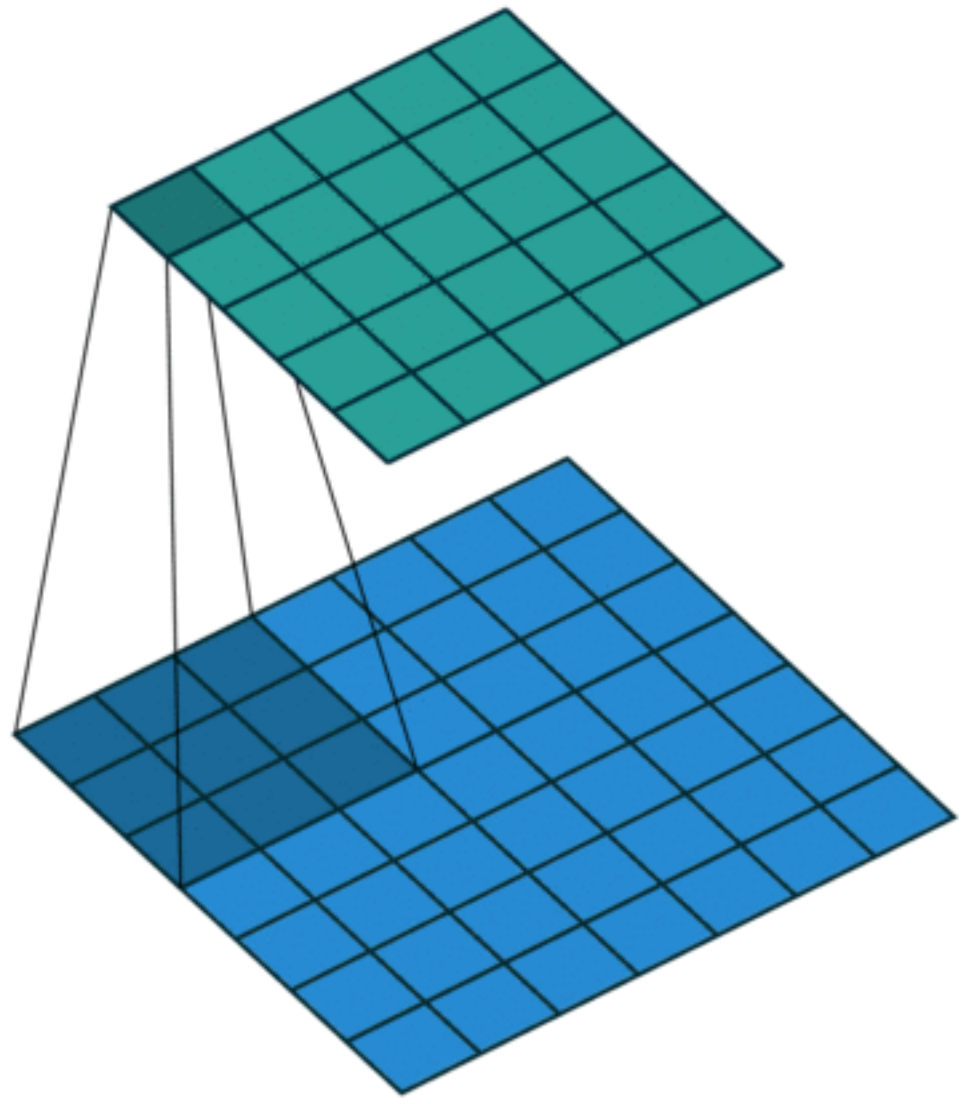
Physics-Informed Inductive Biases in Deep Learning



Miles Cranmer (Princeton)
Shirley Ho (Flatiron, NYU, CMU, Princeton)

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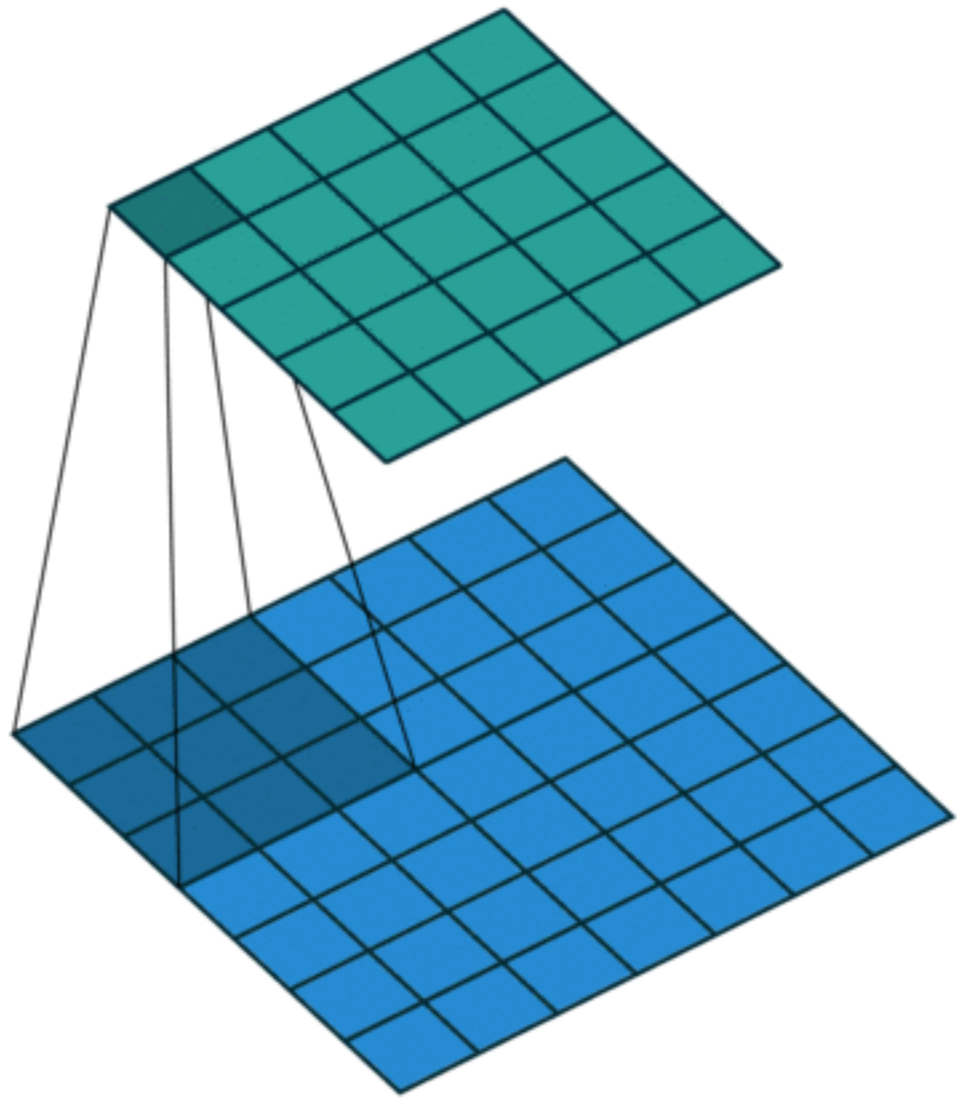

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Main Ideas

- Physics has informed many inductive biases in deep learning, both **explicitly and implicitly**
    - Success of these often due to fact that deep learning seeks models of the physical world; using physics as a prior can directly or indirectly benefit these models.
- Formalizing these in a physics language often leads to **new insights**

First, some history

- An early physics-motivated inductive bias: **Hopfield networks**
- Based on **Ising Model**

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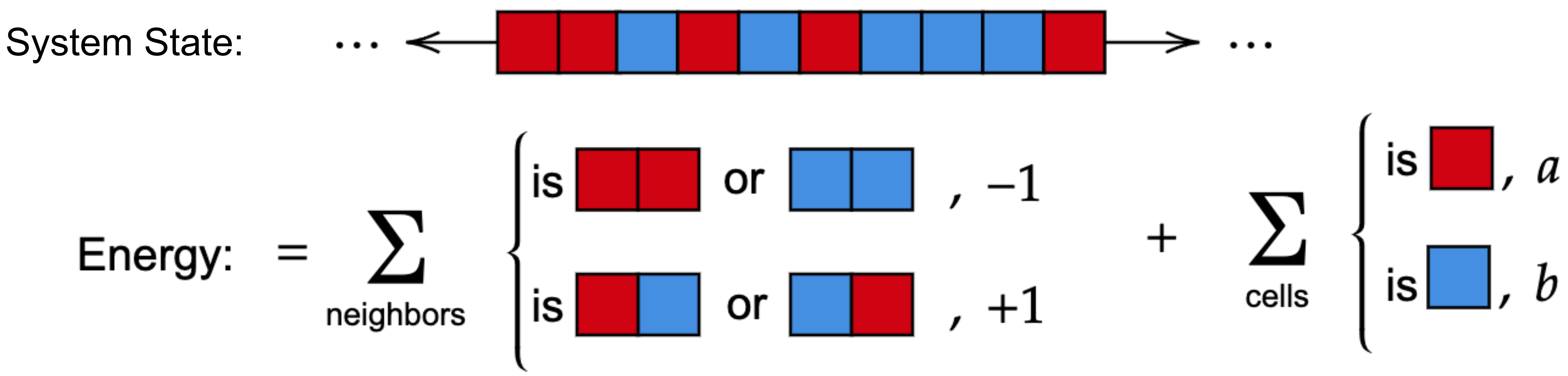

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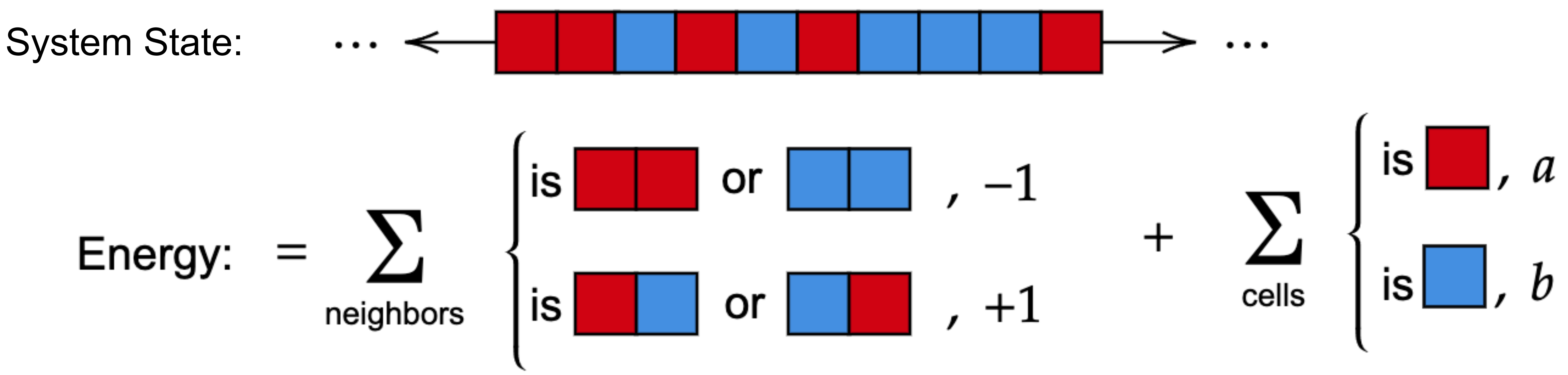

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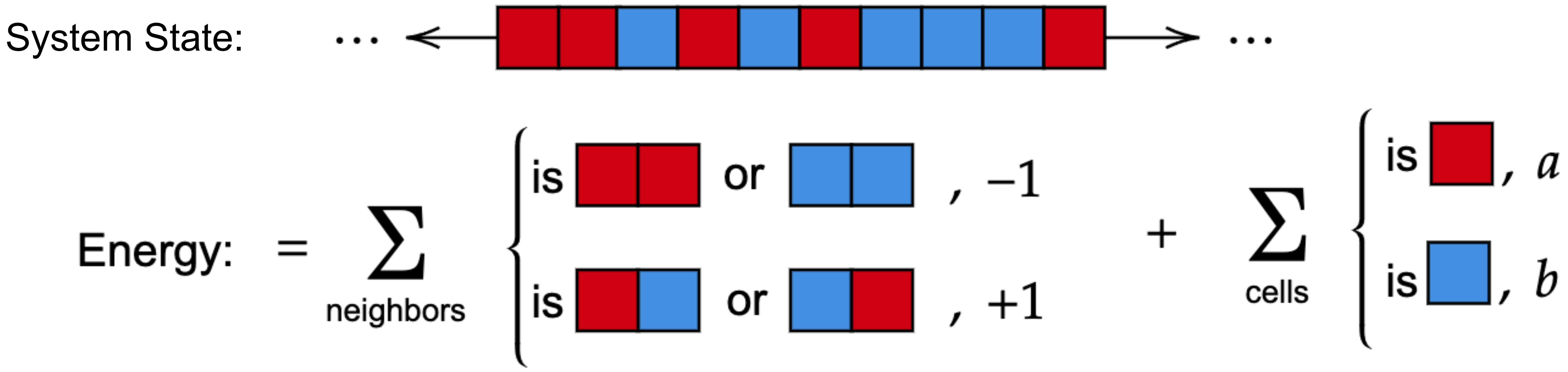
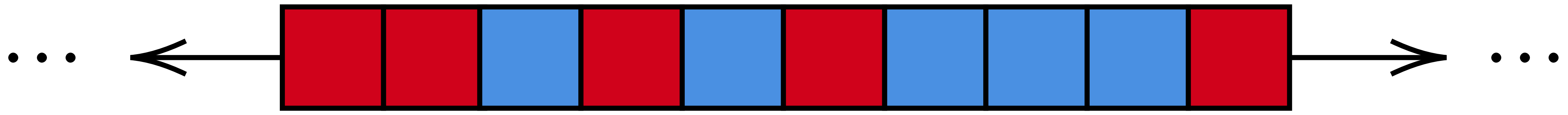


$$p(\textbf{State}) \propto \exp(-\textbf{Energy}/\textbf{Temperature})$$

In higher dimension - additional neighbors!

Ising Model

System State: 

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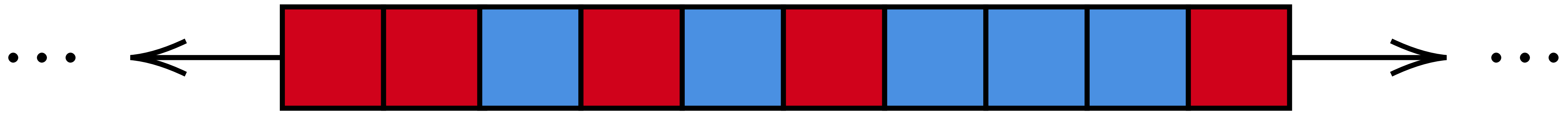

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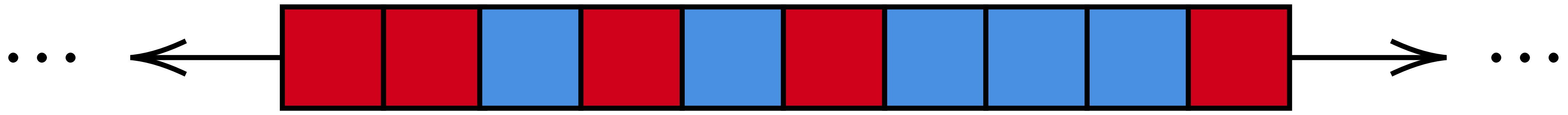

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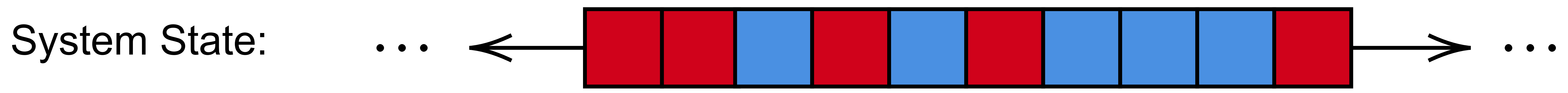

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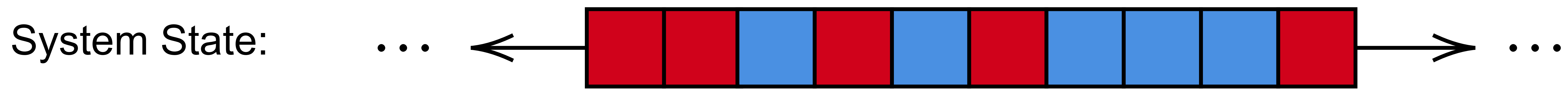

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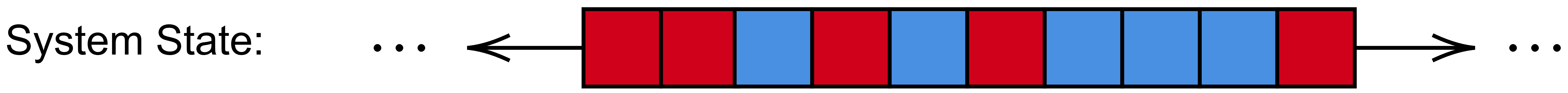

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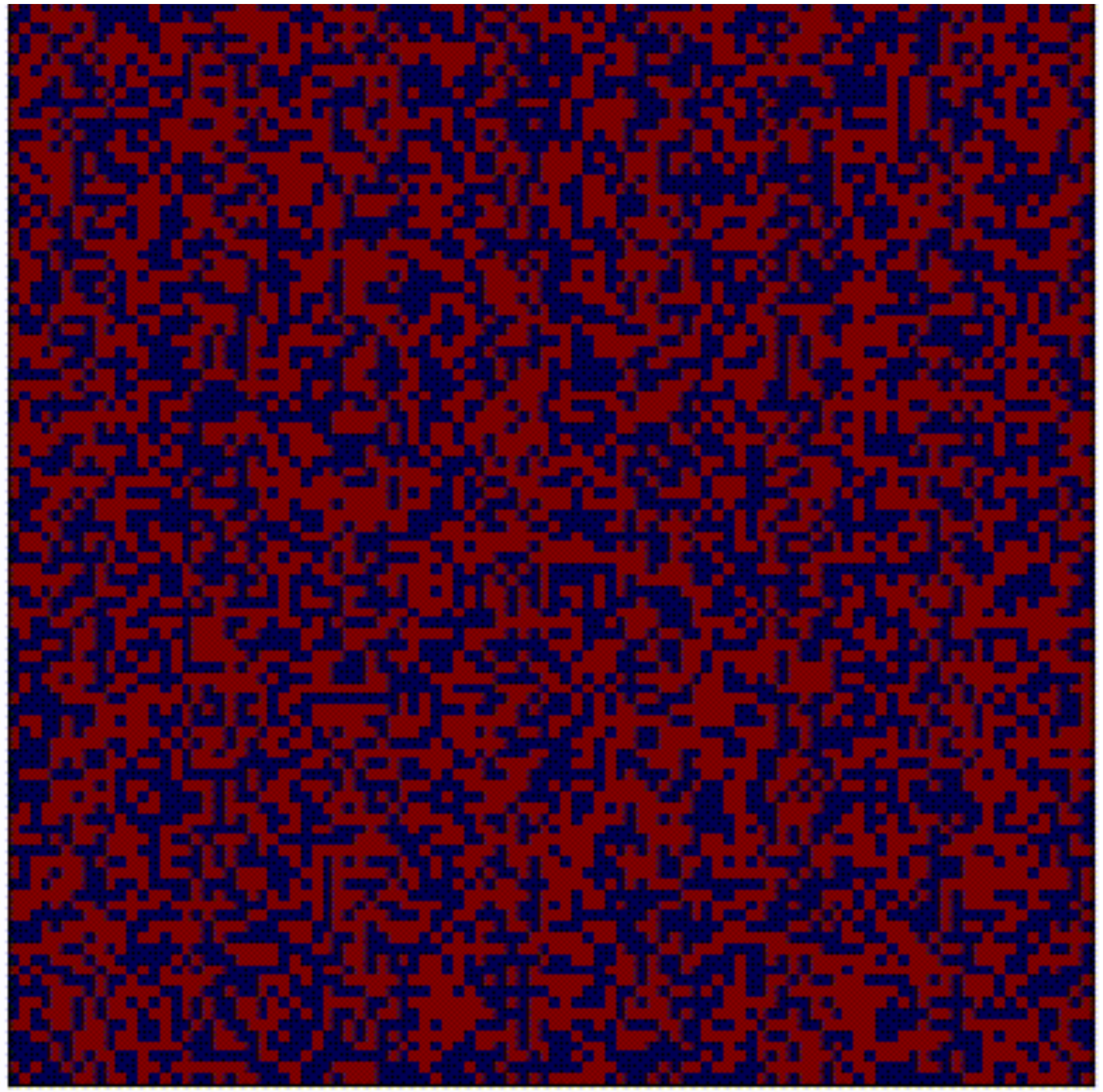
2D (4 neighbors for every cell)



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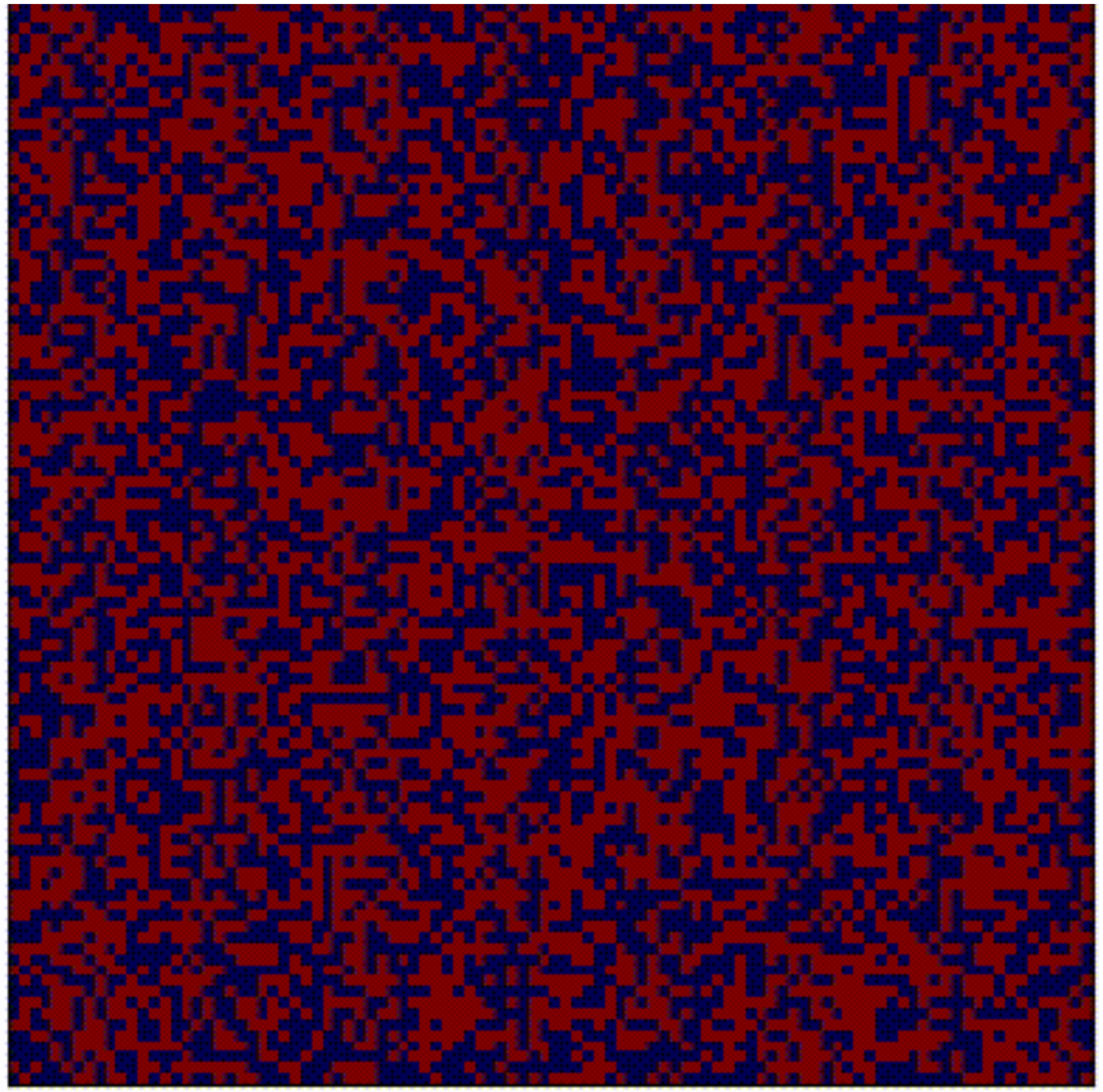

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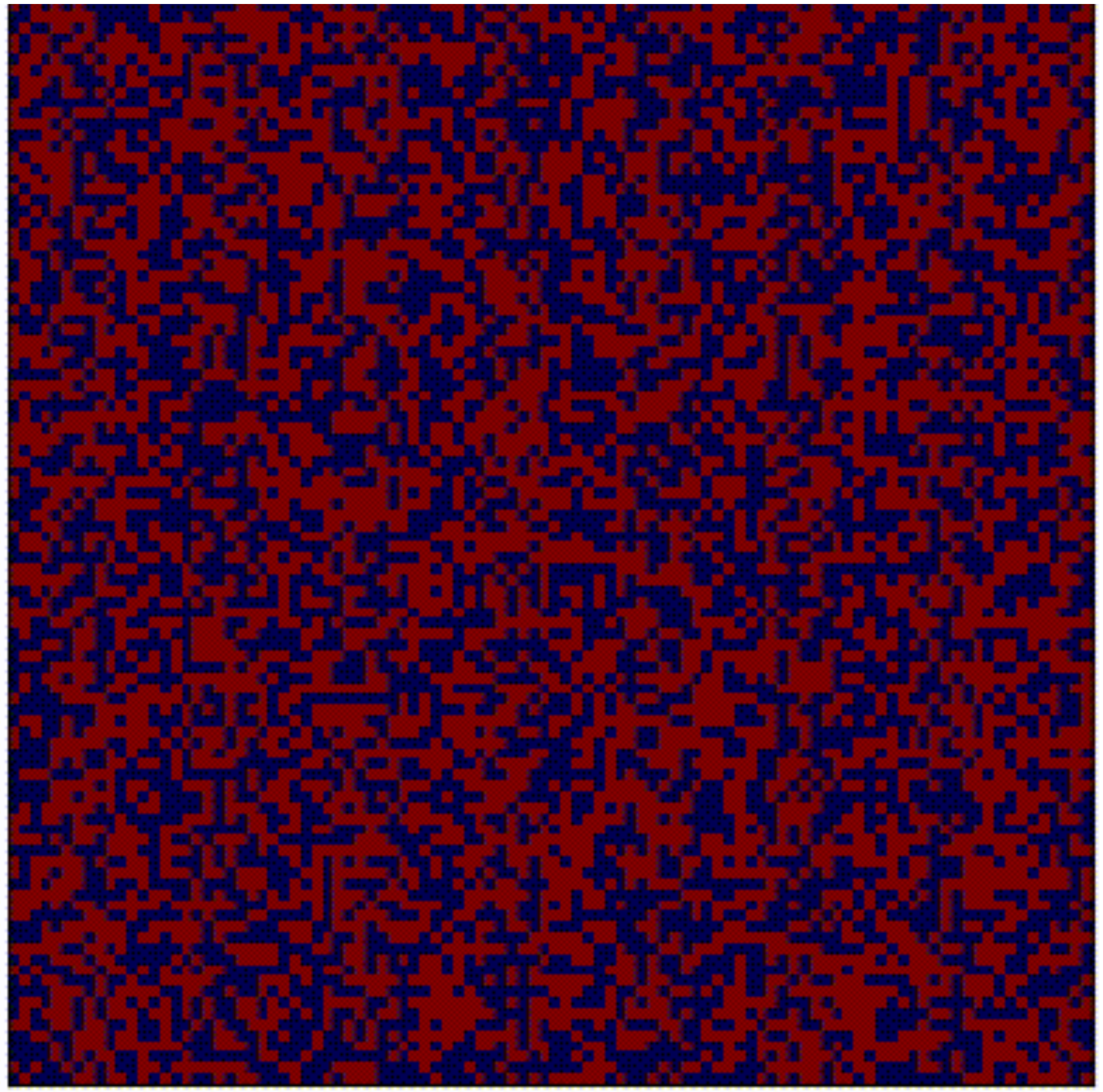

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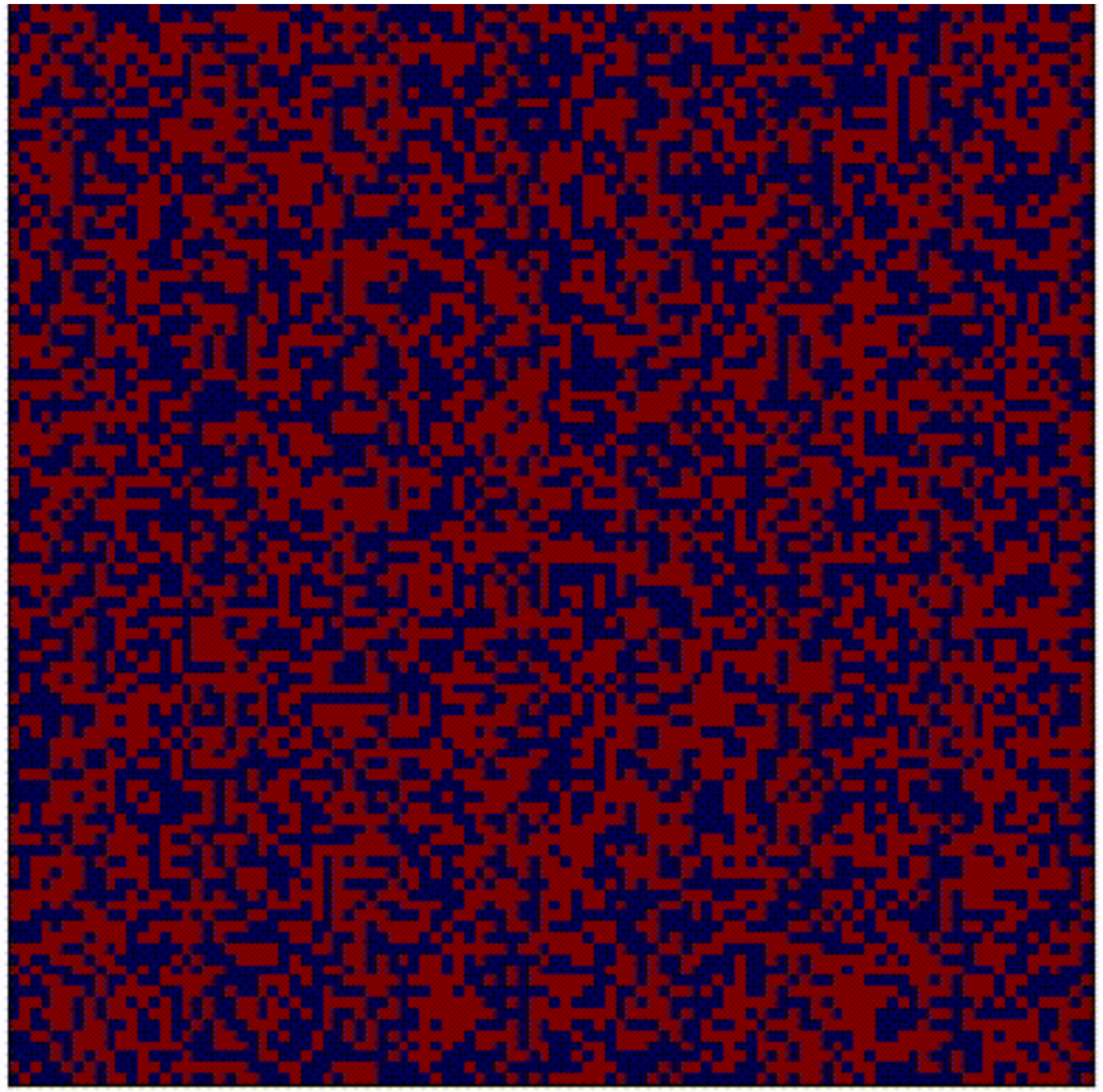

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  - Non-physics: social networks, human memory (Hopfield network!), etc.

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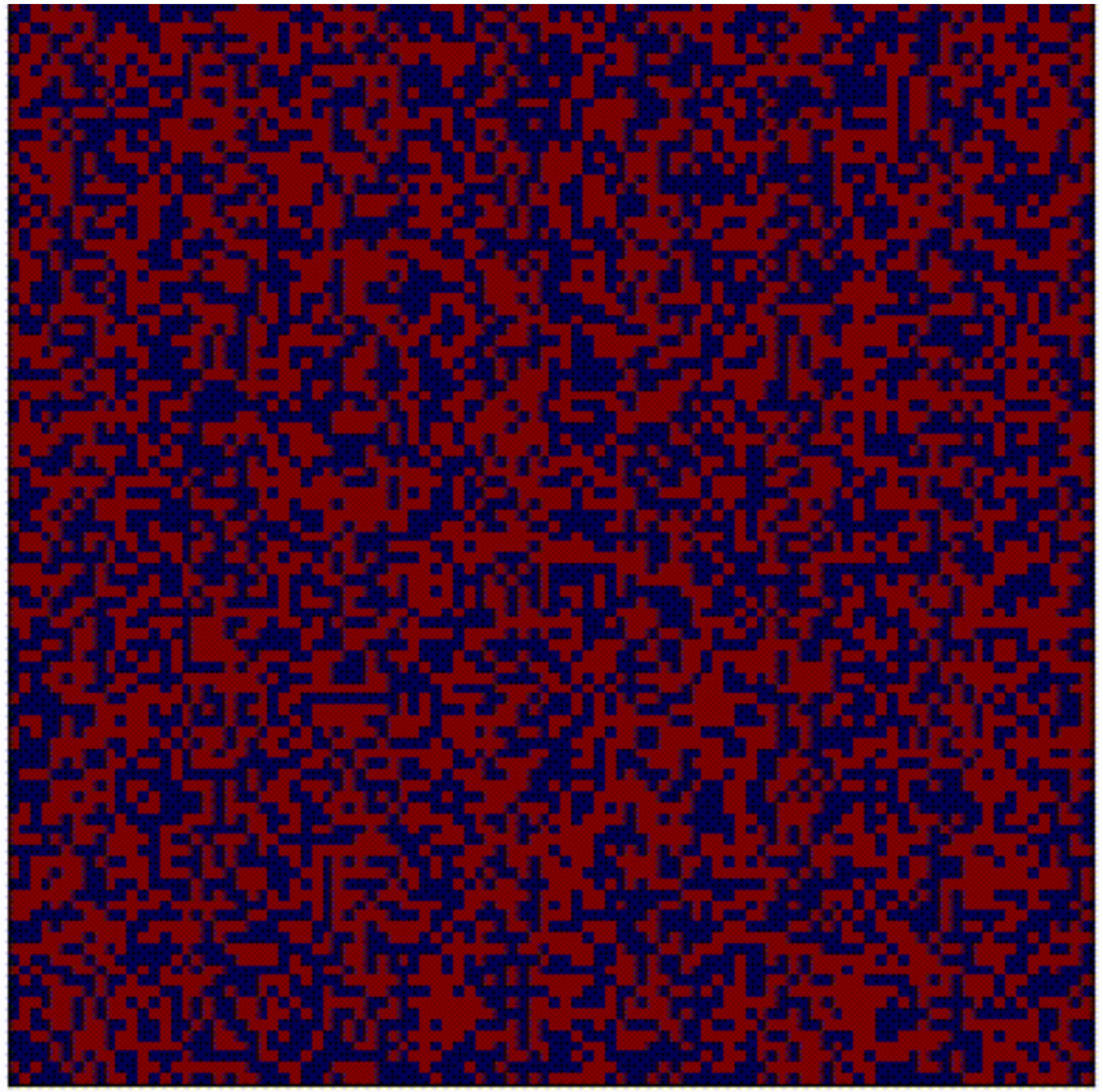

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Hopfield Networks & Boltzmann Machines

“Neighbor” $\Rightarrow$”Connection”

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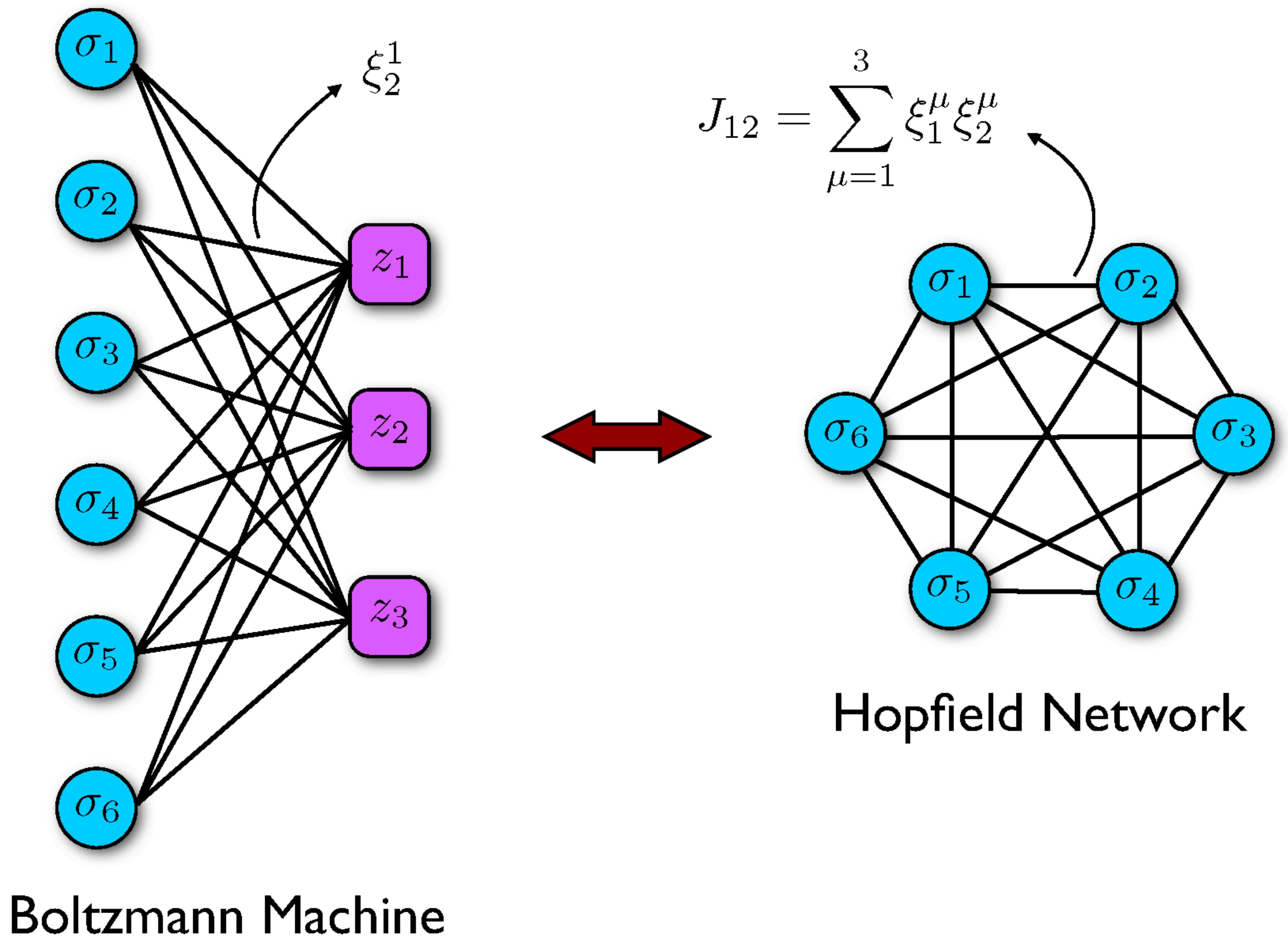

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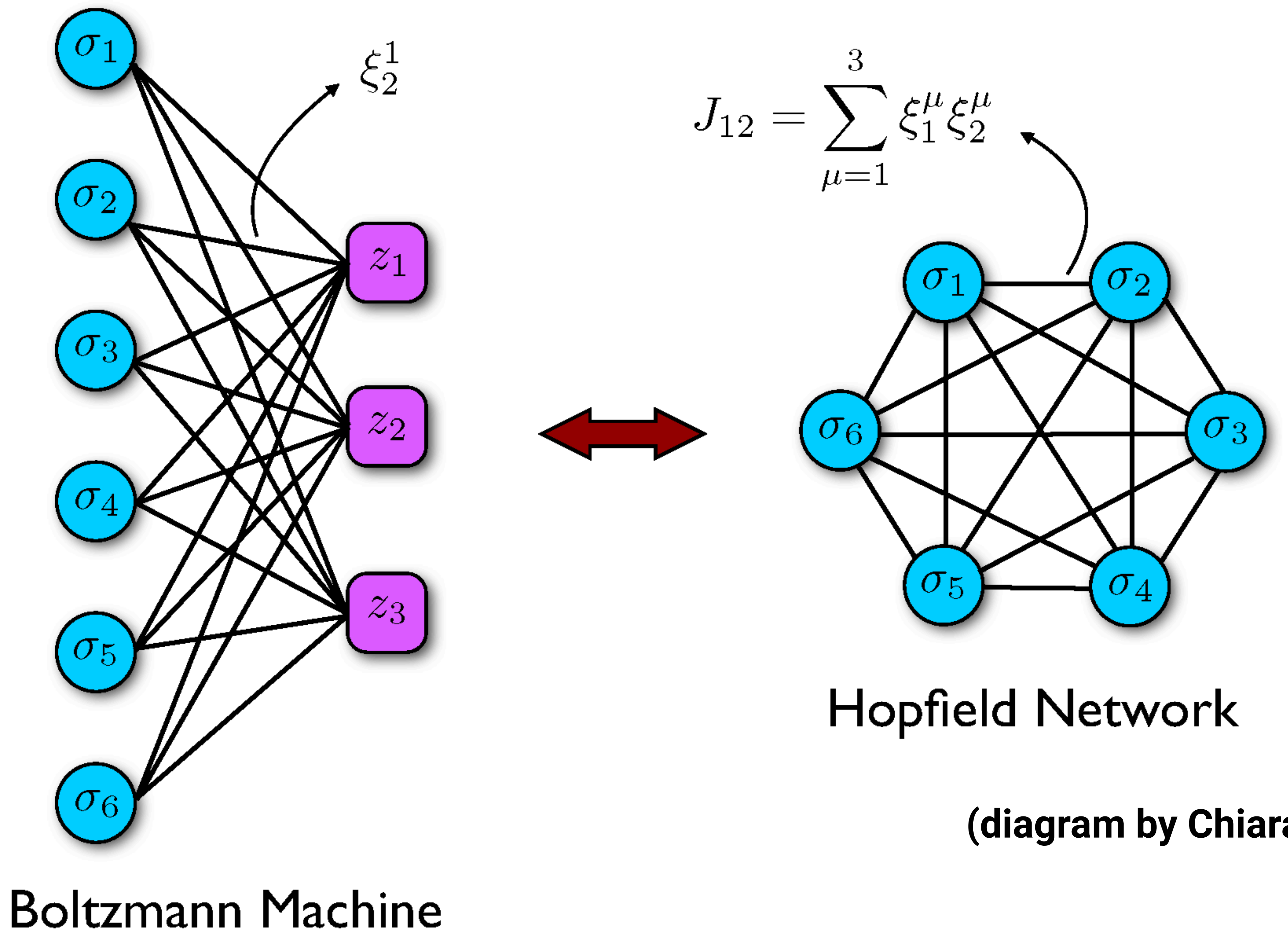

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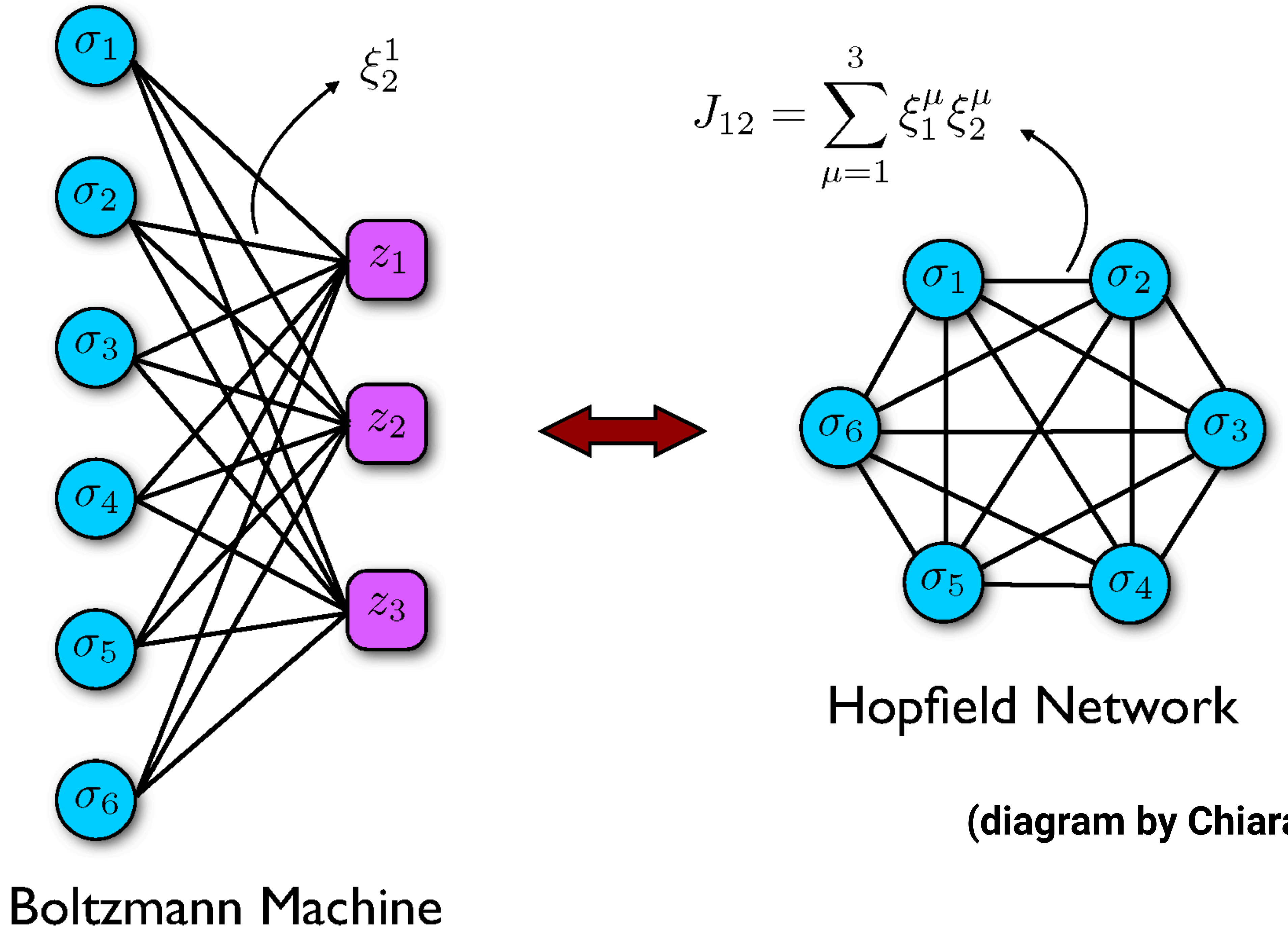

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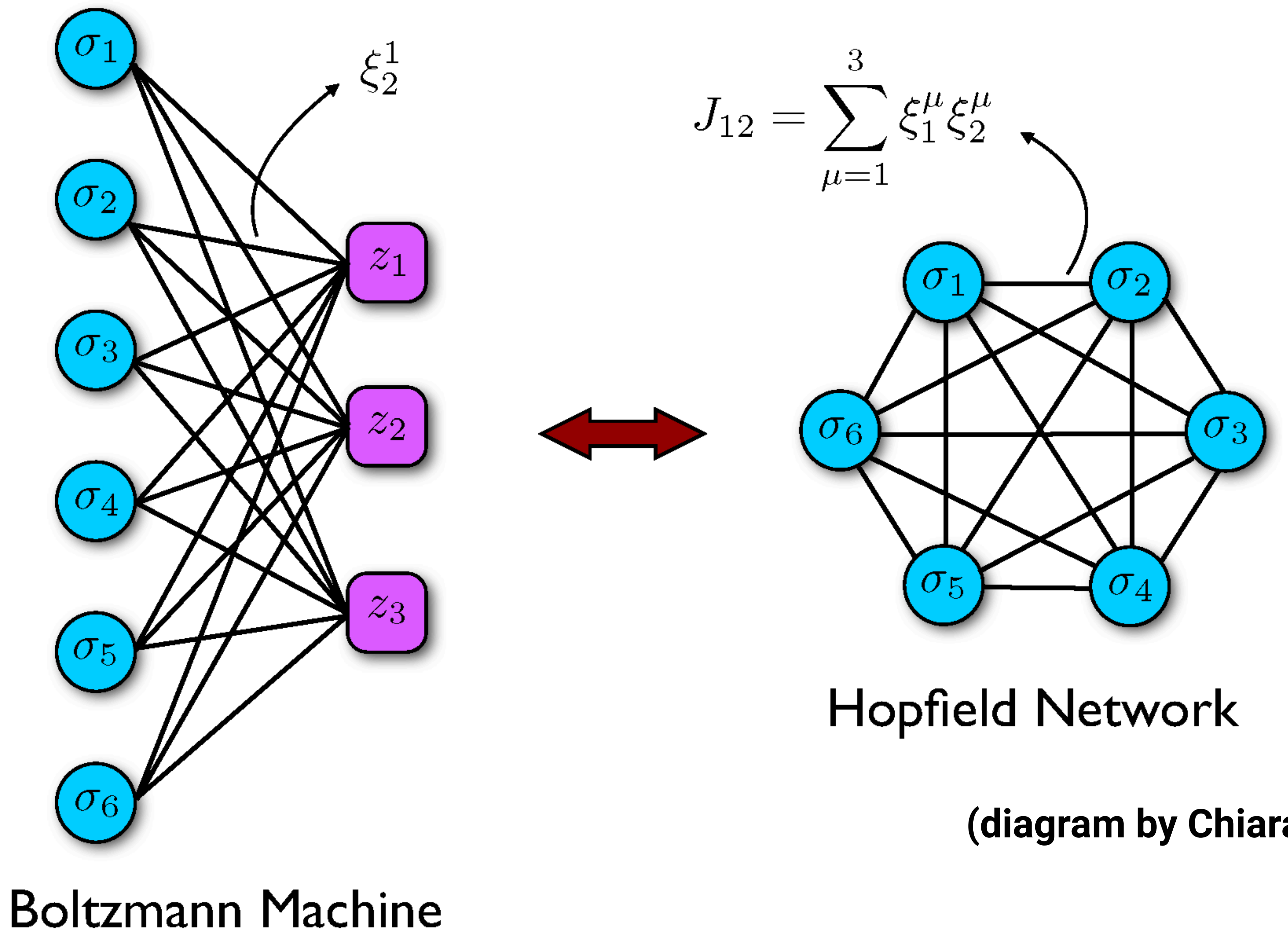

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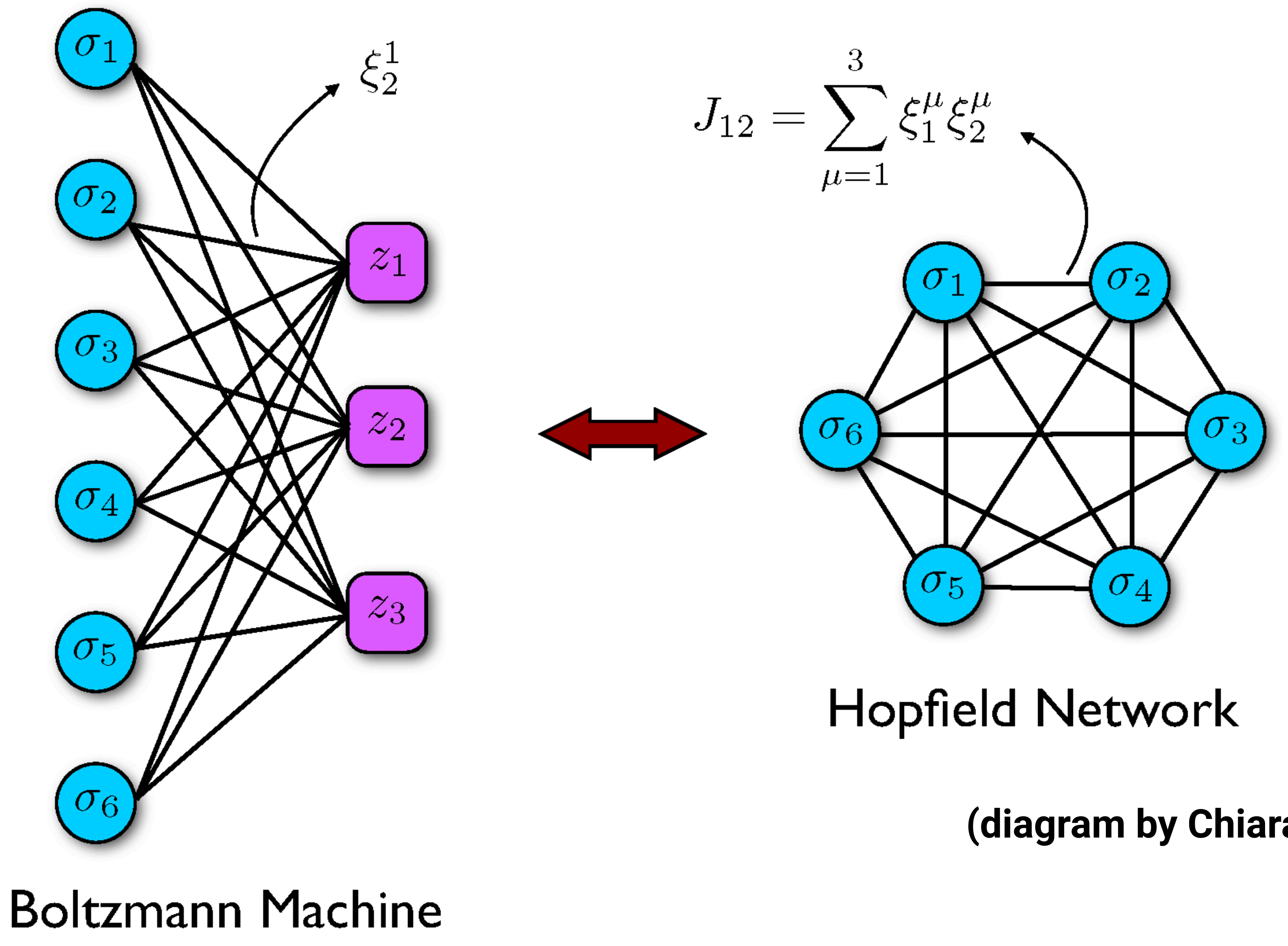

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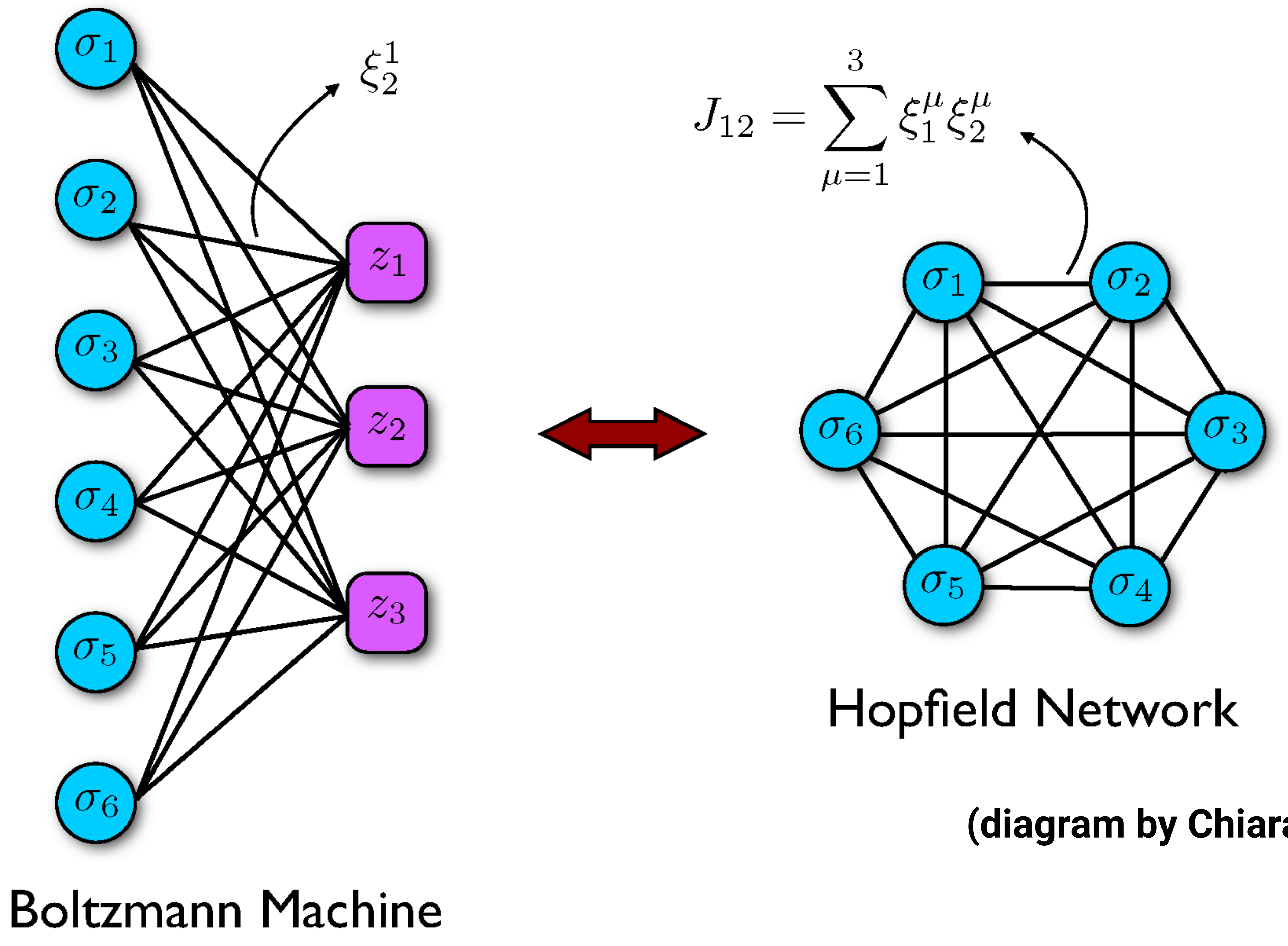

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  - **Hopfield Networks is All You Need** (2020)**,** Hubert Ramsauer, et al., successfully applies a variant of modern Hopfield Networks to classification, NLP, and drug design problems, with great performance.

(A Small Selection of)

Physics-Informed Inductive Biases in the modern era

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Categories:

1. Energy
2. Geometry
3. Differential Equations

Why Inductive Biases?

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- However, this prior is not enough. Physically-motivated inductive biases define additional priors on this function space.

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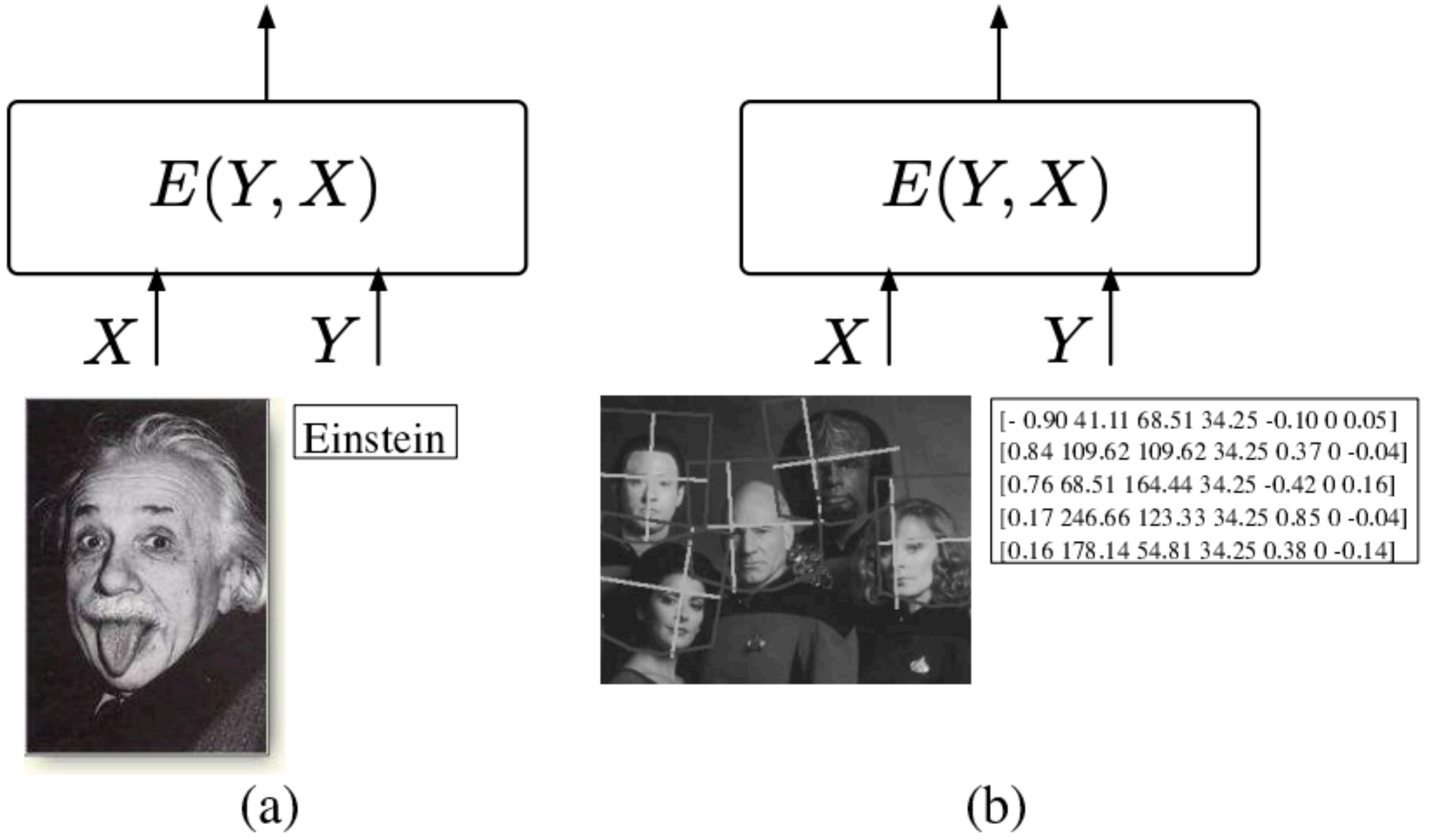

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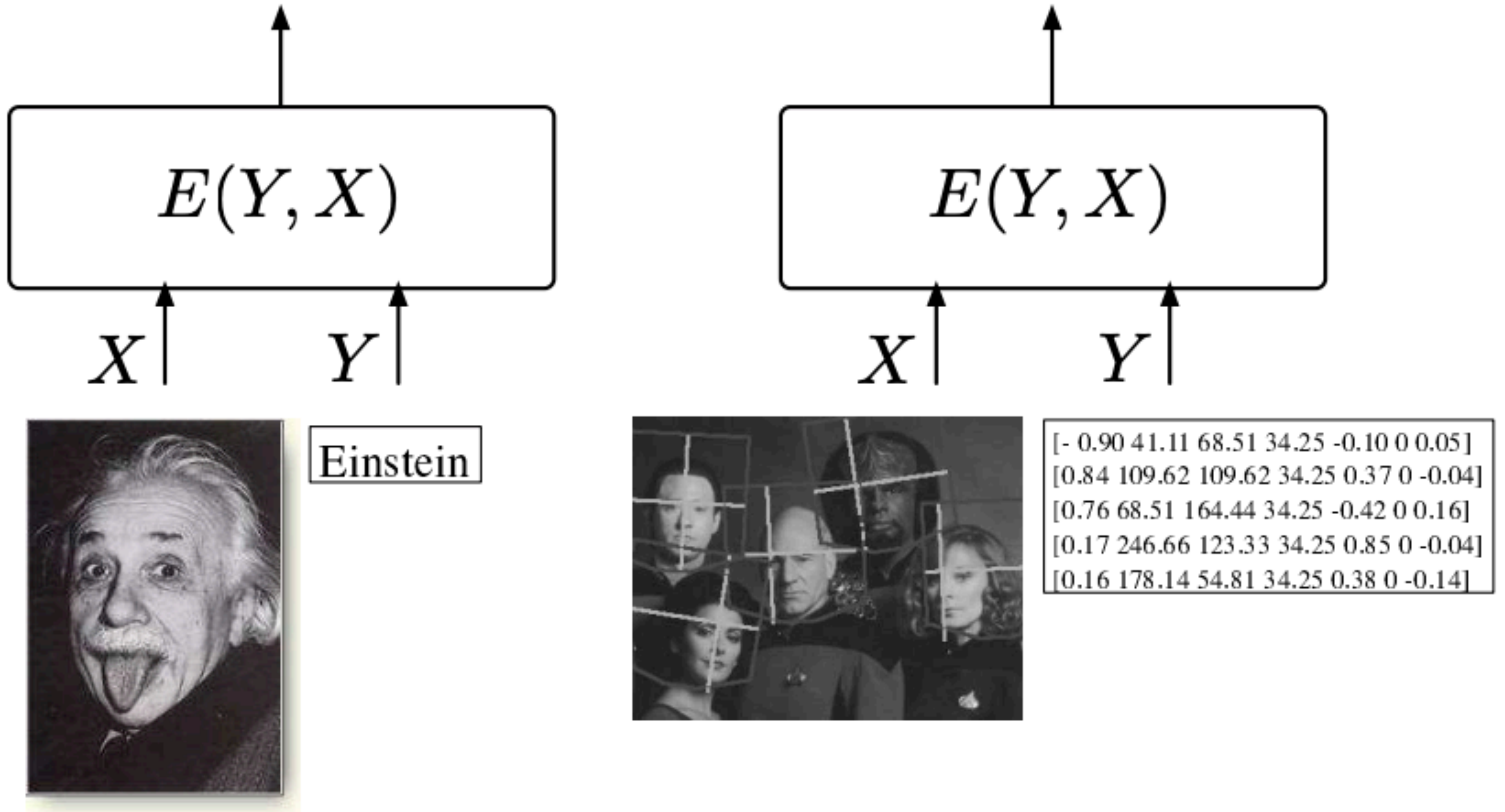

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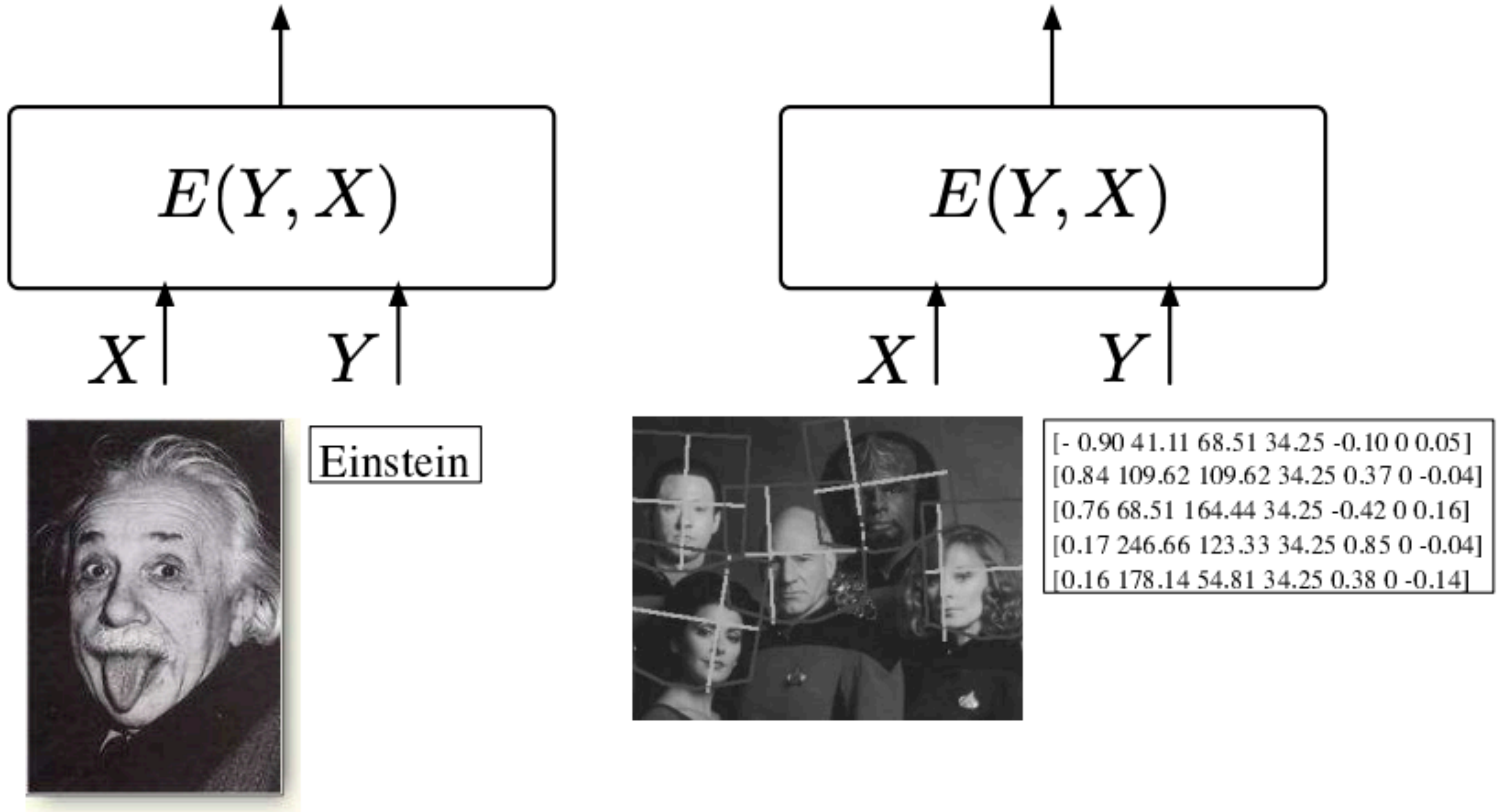

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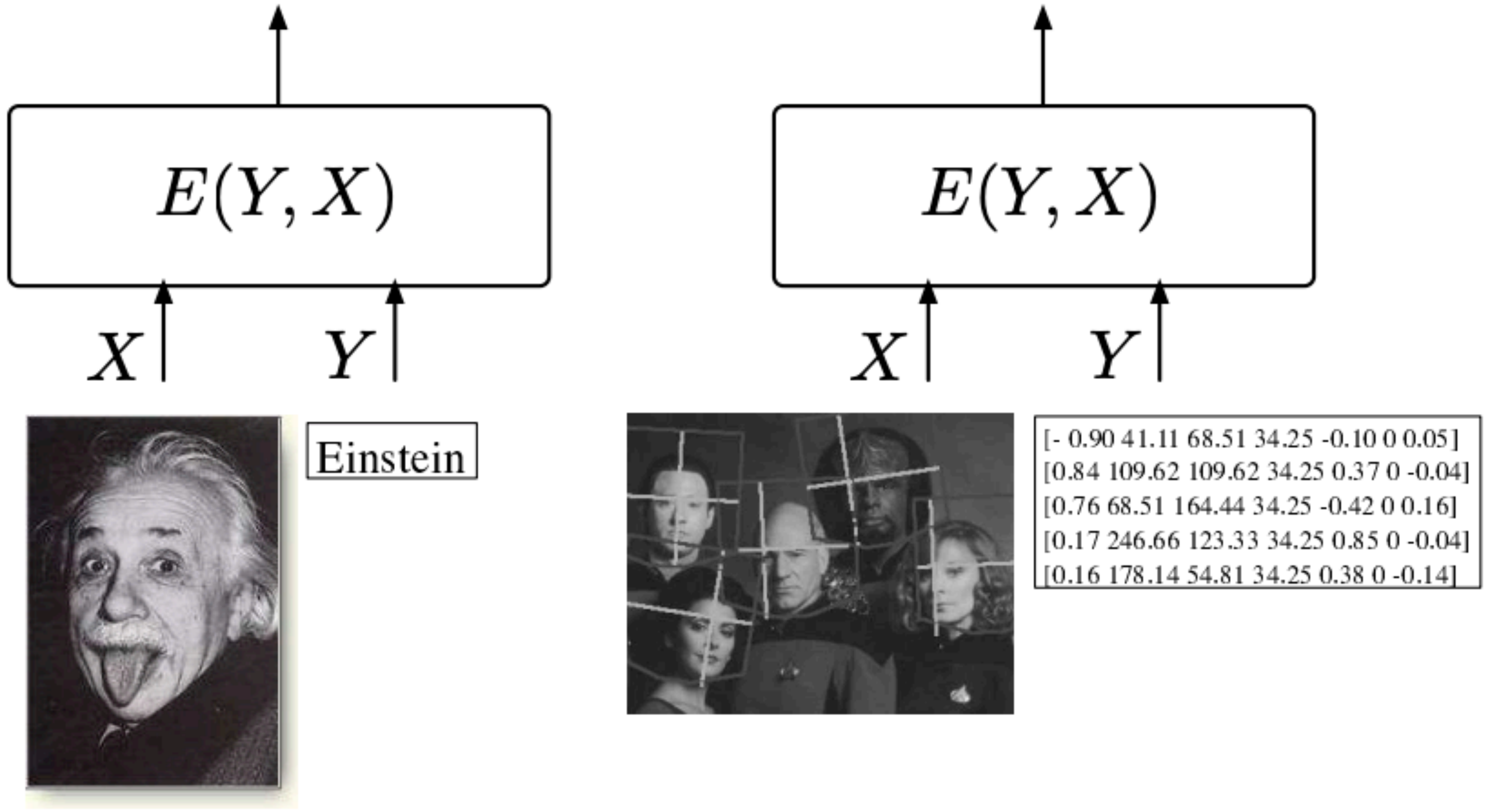

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Energy surface

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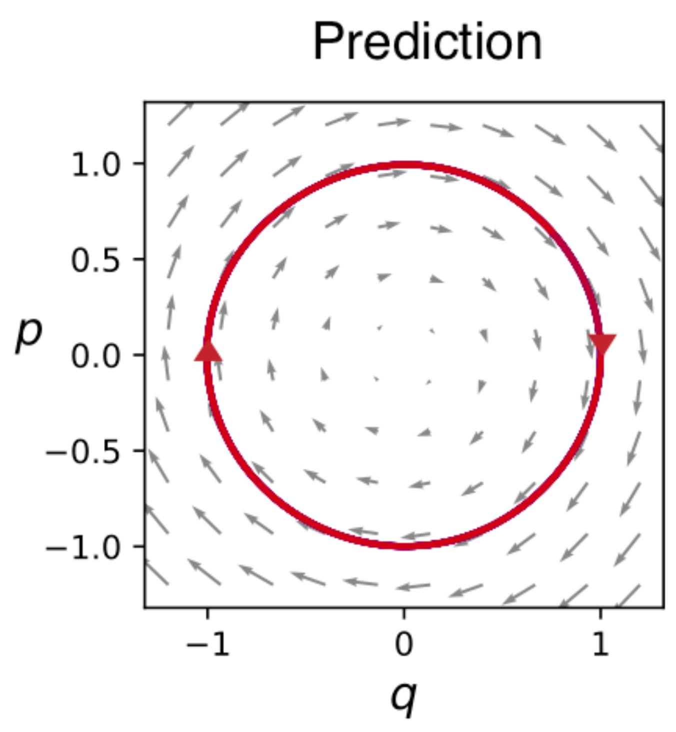

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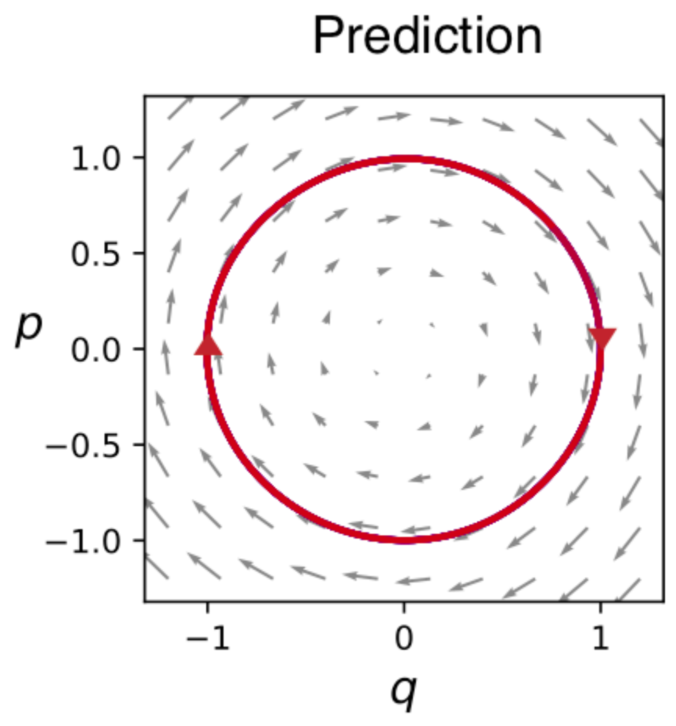

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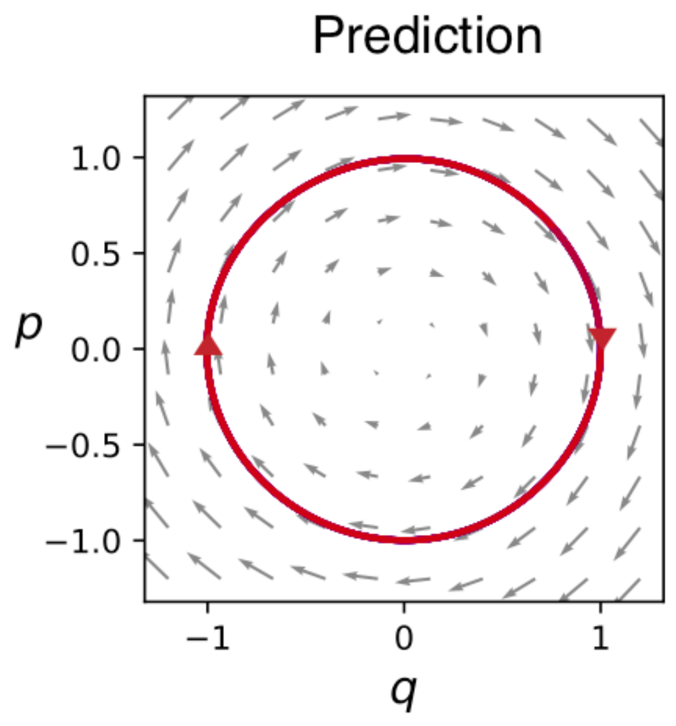

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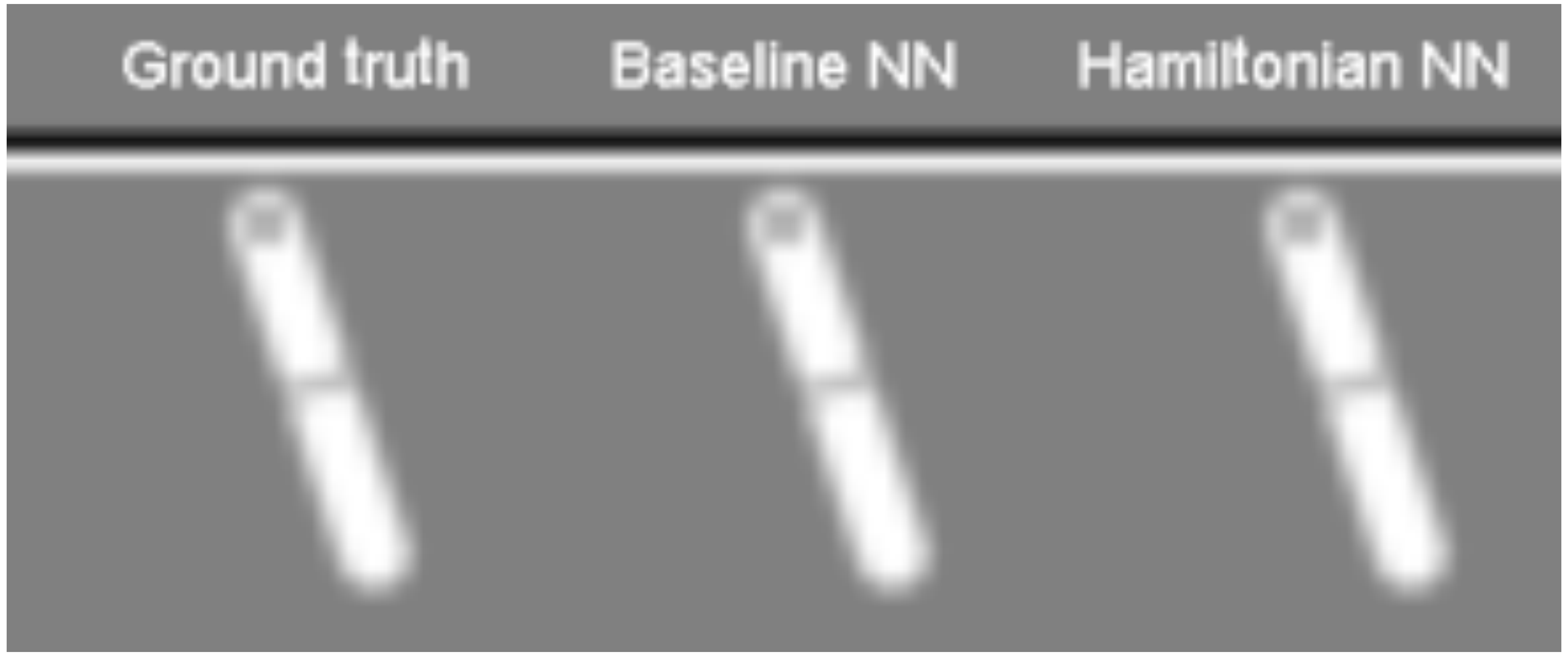

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$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_j} = \frac{\partial \mathcal{L}}{\partial q_j} \qquad \text{Euler-Lagrange (5)}$$

$$\frac{d}{dt}\nabla_{\dot{q}}\mathcal{L} = \nabla_q \mathcal{L} \qquad \text{vectorize (6)}$$

$$\nabla_q \mathcal{L} = (\nabla_{\dot{q}}\nabla_{\dot{q}}^{\top}\mathcal{L})\ddot{q} + (\nabla_q \nabla_{\dot{q}}^{\top}\mathcal{L})\dot{q} \qquad \text{expand } \frac{d}{dt} \text{ (7)}$$

$$\ddot{q} = (\nabla_{\dot{q}}\nabla_{\dot{q}}^{\top}\mathcal{L})^{-1}[\nabla_q \mathcal{L} - (\nabla_q \nabla_{\dot{q}}^{\top}\mathcal{L})\dot{q}] \qquad \text{solve for } \ddot{q} \text{ (8)}$$

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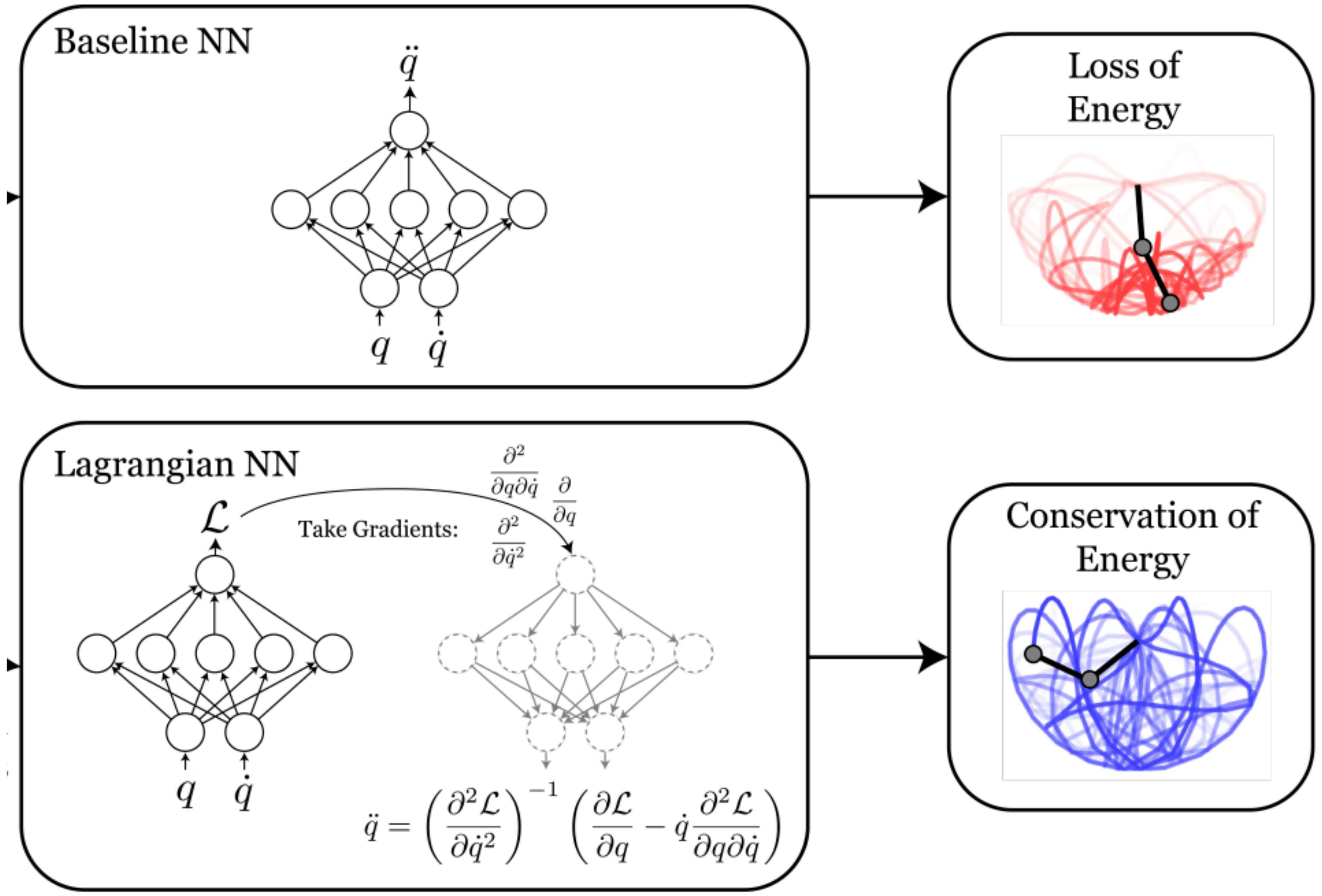

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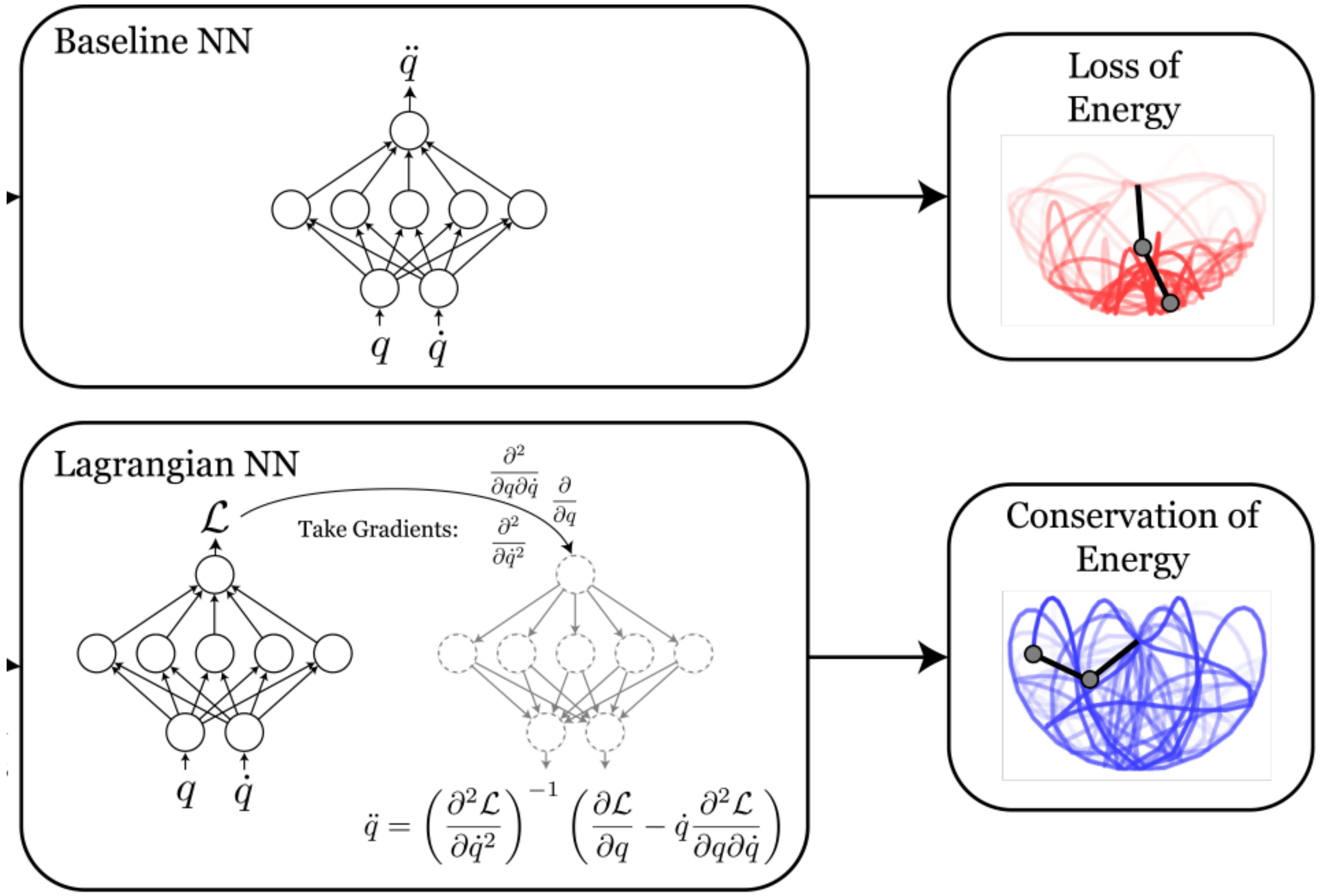

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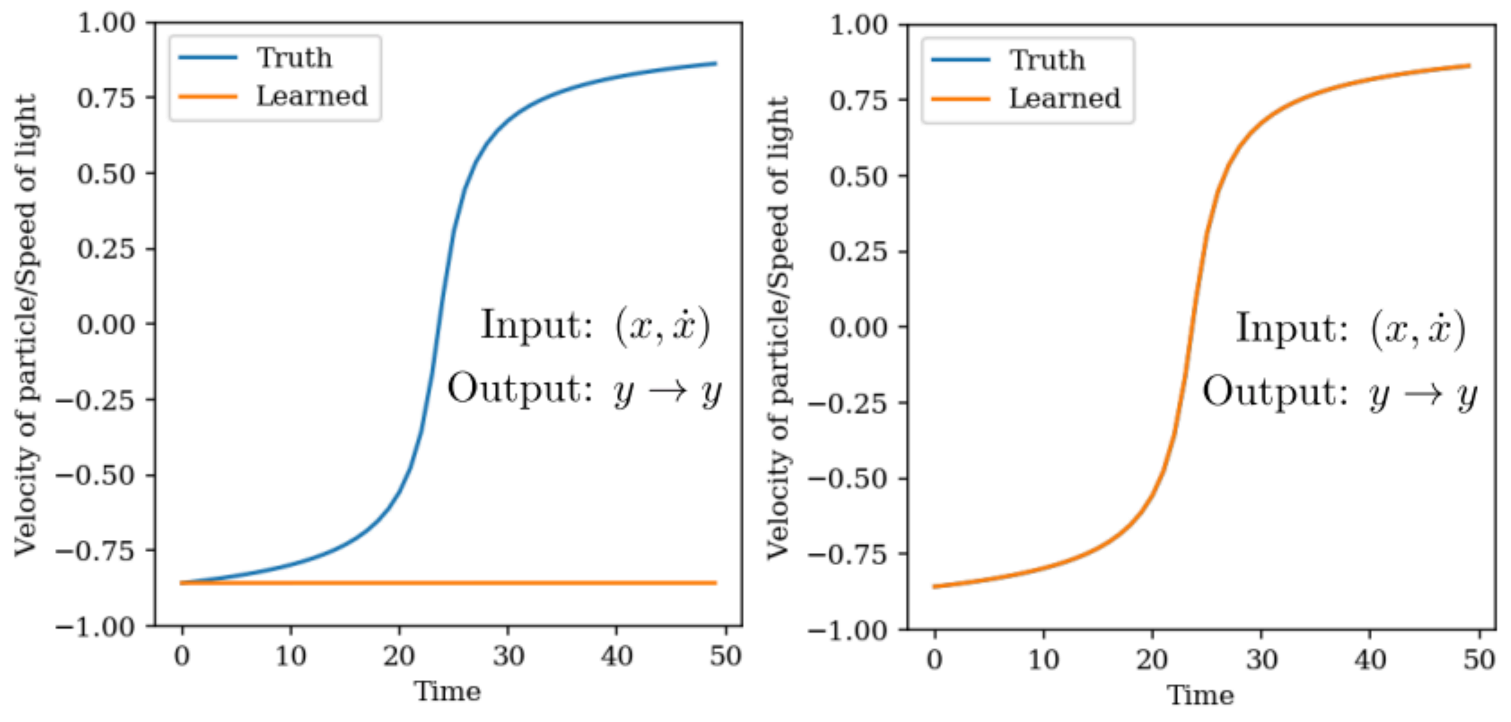
Without known kinetic energy:



HNN LNN

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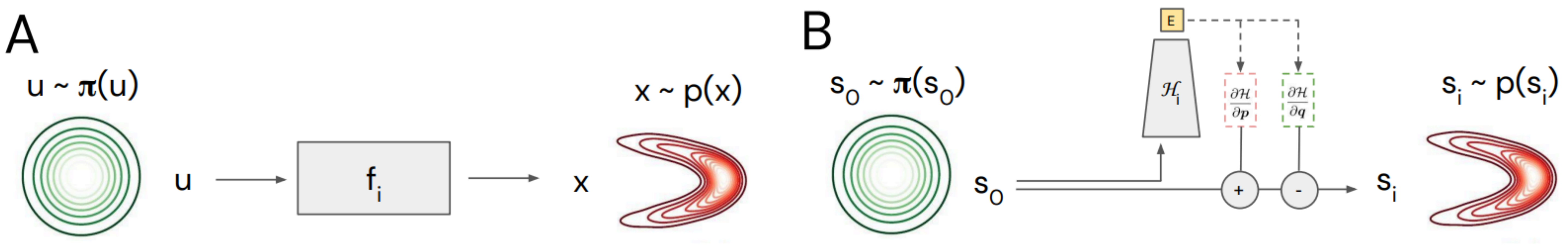
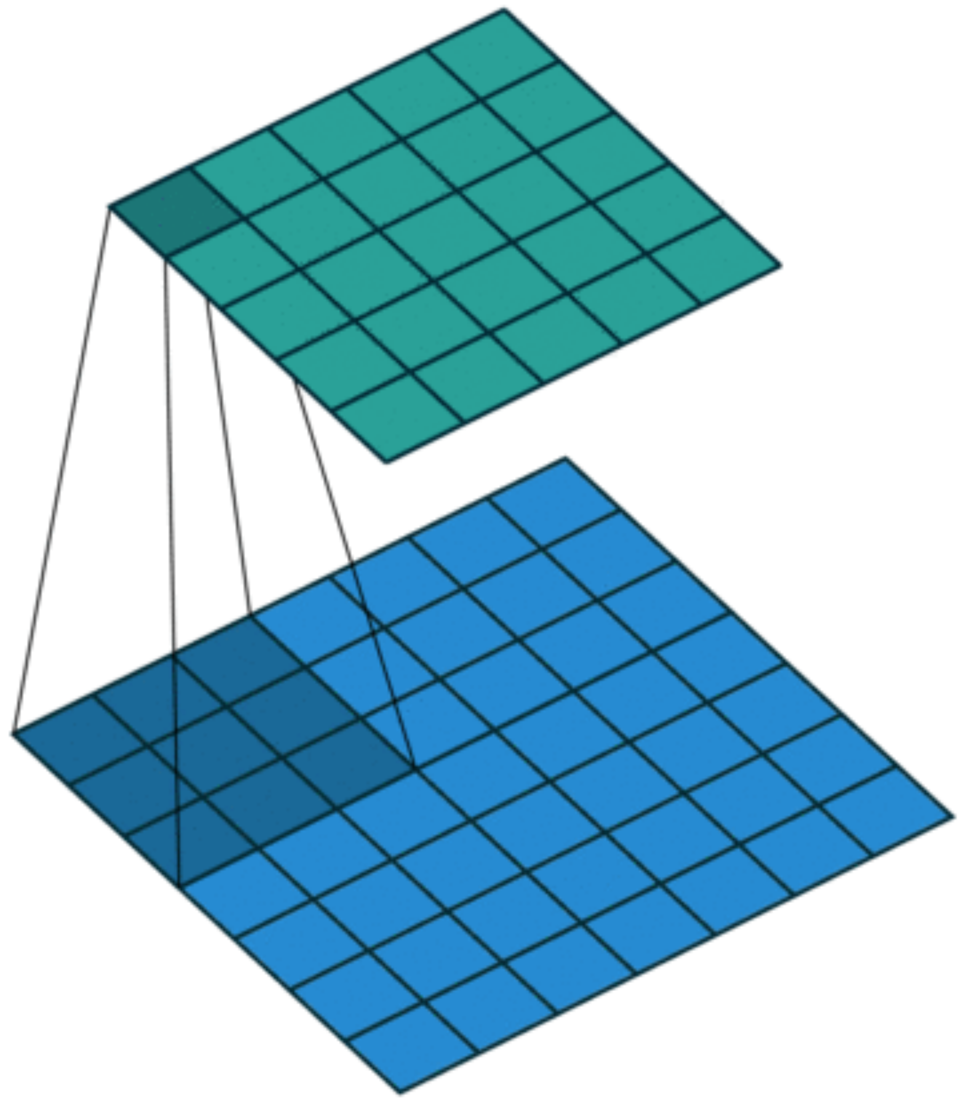


Figure 3: **A**: standard normalising flow, where the invertible function f_i is implemented by a neural network. **B**: Hamiltonian flows, where the initial density is transformed using the learned Hamiltonian dynamics. Note that we depict Euler updates of the state for schematic simplicity, while in practice this is done using a leapfrog integrator.

Inductive Biases which Specify <u>Geometry</u>



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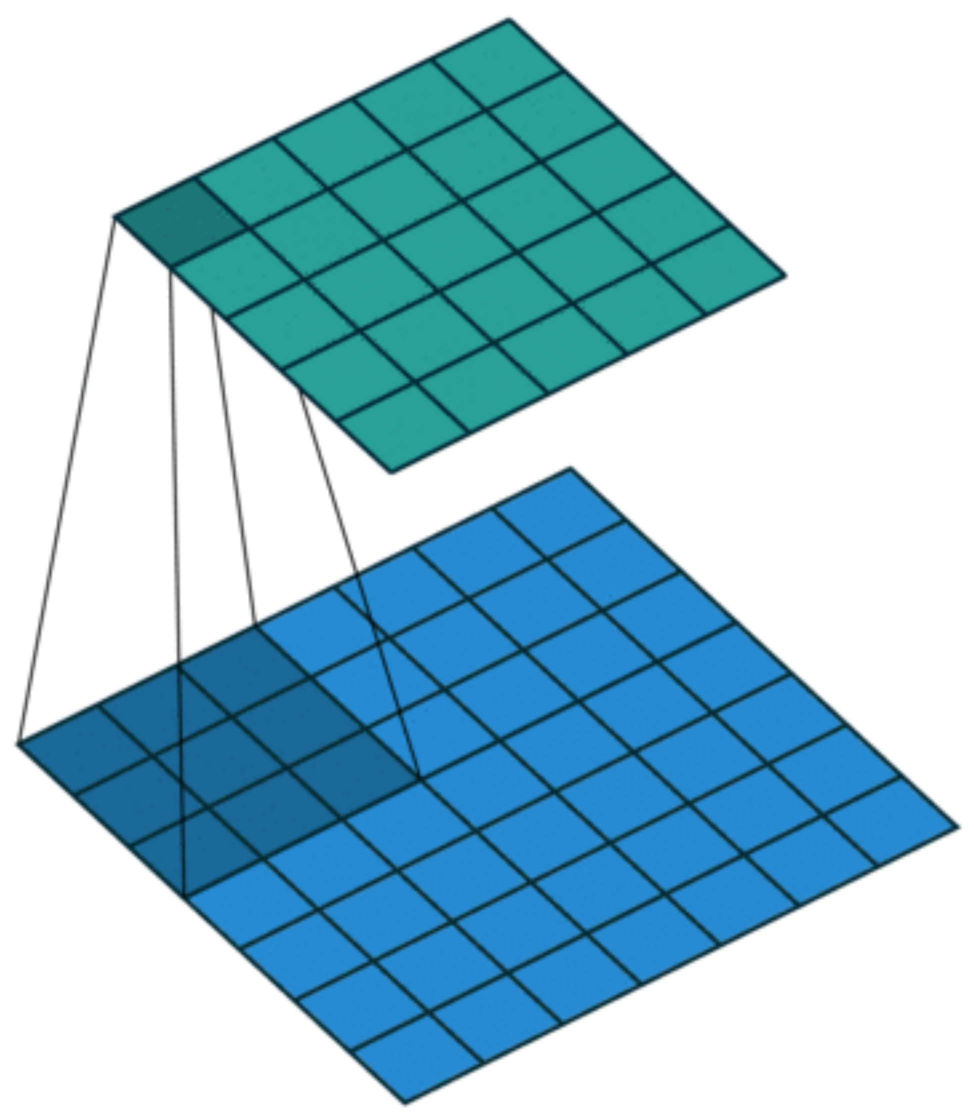

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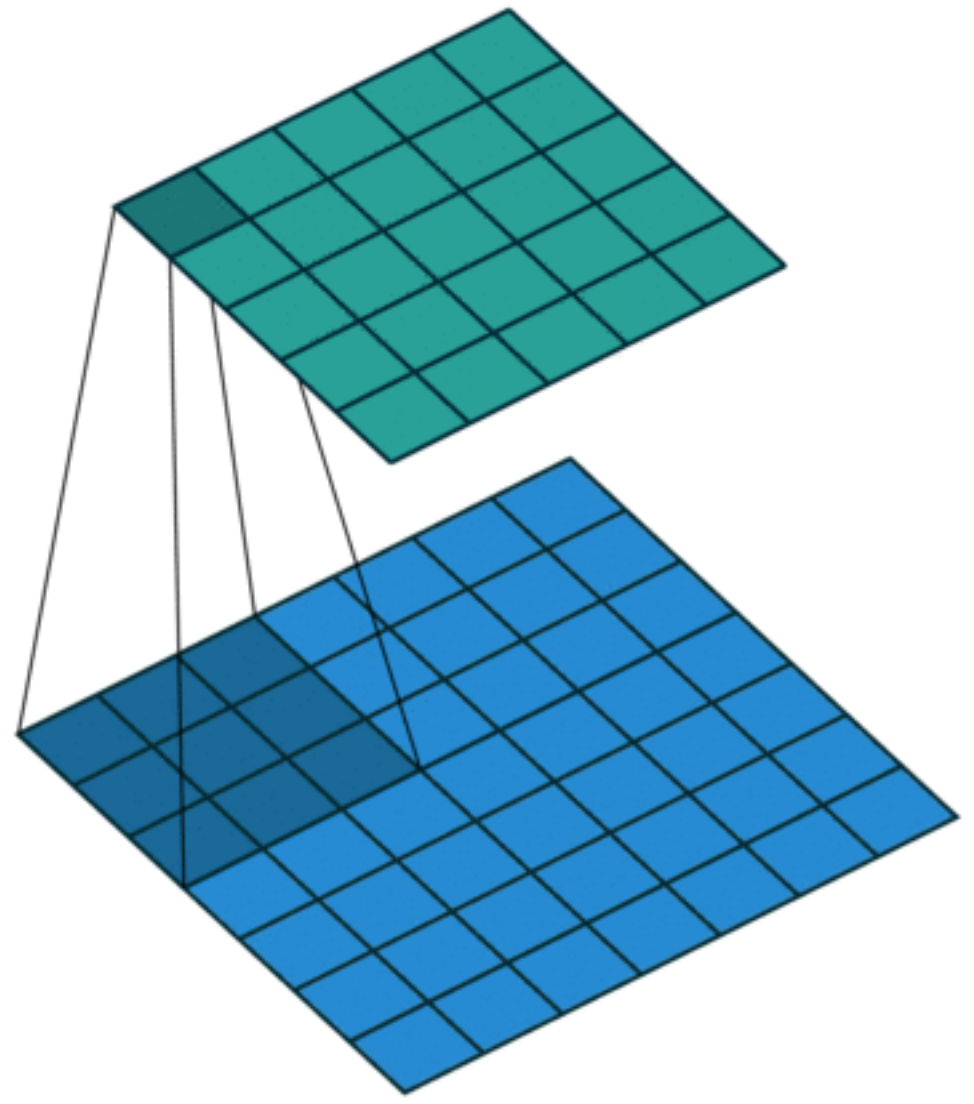

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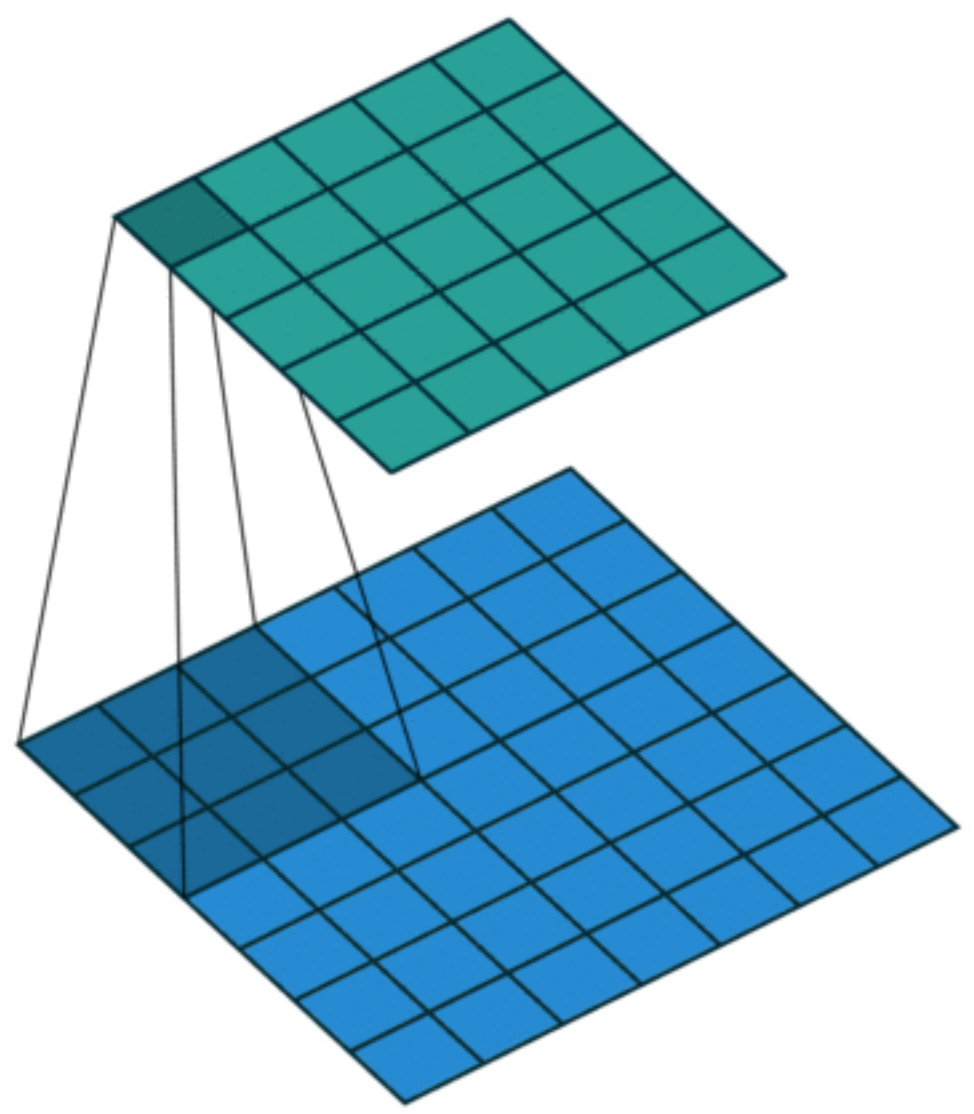
- Convolutional Neural Networks are translationally **equivariant**



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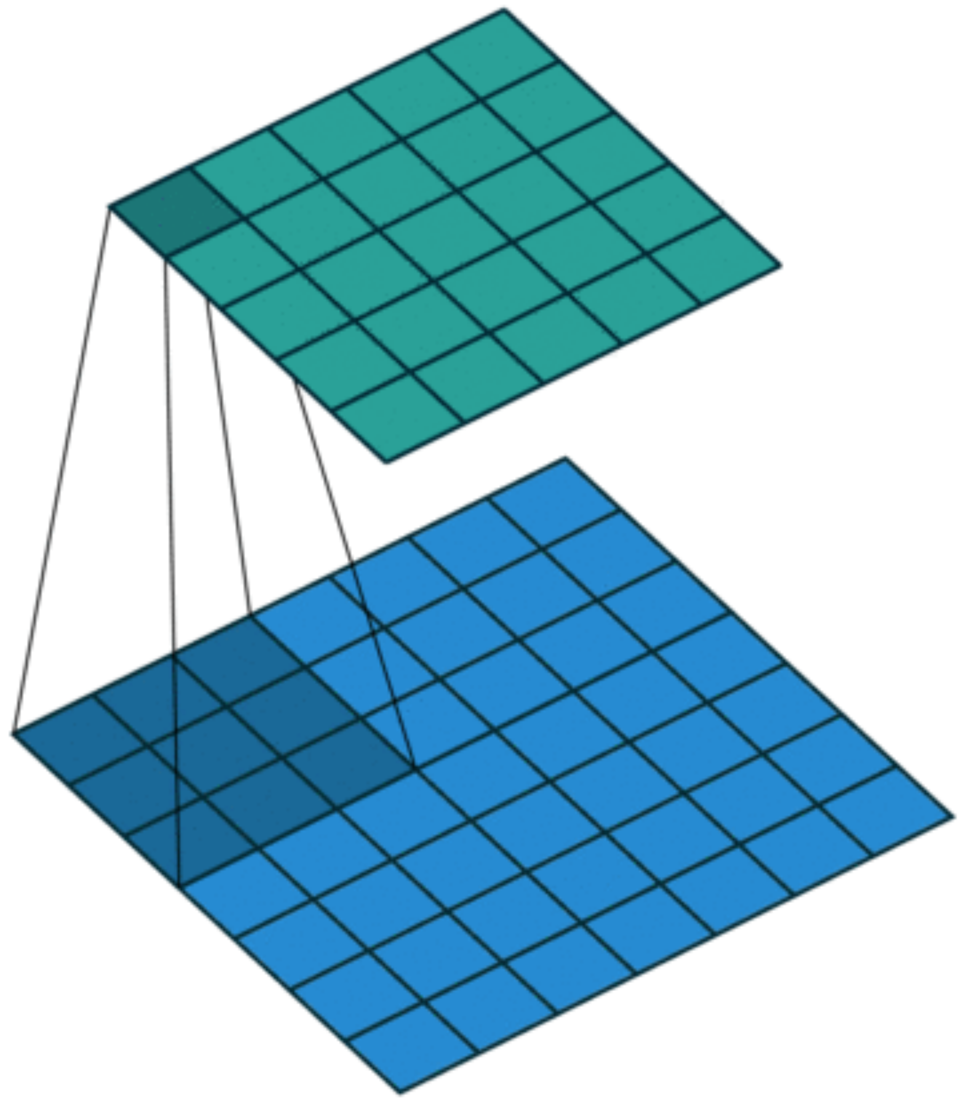

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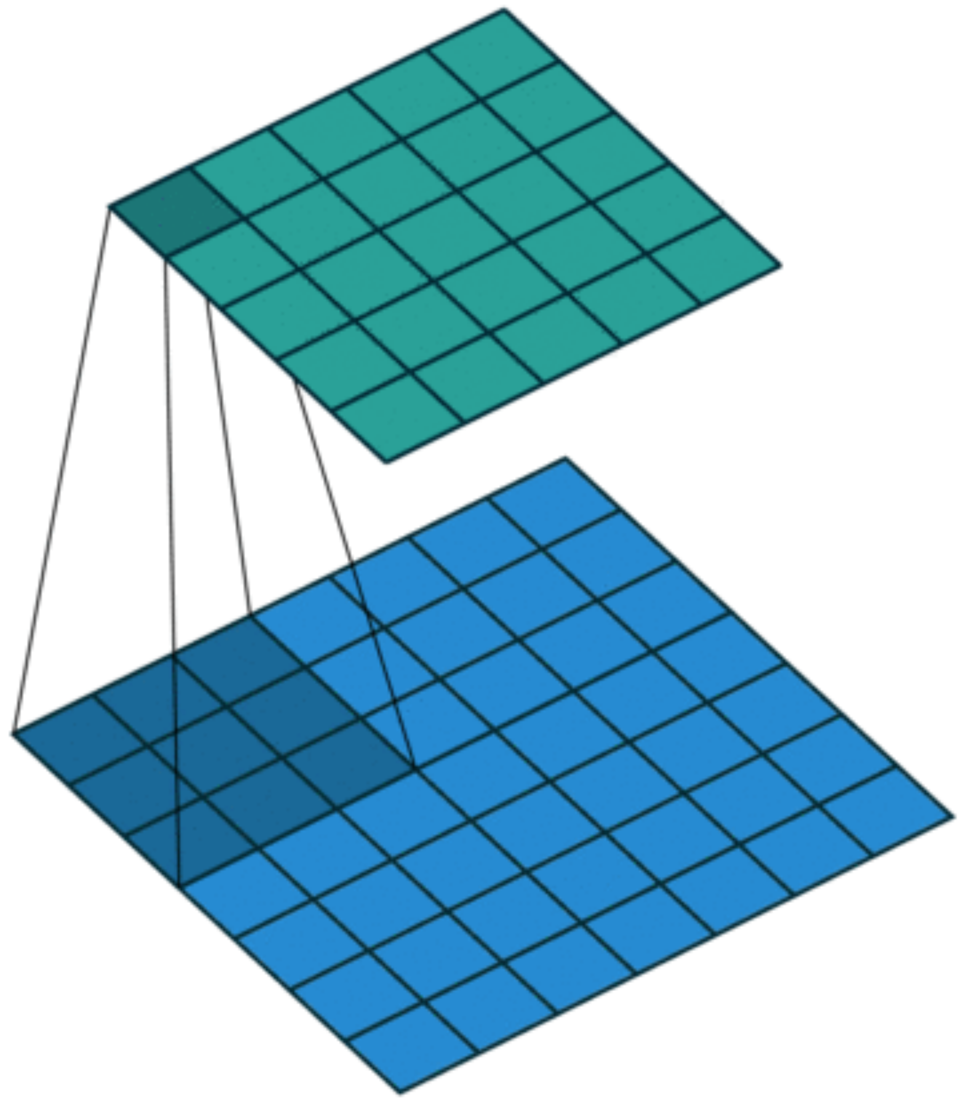

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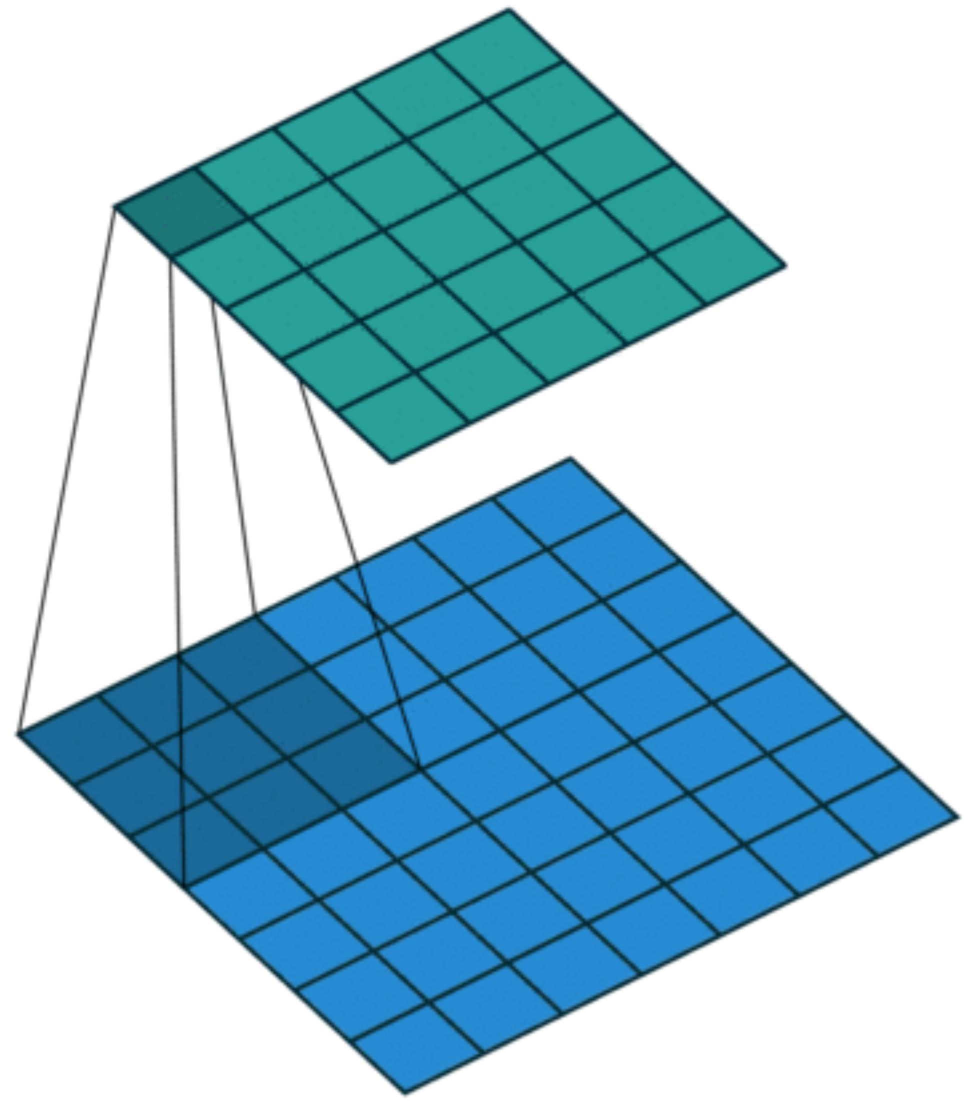

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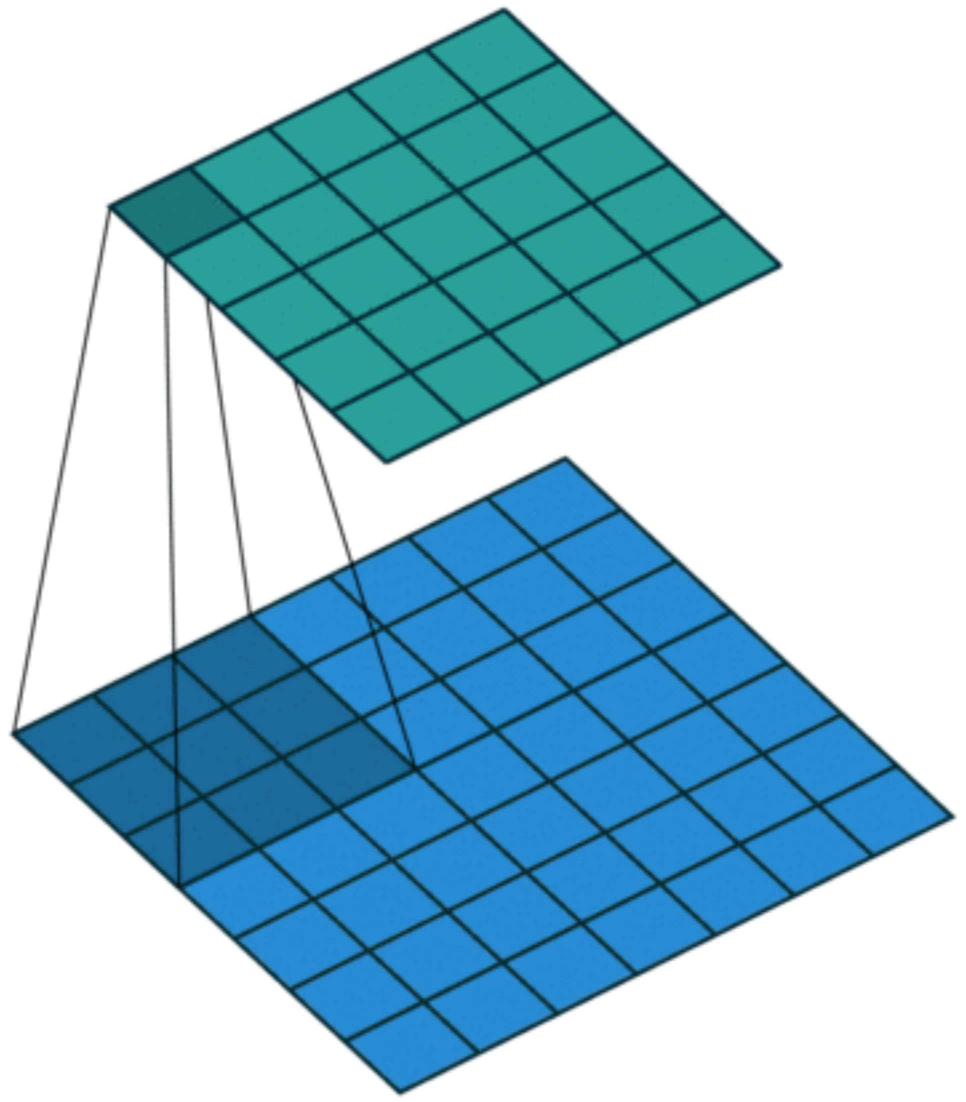
- This symmetry is intuitive because we have been living with these physical laws. Perhaps it would not be as intuitive if the laws of physics changed at every point of space!



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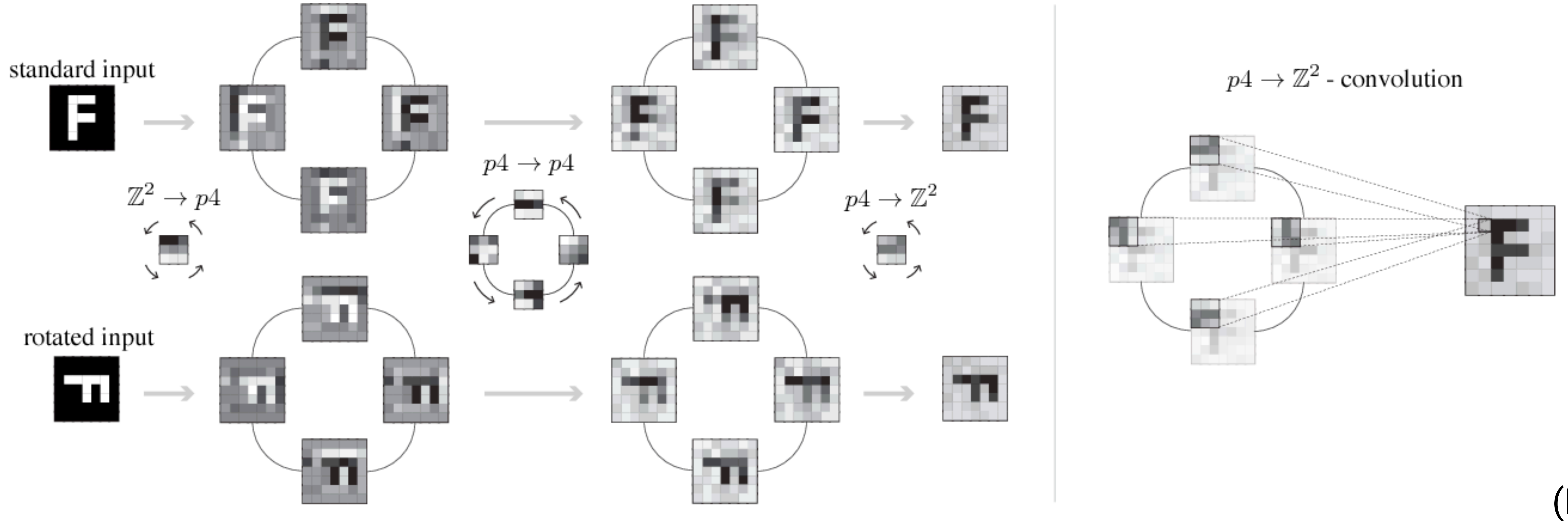

(Note that rotational symmetry is also a symmetry of the universe)

Graph Nets

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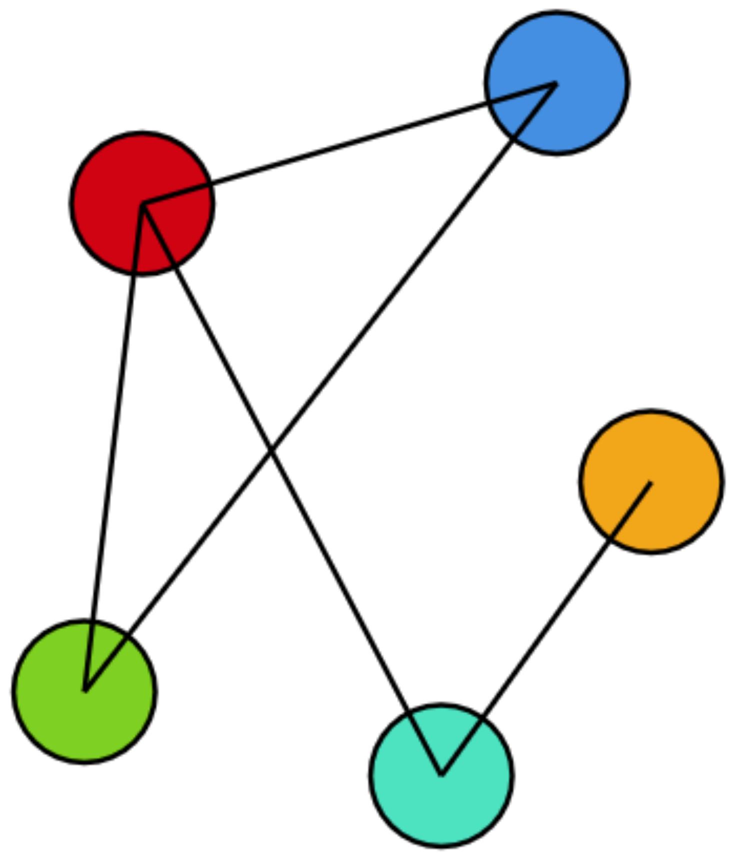
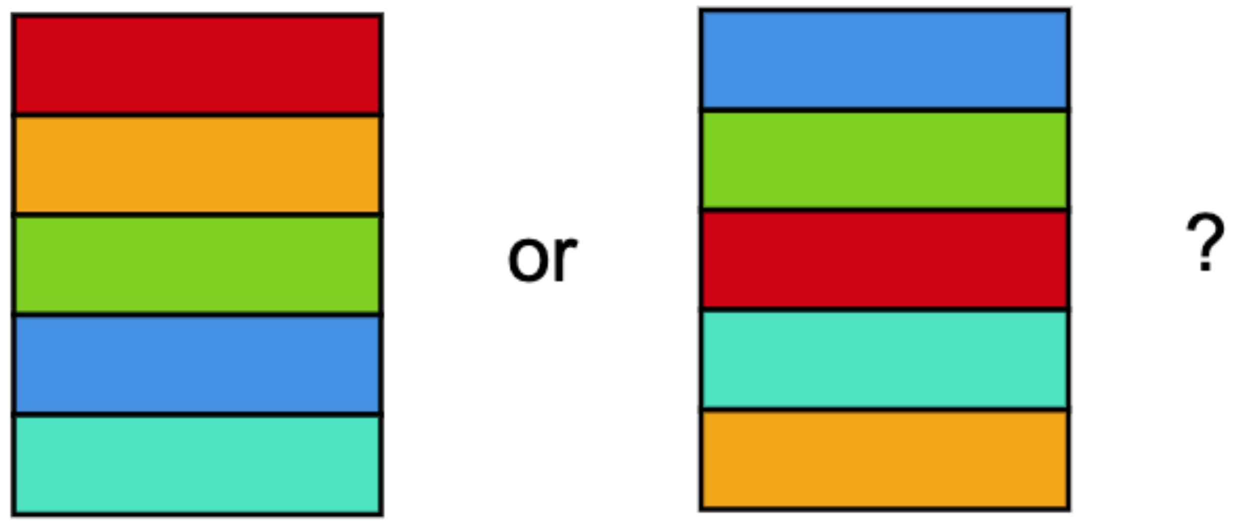


How should we pass this graph to a model?



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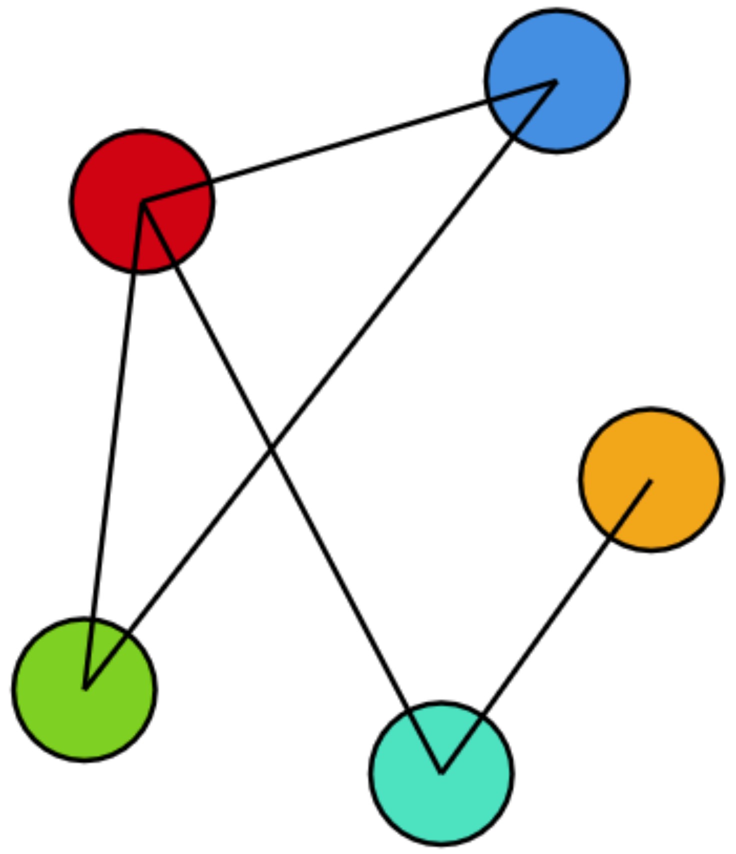

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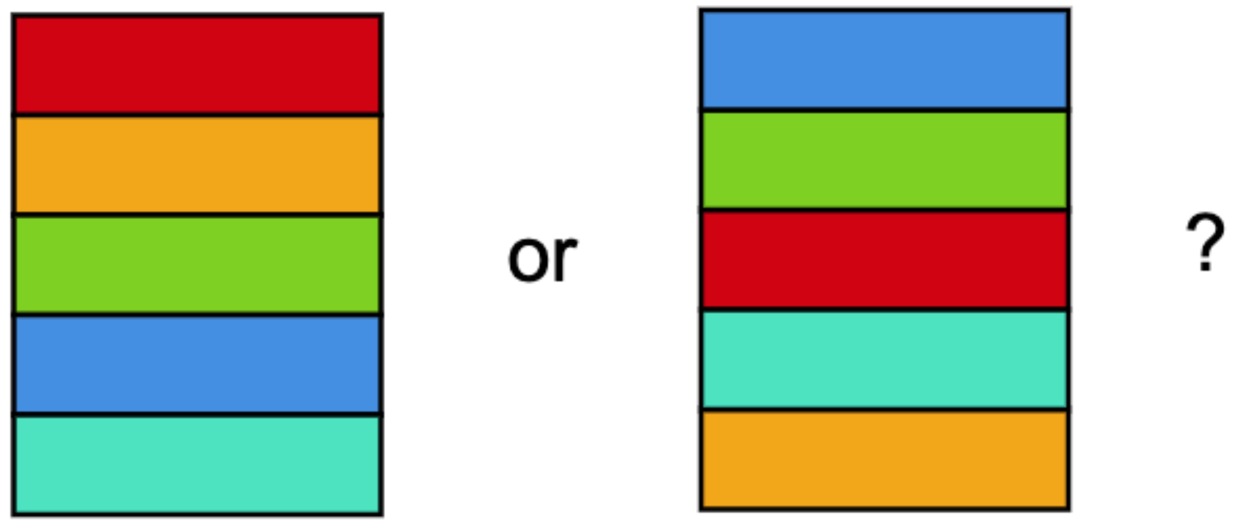

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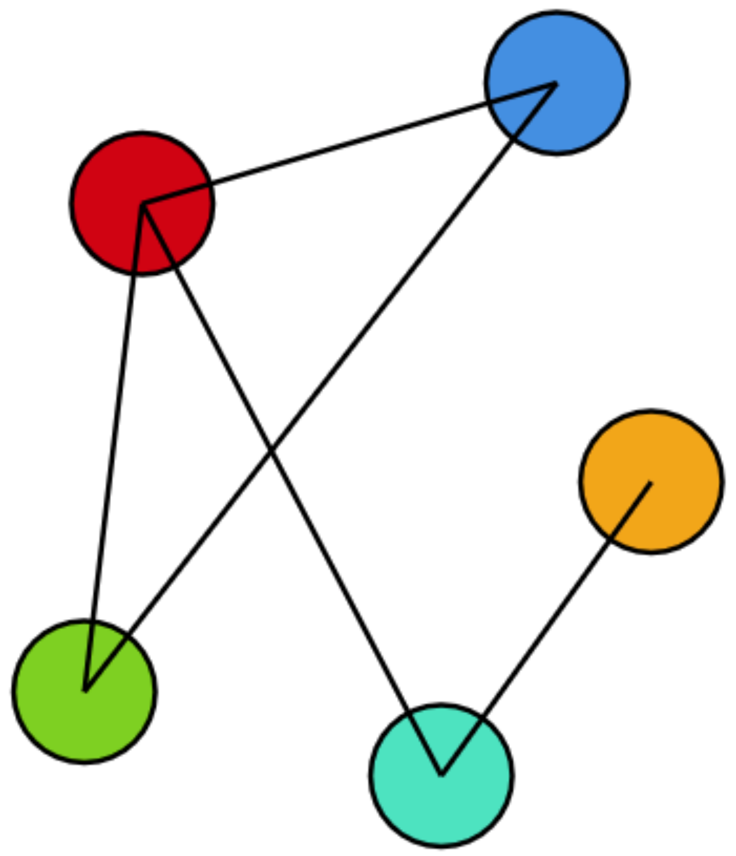

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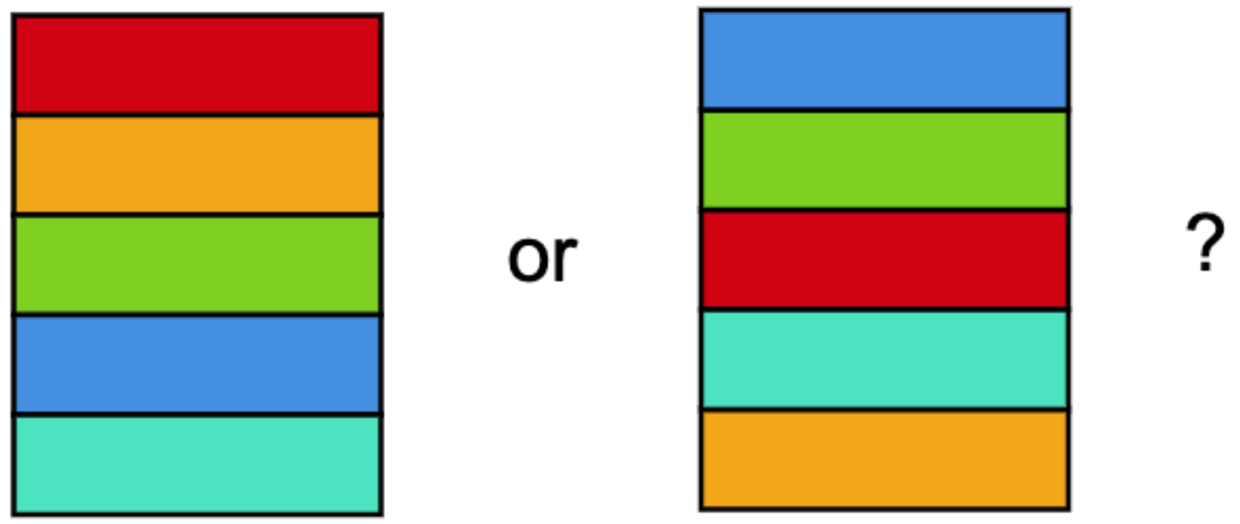

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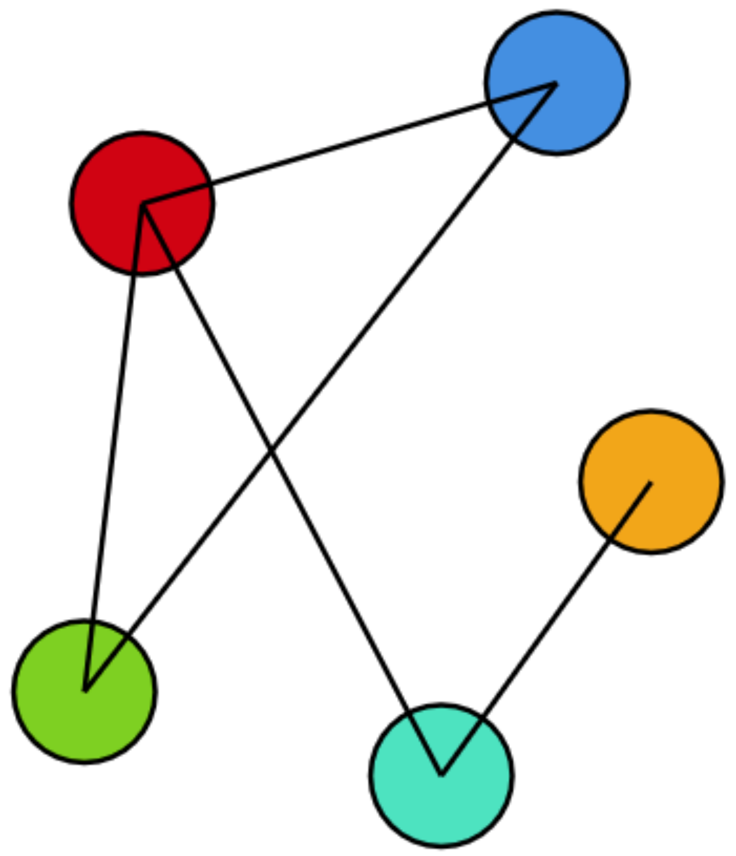

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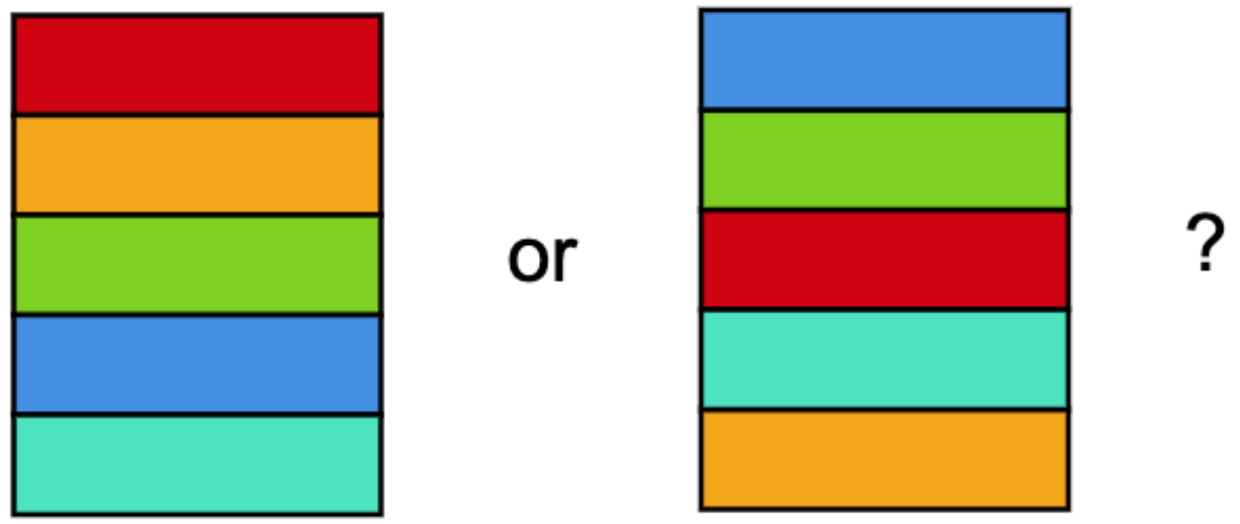

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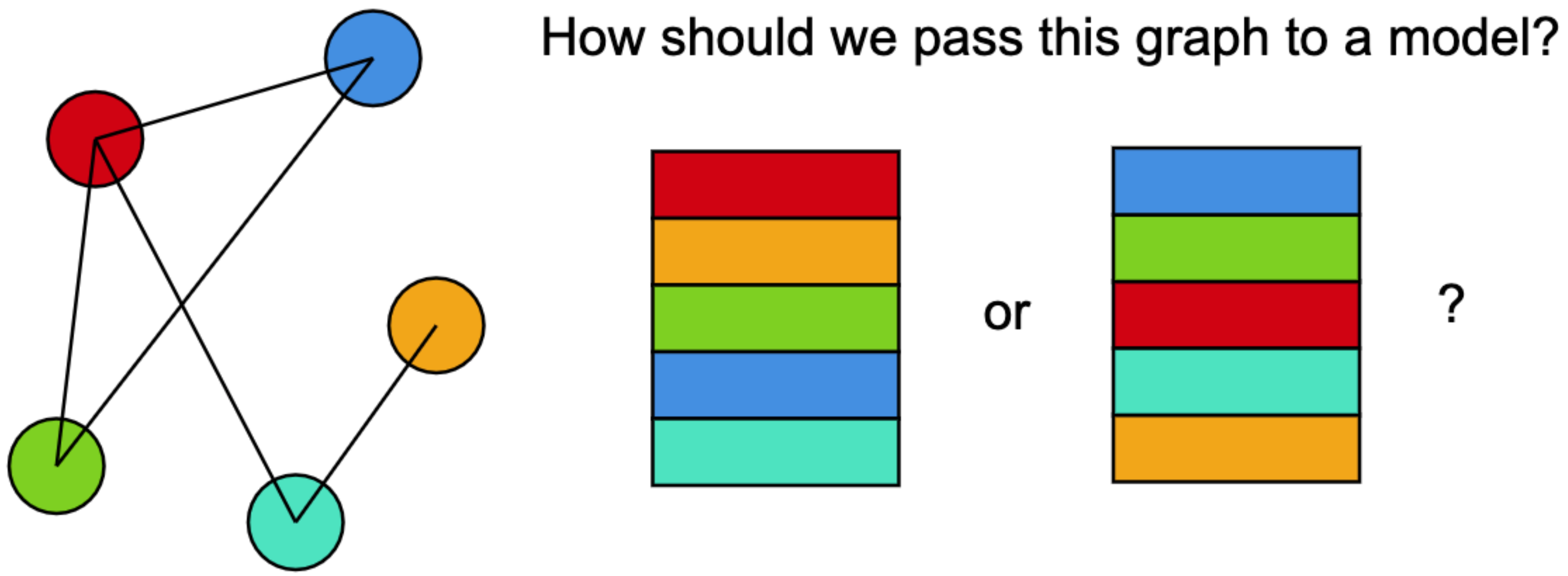

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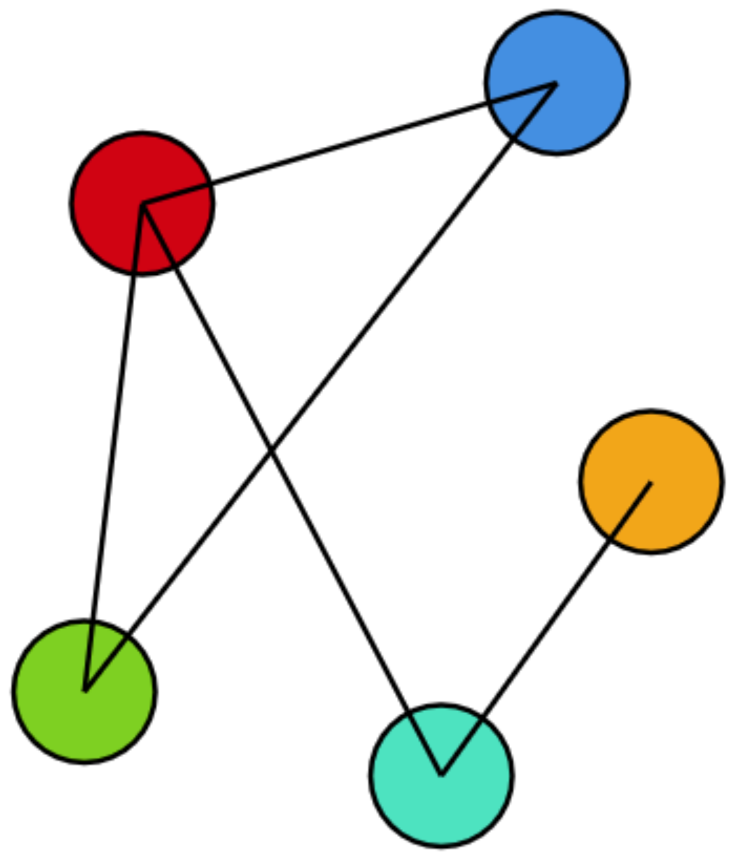

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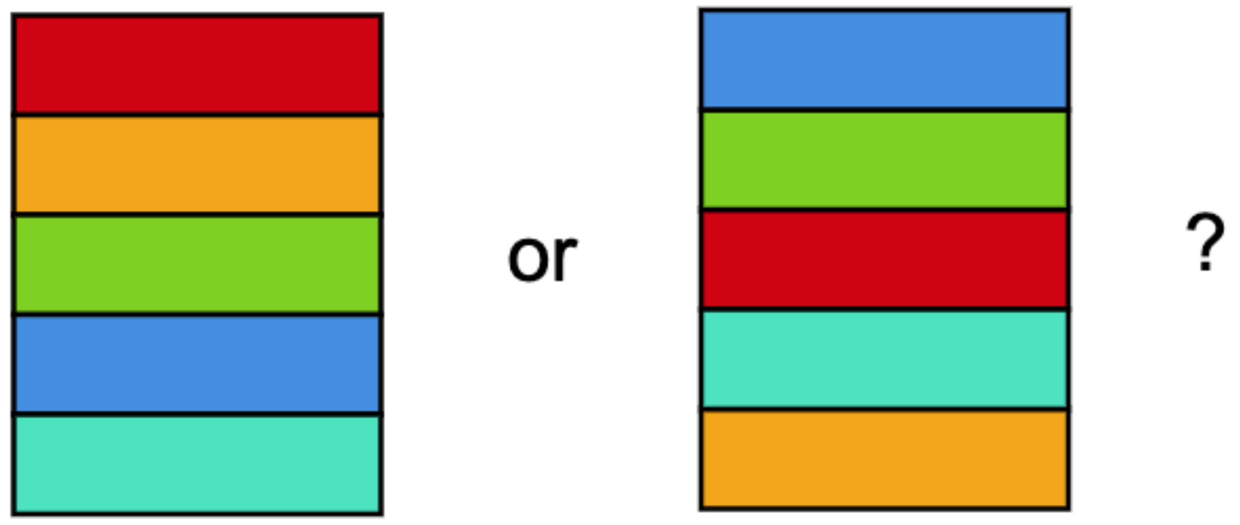

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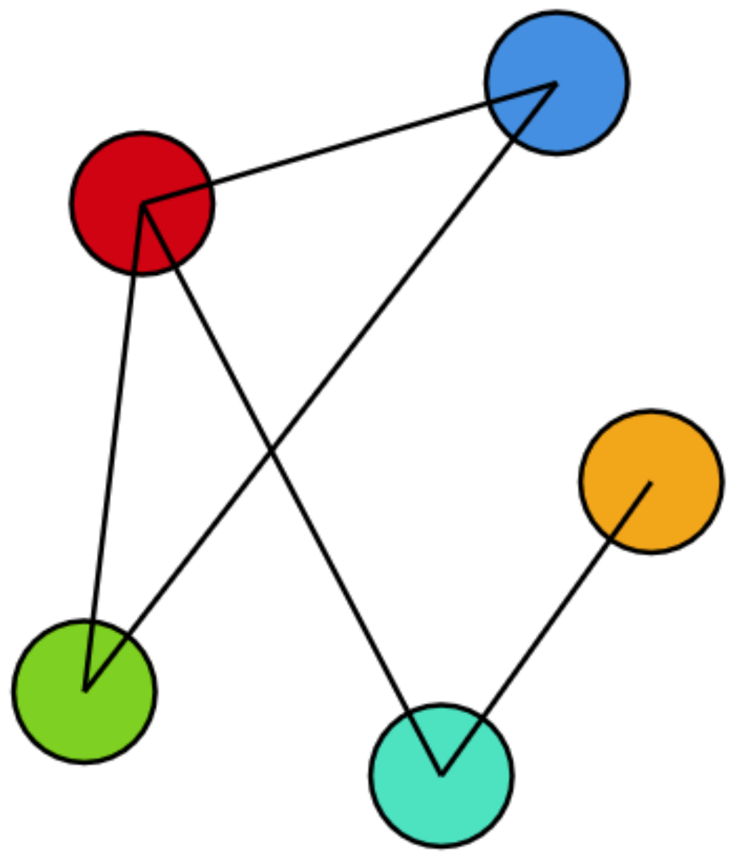

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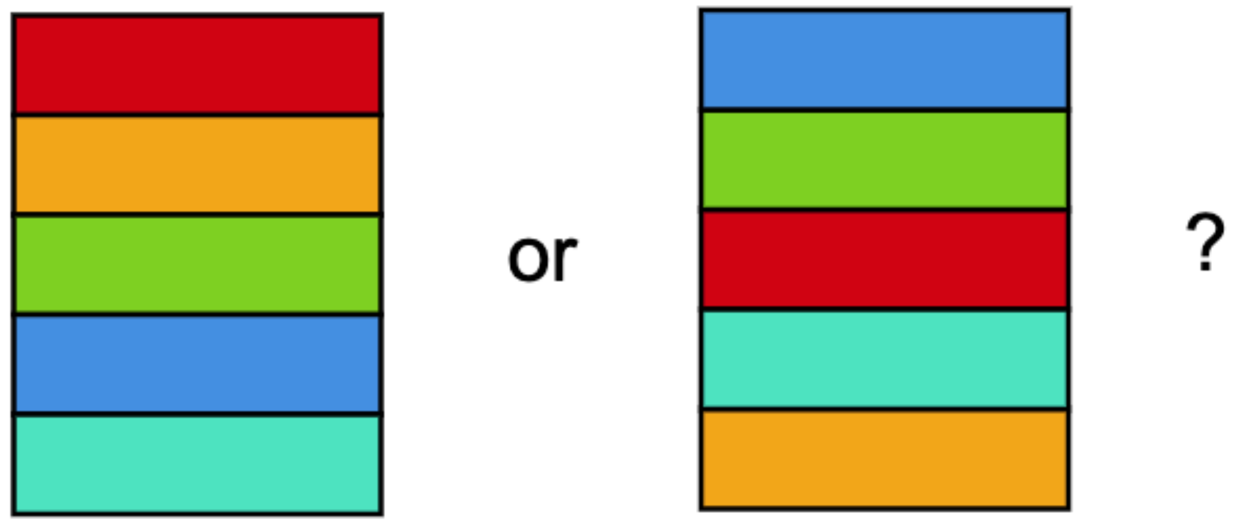

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(Can even exploit this relation to classical mechanics, and distill force laws - see M Cranmer et al., 2020)

For the ultimate book on geometry in deep learning, see geometricdeeplearning.com (Bronstein, Bruna, Cohen, Veličković)

Differential Equations - Neural ODEs

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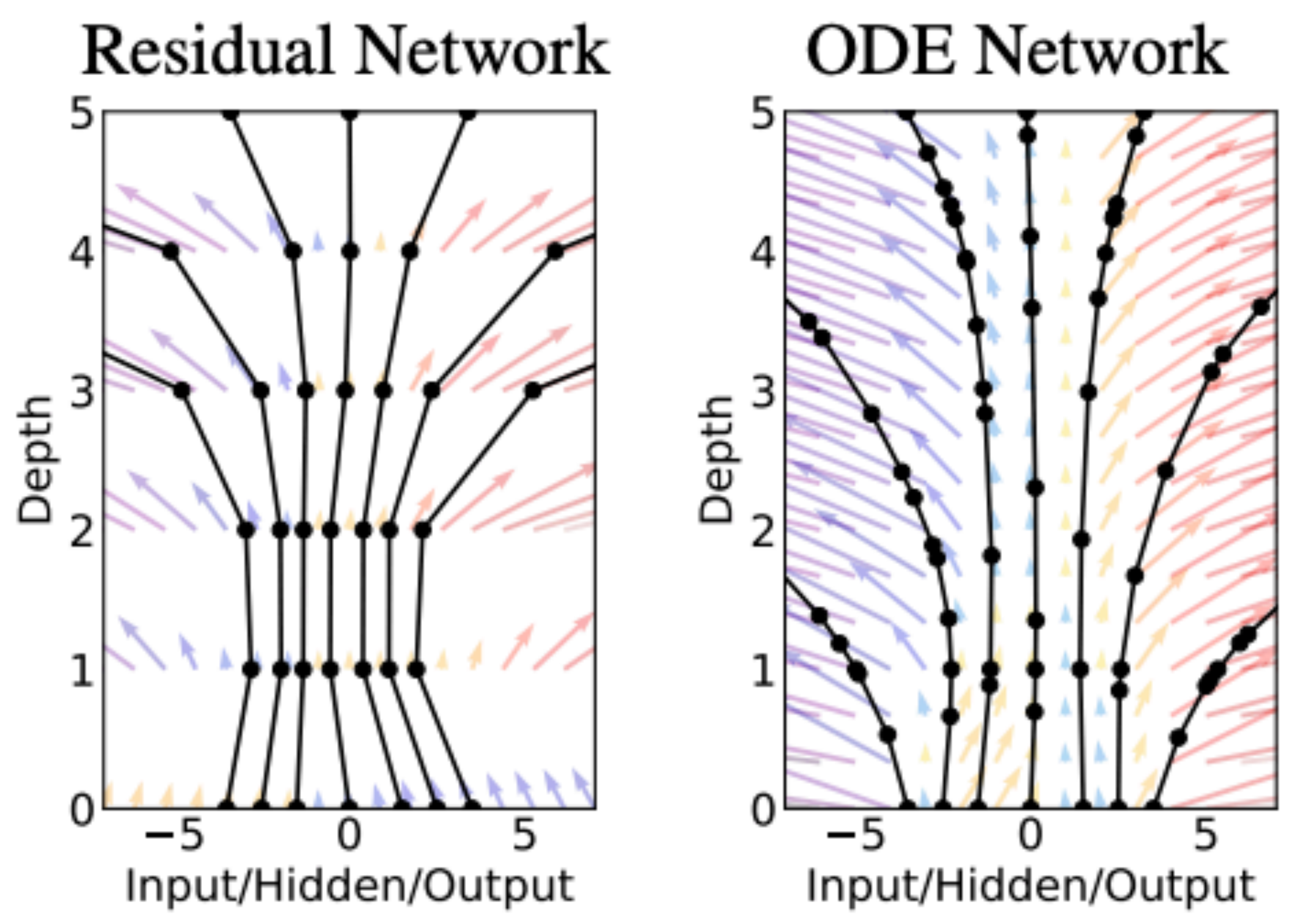

Figure 1: *Left:* A Residual network defines a discrete sequence of finite transformations. *Right:* A ODE network defines a vector field, which continuously transforms the state. *Both:* Circles represent evaluation locations.

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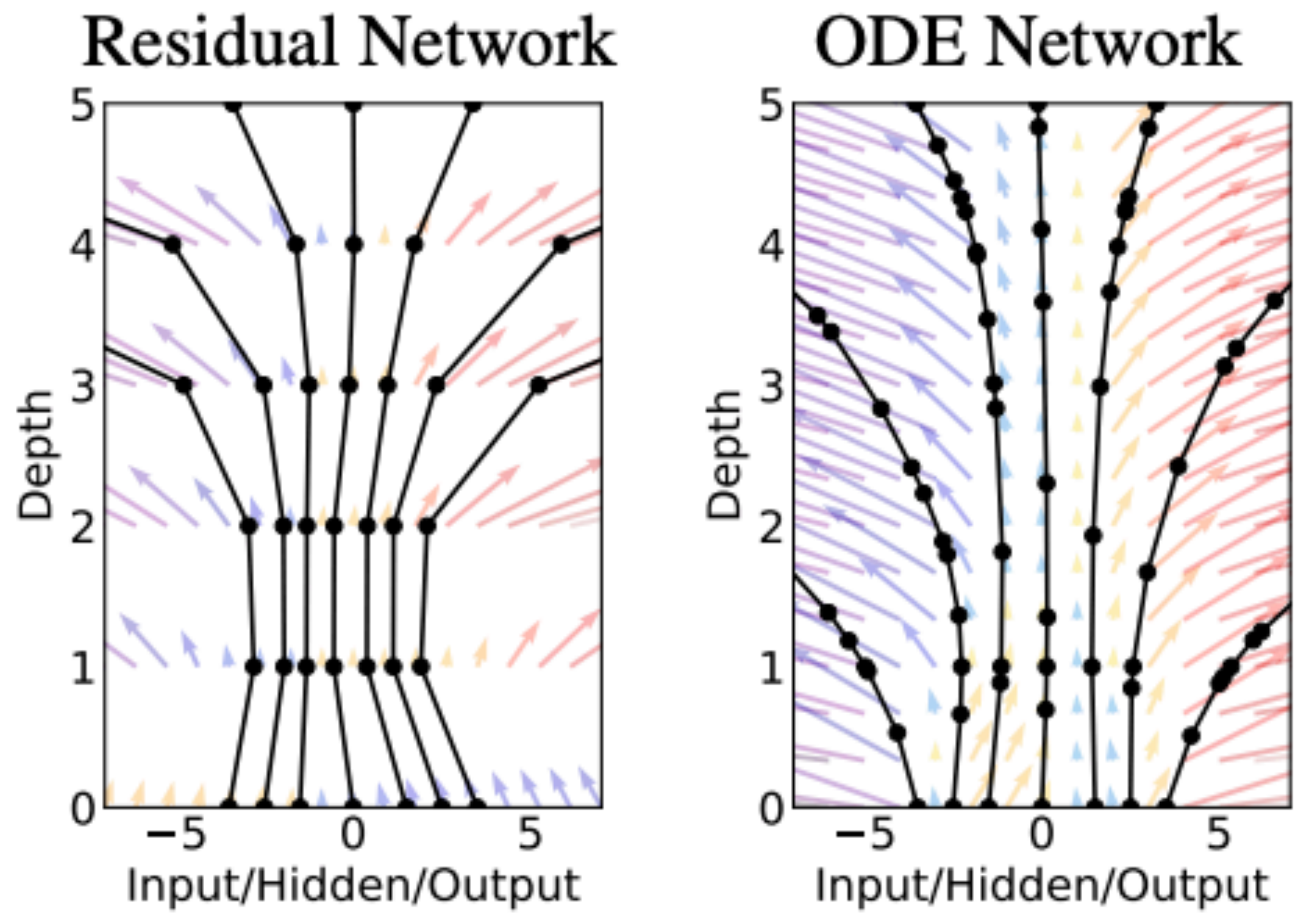
- With the obvious applicability to learning time series, can be applied to learning for general problems



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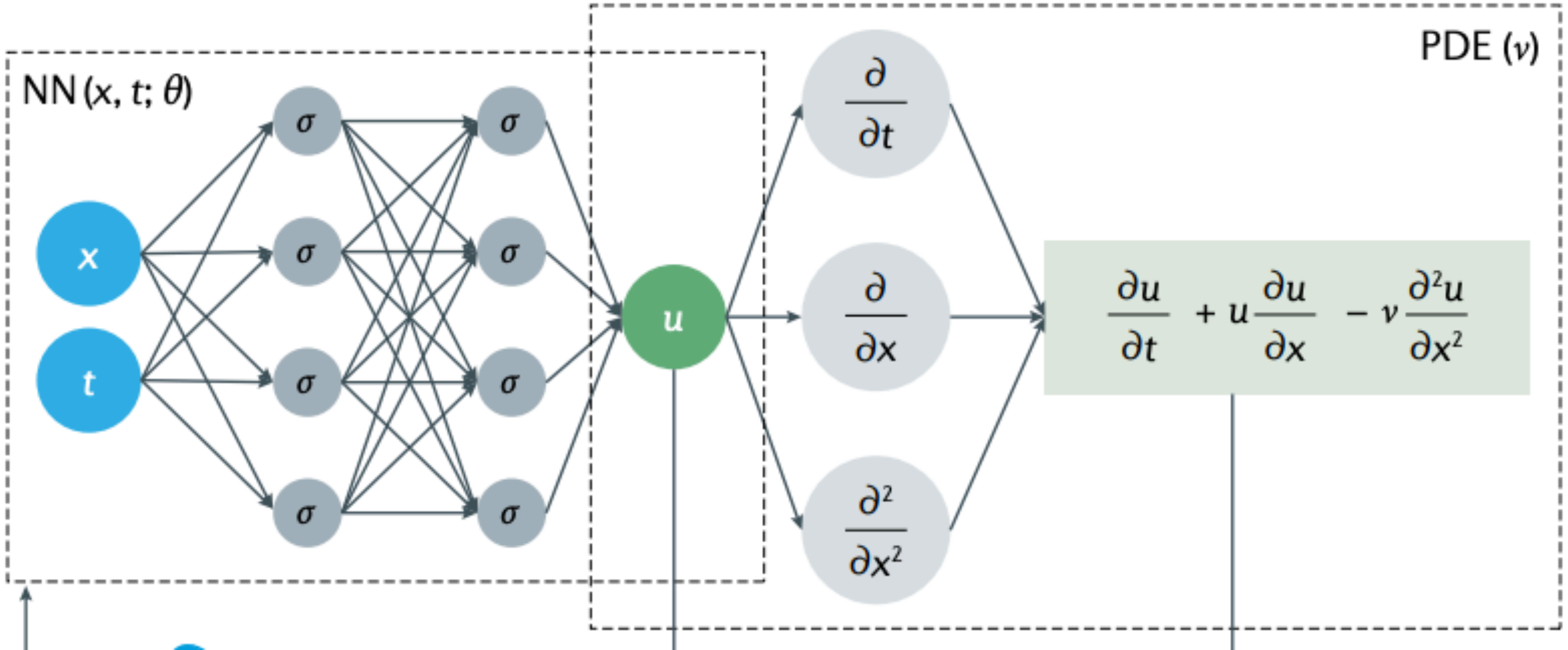
Truth: $\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = v\frac{\partial^2 u}{\partial x^2}$

Compute error in PDE



See Karniadakis, et al., (2021) for a good review.

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- For some inductive biases, hard constraints may be intractable to create. Soft constraints are useful when a symmetry might be slightly violated.

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  - e.g., large learning rates and small batch sizes define an implicit regularization term (e.g., Sam Smith et al., 2021 and references therein)
- Generally, it seems that making an inductive bias **explicit** in a formal framework, such as physics, leads to new insights, and allows one to use existing methods. Also allows one to control it.

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- Application-specific: an inductive bias created for a particular physical problem
  - For example, a PINN’s inductive bias is the ODE describing the underlying data; whereas some Neural ODE regularizations are very general (e.g., J Kelly et al., 2020 and C Finlay et al., 2020)

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Code tutorial

https://astroautomata.com/inductive_biases_tutorial.html