Machine Learning Physics

From Quantum Mechanics to Holographic Duality

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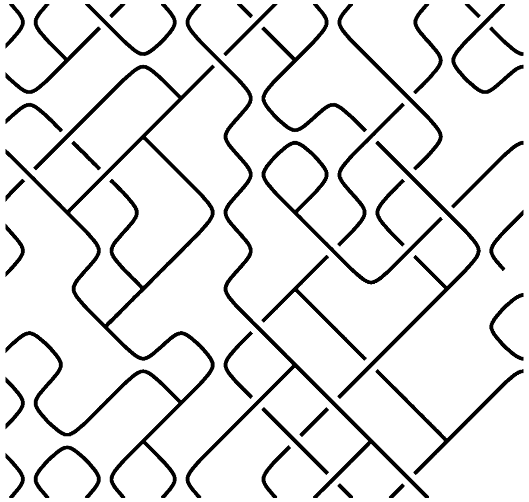
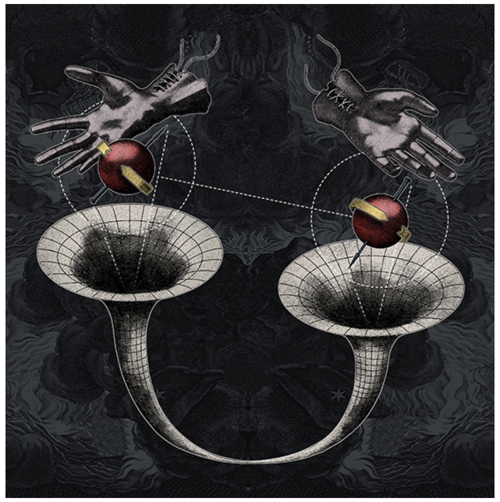
Machine Learning Physics

- Emergent phenomenon — a central theme of condensed matter physics.

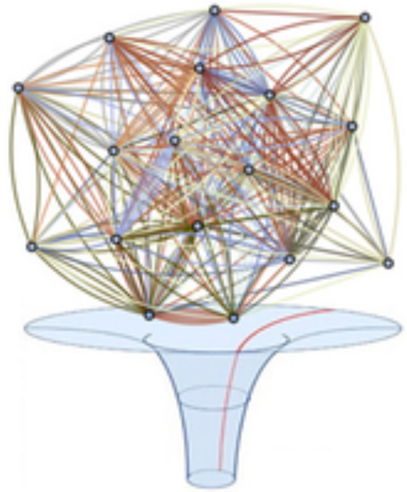
Weyl semimetal
(emergent particle)



String net condensation
(emergent force)



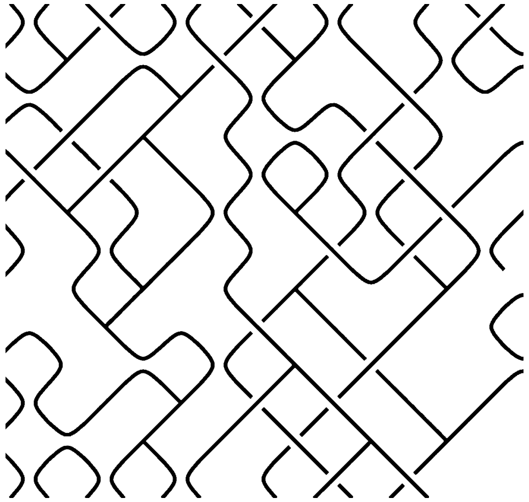
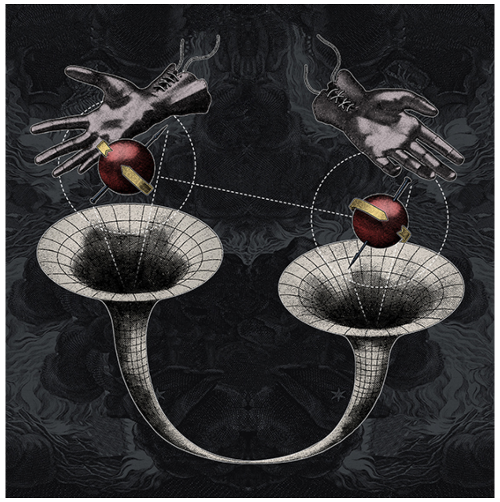
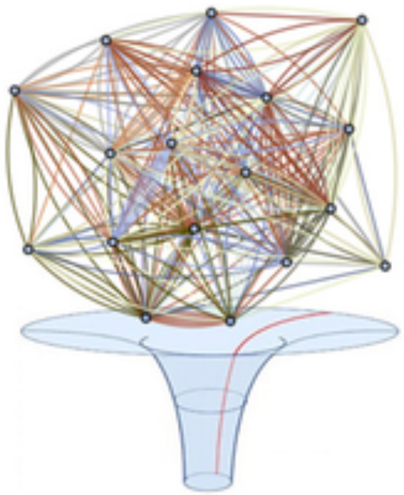
ER = EPR
(emergent spacetime)



SYK model
(emergent gravity)

Machine Learning Physics

- Aren't all these physics theories themselves also emergent phenomena?

Machine Learning Physics

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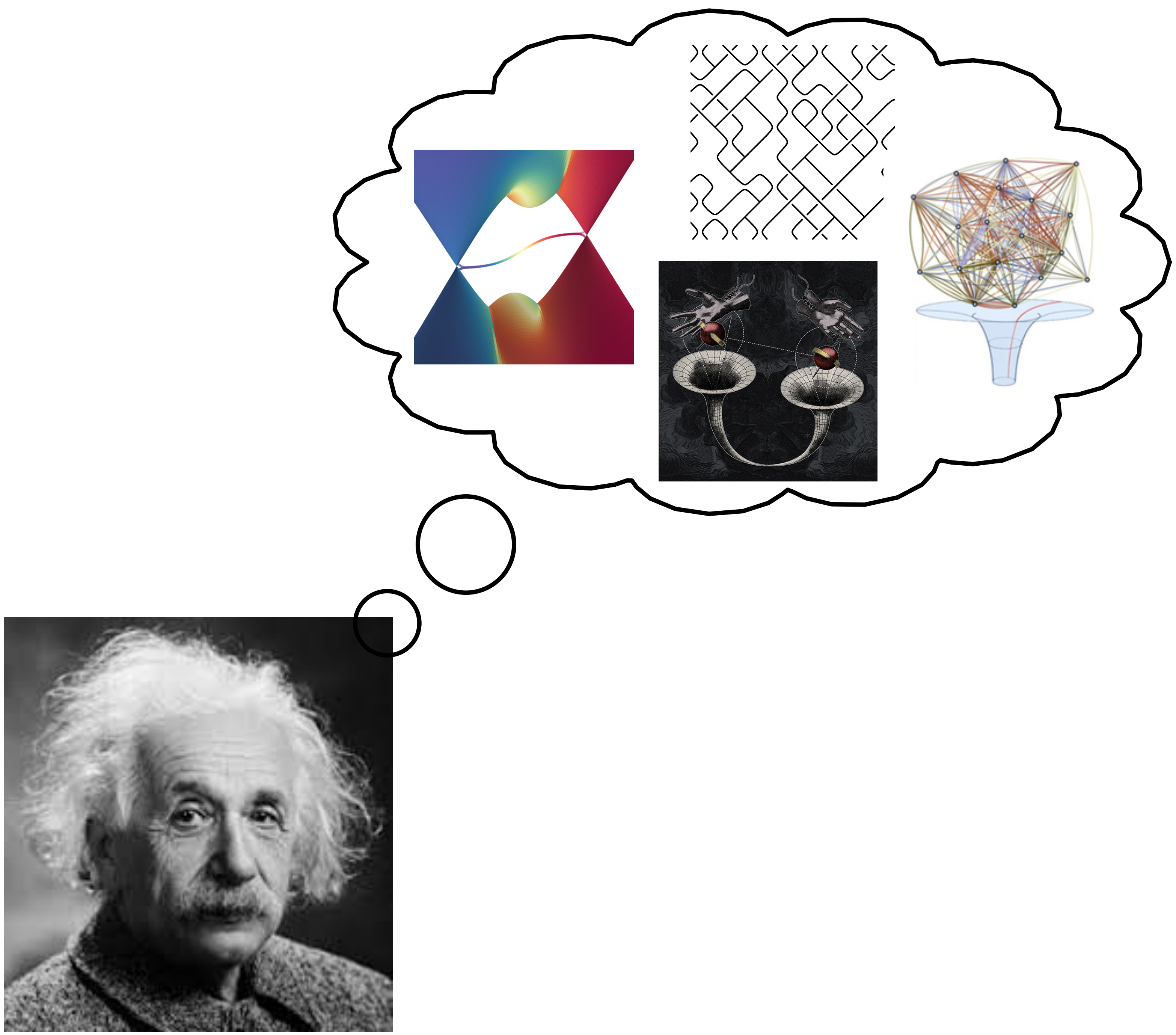

Machine Learning Physics

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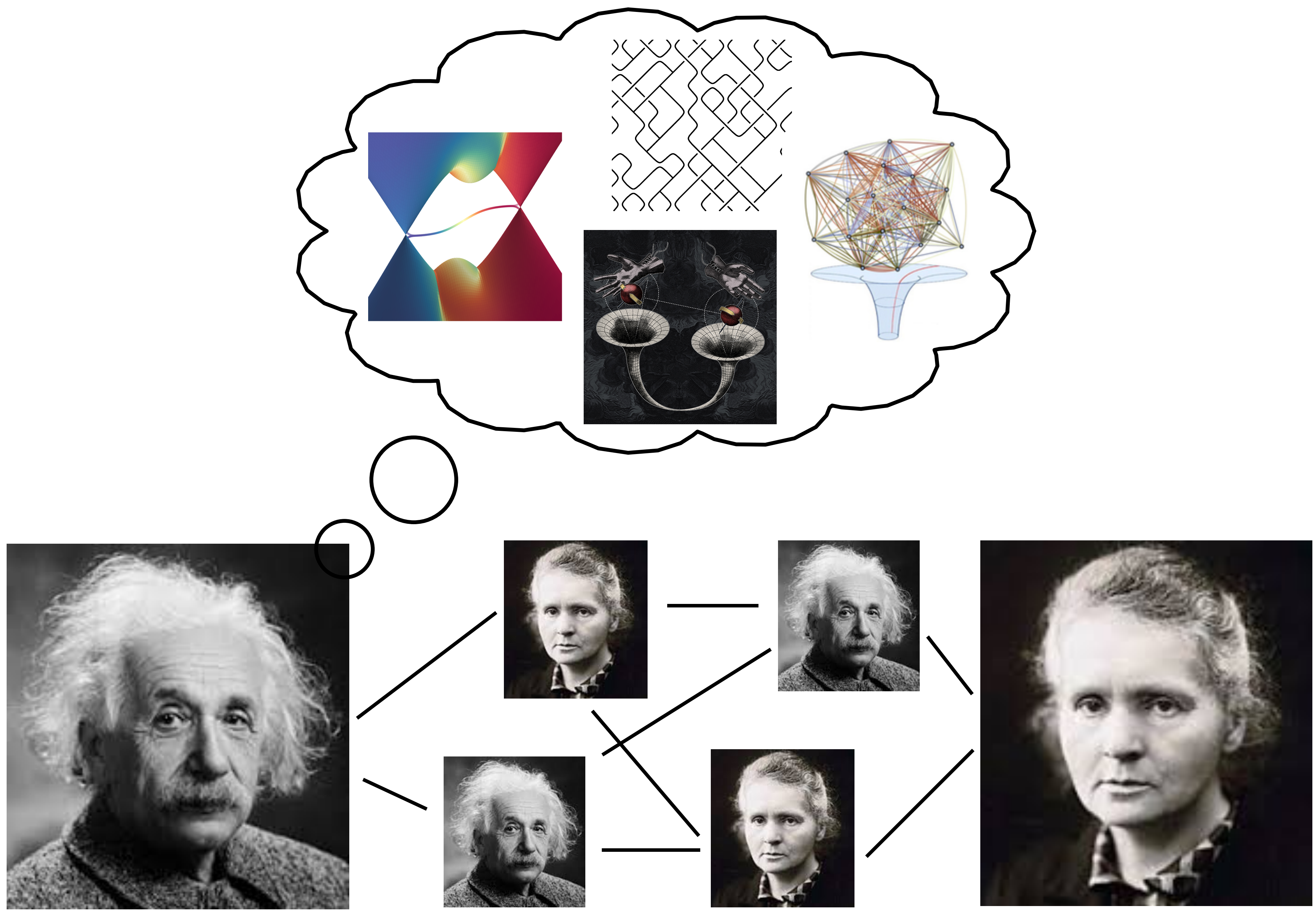
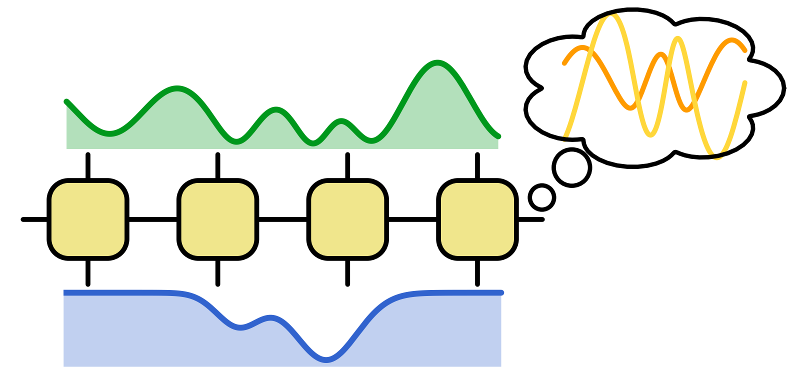


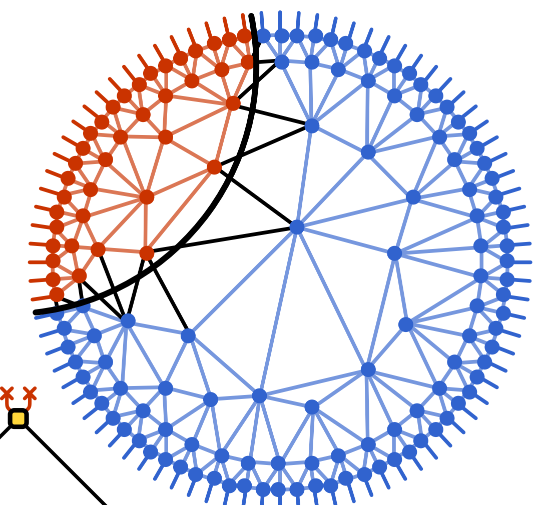
Machine Learning Physics

- Goal: investigate whether artificial neural networks can be used to discover physical concepts and laws from observation data.



- Examples
    - Machine learning quantum mechanics — recurrent autoencoder

      C Wang, H Zhai, Y-Z You. arXiv: 1901.11103

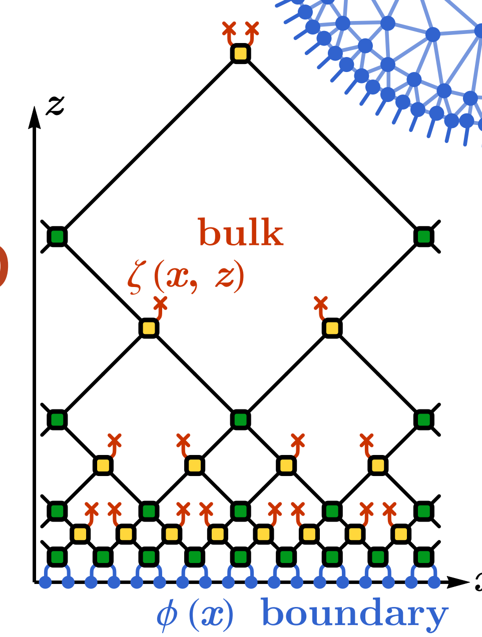


    - Machine learning holographic geometry — deep Boltzmann machine

      Y-Z You, Z Yang, X-L Qi. PRB 97, 045153 (2018)

    - Machine learning renormalization group — flow-based deep generative model

      H Hu, S-H Li, L Wang, Y-Z You. arXiv: 1903.00804



Machine Learning
Quantum Mechanics

Potential and Density Data

- Suppose quantum mechanics has not been formulated so far
- Yet, amazingly, we know how to perform cold atom experiments of Bose-Einstein condensate (BEC)

Potential profile
(optical speckles,
optical tweezers …)

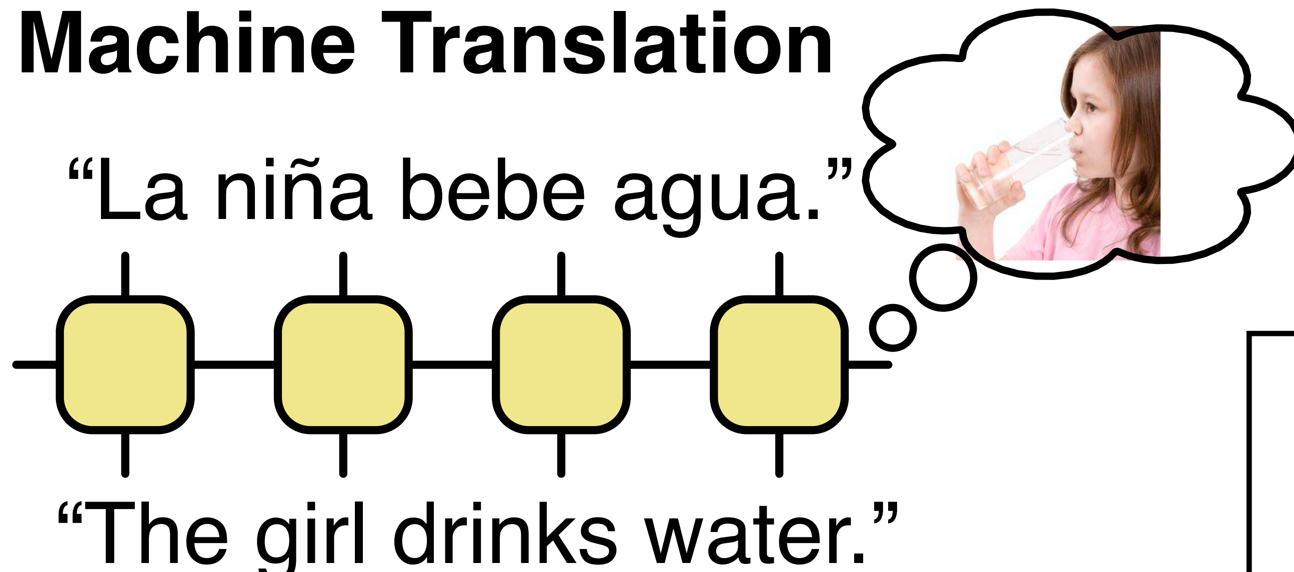
BEC Density profile
(in-situ measurement)

- Questions
  - Can quantum mechanics (QM) be discovered as the most natural theory to explain the experiment?
  - Will the machine develop alternative form of QM?

Inspiration from Machine Translation

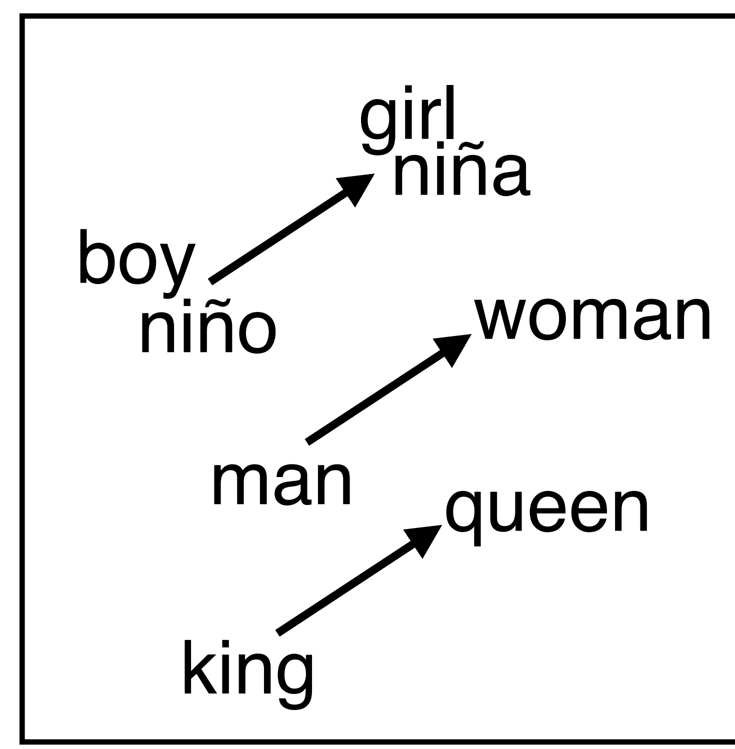
- Motivation: developments in machine translation
  - Sequence-to-sequence mapping (RNN, LSTM …)

Machine Translation



- Representation learning (word2vec …)

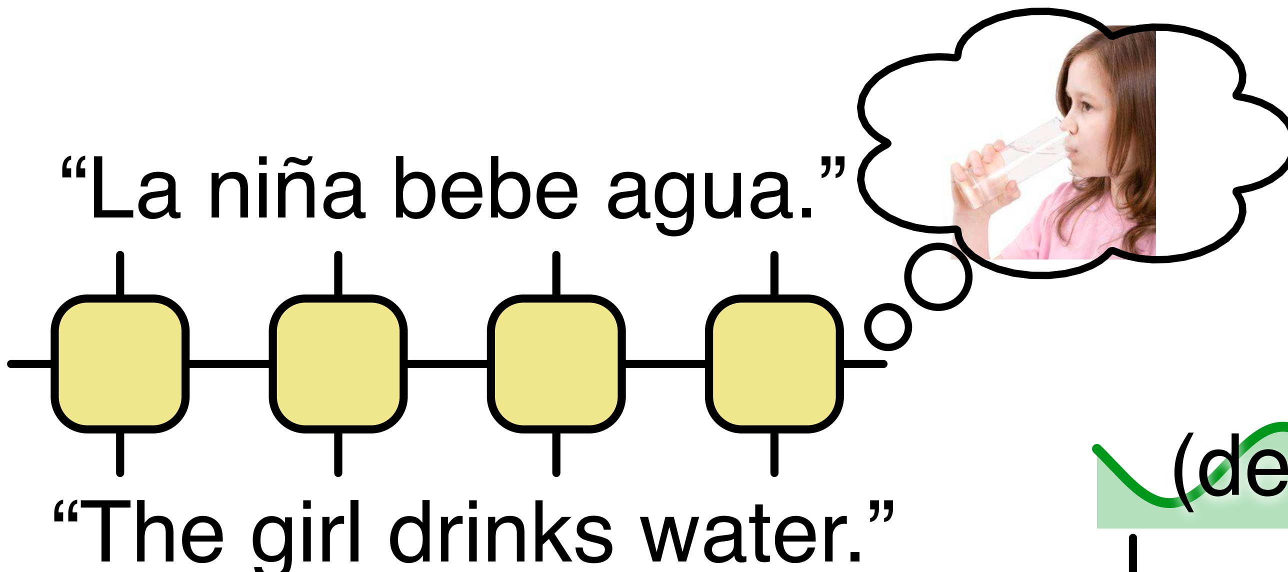
king – man + woman ≈ queen

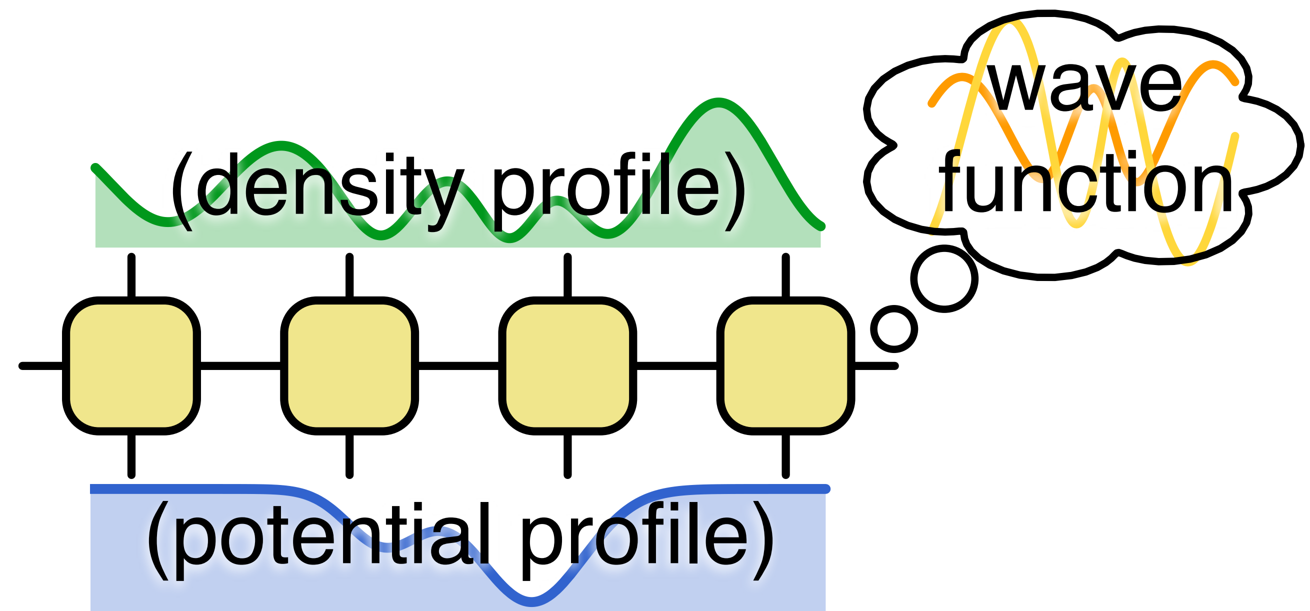


T Mikolov, SW Yih, G Zweig. NAACL-HLT-2013

Inspiration from Machine Translation

- Motivation: developments in machine translation
  - Train the neural network model to perform a task
  - Discover concepts and relations in representation space

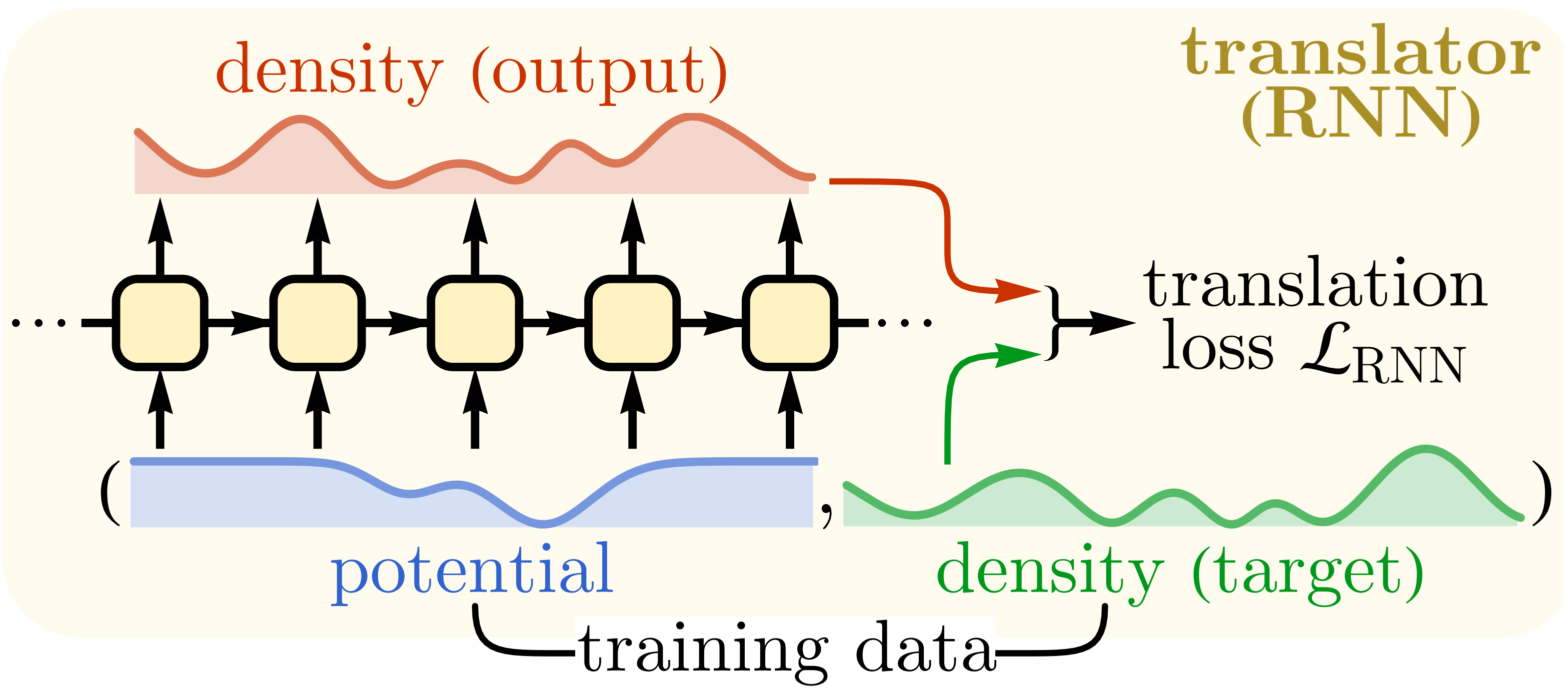


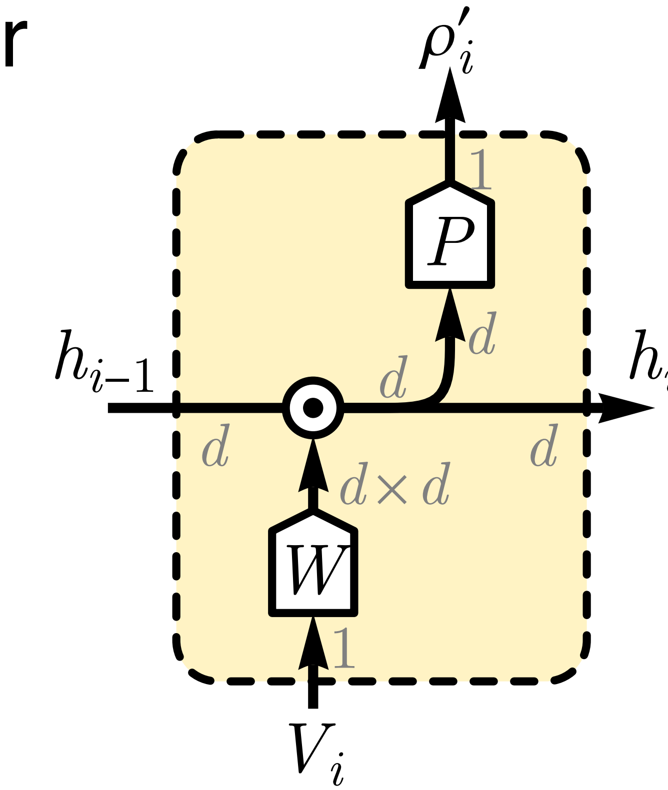


- **Task**: potential-to-density mapping
- **Latent variables**: wave function?

Potential-to-Density Translator

- Recurrent neural network (RNN) translator

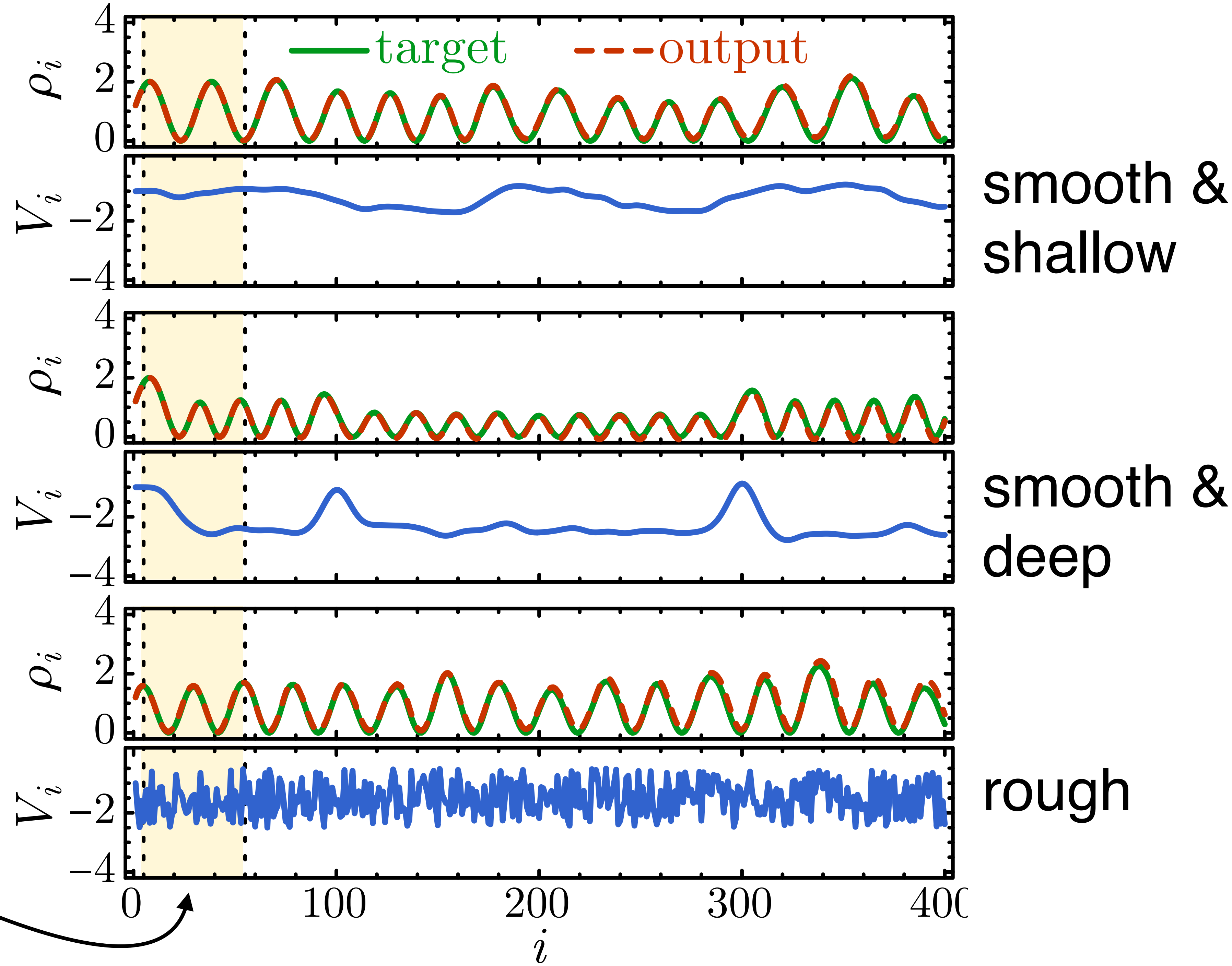




  - Discretize the 1D space, collect training data by simulation
  - Input: potential sequence V_i
  - Update: hidden state $h_i = W(V_i) \cdot h_{i-1}$
  - Output: density sequence $\rho'_i = P(h_i)$
  - Minimize translation loss $\mathcal{L}_{\text{RNN}} = \sum_{i \in \text{window}} (\rho'_i - \rho_i)^2$

Performance of the Translator

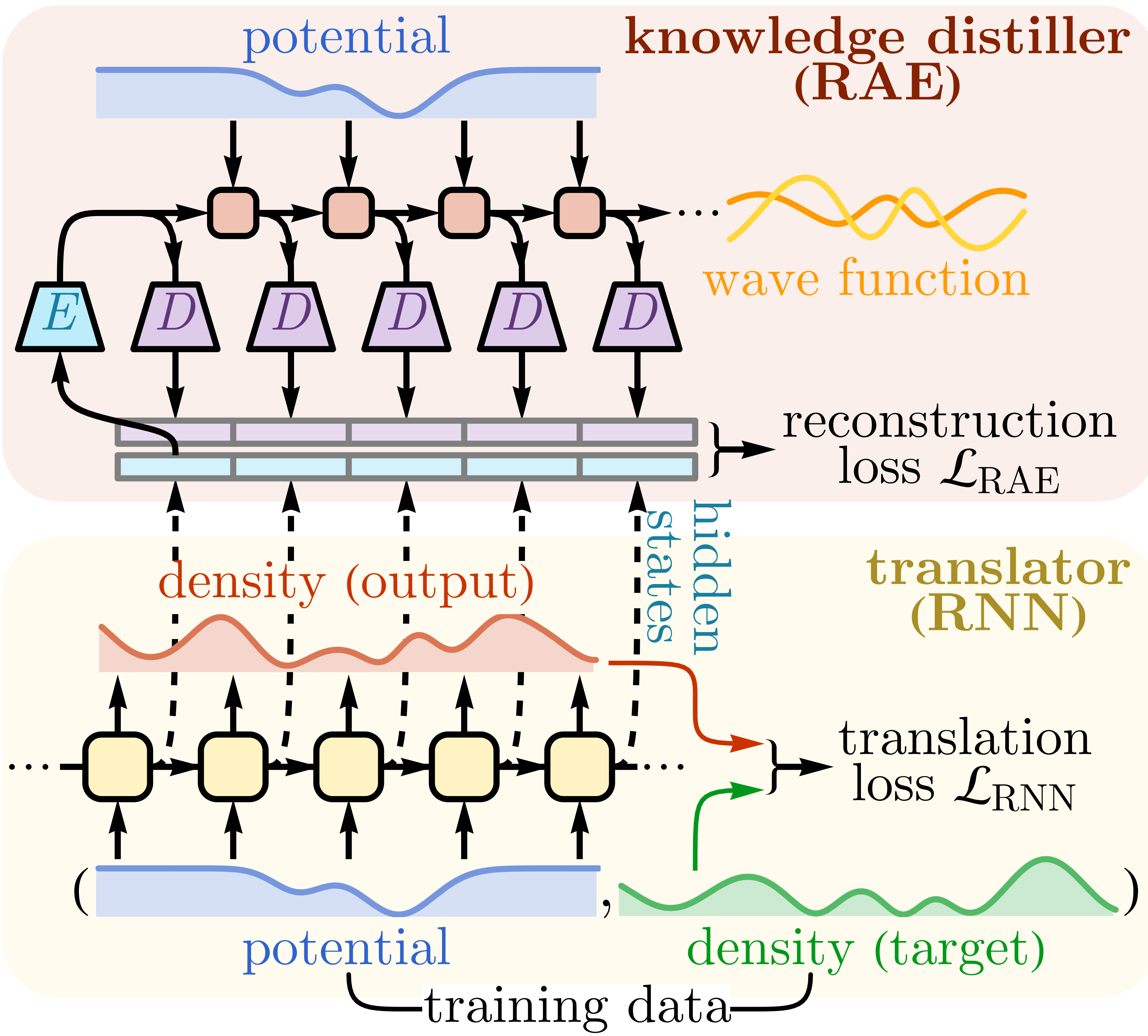
- Performance of the RNN translator



Trained over window of 50

Introspective Learning

- Introspective Learning

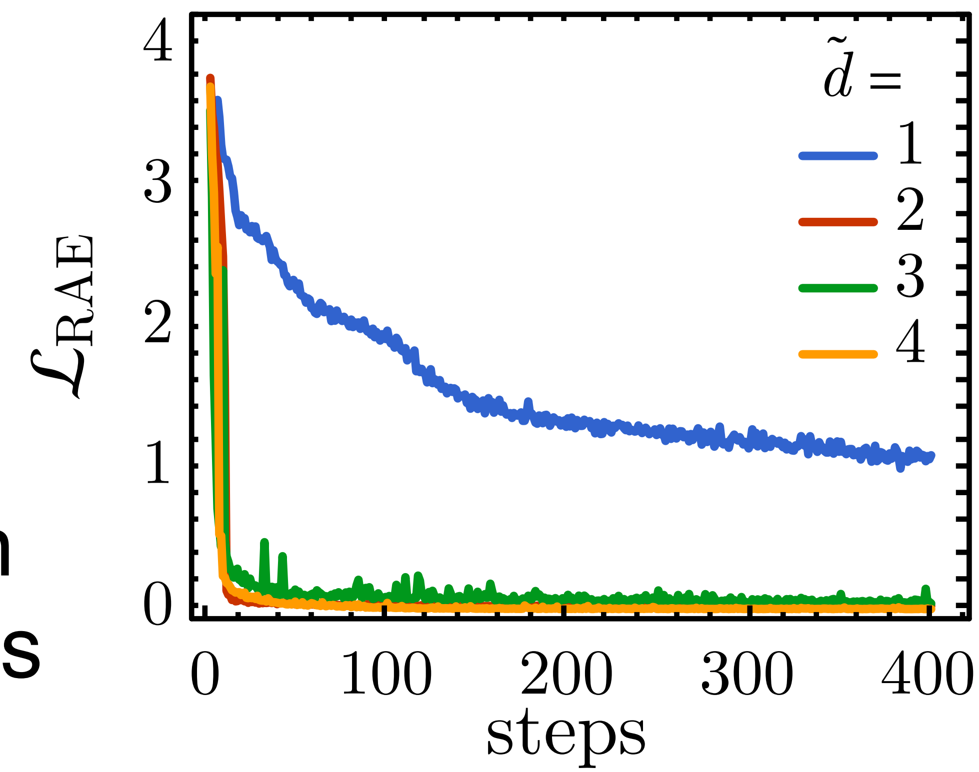


High-level machine only interface with the neural activation of the low-level machine

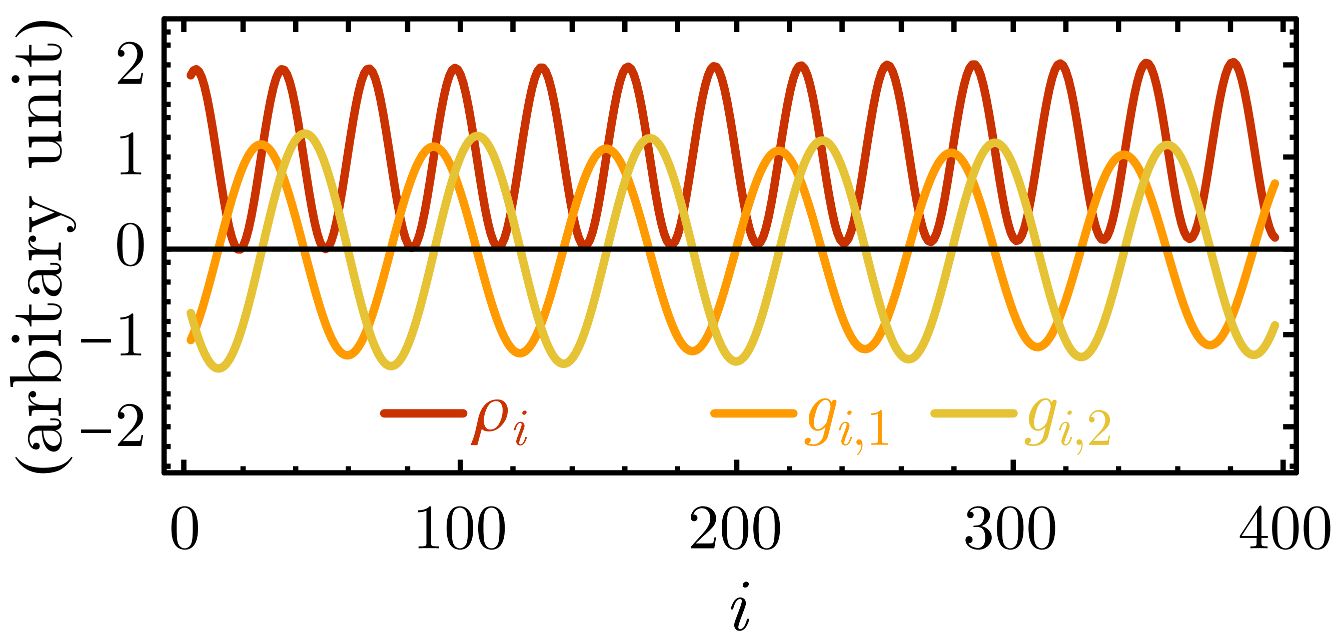
Low-level machine deal with training / experimental data

Emergent Quantum Mechanics

- Imposing information bottleneck
  - Squeezing the latent space dim
  - Monitor the reconstruction loss of the knowledge distiller
  - Abrupt increase of loss only when latent dim < 2 ⇒ two real variables



- Quantum wave function and its 1st order derivative



Update rules

$$\begin{bmatrix} g_{i+1,1} \\ g_{i+1,2} \end{bmatrix} = \begin{bmatrix} 1 & a \\ aV_i & 1 \end{bmatrix} \begin{bmatrix} g_{i,1} \\ g_{i,2} \end{bmatrix}$$

matching Schrödinger Eq.

$$\partial_x^2 \psi(x) = V(x)\psi(x)$$

Alternative Forms of Quantum Mechanics

- If we relax the information bottle neck → alternative forms of quantum machines can also emerge, e.g.

$$\partial_x \begin{bmatrix} \rho(x) \\ \rho'(x) \\ \rho''(x) \end{bmatrix} = \begin{bmatrix} 0 & 2 & 0 \\ V(x) & 0 & 1 \\ 0 & 2V(x) & 0 \end{bmatrix} \begin{bmatrix} \rho(x) \\ \rho'(x) \\ \rho''(x) \end{bmatrix}$$

  - Hidden variables: density $\rho(x) = |\psi(x)|^2$ and derivatives
  - In spirit of density functional theory
  - But requires at least three real variables

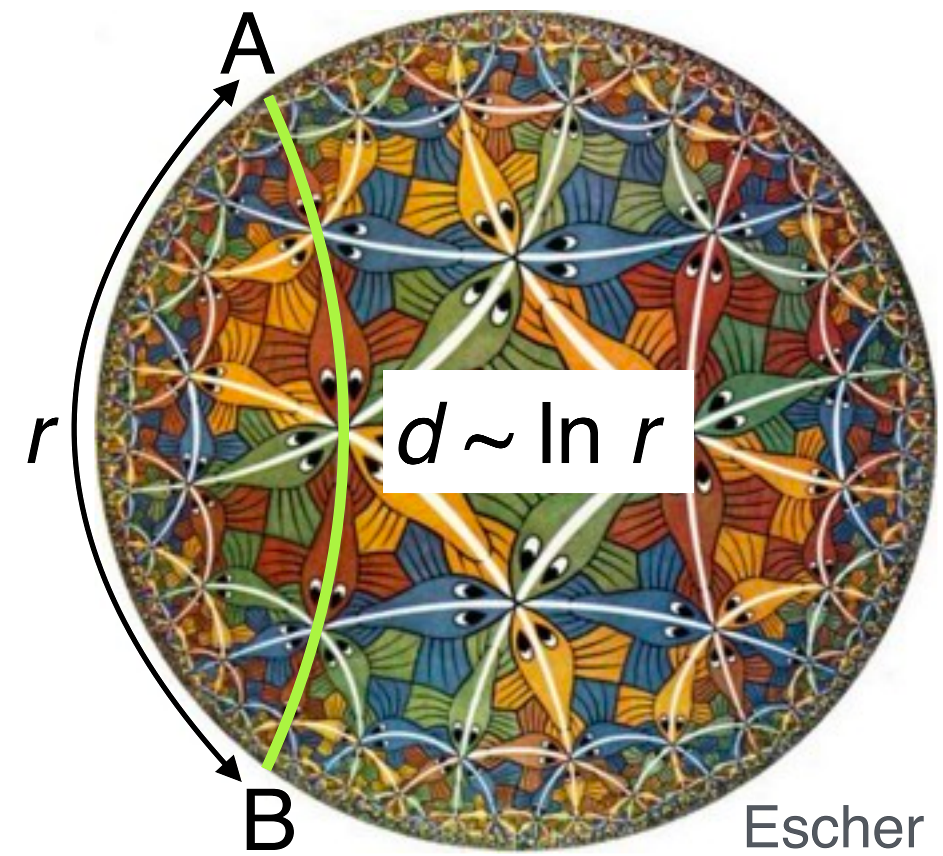
- Wave function + Schrödinger equation formulation of QM is indeed the most parsimonious theory that have emerged in our neural network.

Machine Learning Holography

Holographic Duality

Maldacena 97; Witten 98; Gubser, Klebanov, Polyakov 98

- Holographic Duality (AdS/CFT)
  - Conformal field theory (CFT)
    scale-free, critical, gapless
    $$\langle \phi_A \phi_B \rangle \sim r_{AB}^{-\alpha} \quad \text{(power-law)}$$
  - Anti-de Sitter (AdS) space
    negative curvature, tree network
    $$\langle \zeta_A \zeta_B \rangle \sim e^{-d_{AB}/\xi_{\text{blk}}} \sim r_{AB}^{-\alpha}$$
- Extra dimension: RG scale
- Mass deformation away from CFT
  - IR region capped off at $z_{\text{cut}} \sim \ln \xi_{\text{bdy}} = -\ln m$
  - Correlation decays exponentially
    $$\langle \zeta_A \zeta_B \rangle \sim e^{-d_{AB}/\xi_{\text{blk}}} \sim e^{-r_{AB}/\xi_{\text{bdy}}}$$



Escher

Holographic Duality

Maldacena 97; Witten 98; Gubser, Klebanov, Polyakov 98

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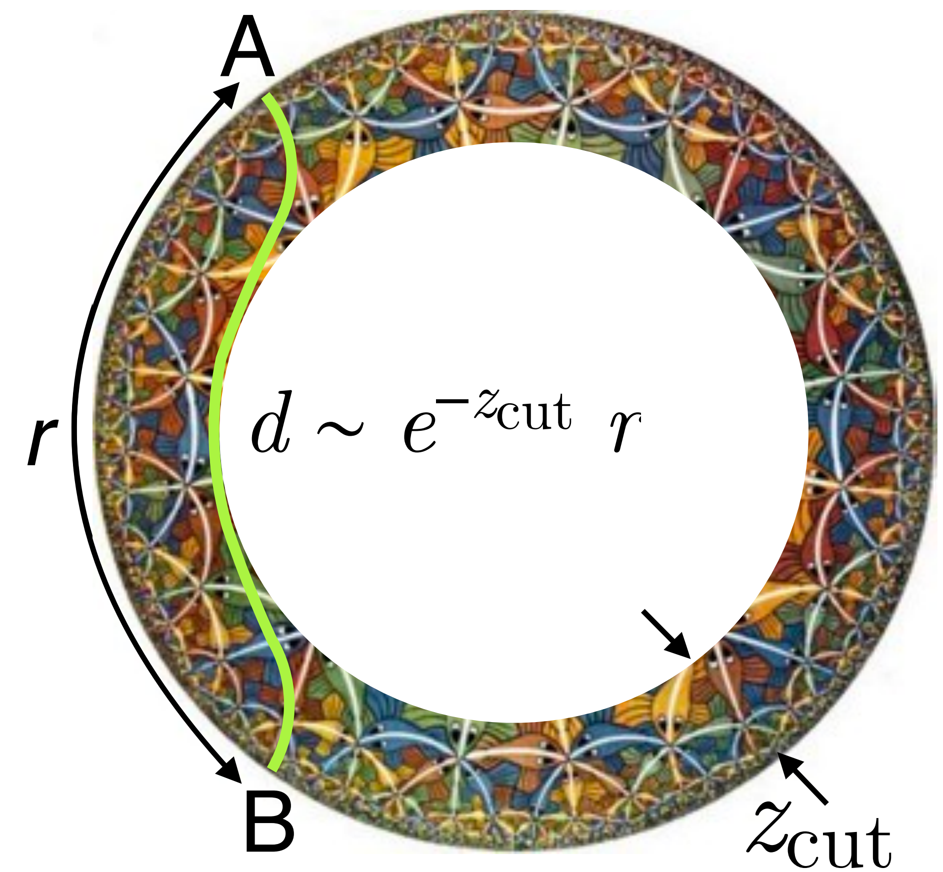
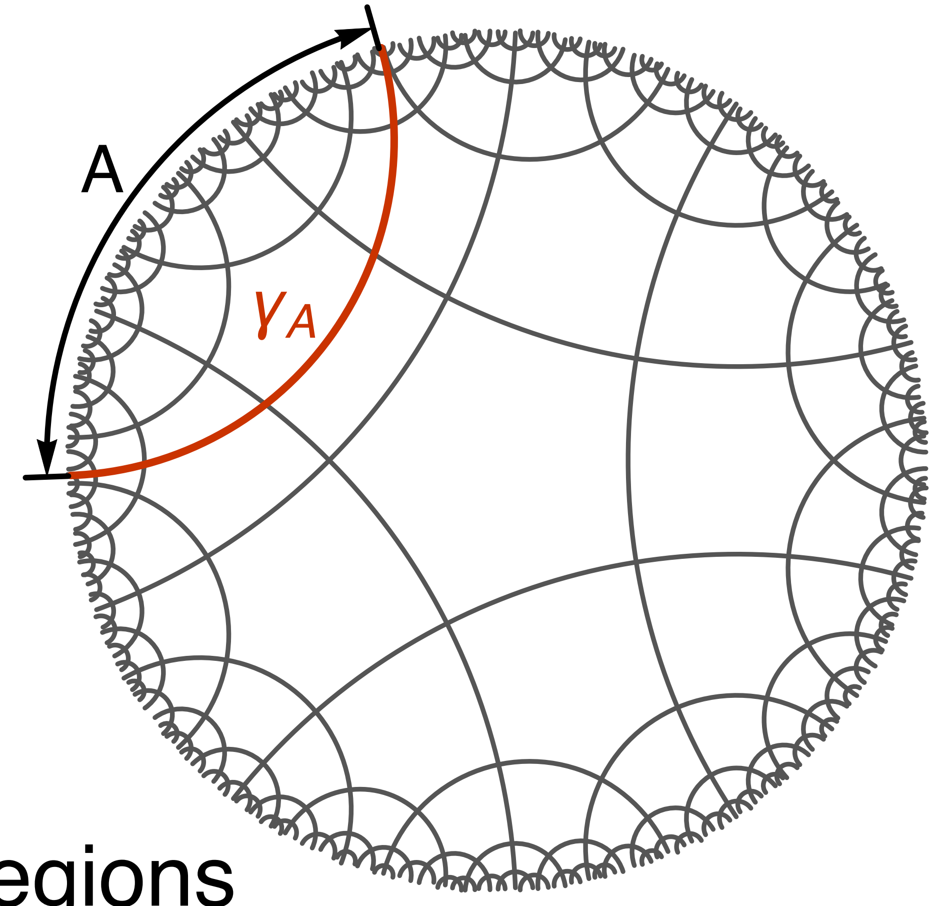


Entanglement and Geometry

- One prominent feature of holographic duality is the deep relation between:
  - Boundary quantum entanglement structure
  - Bulk spatial geometry structure
- Entanglement entropy = minimal cut

$$S_E(A) = \frac{1}{4G_N}|\gamma_A|$$

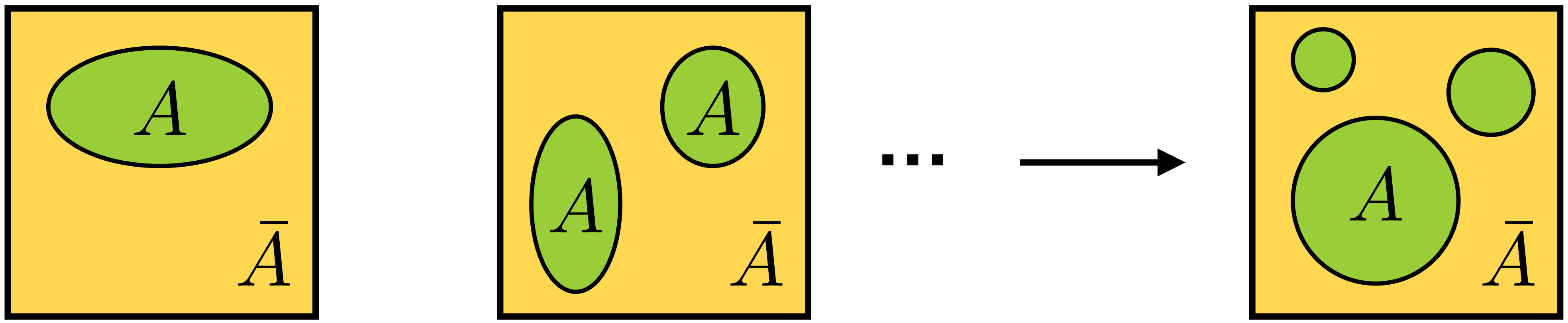
Ryu, Takayanagi (2006)



- Geometry is encoded in $S_E(A)$ data
- Task: predict $S_E(A)$ over different regions using a neural network model (that represents the geometry)
- Bulk geometry will emerge as training builds up the network

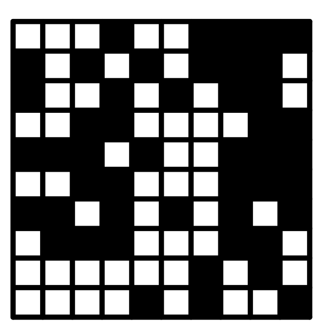
Entanglement Feature Learning

- Task: predict entanglement entropy for different regions



$S_E(A) = 2.8\text{bit}$ $S_E(A) = 3.5\text{bit}$ $S_E(A) = ?$

- How to formulate this problem?
  - Specify the entanglement region by an Ising configuration
  - Treat the entanglement entropy as an energy associated to the Ising configuration

$A \to [\tau] =$ 

$S_E(A) \to F[\tau]$

Entanglement Big Data

- How many different choice of region A?
  - A system of N sites → 2^N choices of $[\tau] = (\tau_1, \tau_2, \cdots)$

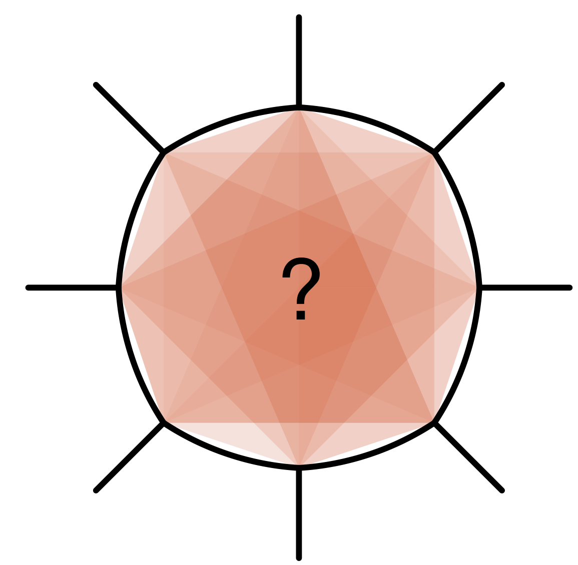
$$\tau_i = \begin{cases} +1 & i \in A \\ -1 & i \in \bar{A} \end{cases}$$

(like Ising variables)

  - Each Ising configuration (entanglement region) is associated with an entanglement entropy → big data…
- A naive energy-based model (generally non-local!)

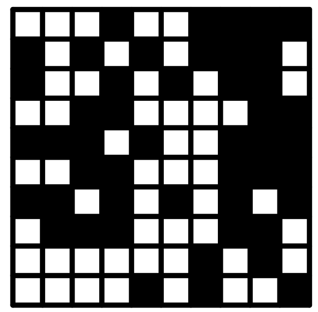
$$S_E(A) = F[\tau] = S_0 - \sum_{ij} J_{ij}\tau_i\tau_j - \sum_{ijkl} J_{ijkl}\tau_i\tau_j\tau_k\tau_l + \cdots$$

- Multi-spin interaction in the Ising model reflects the non-local structure of many-body entanglement



Deep Boltzmann Machine

- How do we decode the structure behind this Ising model of quantum many-body entanglement?

$$A \rightarrow [\tau] =$$  $$P[\tau] \propto e^{-F[\tau]} = e^{-S_E(A)}$$

- **Machine learning**: how do we represent a complicated joint probability distribution of pixels in an image dataset?
  - We train a generative model …

Deep Boltzmann Machine

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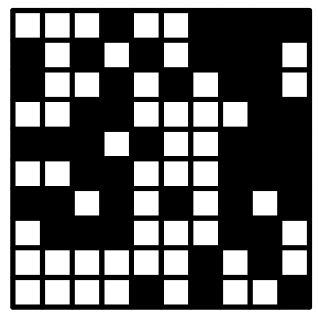
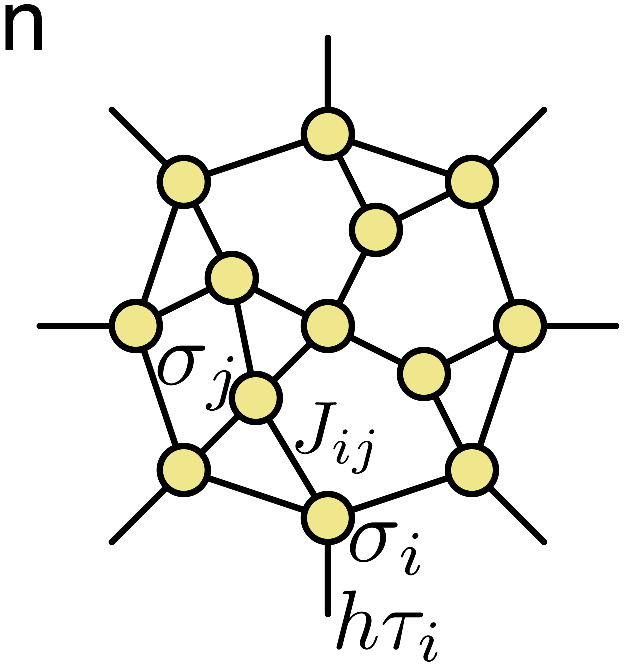
$$A \to [\tau] =$$  $$P[\tau] \propto e^{-F[\tau]} = e^{-S_E(A)}$$

- **Machine learning**: how do we represent a complicated joint probability distribution of pixels in an image dataset?
  - In particular, we can train a deep Boltzmann machine by introducing hidden neurons σ_i

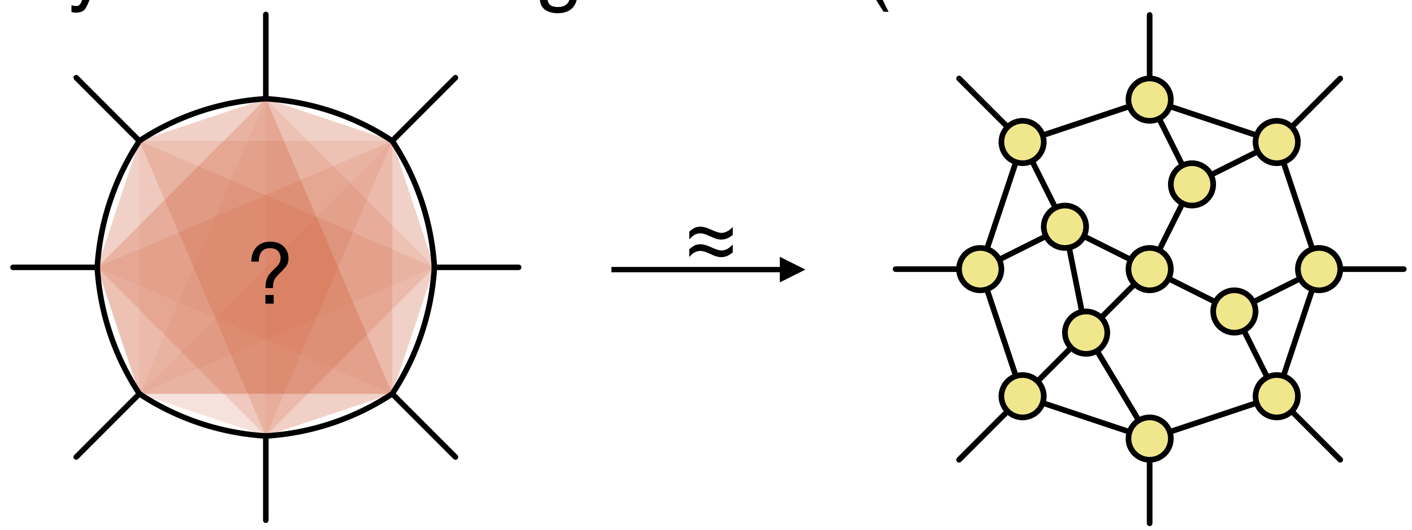


$$e^{-F[\tau]} = \sum\nolimits_{[\sigma]} e^{-E[\sigma,\tau]}$$

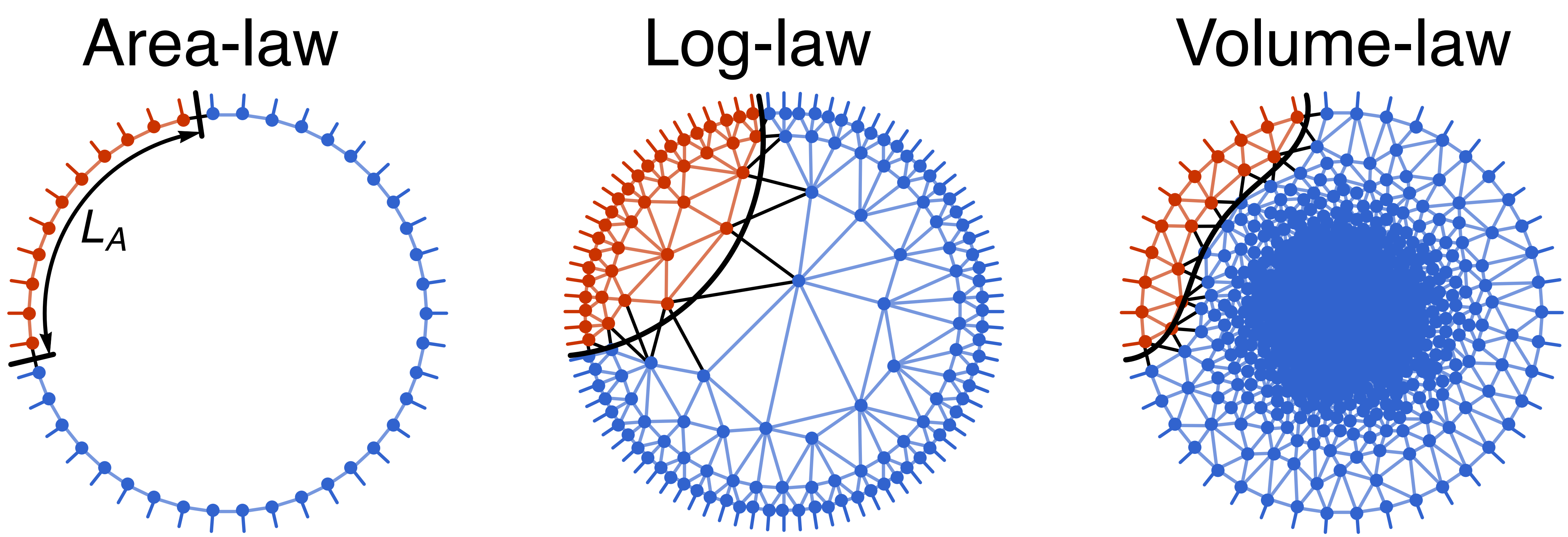
$$E[\sigma, \tau] = -\sum_{\langle ij \rangle} J_{ij}\sigma_i\sigma_j - \sum_{i \in \partial} h\tau_i\sigma_i$$

Holographic Duality

- Resolve the non-local entanglement structure on the boundary by a local Ising model (neural network) in the bulk.



You, Yang, Qi
arXiv:1709.01223
Vasseur, Potter, You, Ludwig
arXiv: 1807.07082



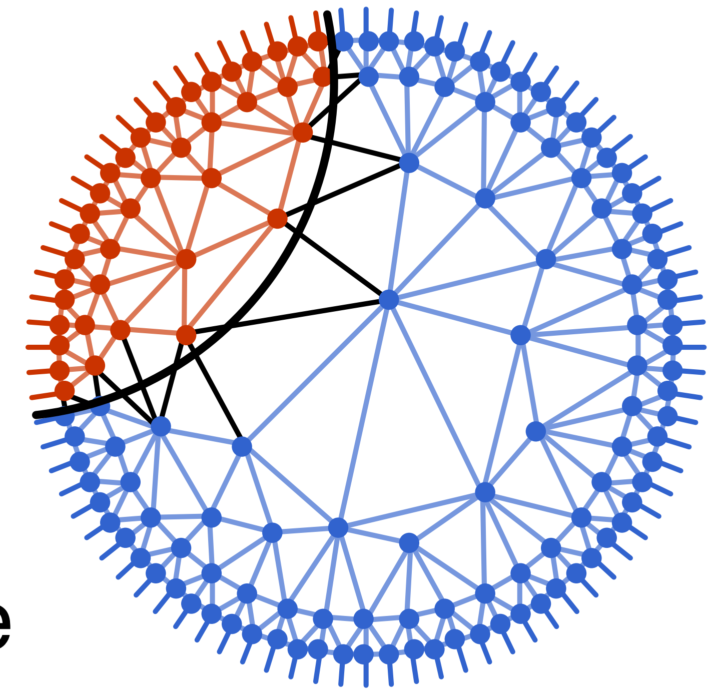
- Holographic network geometry emerges from learning!

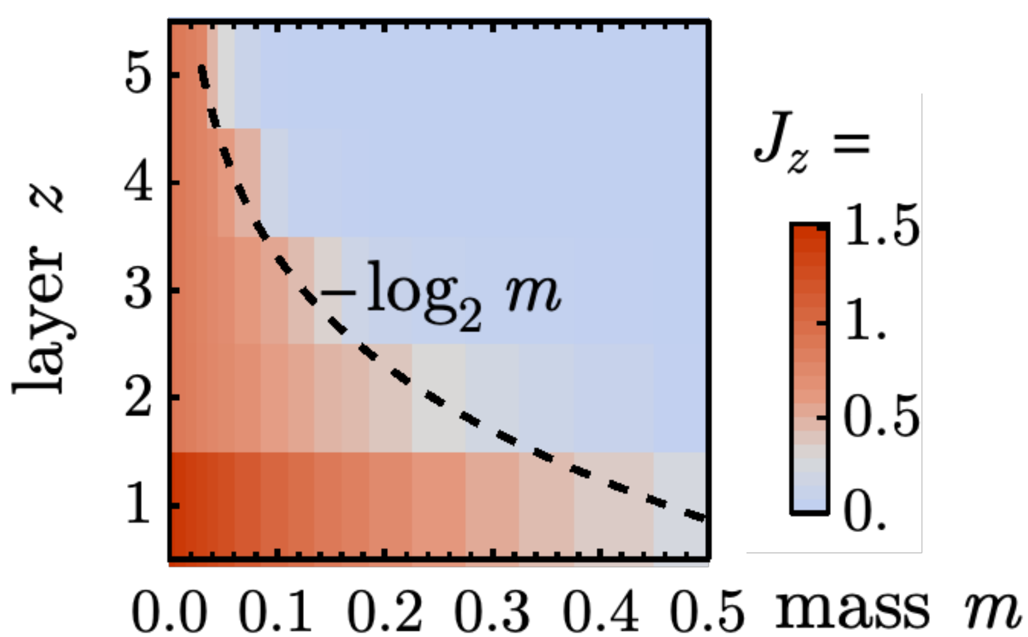
Entanglement Feature Learning

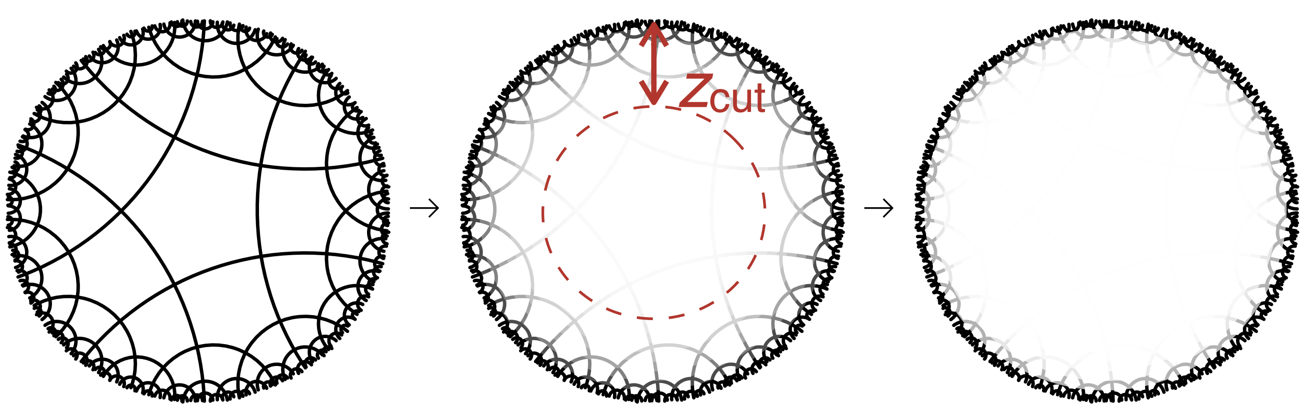
- Network design
  - Entanglement entropy ~ minimal cut ~ energy cost of Ising domain wall

$$S_E^{(2)}(A) \sim F(A)$$

  - Ising model → deep Boltzmann machine
- Model parameter: weights (Ising couplings)
- Objective: clamped free energy ~ entanglement entropy



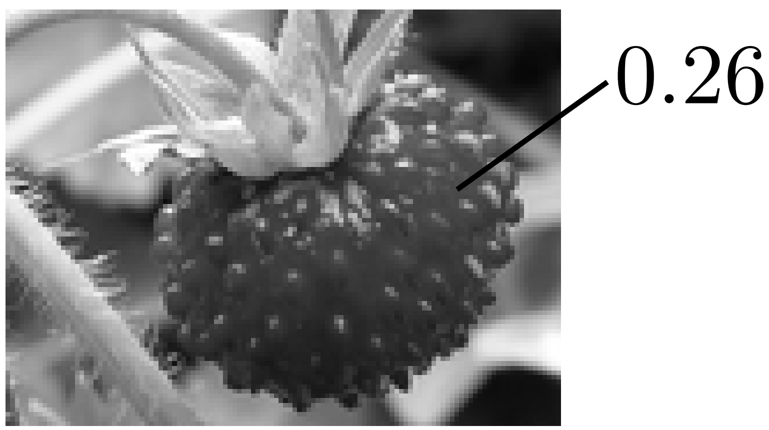




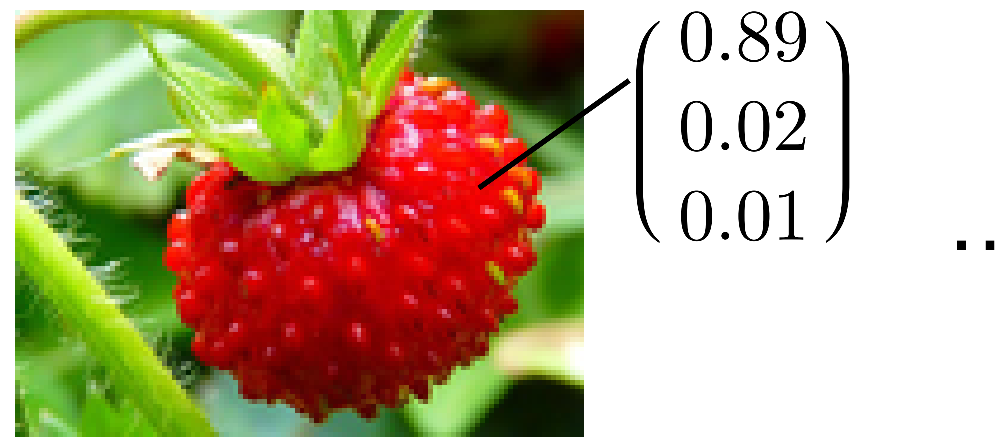
Machine Learning Renormalization Group

Quantum Field Theory as Image Dataset

- A field: a mapping from spacetime to some target manifold

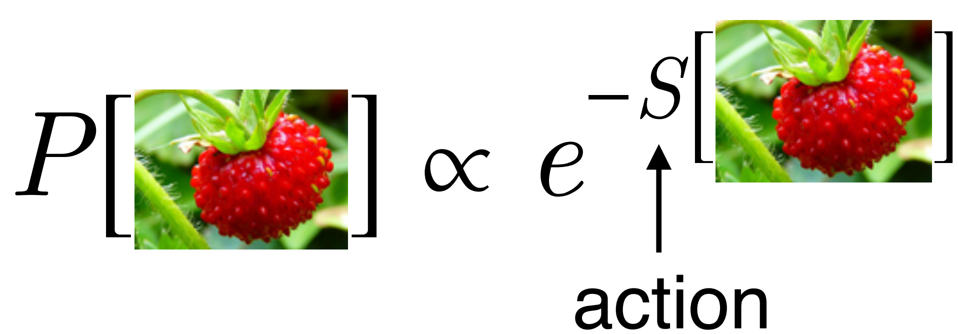


Scalar fields



Vector fields

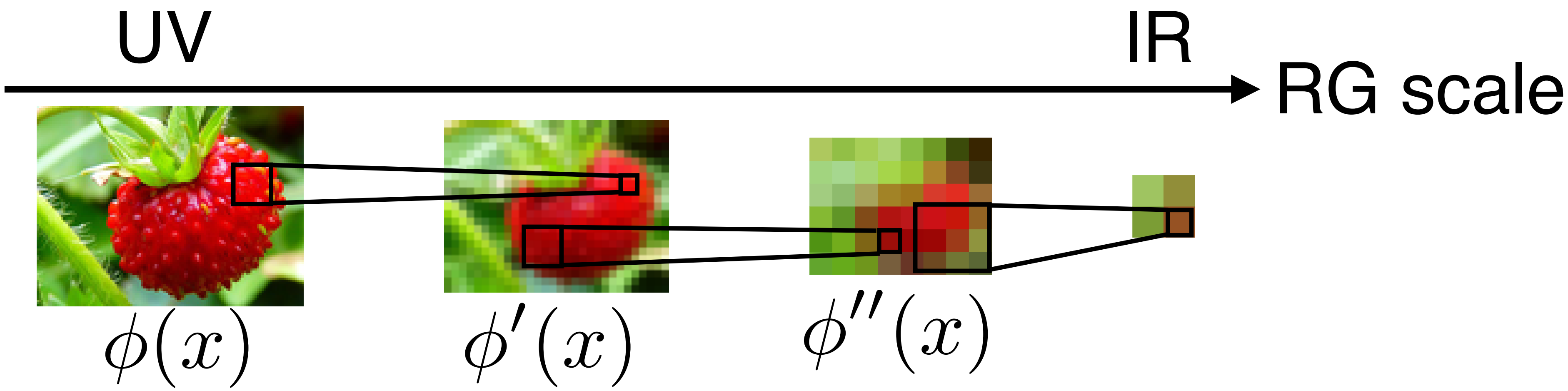
- A quantum field theory (QFT): a model that assigns an action (= negative log likelihood) to every field configuration.



- Can we train a generative model to represent the QFT?

Renormalization Group as Generative Model

- Renormalization "group" (RG): progressively coarse-graining the field (like a convolutional neural network)



Renormalization Group as Generative Model

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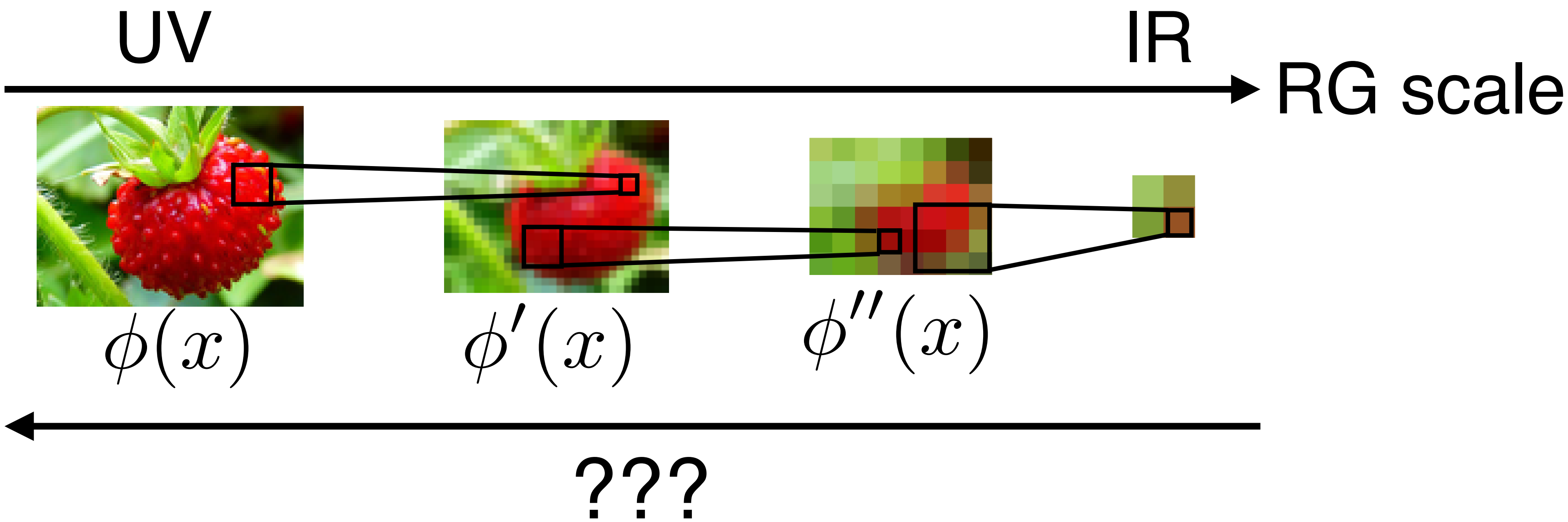
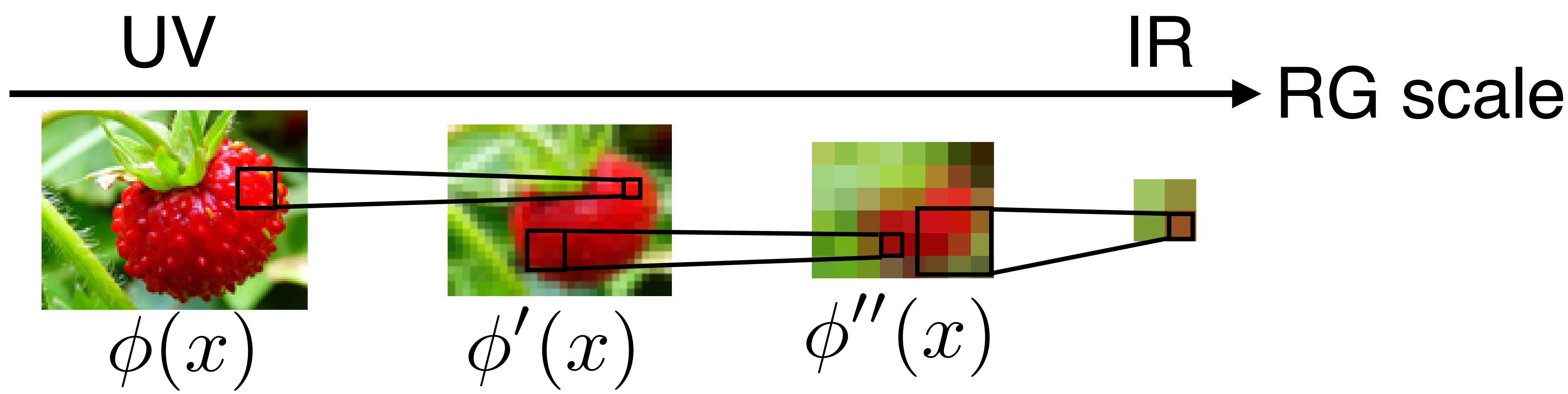


Traditional RG is not invertible…

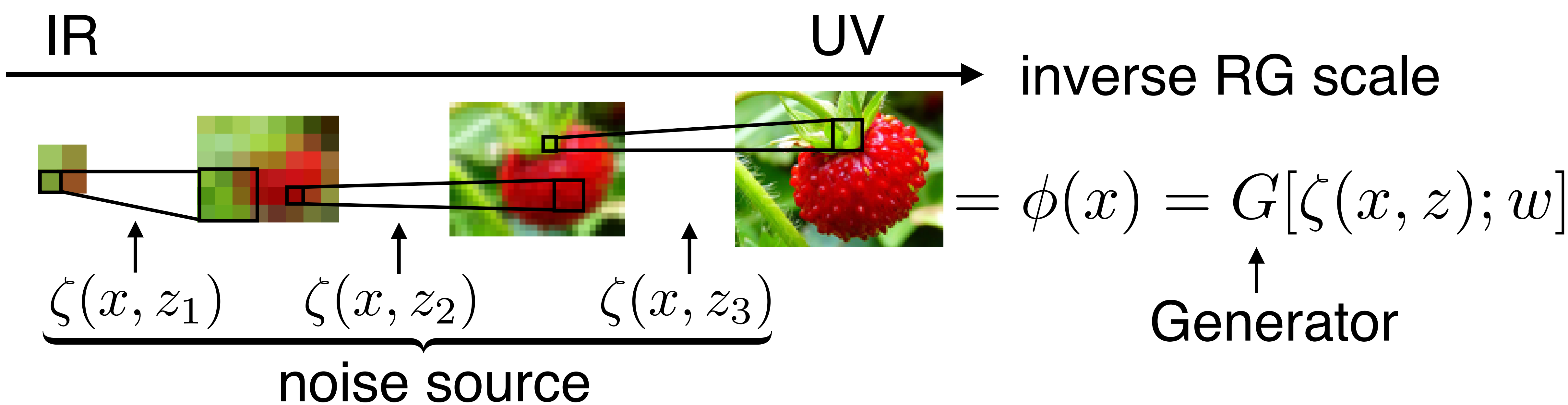
Renormalization Group as Generative Model

- Renormalization "group" (RG): progressively coarse-graining the field, similar in spirit to a convolutional neural network



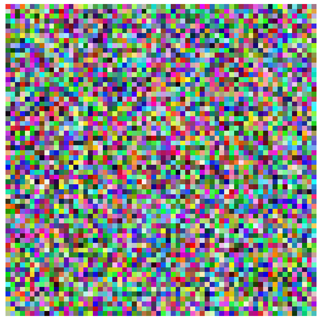
- Inverse RG: a hierarchical generative model

Beny (2013)

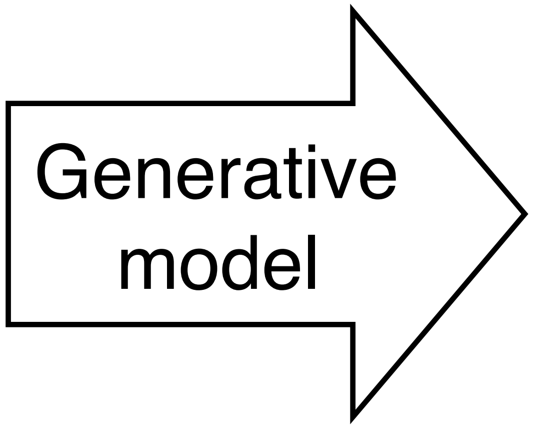


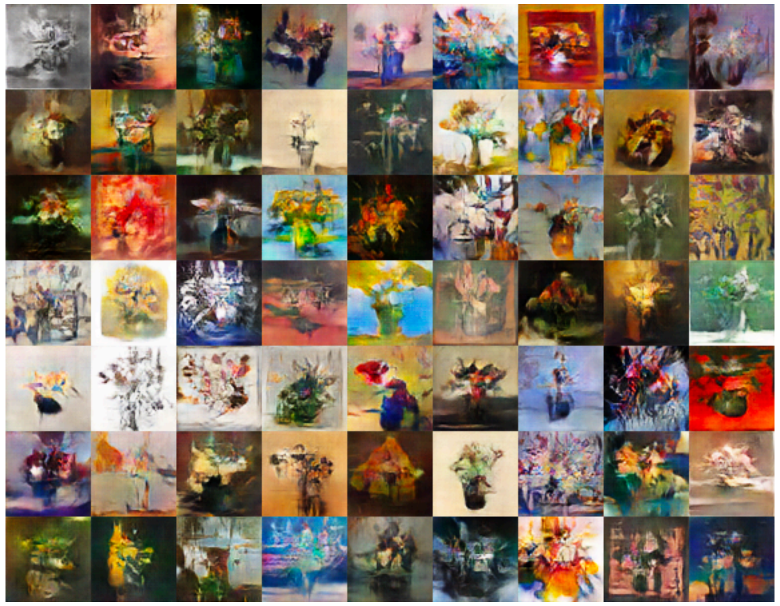
Generative Models

- Differentiable generative model: generate images from noise (latent variables) by a non-linear transformation



Random noise

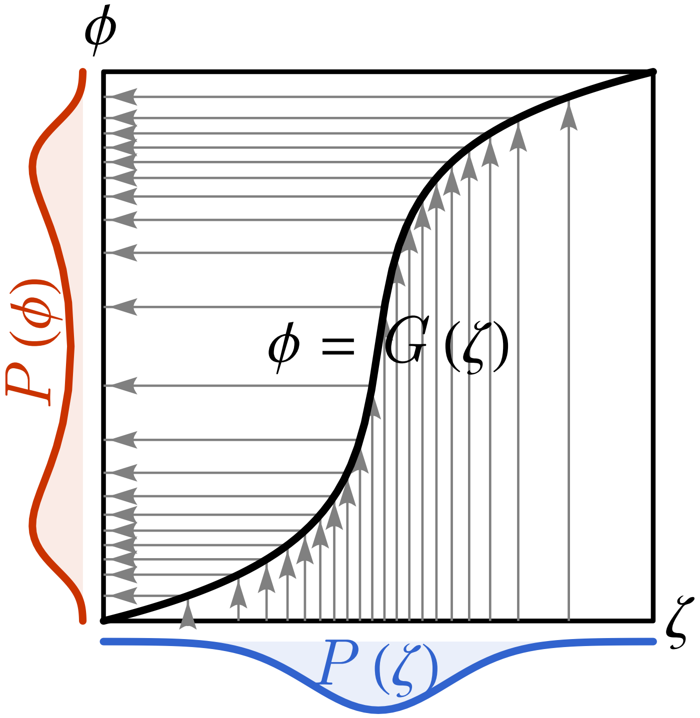




- Generative model deforms the probability distribution, sample ζ to generate ϕ

$$\phi = G(\zeta)$$

$$P(\phi) = P(\zeta)\left(\frac{\partial G(\zeta)}{\partial \zeta}\right)^{-1}$$



Optimal mass transport - Lei, Su, Cui, Yau, Gu (2017)

Deep Generative Model

- Generative model deforms noise to QFT

Li, Wang (2018), Hu, Li, Wang, You (2109)

Posterior (boundary) ↓ Prior (bulk) ↓ Generator ↓

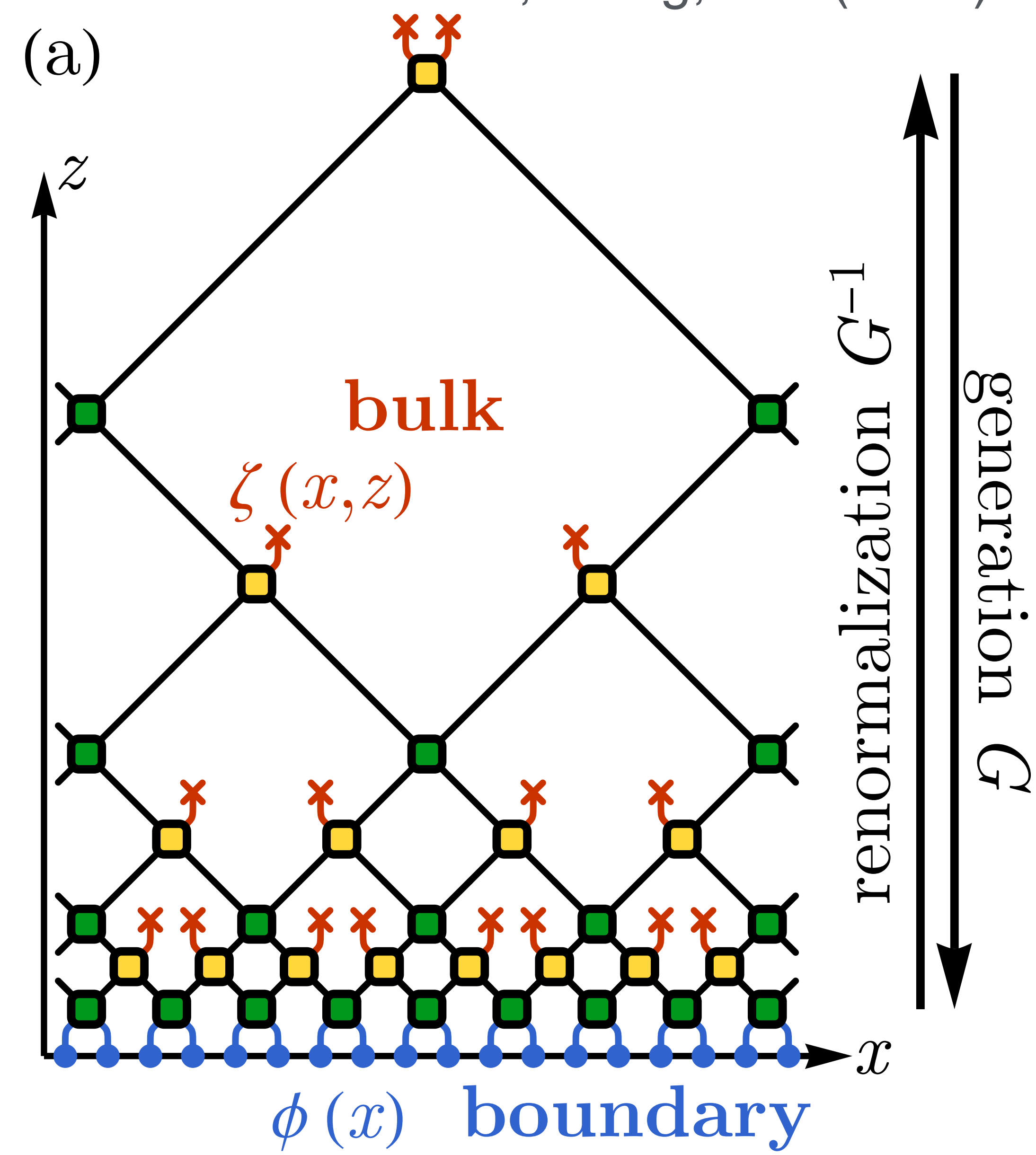
$$P_\partial[\phi] = P[\zeta]\det\left(\frac{\delta G[\zeta]}{\delta \zeta}\right)^{-1}$$

Model

↕ Minimize KL divergence

Target (QFT)

$$e^{-S[\phi]}/Z$$



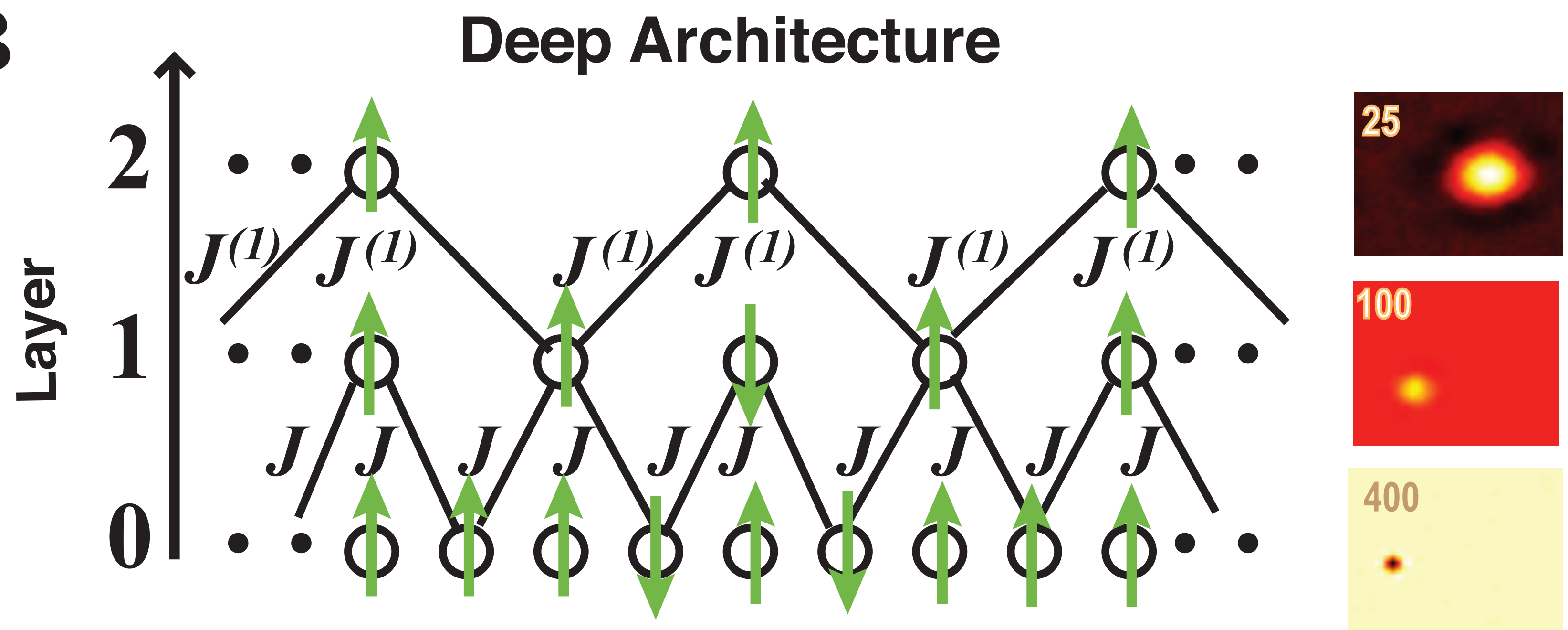
MERA network - Vidal (2006)

- How to choose the prior?
  Our choice: independent Gaussian $P[\zeta] \propto e^{-\zeta^2}$ (Why?)

Information Theoretic Goal of RG

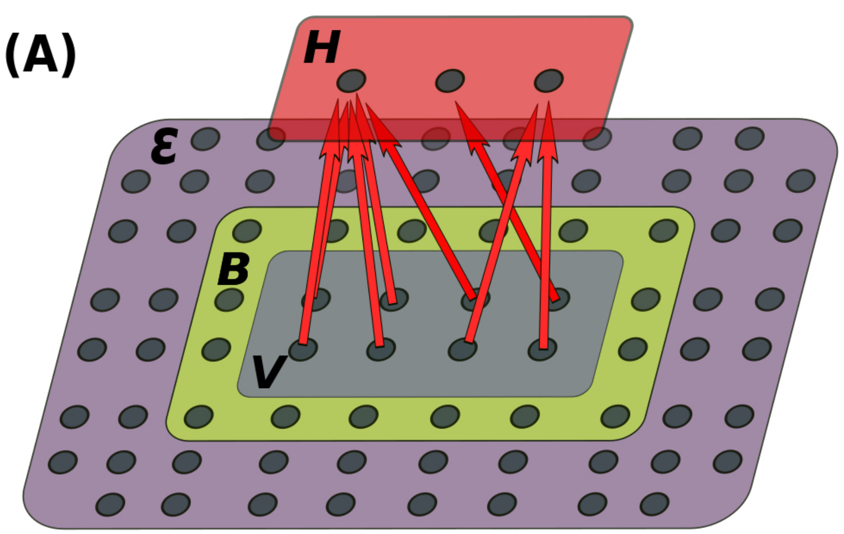
- Renormalization Group = Deep Learning? Mehta, Schwab (2014)

B



- Maximal Real-Space Mutual Information (maxRMI) principle

(A)



Koch-Janusz, Ringel (2017)

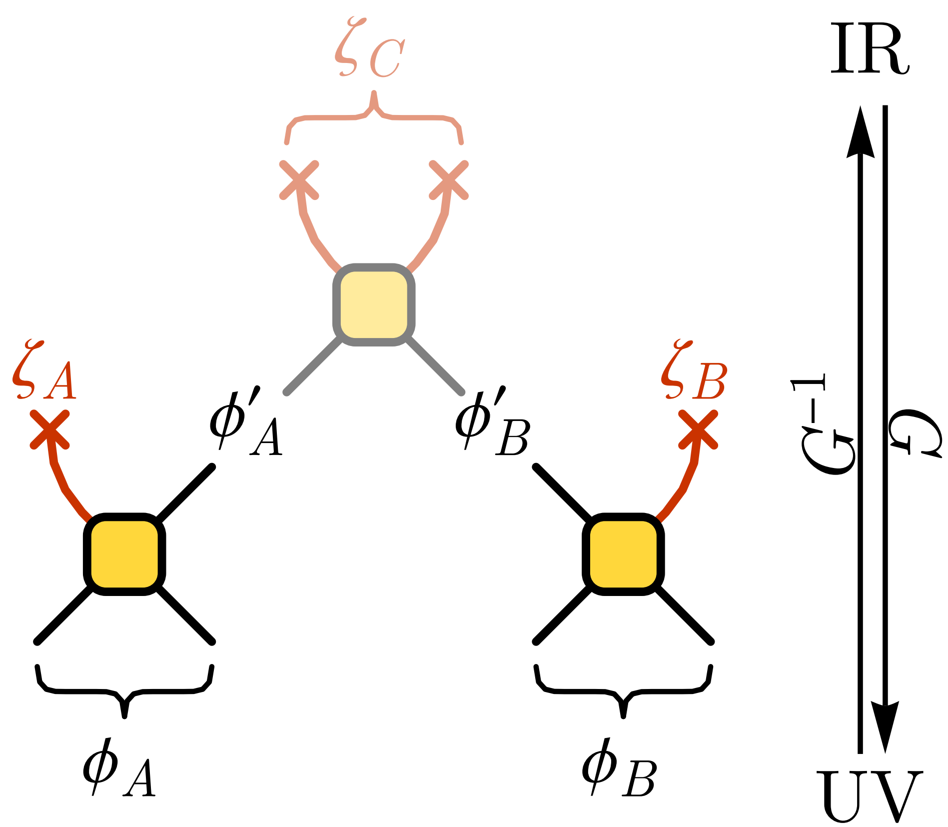
$$\max I(H, \mathcal{E})$$

Coarse-grained freedom

Environment

Information Theoretic Goal of RG

- Minimal Bulk Mutual Information (minBMI) principle



- maxRMI: $\max I(\phi'_A : \phi_B)$
- minBMI: $\min I(\zeta_A : \zeta_B)$

Two objectives are equivalent

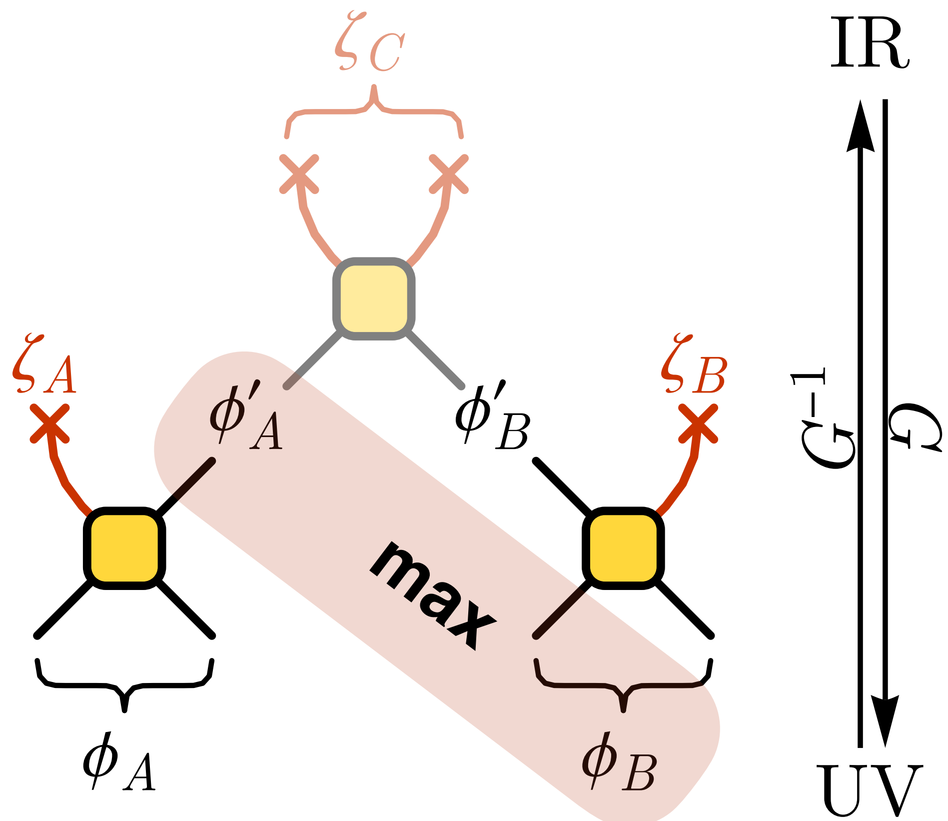
$$I(\phi'_A : \phi_B) + I(\zeta_A : \zeta_B)$$
$$= I(\phi_A, \phi_B) = \text{const.}$$

Hu, Li, Wang, You (2109)

- The objectives are two-folded
  - Generate the QFT on the boundary
  - Disentangle the QFT in the bulk

Information Theoretic Goal of RG

- Minimal Bulk Mutual Information (minBMI) principle



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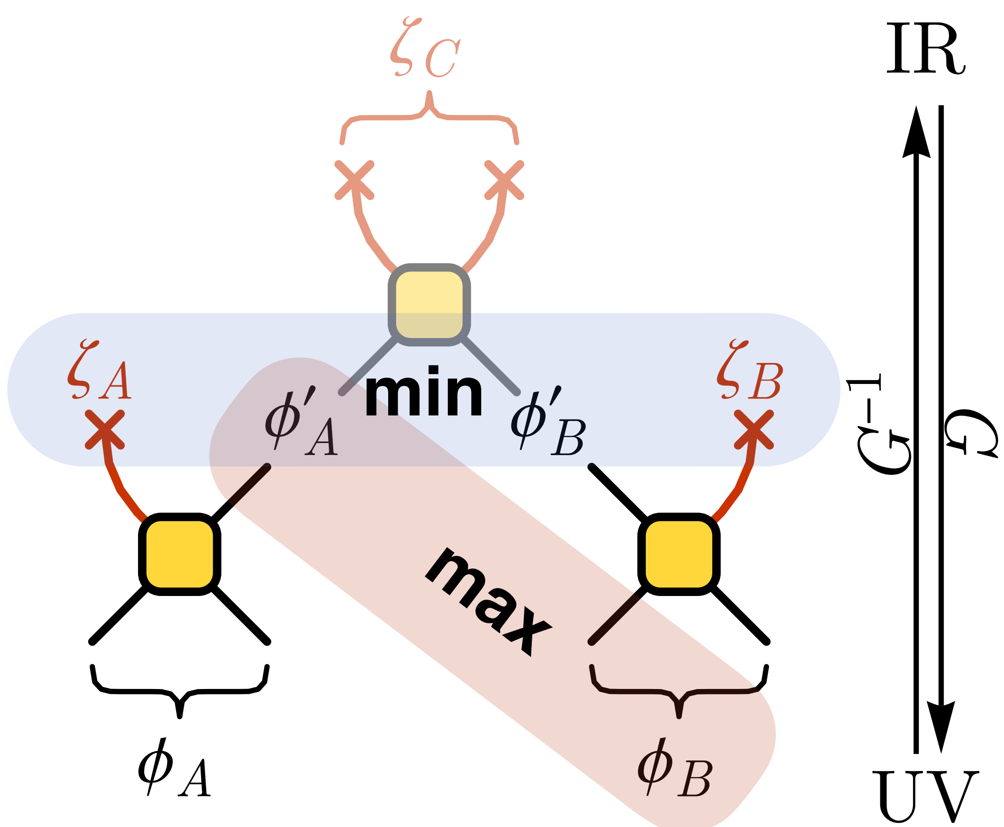

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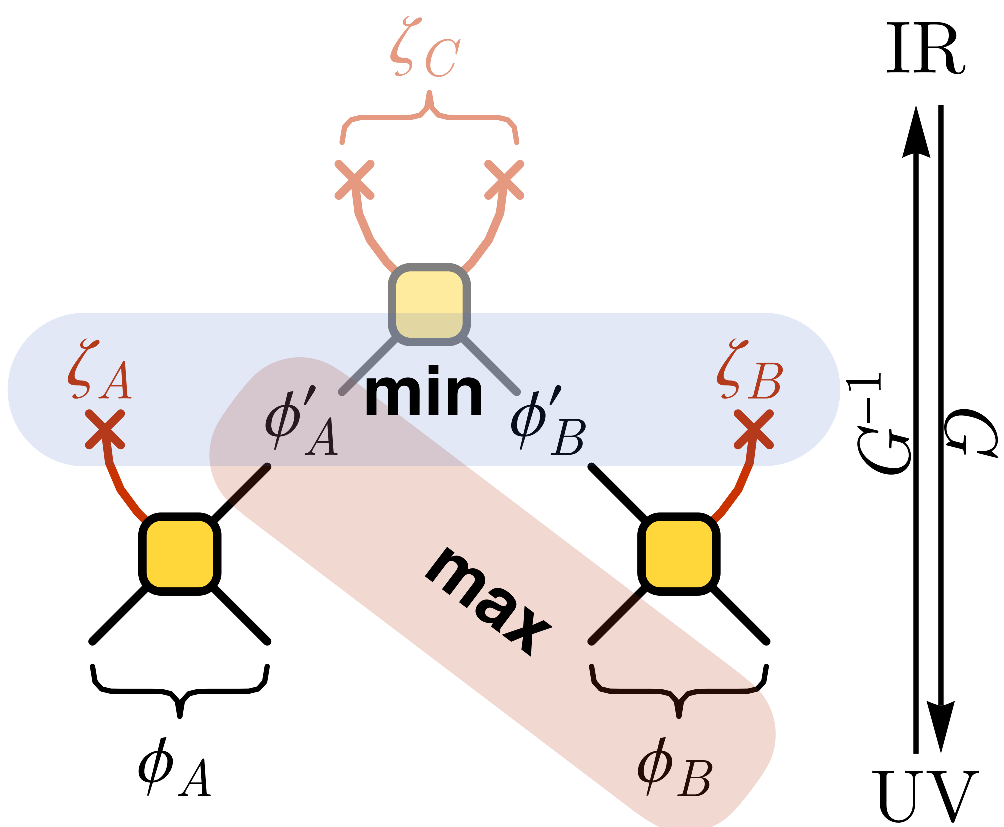

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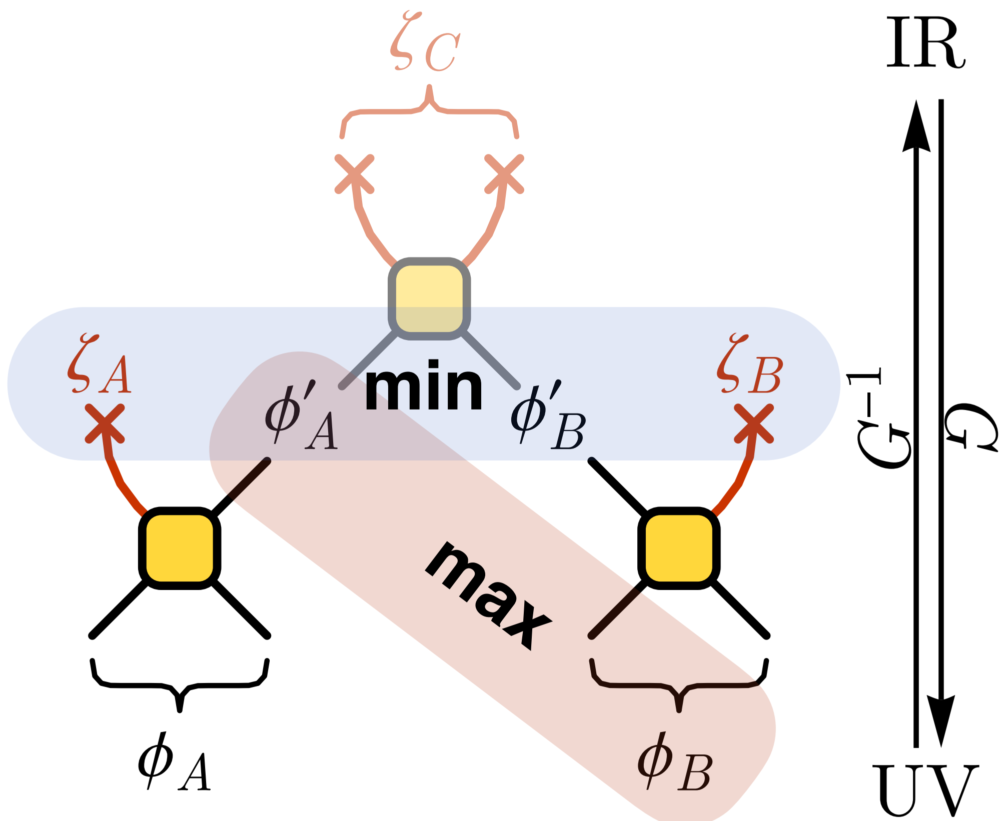
- The objectives are two-folded
  - Generate the QFT on the boundary

$$\min \mathrm{KL}(P[\zeta] \det(\delta_\zeta G[\zeta])^{-1} || e^{-S[\phi]})$$

  - Disentangle the QFT in the bulk

Information Theoretic Goal of RG

- Minimal Bulk Mutual Information (minBMI) principle



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Hu, Li, Wang, You (2109)

- The objectives are two-folded
  - Generate the QFT on the boundary
  $$\min \mathsf{KL}(P[\zeta] \det(\delta_\zeta G[\zeta])^{-1} || e^{-S[\phi]})$$
  - Disentangle the QFT in the bulk $P[\zeta] \propto e^{-\zeta^2}$

Machine Learning Holography

- Training a generative model establishes a holographic duality

$$\min \mathsf{KL}(P[\zeta]\det(\delta_\zeta G[\zeta])^{-1} || e^{-S[\phi]})$$

CFT (boundary) | **AdS** (bulk)

$$Z = \mathrm{Tr}_{[\phi]}\, e^{-S[\phi]} \longleftrightarrow Z = \mathrm{Tr}_{[\zeta]}\, P[\zeta]\det(\delta_\zeta G[\zeta])^{-1}$$

Field theory in flat space

- massless field $\phi(x)$

(Classical) gravity + matter

- massive matter $\zeta(x, z)$
- on background $G[\cdot; w]$

Features in dataset

- image $\phi(x)$

Deep generative model

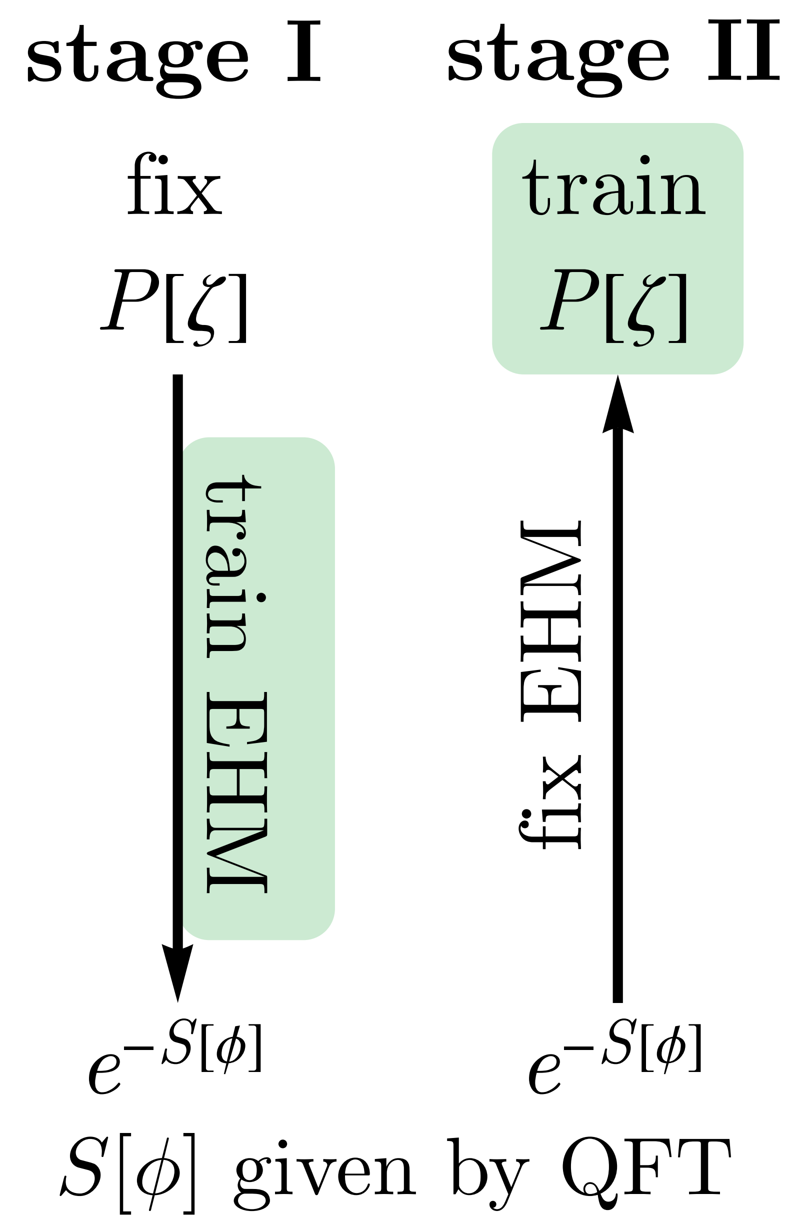
- latent representation $\zeta(x, z)$
- neural network $G[\cdot; w]$

Probing Holographic Bulk Geometry

- What can we learn from the bulk?
- Pushing the QFT into the bulk, bulk field will have residual correlation
  - Pessimist: insufficient model capacity and training loss …
  - Optimist: bulk field correlation contains important information about bulk geometry!
- Probing geometry by matter X-L Qi (2013)

$$I(\zeta_i : \zeta_j) \sim e^{-d(\zeta_i:\zeta_j)/\xi}$$

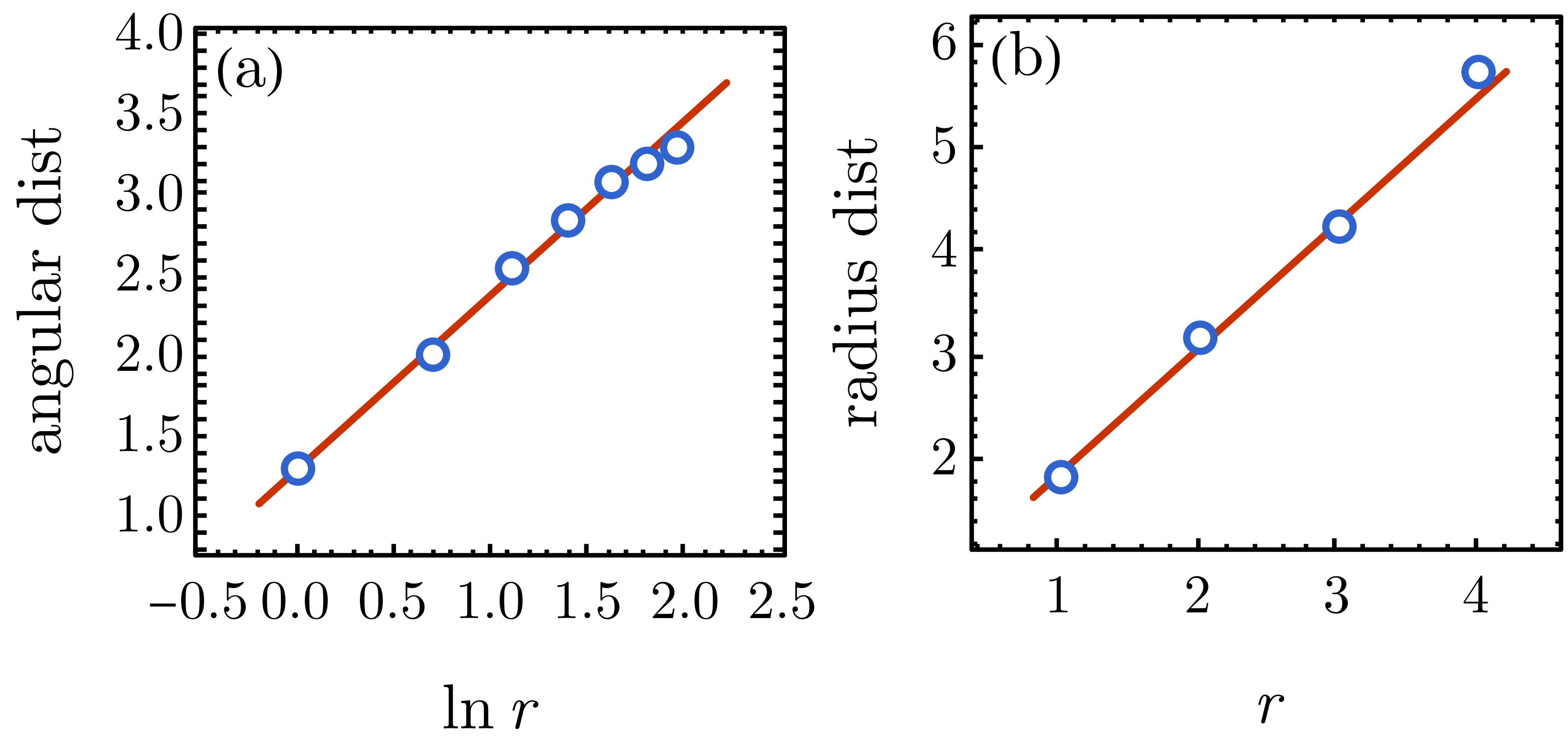
↑ residual mutual information ↑ geodesic distance



Probing Holographic Bulk Geometry

- Apply to Luttinger liquid CFT, measure the bulk distance

$$d(x,y,z|x+r,y,z) \sim \ln r \qquad d(x,y,z|x,y,z+r) \sim r$$



- Result matches hyperbolic geometry ~ AdS

$$\mathrm{d}s^2 = \frac{1}{z^2}(\mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^2)$$

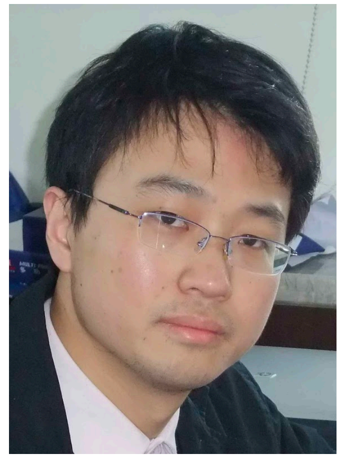
Summary

- We demonstrated several examples of machine learning physics. The common theme:
  - Train the machine on a task (but we don't use it!)
  - Open up the neural network for emergent physics

	Task	Emergent physics
ML Quantum Mechanics arXiv: 1901.11103	Potential-density mapping	Wave function + Schrödinger eq.
ML many-body entanglement arXiv:1709.01223	Entanglement entropy prediction	Holographic bulk geometry
ML holographic mapping arXiv:1903.00804	Quantum field generation	RG scheme, bulk effective theory

Acknowledgment

- ML Quantum Mechanics

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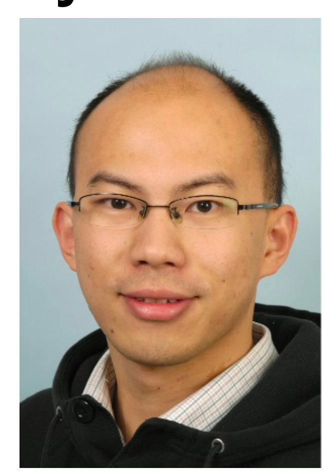
- Quantum Entanglement


Zhao Yang Xiao-Liang Qi

(Stanford University)

- Neural-RG and Holography





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