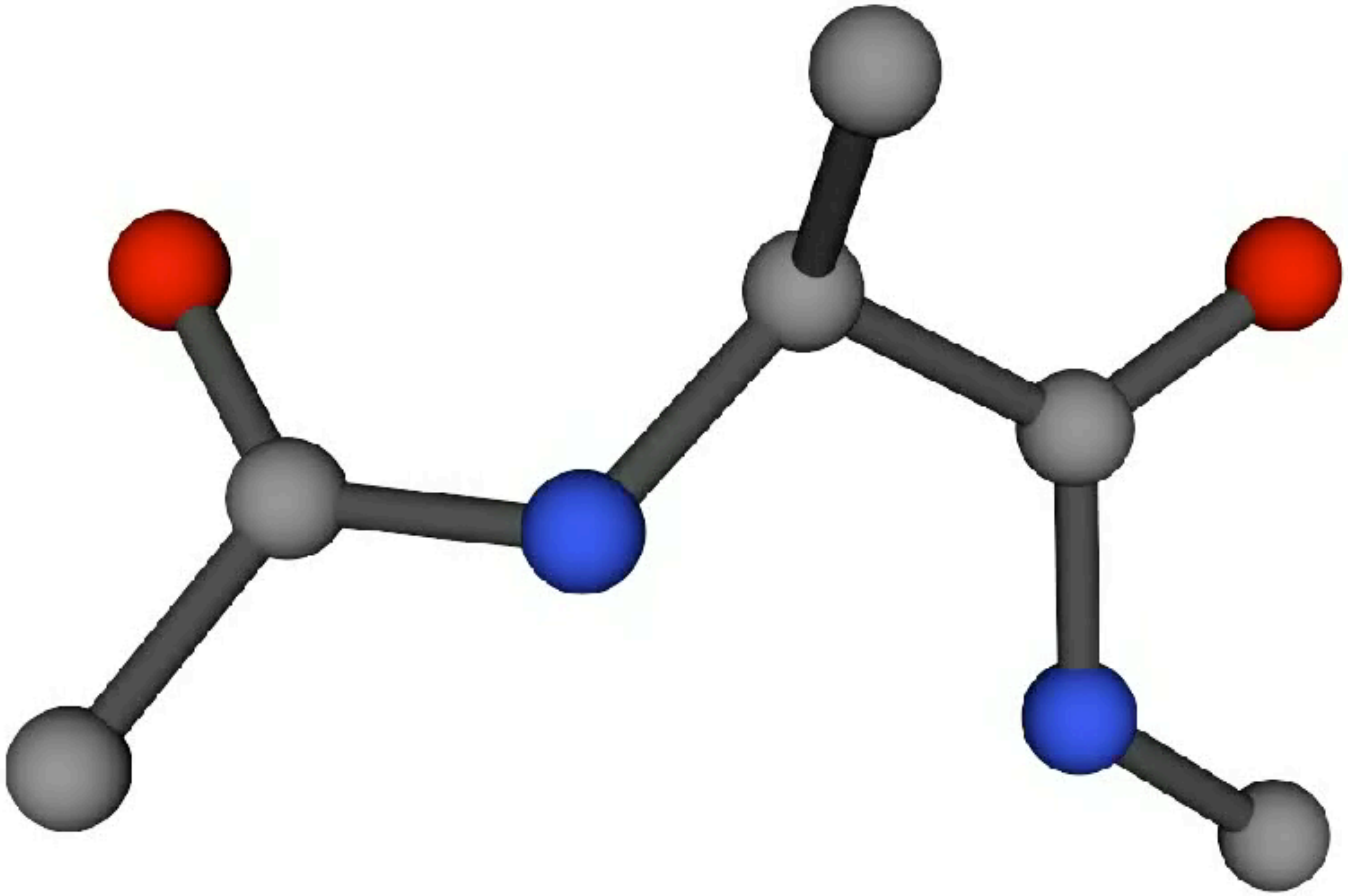
Example 2: Alanine Dipeptide



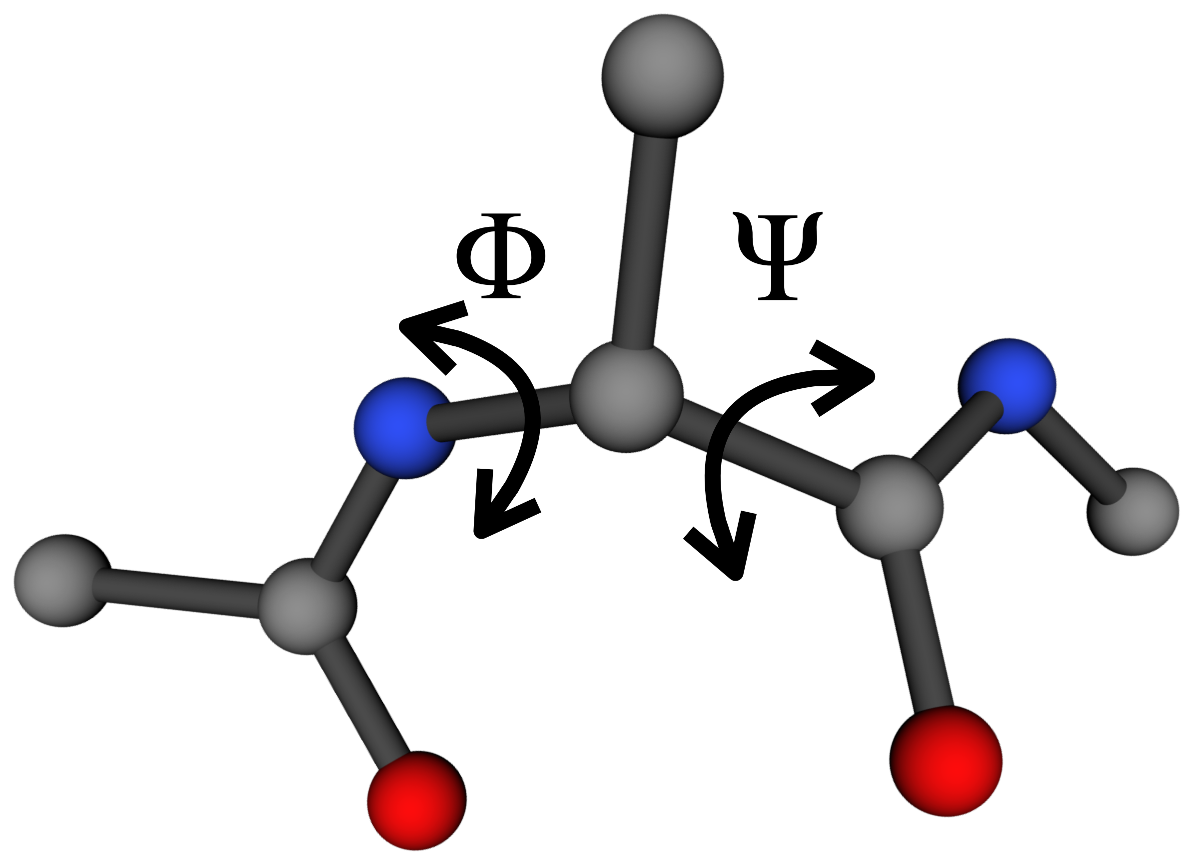
250 ns molecular dynamics simulation data at 300 K

https://markovmodel.github.io/mdshare/ALA2/#alanine-dipeptide

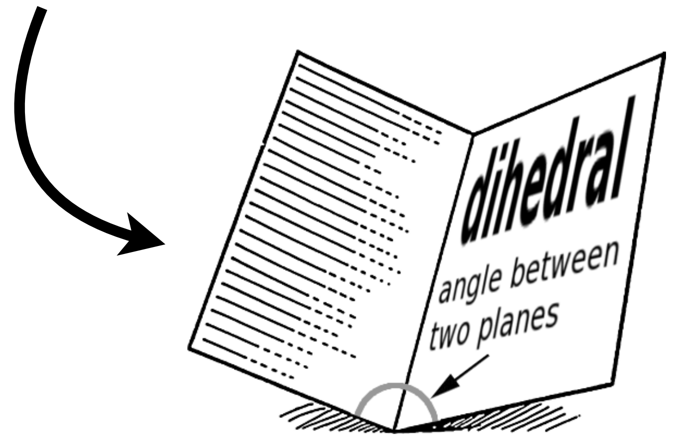
More than 3 hours of video …

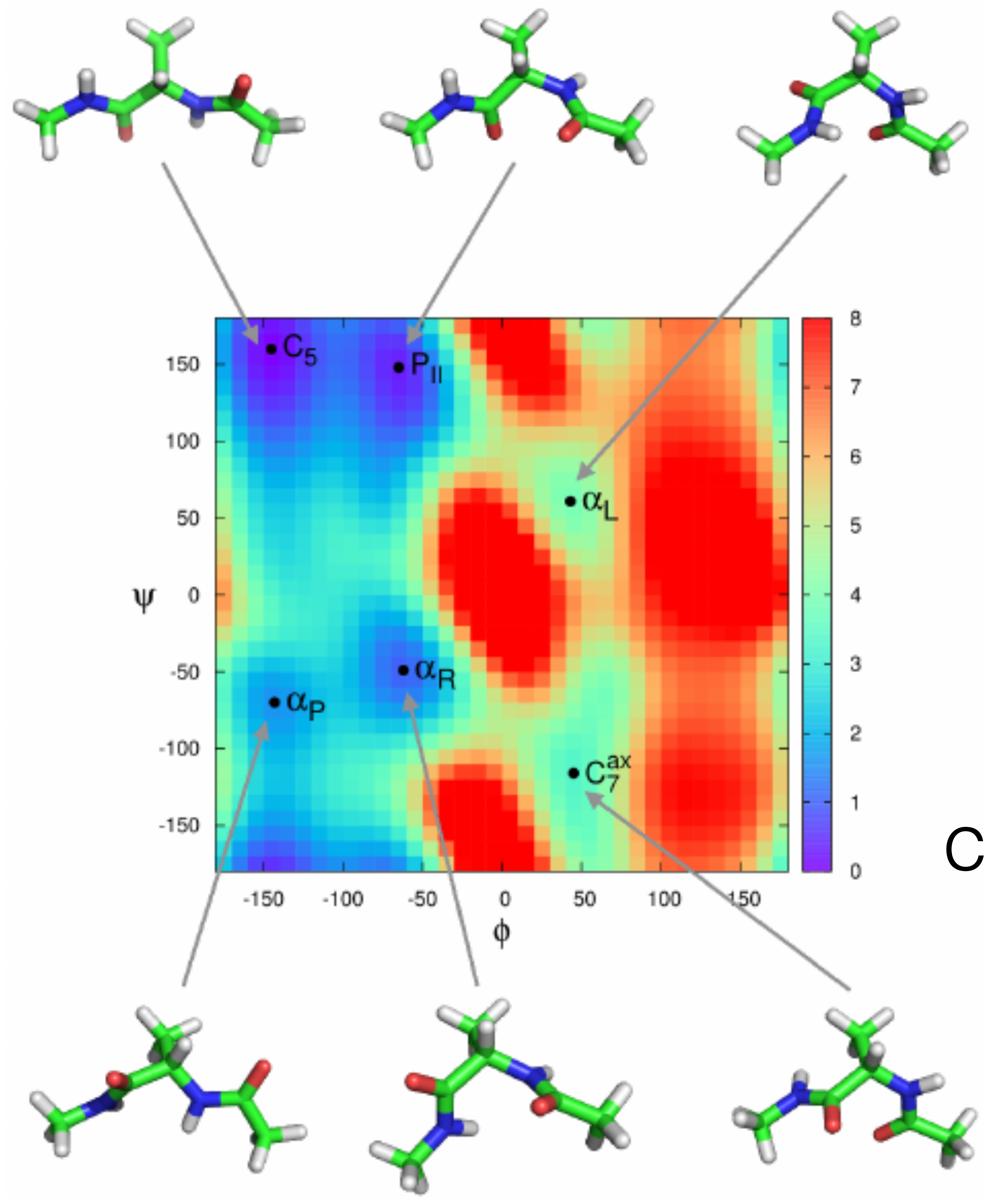


What do biologists see ?



slow motion of the
two torsion angles

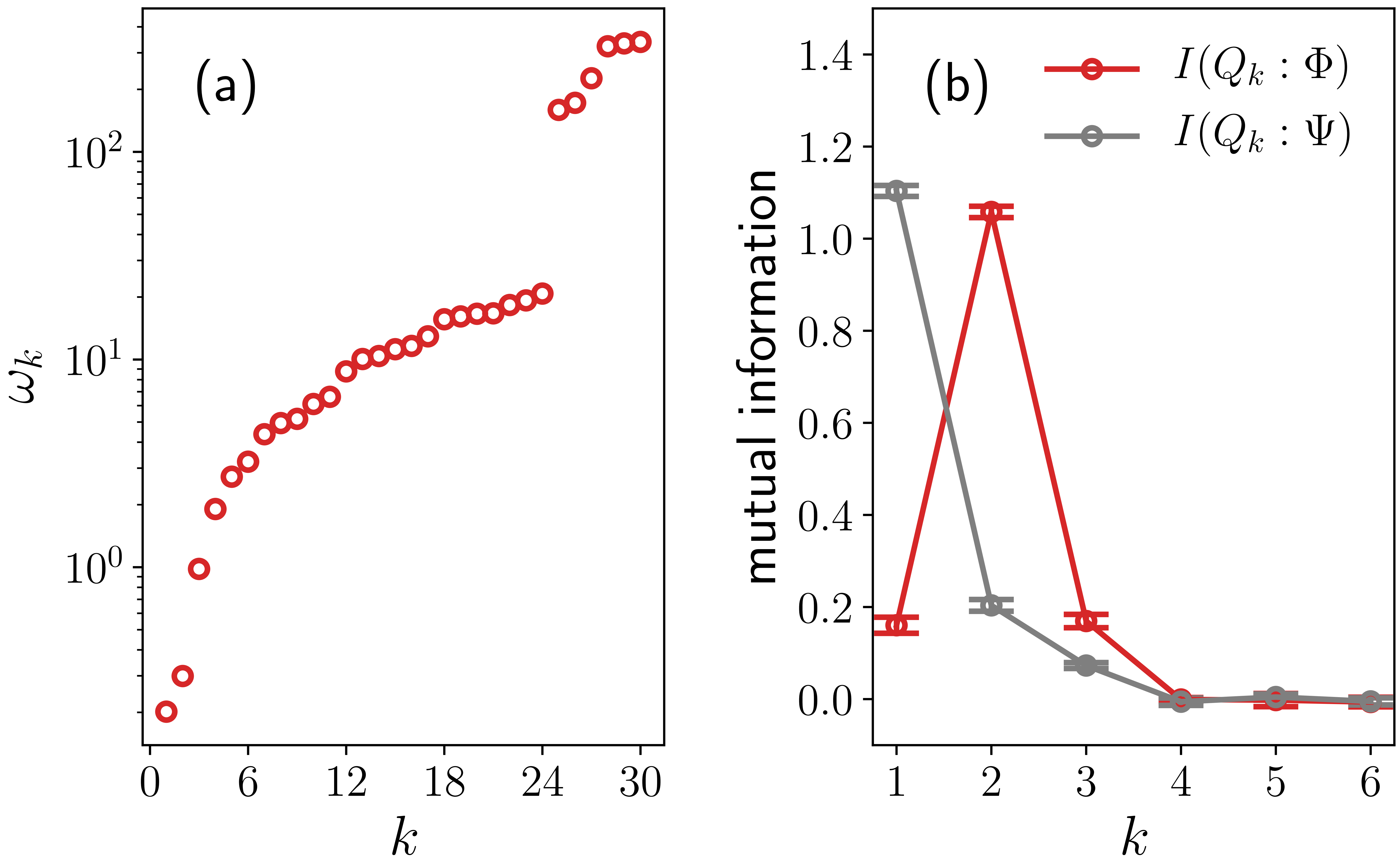




stable
conformations

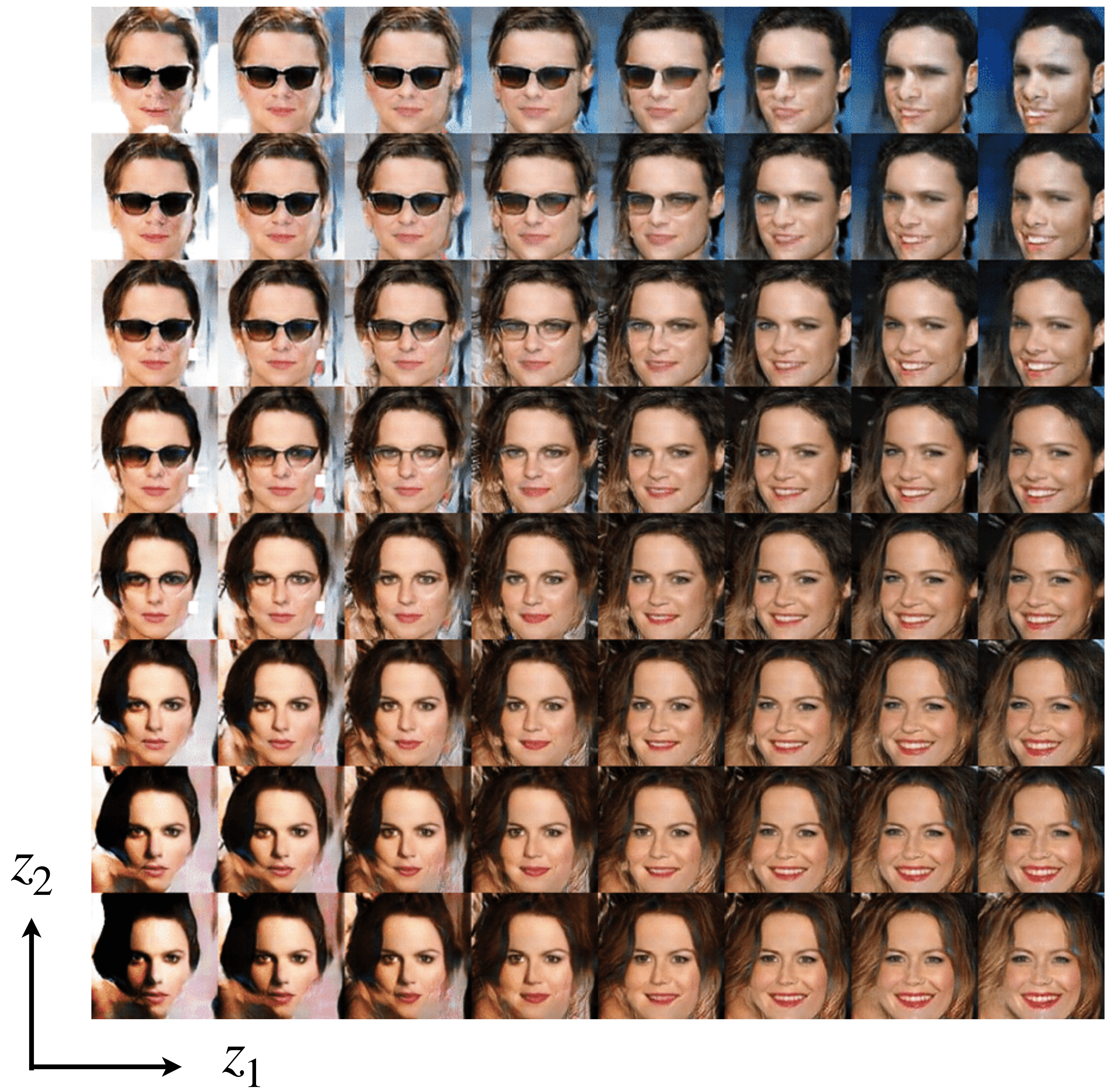
“Dimensional reduction” to manually designed collective variables

What does the neural net see ?

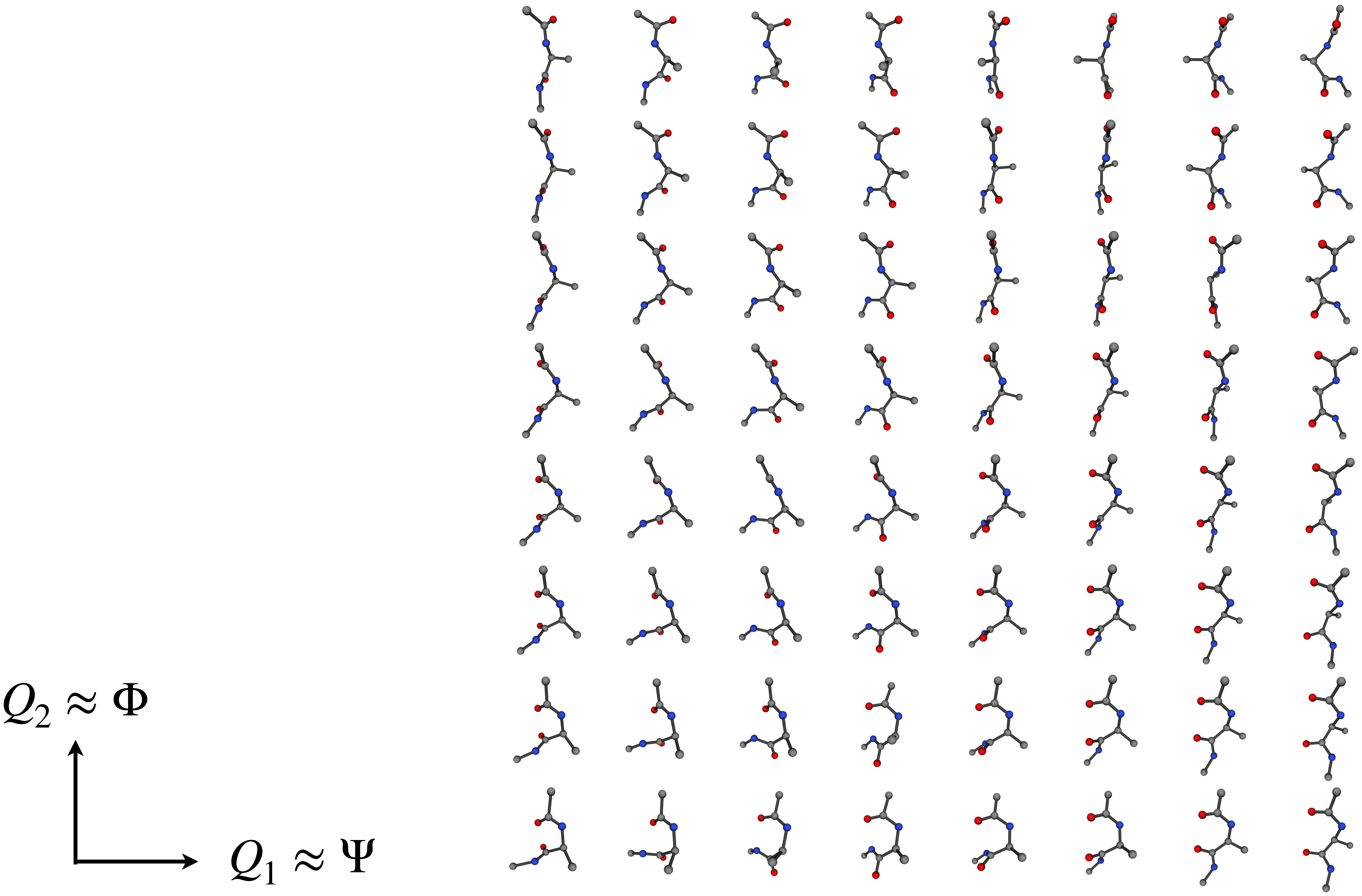


Unsupervised learning of slow & nonlinear collective variables from data

Latent space interpolation



Latent space interpolation



Example 3: MNIST

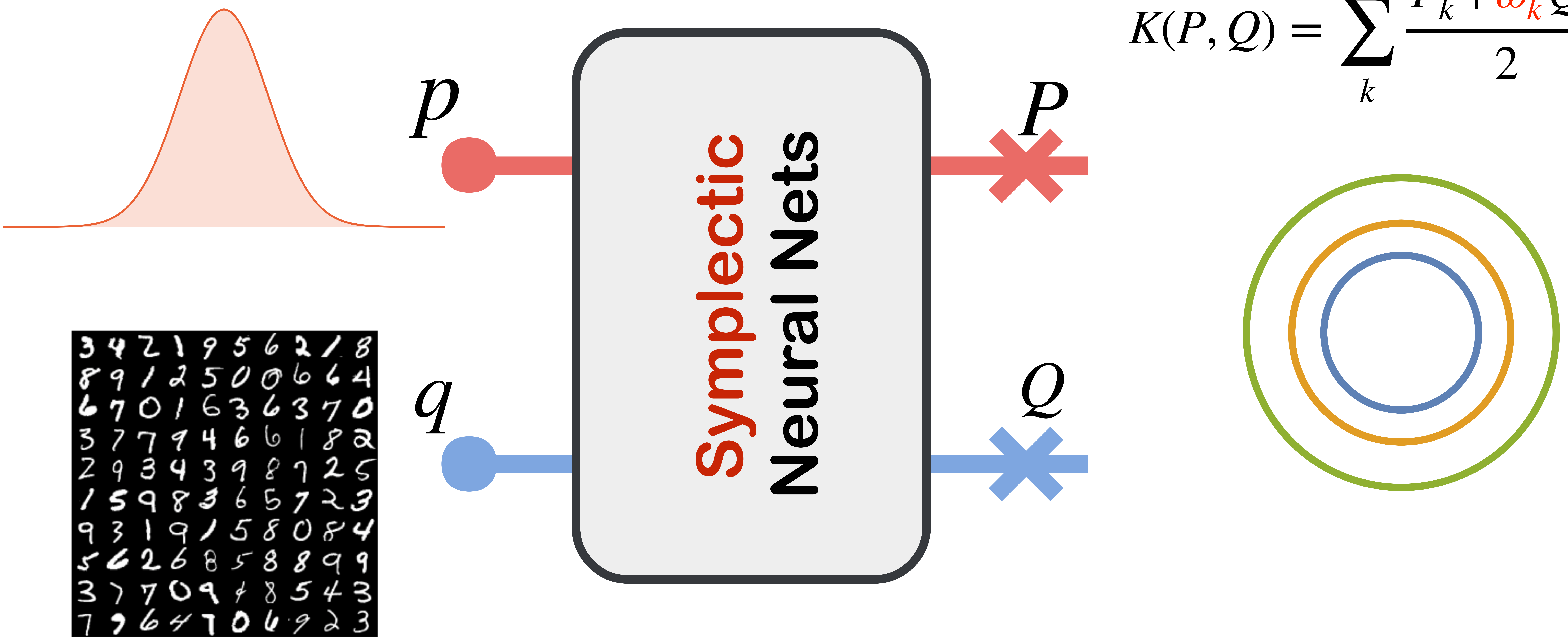
Data scientists:

“50,000 grayscale images with 28x28 pixels”

Physical Chemists:

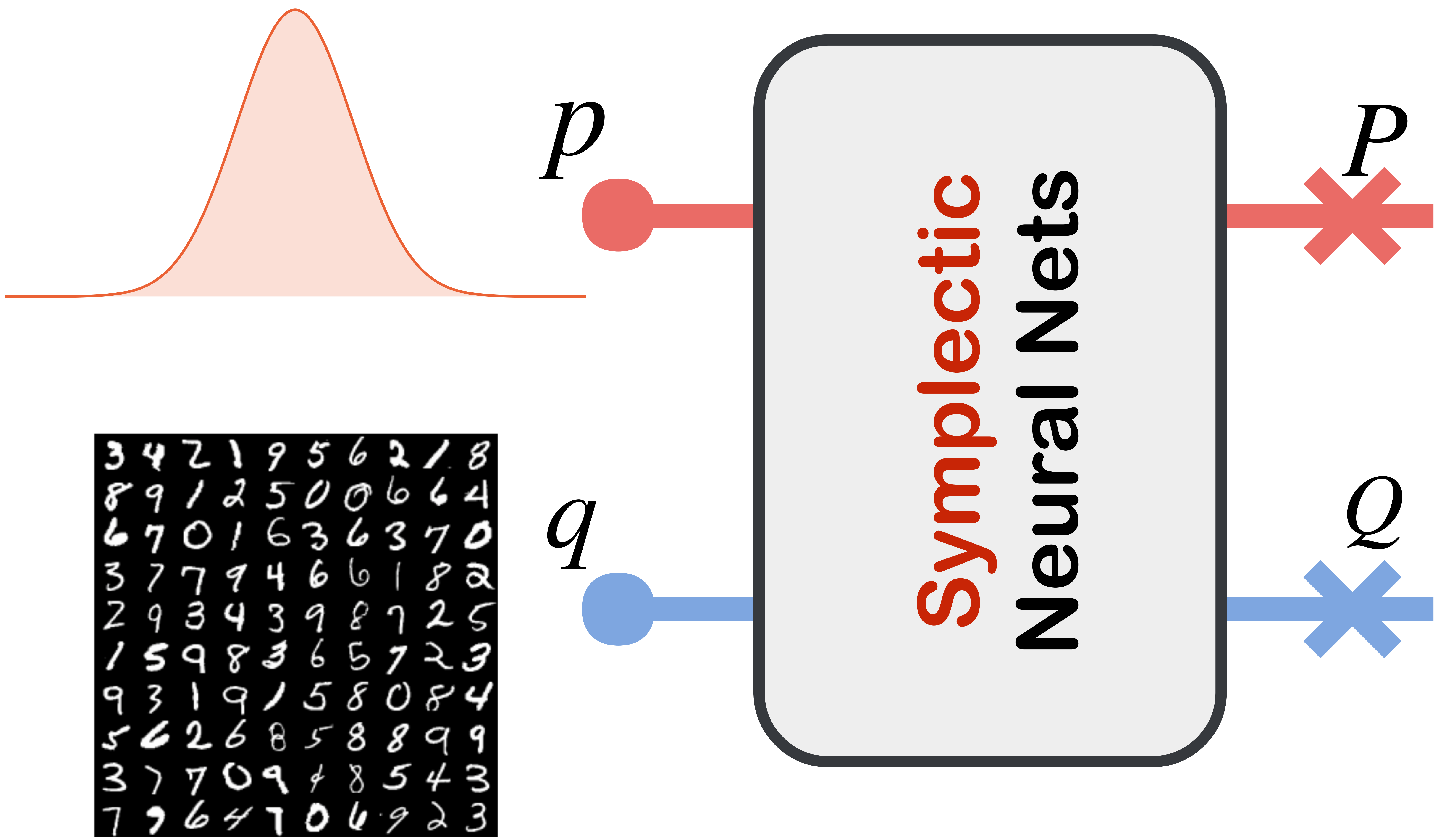
“Stable conformations of a molecule with 784 degrees of freedom”

Learning slow variables of MNIST

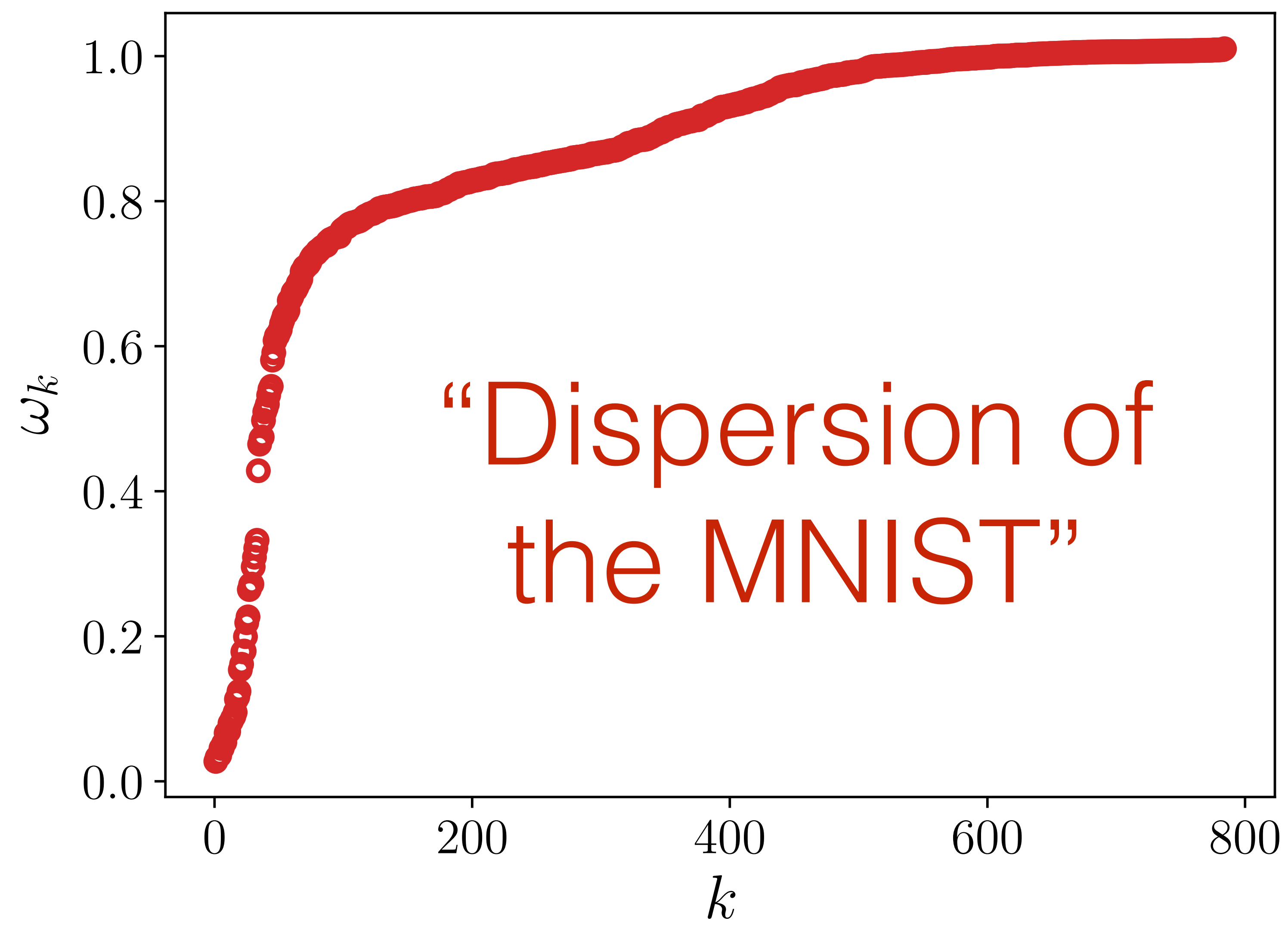


$$K(P,Q) = \sum_k \frac{P_k^2 + \omega_k^2 Q_k^2}{2}$$

Learning slow variables of MNIST

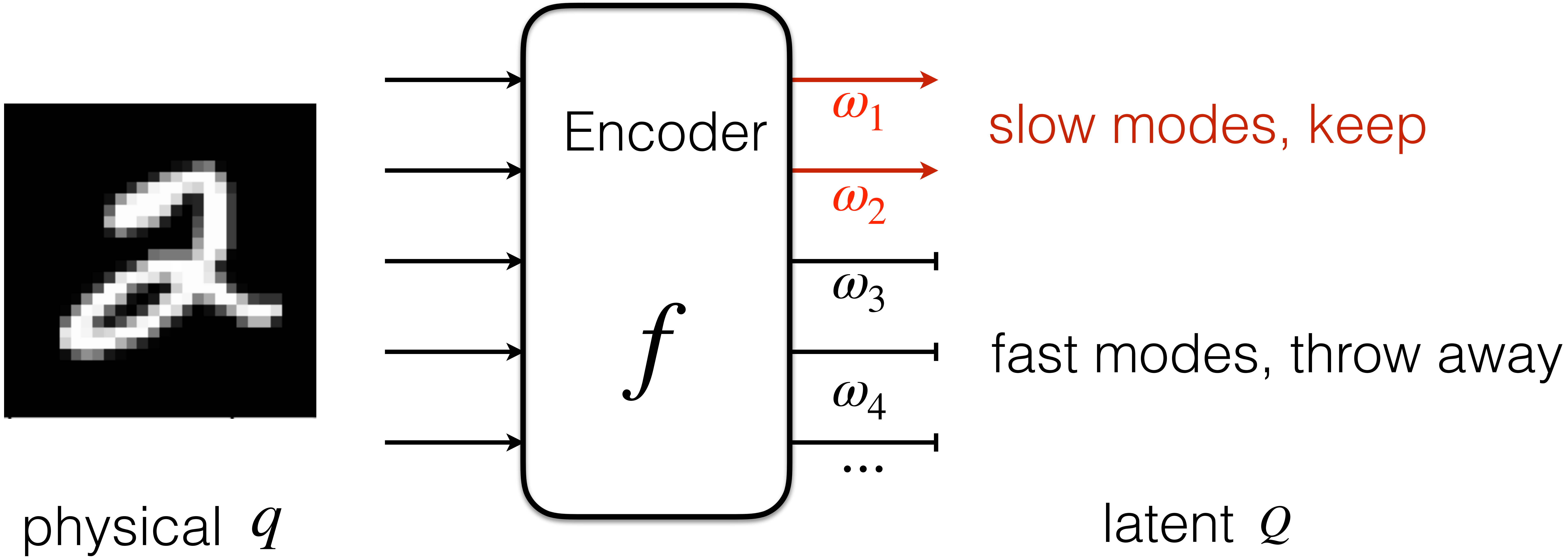


$$K(P,Q) = \sum_k \frac{P_k^2 + \omega_k^2 Q_k^2}{2}$$



Conceptual Compression

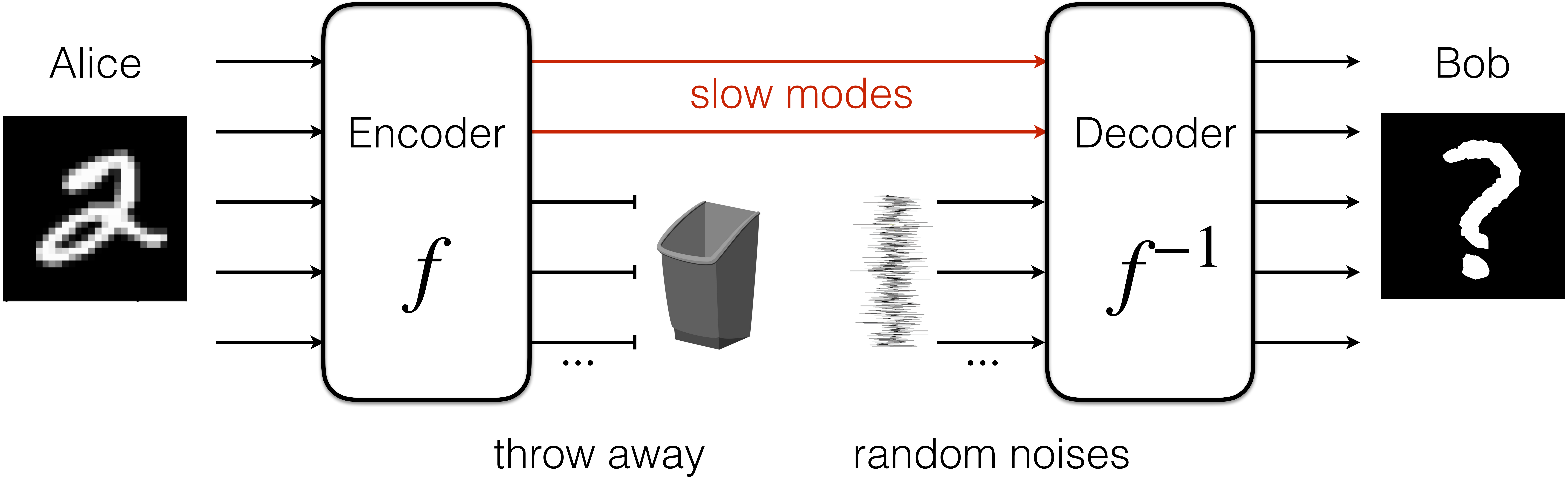
$$\omega_1 < \omega_2 < \omega_3 < \omega_4 < \cdots$$



Compress by keeping slow collective variables

Kingma et al, 1312.6114 Gregor et al, 1604.08772 Dinh et al, 1605.08803
autoencoders/hierarchical network architecture/hyperbolic latent space…

Neural Alice-Bob game



Conceptual Compression of MNIST

Original

1/784 kept

Conceptual Compression of MNIST

Original

2/784 kept

Conceptual Compression of MNIST

Original

3/784 kept

Conceptual Compression of MNIST

Original

4/784 kept

Conceptual Compression of MNIST

Original

5/784 kept

Conceptual Compression of MNIST

Original

10/784 kept

Conceptual Compression of MNIST

Original

15/784 kept

Conceptual Compression of MNIST

Original

20/784 kept

“A Hamiltonian Extravaganza”

—Danilo J. Rezende@DeepMind

Sep 25 **ICLR 2020 Paper Submission deadline**

Sep 26 *Symplectic ODE-Net*, 1909.12077

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

Thank You!

Neural Canonical Transformation with Symplectic Flows, 1910.00024

Shuo-Hui Li 李烁辉
IOP CAS

Chen-Xiao Dong 董陈潇
IOP CAS

Linfeng Zhang 张林峰
Princeton